Supplementary Information

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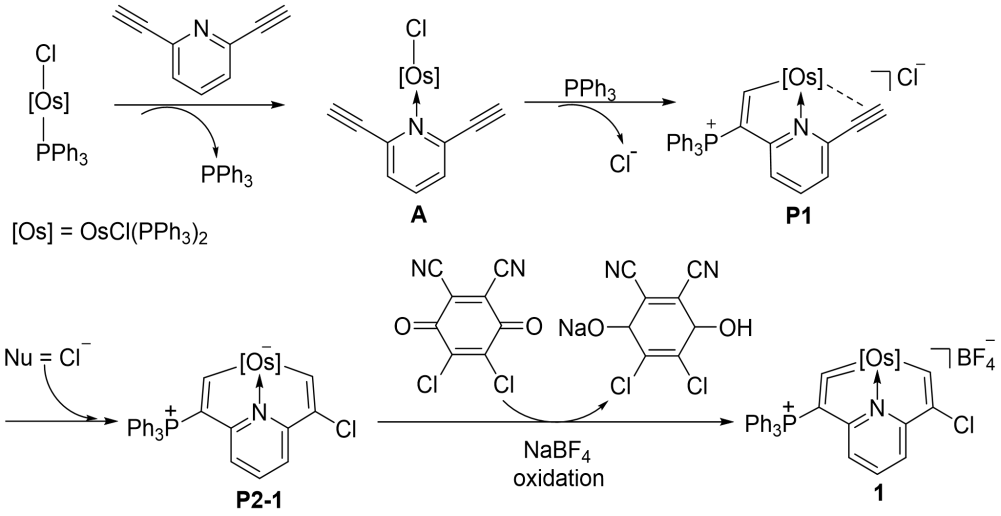
1. Proposed Mechanisms and Validation Experiment Spectra

Scheme S1. A possible mechanism for the formation of 1.



A plausible mechanism for the formation of osmium vinylidene complex **1** is proposed in Scheme S1. The process initiated with the coordination of 2,6-diethynylpridine to the metal center, associated with the dissociation of a PPh_3 ligand, resulting in intermediate **A**. Subsequently, nucleophilic addition of PPh_3 to the C≡C triple bond, followed by the removal of a chloride ion, led to the formation of the osmium vinyl intermediate **P1**. Then, another nucleophile (chloride ion) was added to the alkynyl group generated a metallacycle intermediate **P2-1**. Finally, the oxidative dehydrogenation of **P2-1** by DDQ, followed by the addition of $NaBF_4$, yielded cyclic osmium vinylidene complex **1**. The expected intermediate **P2-1** could be detected by ESI-MS.

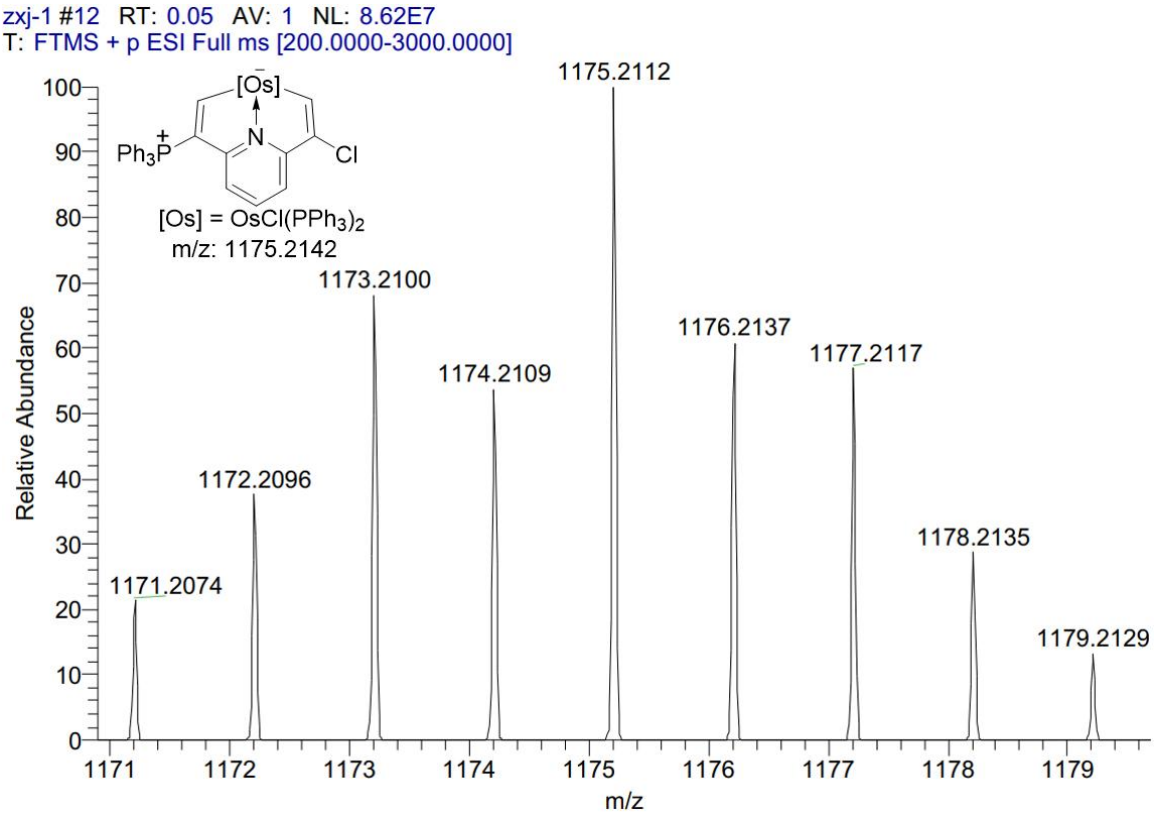
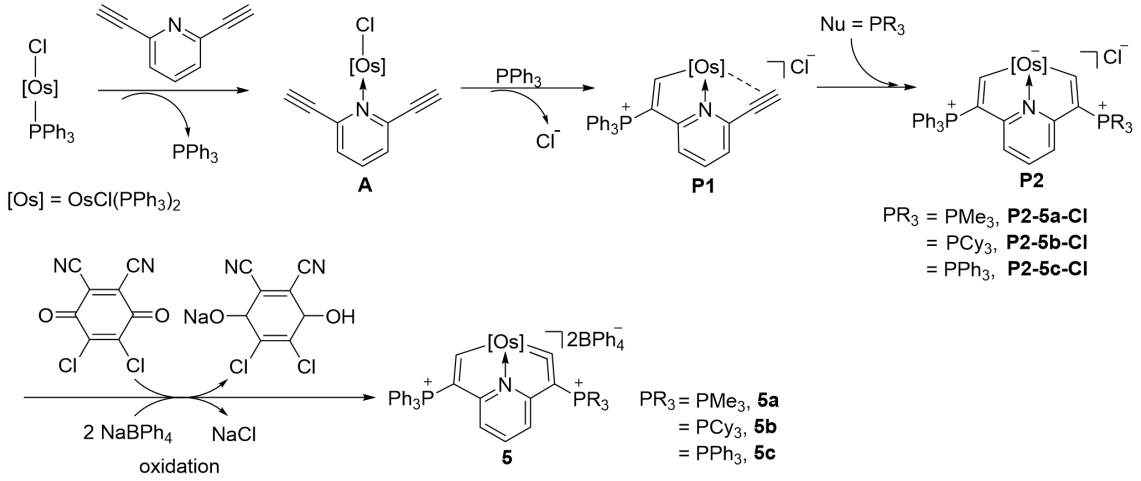


Figure S1. Positive-ion ESI-MS spectrum of [**P2-1**] measured in methanol.

Scheme S2. A possible mechanism for the formation of 5.



A plausible mechanism for the formation of osmium vinylidene complexes **5** is proposed in Scheme S2. The process before **P1** was the same with the formation of osmium vinylidene complex **1**. Another nucleophiles (tertiary phosphines, PMe_3, PCy_3, PPh_3) were added to the alkynyl group generated metallacycle intermediates **P2,** respectively. Finally, the oxidative dehydrogenation of **P2** with DDQ, followed by the addition of $NaBPh_4$, yielded a series of cyclic osmium vinylidene complexes **5**. The expected intermediates **P2-5a**, **P2-5b** and **P2-5c** could be detected by ESI-MS.

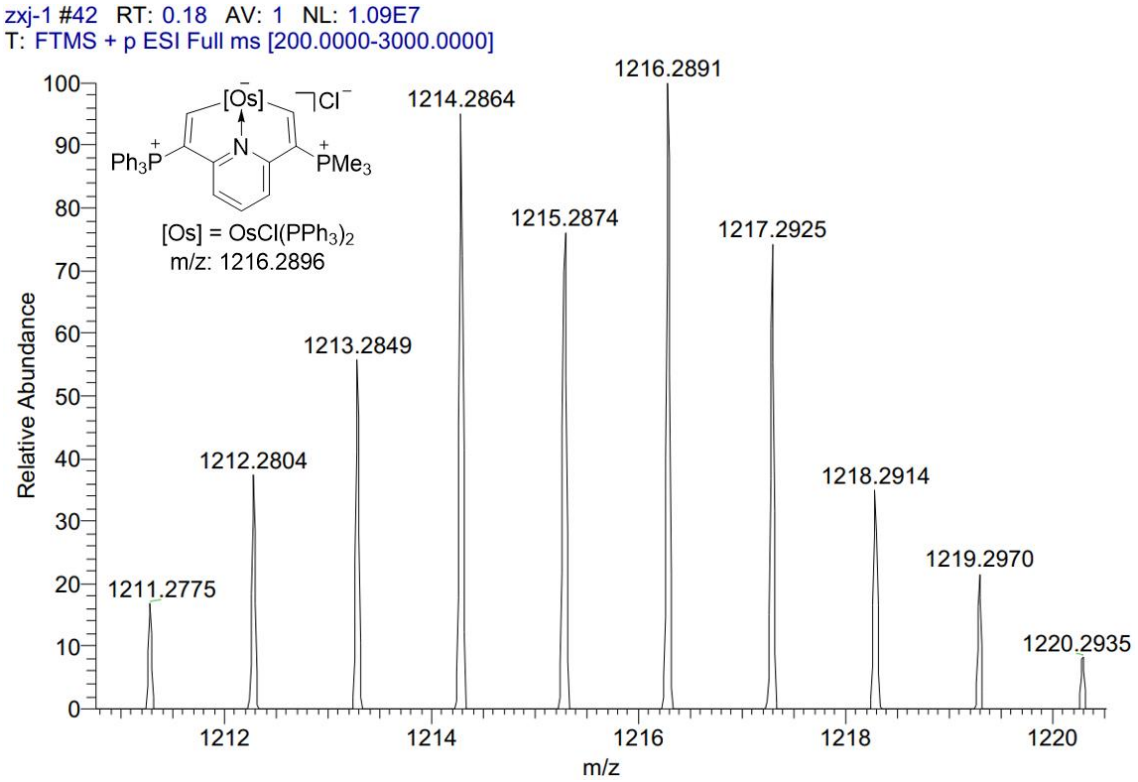


Figure S2. Positive-ion ESI-MS spectrum of [**P2-5a**]$^+$ measured in methanol.

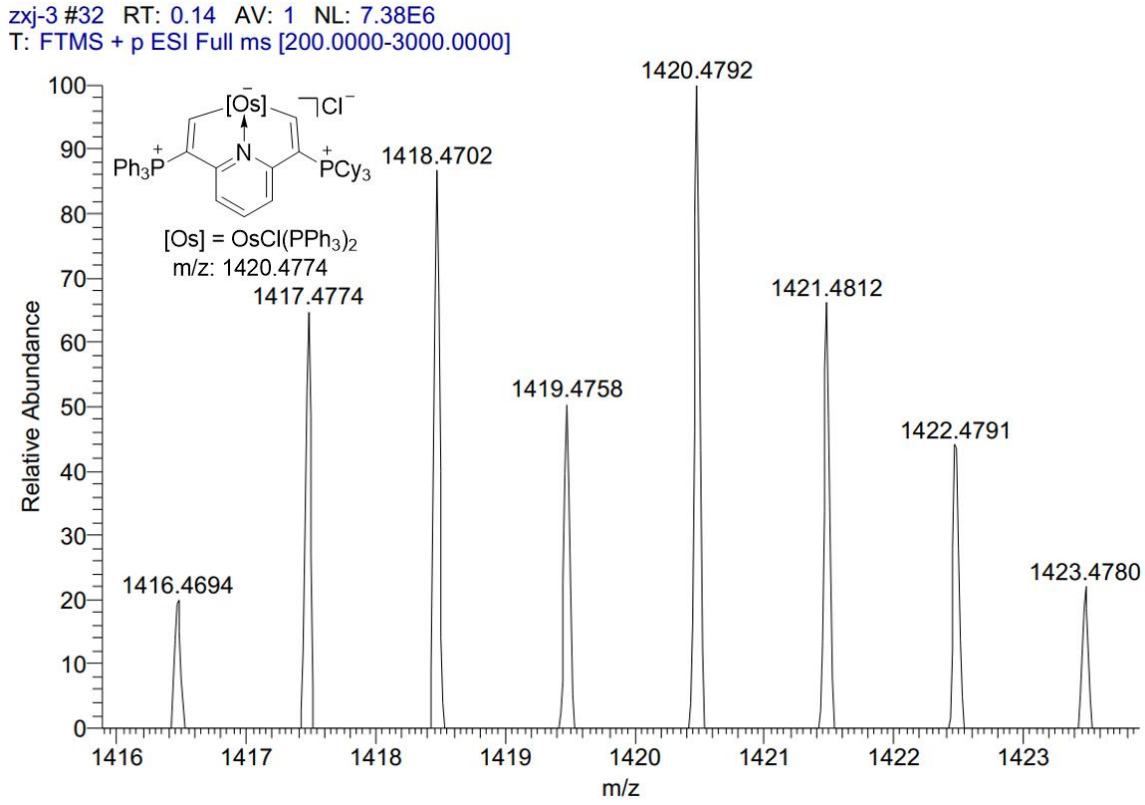


Figure S3. Positive-ion ESI-MS spectrum of [**P2-5b**]$^+$ measured in methanol.

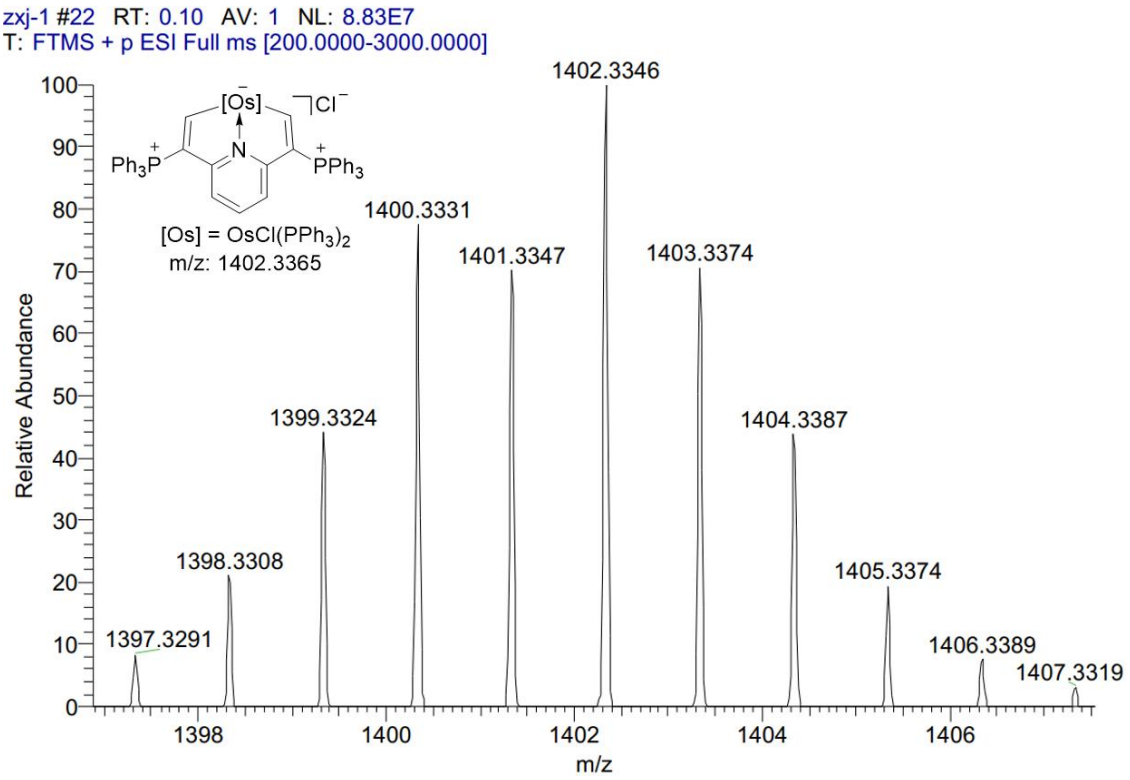
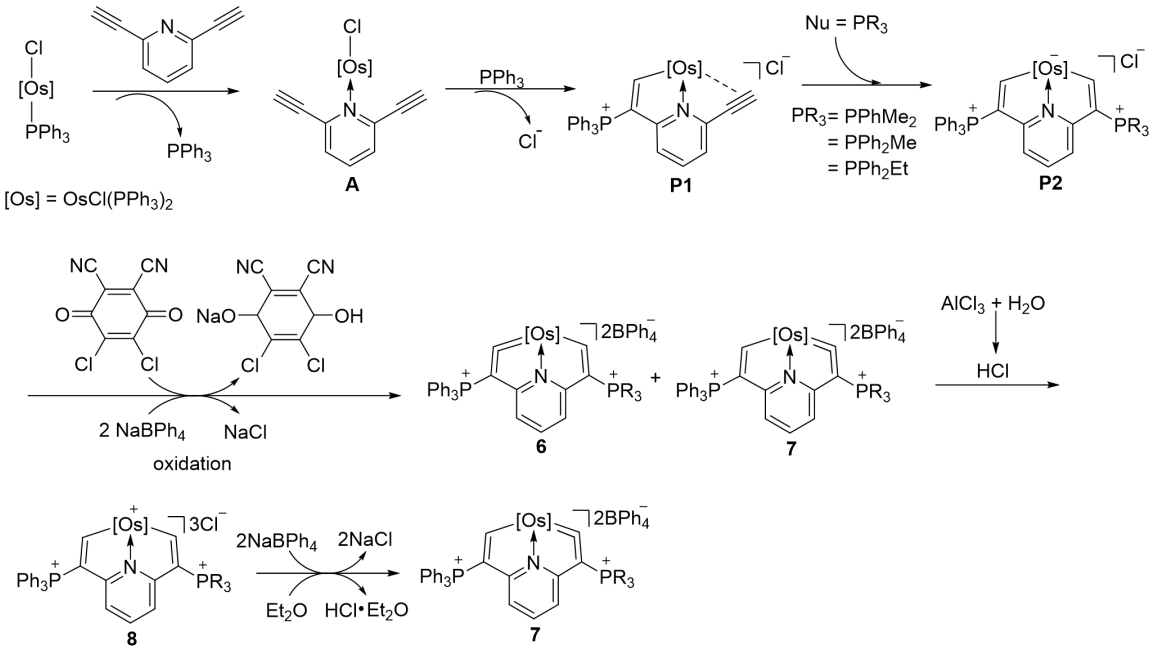


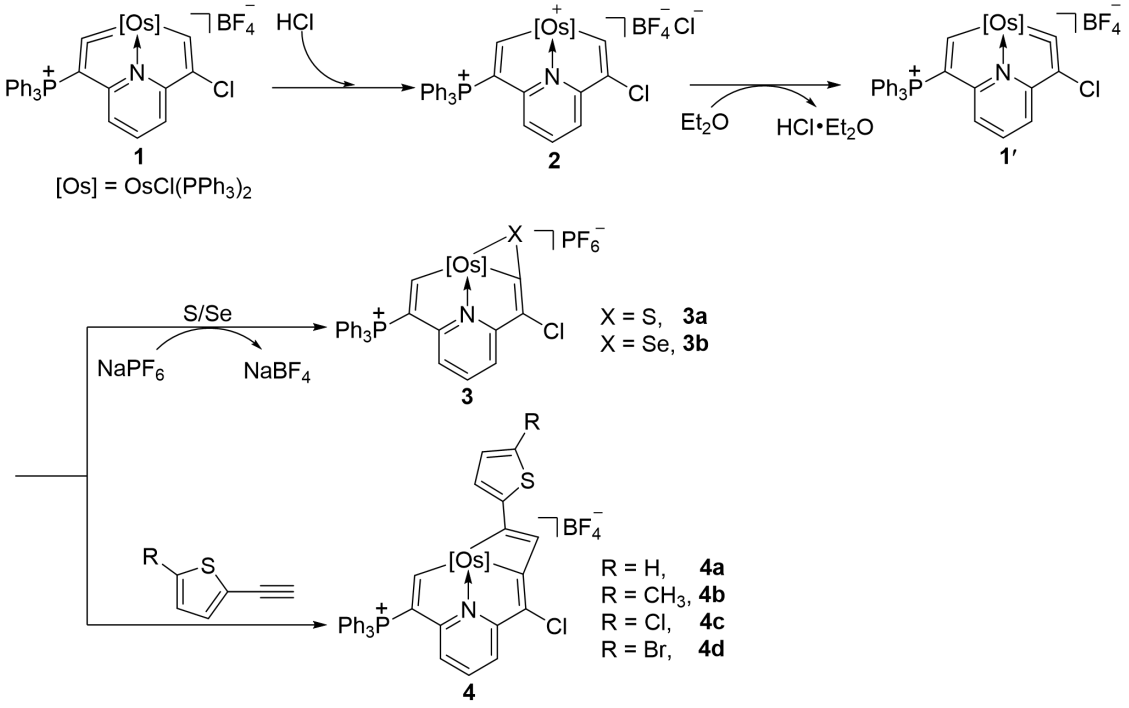
Figure S4. Positive-ion ESI-MS spectrum of [**P2-5c**]$^{+}$ measured in methanol.

Scheme S3. A possible mechanism for the formation of isomers (6 and 7) and their transformation to single species 7.



A plausible mechanism for the formation of isomers (**6** and **7**) and their transformation to single species 7 is proposed in Scheme S3. The process before **P2** was the same with the formation of osmium vinylidene complexes **5** by using different tertiary phosphines ($PPhMe_2$, PPh_2Me, PPh_2Et). Then, the oxidative dehydrogenation of **P2** with DDQ, followed by the addition of $NaBPh_4$, yielded a series of cyclic osmium vinylidene isomers (**6** and **7**). Subsequently, The addition of protons with HCl (generated from the hydrolysis of $AlCl_3$) at osmium vinylidene units of isomers (**6** and **7**) gave the complexes **8**. Finally, the removal of protons by Lewis base Et_2O, coupled with exchange of the counter ions by $NaBPh_4$, afforded the final products **7**.

Scheme S4. A possible mechanism for the formation of 3 and 4.



A plausible mechanism for the formation of complexes **3** and **4** is presented in Scheme S4. The addition of protons at osmium vinylidene units of complex **1** gave the complex **2**. Subsequently, the substraction of protons afforded the complex **1'**. Finally, the products **3** were formed via the [2+1] cycloaddition reaction accompanied with the exchange of the counterion by $NaPF_6$ and the products **4** were formed through the [2+2] cycloaddition reaction.

Table S1. The transformation of osmium vinylidene complex 1 to cycloaddition products 3a with different amounts of acid and temperature.

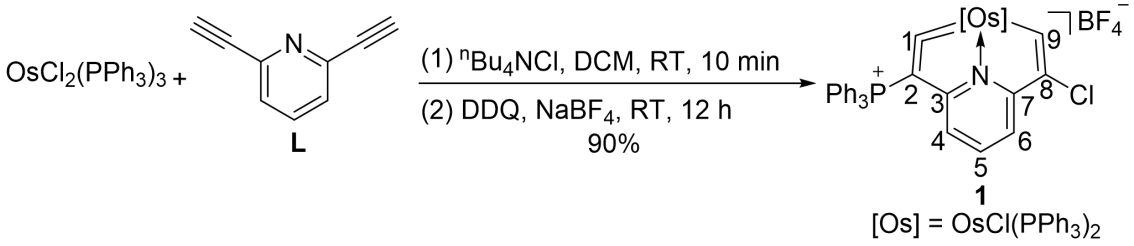
Entry	Equivalent of acids	Temperature (°C)	Yield (%)[a]
1	1 eq. CF_3COOH	40	trace
2	1 eq. $HBF_4 \bullet Et_2O$	40	16
3	1 eq. $HCl \bullet H_2O$	40	10
4	1 eq. $HCl \bullet Et_2O$	40	28
5	1 eq. $HCl \bullet Et_2O$	50	42
6	1 eq. $HCl \bullet Et_2O$	60	53
7	1.5 eq. $HCl \bullet Et_2O$	60	45
8	0.5 eq. $HCl \bullet Et_2O$	60	65
9	0.3 eq. $HCl \bullet Et_2O$	60	50

[a]Reaction conditions: A mixture of compound **1** (15 mg, 0.012 mmol) and S (3.8 mg, 0.12 mmol) were dissolved in CH_2Cl_2 (0.5 mL) by stirring for 48 hours.

2. Experimental Procedures

General Information: All syntheses were carried out under an inert atmosphere (N_2) using standard Schlenk techniques, unless otherwise stated. Solvents were distilled from sodium/benzophenone (diethyl ether) or calcium hydride (dichloromethane) under N_2 prior to use. $OsCl_2(PPh_3)_3$[1] and 2,6-diethynylpyridine (**L**)[2] were prepared according to the previously published procedure. Other reagents were used as received from commercial sources without further purification. Nuclear magnetic resonance (NMR) experiments were performed on a Bruker Ascend 400 spectrometer (^{1}H, 400.1, ^{13}C, 100.6, ^{31}P, 161.9 MHz) and Bruker Ascend III 600 spectrometer (^{1}H, 600.1, ^{13}C, 150.9, ^{31}P, 242.9 MHz) at room temperature. ^{1}H and ^{13}C NMR chemical shifts (δ) are relative to tetramethylsilane, and ^{31}P NMR chemical shifts are relative to 85% H_3PO_4. Two-dimensional is abbreviated as HMBC (heteronuclear multiple bond coherence) and HSQC (heteronuclear single quantum coherence). The absolute values of the coupling constants are given in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), and broad (br). High-resolution mass spectroscopy (HRMS) experiments were conducted on a Thermo Scientific Q Exactive instrument. Elemental analyses were performed on a Vario EL III elemental analyzer.

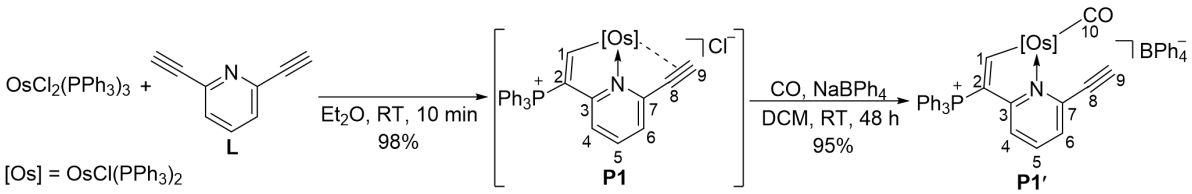
Synthesis and characterization of 1



A mixture of $OsCl_2(PPh_3)_3$ (150 mg, 0.14 mmol), ^{n}Bu$_4$NCl (39 mg, 0.14 mmol) and 2,6-diethynylpyridine (18 mg, 0.14 mmol) were dissolved in DCM (5 mL). The reaction mixture was stirred for 10 minutes at room temperature, DDQ (32 mg, 0.14 mmol) and $NaBF_4$ (77 mg, 0.70 mmol) were added subsequently. The reaction mixture was stirred for 12 hours at room temperature to give a brownish-

yellow suspension and the solid suspension was removed through a filter. The filtrate was evaporated to 2 mL recrystallized from CH_2Cl_2/Et_2O 10/1 mixture. The compound **1** was obtained in 90% yield (159 mg) as a yellow solid. ^{1}H-NMR (600.1 MHz, $CDCl_3$, δ ppm): 9.23 (s, 1H, C^9*H*), 6.93 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.22 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 5.77 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 7.83-7.07 (m, 45H, other aromatic protons). ^{31}P-NMR (242.9 MHz, $CDCl_3$, δ ppm): 2.59 (s, C*P*Ph_3), 2.47 (s, Os*P*Ph_3). ^{13}C-NMR (150.9 MHz, $CDCl_3$,δ ppm): 327.96 (td apparent q, $J_{P\text{-}C}$ = 11.5 Hz, $J_{P\text{-}C}$ = 12.1 Hz, C^1), 173.06 (t, $J_{P\text{-}C}$ = 10.5 Hz, C^9), 162.70 (s, C^7), 158.06 (d, $J_{P\text{-}C}$ = 21.1 Hz, C^3), 141.62 (s, C^5), 121.76 (s, C^8), 111.10 (s, C^4), 110.74 (s, C^6), 91.19 (d, $J_{P\text{-}C}$ = 116.2 Hz, C^2), 135.0-118.8 (m, PPh_3). HRMS (ESI): m/z calcd for $[C_{63}H_{49}Cl_2NOsP_3]^+$, 1174.2064; Found: 1174.2045. Anal. Calcd. for $C_{63}H_{49}BCl_2F_4NOsP_3$: C, 60.01; H, 3.92; N, 1.11. Found: C, 59.82; H, 4.22; N, 1.37.

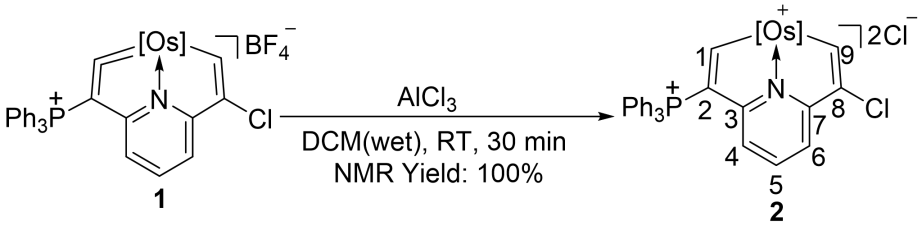
Synthesis and characterization of P1 and P1'



A mixture of $OsCl_2(PPh_3)_3$ (150 mg, 0.14 mmol) and 2,6-diethynylpyridine (22 mg, 0.17 mmol) was dissolved in Et_2O (5 mL). The reaction mixture was stirred for 10 minutes at room temperature to give a brownish-yellow suspension. The solid was collected by filtration, washed with Et_2O (3×2 mL) and then dried under vacuum. The compound **P1** was obtained in 98% yield (161 mg) as a brownish-yellow solid as shown in the picture. A mixture of **P1** (150 mg, 0.13 mmol) and $NaBPh_4$ (133 mg, 0.39 mmol) was dissolved in CH_2Cl_2 (5 mL) and stirred for 48 hours at room temperature in an atmosphere of CO. Then the solid suspension was removed through a filter and the residue was recrystallized from

CH_2Cl_2/Et_2O 1/10 mixture. The compound **P1'** was obtained in 95% yield (184 mg) as a red solid. **P1** exhibits poor solubility in commonly used solvents such as DCM, $CHCl_3$, DCE, MeOH, EtOH, Et_2O, THF, Acetone, CH_3CN, even DMF and DMSO. Furthermore, it demonstrates instability in its solid state after just 3 hours let alone in solution. Consequently, efforts to obtain a comprehensive characterization of **P1**, including NMR experiments and high-resolution mass spectroscopy, have proven unsuccessful. In contrast, **P1'** can be fully characterized without such limitations. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.60 (d, $J_{P\text{-}H}$ = 25.8 Hz, 1H, C^1*H*), 6.65 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.38 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 6.36 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 3.32 (s, 1H, C^9*H*), 7.80-6.82 (m, 65H, other aromatic protons). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.92 (s, C*P*Ph$_3$), -7.64 (s, Os*P*Ph$_3$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 237.82 (m, C^1), 191.19 (m, C^{10}), 166.81 (d, $J_{P\text{-}C}$ = 33.2 Hz, C^3), 149.75 (s, C^7), 134.26 (s, C^5), 129.96 (s, C^6), 121.02 (s, C^4), 118.24(d, $J_{P\text{-}C}$ = 75.5 Hz, C^2), 89.60 (s, C^9), 83.03 (s, C^8), 136.2-118.4 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{64}H_{50}ClNOOsP_3]^+$, 1168.2403; Found: 1168.2393. Anal. Calcd. for $C_{88}H_{70}BClNOOsP_3$: C, 71.08; H, 4.75; N, 0.94. Found: C, 70.92; H, 4.92; N, 1.12.

Synthesis and characterization of 2



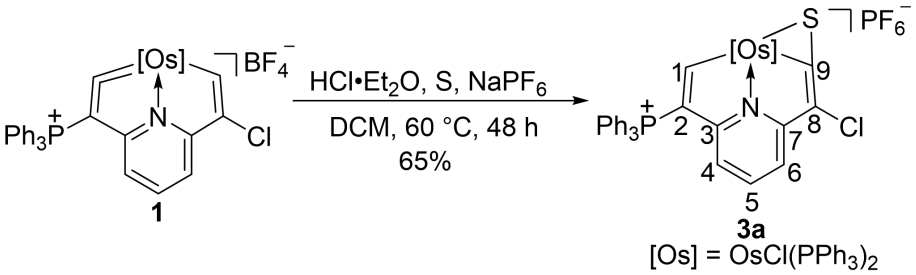
1 **2**

[Os] = OsCl(PPh$_3$)$_2$

A mixture of **1** (150 mg, 0.12 mmol) and $AlCl_3$ (284 mg, 1.8 mmol) were dissolved in DCM (wet, 2 mL). The reaction mixture was stirred for 30 minutes at room temperature to give an orange suspension, the solid suspension was removed through a filter to give an orange solution of **2** (approximately 100% yield based on ^{1}H and ^{31}P{1H} NMR). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 10.10 (dd, $J_{P\text{-}H}$ = 11.4 Hz, $J_{H\text{-}H}$ = 4.2 Hz, 1H, C^1*H*), 8.33 (d, $J_{H\text{-}H}$ = 4.0 Hz, 1H, C^9*H*), 7.42 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.10 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 5.99 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 8.03-6.95 (m, other aromatic protons plus C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 16.57 (s, Os*P*Ph$_3$), 10.92 (s, C*P*Ph$_3$). ^{13}C-NMR (150.9 MHz,

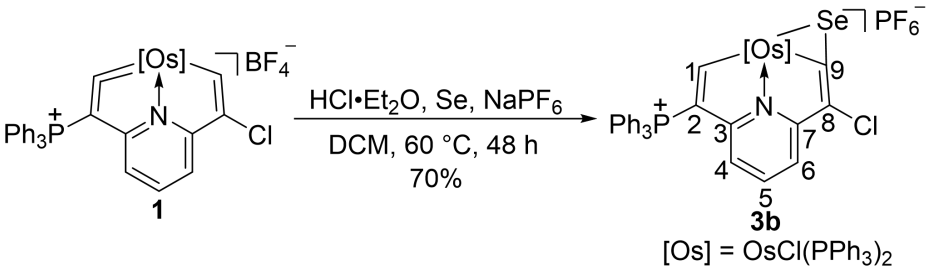
CD_2Cl_2, δ ppm): 210.79 (td apparent t, $J_{P\text{-}C}$ = 5.3 Hz, C^1), 182.03 (td apparent t, $J_{P\text{-}C}$ = 8.3 Hz, C^9), 157.54 (s, C^7), 156.67 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^3), 144.51 (s, C^5), 129.72 (s, C^8), 120.27 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^2), 119.78 (s, C^6), 119.63 (s, C^4), 137.3-128.7 (m, other aromatic carbons).

Synthesis and characterization of 3a



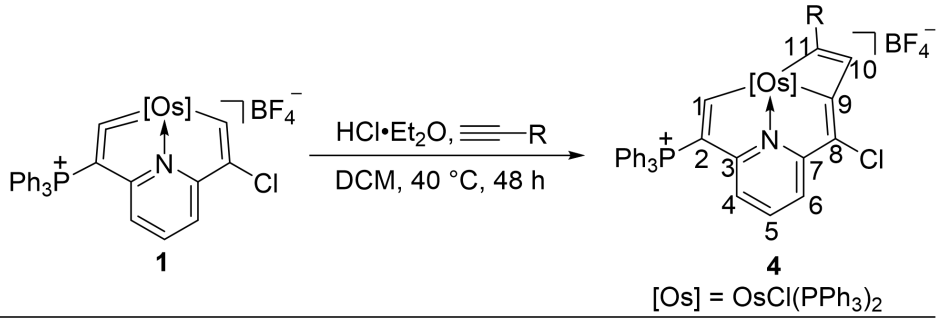
A mixture of compound **1** (150 mg, 0.12 mmol), HCl·Et_2O (30 μL, 2M, 0.06 mmol) and S (38 mg, 1.20 mmol) were dissolved in CH_2Cl_2 (5 mL). After stirring for 48 hours at 60 ℃, The excess S_8 was removed by filtration, and the filtrate was evaporated to 2 mL and then washed with Et_2O (1×20 mL). The compound **3a** was obtained as a brown solid in 65% yield (105 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.18 (d, $J_{P\text{-}H}$ = 19.8 Hz, 1H, C^1H), 6.85 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 6.09 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4H), 5.99 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6H), 7.87-6.97 (m, 45H, other aromatic protons). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.22 (s, C*P*Ph_3), -20.85 (s, Os*P*Ph_3), -144.50 (septet, *P*F_6). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 230.23 (t, $J_{P\text{-}C}$ = 6.7 Hz,, C^1), 203.52 (br, C^9), 168.66 (s, C^7), 164.74 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^3), 135.62 (s, C^5), 113.16 (s, C^6), 109.99 (s, C^4), 109.53 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^2), 105.86 (s, C^8), 135.1-117.8 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{63}H_{49}Cl_2NP_3OsS]^+$, 1206.1785; Found: 1206.1744. Anal. Calcd. for $C_{63}H_{49}F_6Cl_2NP_4OsS$: C, 56.00; H, 3.66; N, 1.04; S, 2.37. Found: C, 56.32; H, 3.85; N, 1.14. ; S, 2.55.

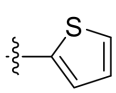
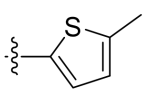
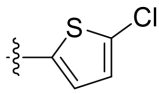
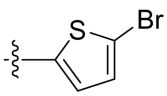
Synthesis and characterization of 3b



A mixture of compound **1** (150 mg, 0.12 mmol), $HCl{\cdot}Et_2O$ (30 μL, 2M, 0.06 mmol) and Se (95 mg, 1.20 mmol) were dissolved in CH_2Cl_2 (5 mL). After stirring for 48 hours at 60 ℃, The excess Se was removed by filtration, and the filtrate was evaporated to 2 mL and then washed with Et_2O (1×20 mL). The compound **3b** was obtained as a brown solid in 70% yield (117 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.05 (d, $J_{P\text{-}H}$ = 19.8 Hz, 1H, C^1*H*), 6.82 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.03 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 5.94 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 7.88-6.92 (m, 45H, other aromatic protons). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 13.91 (s, C*P*Ph$_3$), -25.54 (s, Os*P*Ph$_3$), -144.49 (septet, *P*F$_6$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 230.31 (t, $J_{P\text{-}C}$ = 6.8 Hz, C^1), 211.98 (t, $J_{P\text{-}C}$ = 3.3 Hz, C^9), 168.57 (s, C^7), 164.96 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^3), 137.31 (s, C^5), 115.92 (s, C^8), 112.69 (s, C^6), 109.57 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^2), 109.69 (s, C^4), 135.5-118.0 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{63}H_{49}Cl_2NP_3OsSe]^+$, 1254.1229; Found: 1254.1198. Anal. Calcd. for $C_{63}H_{49}F_6Cl_2NP_4OsSe$: C, 54.12; H, 3.53; N, 1.00. Found: C, 53.98; H, 3.61; N, 1.12.

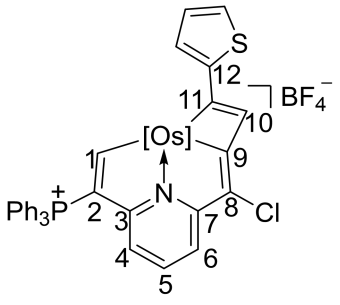
General Procedure for the Synthesis of 4 (Procedure 1)



Complexes	**4a**	**4b**	**4c**	**4d**
R				
Yield	75%	78%	76%	75%

A mixture of compound **1** (150 mg, 0.12 mmol), $HCl{\cdot}Et_2O$ (30 μL, 2M, 0.06 mmol) and aromatic terminal alkynes (0.60 mmol) were dissolved in CH_2Cl_2 (5 mL). After stirring for 48 hours at 40 ℃, the solution was evaporated to 2 mL and recrystallized from CH_2Cl_2/Et_2O= 5/1 mixture. The compound **4** was obtained in 75~78% yield as an orange solid.

Synthesis and characterization of 4a

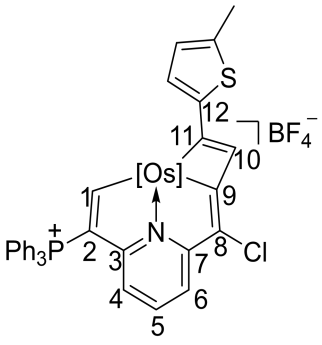


4a

[Os] = $OsCl(PPh_3)_2$

4a was synthesized according to **Procedure 1** and obtained in 75% yield (123 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.88 (d, $J_{P\text{-}H}$ = 21.6 Hz, 1H, C^1*H*), 7.91 (br, 1H, C^{10}*H*), 6.93 (br, C^5*H*), 6.44 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 6.16 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 7.87-6.67 (m, 50H, other aromatic protons plus C^{10}*H*, C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 13.45 (s, C*P*Ph_3), -25.13 (s, Os*P*Ph_3). ^{13}C NMR (150.9 MHz, CD_2Cl_2, δ ppm): 234.10 (m, C^1), 165.70 (d, $J_{P\text{-}C}$ = 30.2 Hz, C^3), 164.56 (s, C^7), 151.14 (t, $J_{P\text{-}C}$ = 5.4 Hz, C^9), 148.83 (t, $J_{P\text{-}C}$ = 8.2 Hz, C^{11}), 147.98 (s, C^{12}), 136.06 (s, C^5), 135.50 (s, C^{10}), 115.74 (s, C^6), 111.75 (d, $J_{P\text{-}C}$ = 87.5 Hz, C^2), 110.92 (s, C^4), 108.95 (s, C^8), 135.5-118.5 (m, PPh_3). HRMS (ESI): m/z calcd for $[C_{69}H_{53}Cl_2NOsP_3S]^+$, 1282.2103; Found: 1282.2085. Anal. Calcd. for $C_{69}H_{53}BCl_2F_4NOsP_3S$: C, 60.53; H, 3.90; N, 1.02; S, 2.34. Found: C, 60.21; H, 4.21; N, 0.92; S, 2.11.

Synthesis and characterization of 4b



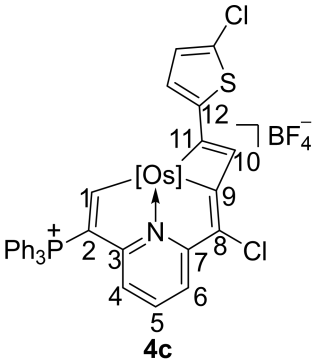
4b

[Os] = $OsCl(PPh_3)_2$

4b was synthesized according to **Procedure 1** and obtained in 78% yield (129 mg) as an yellow solid. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.83 (d, $J_{P\text{-}H}$ = 21.6 Hz, 1H, C^1*H*), 7.83 (br, C^{10}*H*), 7.06 (br, C^5*H*), 6.45 (d, $J_{H\text{-}H}$ = 7.2 Hz, 1H, C^6*H*), 6.16 (d, $J_{H\text{-}H}$ = 7.2 Hz, 1H, C^4*H*), 0.88 (s, 3H, CH_3), 7.89-6.63 (m, 49H, other

aromatic protons plus C[10]*H*, C[5]*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 13.56 (s, C*P*Ph_3), -24.95 (s, Os*P*Ph_3). ^{13}C NMR (150.9 MHz, CD_2Cl_2, δ ppm): 233.44 (m, C[1]), 165.65 (d, J_{P-C} = 30.2 Hz, C[3]), 164.40 (s, C[7]), 150.72 (t, J_{P-C} = 6.4 Hz, C[9]), 149.49 (s, C[12]), 147.47 (t, J_{P-C} = 8.5 Hz, C[11]), 136.29 (s, C[5]), 135.61 (s, C[10]), 115.86 (s, C[6]), 111.99 (d, J_{P-C} = 87.5 Hz, C[2]), 111.17 (s, C[4]), 109.26 (s, C[8]), 135.6-115.7 (m, PPh_3). HRMS (ESI): m/z calcd for $[C_{70}H_{55}Cl_2NOsP_3S]^+$, 1296.2260; Found: 1296.2201. Anal. Calcd. for $C_{70}H_{55}BCl_2F_4NOsP_3S$: C, 60.79; H, 4.01; N, 1.00; S, 2.32. Found: C, 61.02; H, 4.30; N, 1.26; S, 2.65.

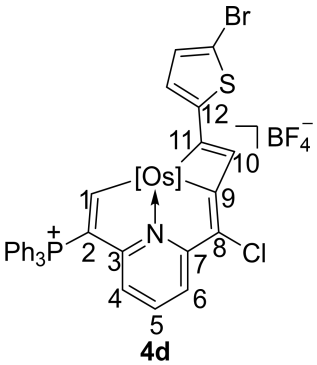
Synthesis and characterization of 4c



4c
[Os] = OsCl(PPh$_3$)$_2$

4c was synthesized according to **Procedure 1** and obtained in 76% yield (128 mg) as a yellow solid. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.83 (d, J_{P-H} = 21.6 Hz, 1H, C[1]*H*), 7.90 (br, C[10]*H*), 6.95 (br, C[5]*H*), 6.46 (d, J_{H-H} = 7.2 Hz, 1H, C[6]*H*), 6.17 (d, J_{H-H} = 7.2 Hz, 1H, C[4]*H*), 7.89-6.48 (m, 49H, other aromatic protons plus C[10]*H*, C[5]*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 13.56 (s, C*P*Ph_3), -24.94 (s, Os*P*Ph_3). ^{13}C NMR (150.9 MHz, CD_2Cl_2, δ ppm): 233.50 (m, C[1]), 165.63 (d, J_{P-C} = 30.2 Hz, C[3]), 164.40 (s, C[7]), 150.64 (t, J_{P-C} = 4.5 Hz, C[9]), 147.58 (t, J_{P-C} = 8.6 Hz, C[11]), 146.62 (s, C[12]), 136.15 (s, C[5]), 135.56 (s, C[10]), 115.82 (s, C[6]), 111.98 (d, J_{P-C} = 87.5 Hz, C[2]), 111.07 (s, C[4]), 109.17 (s, C[8]), 135.5-118.3 (m, PPh_3). HRMS (ESI): m/z calcd for $[C_{69}H_{52}Cl_3NOsP_3S]^+$, 1316.1714; Found: 1316.1672. Anal. Calcd. for $C_{69}H_{52}BCl_3F_4NOsP_3S$: C, 59.05; H, 3.73; N, 1.00; S, 2.28. Found: C,58.77; H, 3.94; N, 1.17; S, 2.35.

Synthesis and characterization of 4d



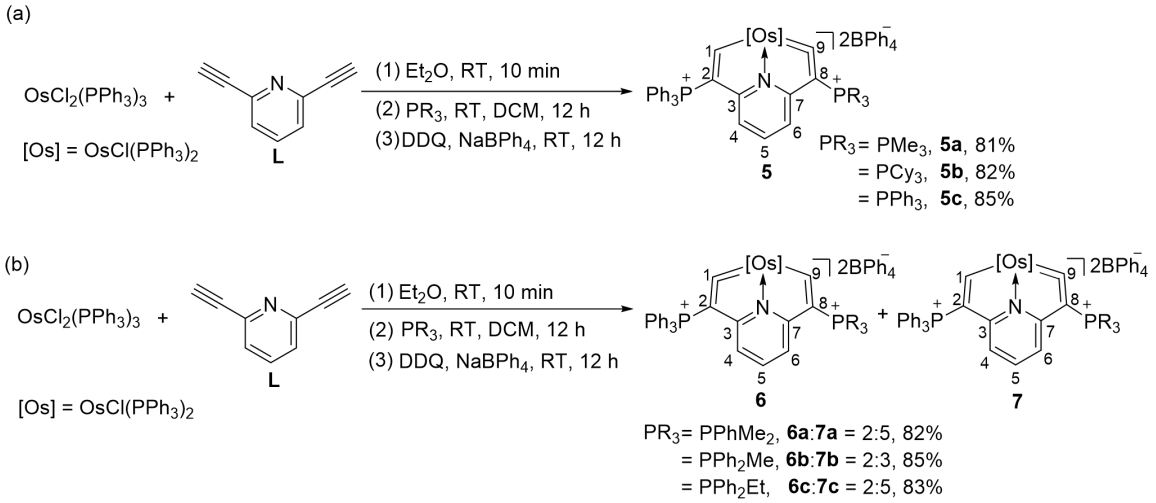
4d
[Os] = OsCl(PPh$_3$)$_2$

4d was synthesized according to **Procedure 1** and obtained in 75% yield (130 mg) as a yellow solid. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 12.84 (d, J_{P-H} = 21.6 Hz, 1H, C[1]*H*), 7.87 (br, C[10]*H*), 6.93 (br, C[5]*H*), 6.45 (d, J_{H-H} = 7.8 Hz, 1H, C[6]*H*), 6.16 (d, J_{H-H} = 7.8 Hz, 1H, C[4]*H*), 7.89-6.62 (m, 49H, other aromatic protons plus C[10]*H*,

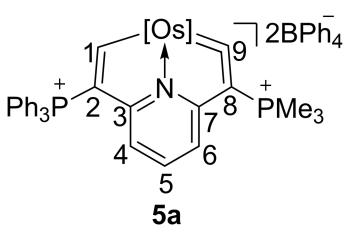
C^5H). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 13.50 (s, $CPPh_3$), -25.04 (s, $OsPPh_3$). ^{13}C NMR (150.9 MHz, CD_2Cl_2, δ ppm): 233.26 (m, C^1), 165.29 (d, J_{P-C} = 30.2 Hz, C^3), 164.09 (s, C^7), 149.11 (s, C^{12}), 150.43 (t, J_{P-C} = 6.9 Hz, C^9), 147.18 (t, J_{P-C} = 8.2 Hz, C^{11}), 135.67 (s, C^5), 134.90 (s, C^{10}), 115.48 (s, C^6), 111.53 (d, J_{P-C} = 86.9 Hz, C^2), 110.65 (s, C^4), 108.91 (s, C^8), 135.1-111.2 (m, PPh_3). HRMS (ESI): m/z calcd for $[C_{69}H_{52}BrCl_2NOsP_3S]^+$, 1360.1209; Found: 1360.1030. Anal. Calcd. for $C_{69}H_{52}BBrCl_2F_4NOsP_3S$: C, 57.23; H, 3.62; N, 0.97; S, 2.21. Found: C,57.52; H, 3.58; N, 1.22; S, 2.35.

General procedure for the synthesis of 5, isomers (6 and 7) (Procedure 2)

A mixture of $OsCl_2(PPh_3)_3$ (150 mg, 0.14 mmol, 1.0 equiv) and 2,6-diethynylpyridine (22 mg, 0.17 mmol, 1.2 equiv) were dissolved in Et_2O (5 mL). The reaction mixture was stirred for 10 minutes at room temperature, then PR_3 (0.42 mmol, 3.0 equiv) was added and stirred at room temperature for 12 hours. DDQ (1.2~4.0 equiv) and $NaBPh_4$ (342 mg, 0.7 mmol, 5.0 equiv) were added subsequently to give a brown suspension and after 12 hours the solid suspension was removed through a filter. The residue was recrystallized from CH_2Cl_2/MeOH 1/10 mixture. The compounds **5** were obtained in 81~85% yield as yellow solids. The compounds **6** and **7** (isomers) were obtained in 82~85% yield as yellow solids.



Synthesis and characterization of 5a

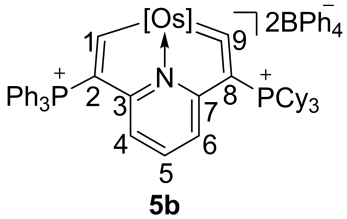


5a

[Os] = $OsCl(PPh_3)_2$

The product was synthesized according to **Procedure 2** with PMe_3 (43 μL, 0.42 mmol) for 12 h and DDQ (38 mg, 0.17 mmol, 1.2 equiv). The compound **5a** was obtained in 81% yield (210 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.35 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1*H*), 6.72 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.09 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 5.47 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 0.80 (d, $J_{P\text{-}H}$ = 13.8 Hz, 9H, C*H*$_3$), 7.86-6.30 (m, 86 H, other aromatic protons plus C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.15 (s, C^2*P*Ph_3), 6.34 (s, Os*P*Ph_3), 1.02 (s, C^8*P*Me_3). ^{13}C-NMR (150.9 MHz, CD_2Cl_2/$(CD_3)_2SO$ = 1/1, δ ppm): 330.68 (br, C^9), 222.52 (br, C^1), 163.60 (br, C^3), 158.62 (d, $J_{P\text{-}C}$ = 21.1 Hz, C^7), 141.60 (s, C^5), 115.43 (d, $J_{P\text{-}C}$ = 86.0 Hz, C^2), 112.21 (s, C^6), 111.36 (s, C^4), 101.32 (d, $J_{P\text{-}C}$ = 105.6 Hz, C^8), 8.50 (d, $J_{P\text{-}C}$ = 57.3 Hz, *C*H$_3$), 135.3-116.0 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{66}H_{58}ClNP_4Os]^{2+}$, 607.6406; Found: 607.6407. Anal. Calcd. for $C_{114}H_{98}B_2ClNP_4Os$: C, 73.88; H, 5.33; N, 0.76. Found: C, 74.08; H, 5.48; N, 0.94.

Synthesis and characterization of 5b



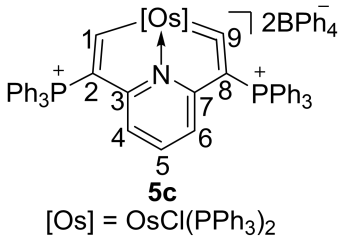
5b

[Os] = $OsCl(PPh_3)_2$

The product was synthesized according to **Procedure 2** with PCy_3 (118 mg, 0.42 mmol) for 12 h and DDQ (128 mg, 0.56 mmol, 4.0 equiv). The compound **5b** was obtained in 82% yield (236 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.20 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1*H*), 7.38 (br, C^5*H*), 6.74 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 6.31 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 7.86-6.63 (m, 87H, other aromatic protons plus C^5*H*, C^6*H*), 1.75-1.13 (m, 33H, Cy). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 22.45 (s, C^8*P*Cy_3), 14.17 (s, C^2*P*Ph_3), 1.36 (s, Os*P*Ph_3). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 336.34 (m, C^9), 223.85 (m, C^1), 165.35 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^3), 161.87 (d, $J_{P\text{-}C}$ = 18.1 Hz, C^7), 143.94 (s, C^5), 119.24 (d, $J_{P\text{-}C}$ = 92.0 Hz, C^2), 113.48 (s, C^6), 112.85 (s, C^4), 94.82 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^8), 141.4-110.9 (m, other aromatic carbons), 35.6-14.2 (m, Cy). HRMS (ESI): m/z calcd for $[C_{81}H_{82}ClNP_4Os]^{2+}$, 709.7345; Found: 709.7318.

Anal. Calcd. for $C_{129}H_{122}B_2ClNP_4Os$: C, 75.30; H, 5.98; N, 0.68. Found: C, 75.52; H, 6.25; N, 0.74.

Synthesis and characterization of 5c

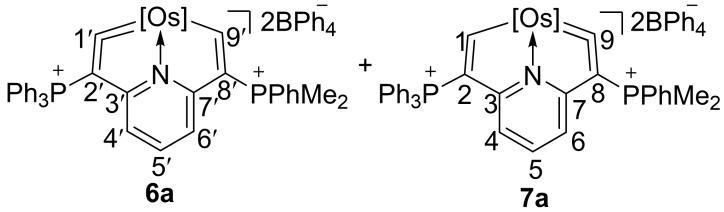


5c

[Os] = $OsCl(PPh_3)_2$

The product was synthesized according to **Procedure 2** with PPh_3 (110 mg, 0.42 mmol) for 12 h and DDQ (96 mg, 0.42 mmol, 3.0 equiv). The compound **5c** was obtained in 85% yield (243 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.29 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1*H*), 6.90 (br, C^5*H*), 6.23 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 5.99 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 7.86-6.39 (m, 101H, other aromatic protons plus C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.67 (s, C^2*P*Ph_3), 3.39 (s, C^8*P*Ph_3), 3.15 (s, Os*P*Ph_3). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 335.08 (m, C^9), 223.39 (m, C^1), 164.80 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^3), 160.84 (d, $J_{P\text{-}C}$ = 21.1 Hz, C^7), 143.02 (s, C^5), 117.50 (d, $J_{P\text{-}C}$ = 84.5 Hz, C^2), 113.02 (s, C^6), 112.98 (s, C^4), 97.87 (d, $J_{P\text{-}C}$ = 113.2 Hz, C^8), 136.3-118.3 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{81}H_{64}ClNP_4Os]^{2+}$, 700.6641; Found: 700.6639. Anal. Calcd. for $C_{129}H_{104}B_2ClNP_4Os$: C, 75.97; H, 5.14; N, 0.69. Found: C, 76.12; H, 5.25; N, 0.84.

Synthesis and characterization of isomers (6a and 7a)



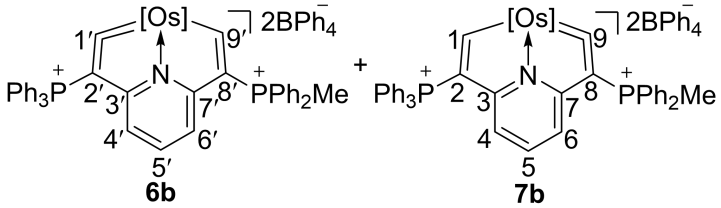
6a **7a**

[Os] = $OsCl(PPh_3)_2$ **6a**:**7a** = 2:5

The product was synthesized according to **Procedure 2** with $PPhMe_2$ (60 μL, 0.42 mmol) for 12 h and DDQ (54 mg, 0.24 mmol, 1.7 equiv). The compound **6a** and **7a** was obtained in 82% yield (220 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.32 (d, $J_{P\text{-}H}$ = 20.4 Hz, 5H, C^1*H*), 10.98 (d, $J_{P\text{-}H}$ = 20.4 Hz, 2H, C$^{9'}$*H*), 6.80-6.75 (m, 7H, C^5*H* plus C$^{5'}$*H*), 6.12 (d, $J_{H\text{-}H}$ = 7.8 Hz, 5H, C^4*H*), 5.93 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, C$^{6'}$*H*), 5.81 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, C$^{4'}$*H*), 5.65 (d, $J_{H\text{-}H}$ = 7.8 Hz, 5H, C^6*H*), 1.20 (d, $J_{P\text{-}H}$ = 12.6 Hz, 12H, C$'H_3$), 1.04 (d, $J_{P\text{-}H}$ = 13.2 Hz, 30H, CH_3), 7.84-6.33 (m, 637H, other aromatic protons plus C^5*H*, C$^{5'}$*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.20 (s, C^2*P*Ph_3), 10.69 (s,

C$^{8'}$*P*PhMe$_2$), 6.19 (s, Os*P*Ph$_3$ of **7a**), 3.94 (s, Os*P*Ph$_3$ of **6a**), 3.18 (s, C$^{2'}$*P*Ph$_3$), -0.82 (s, C^{8}*P*PhMe$_2$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 333.10 (m, C$^{1'}$), 332.92 (m, C^{9}), 224.40 (m, C^{1}), 215.91 (br, C$^{9'}$), 164.64 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^{3}), 162.80 (d, $J_{P\text{-}C}$ = 27.2 Hz, C$^{7'}$), 160.63 (d, $J_{P\text{-}C}$ = 21.1 Hz, C$^{3'}$), 159.27 (d, $J_{P\text{-}C}$ = 22.6 Hz, C^{7}), 142.84 (s, C^{5}), 142.72 (s, C$^{5'}$), 119.62 (d, $J_{P\text{-}C}$ = 86.0 Hz, C$^{8'}$), 116.40 (d, $J_{P\text{-}C}$ = 86.0 Hz, C^{2}), 112.72 (s, C$^{4'}$), 112.18 (s, C^{6}), 112.10 (s, C^{4}), 111.22 (s, C$^{6'}$), 100.94 (d, $J_{P\text{-}C}$ = 110.2 Hz, C^{8}), 97.04 (d, $J_{P\text{-}C}$ = 116.2 Hz, C$^{2'}$), 8.71 (d, $J_{P\text{-}C}$ = 57.3 Hz, *C*H$_3$), 8.41 (d, $J_{P\text{-}C}$ = 57.3 Hz, *C*'H$_3$), 136.3-116.1 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{71}H_{60}ClNP_4Os]^{2+}$, 638.6484; Found: 638.6465. Anal. Calcd. for $C_{119}H_{100}B_2ClNP_4Os$: C, 74.63; H, 5.26; N, 0.73. Found: C, 74.48; H, 5.44; N, 0.85.

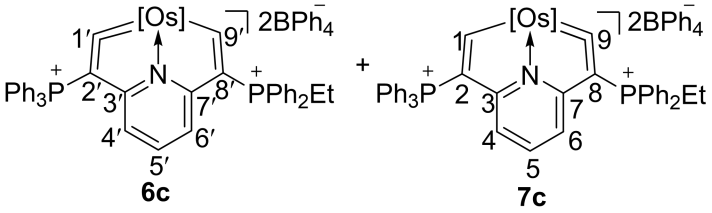
Synthesis and characterization of isomers (6b and 7b)



The product was synthesized according to **Procedure 2** with PPh$_2$Me (78 µL, 0.42 mmol) for 12 h and DDQ (70 mg, 0.31 mmol, 2.2 equiv). The compound **6b** and **7b** was obtained in 85% yield (235 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.23 (d, $J_{P\text{-}H}$ = 21.6 Hz, 3H, C^{1}*H*), 10.89 (d, $J_{P\text{-}H}$ = 19.2 Hz, 2H, C$^{9'}$*H*), 6.88-6.82 (m, 5H, C^{5}*H* plus C$^{5'}$*H*), 6.20 (d, $J_{H\text{-}H}$ = 7.8 Hz, 3H, C^{4}*H*), 6.09 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, C$^{6'}$*H*), 5.89 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, C$^{4'}$*H*), 5.76 (d, $J_{H\text{-}H}$ = 7.8 Hz, 3H, C^{6}*H*), 1.70 (d, $J_{P\text{-}H}$ = 12.6 Hz, 6H, C'*H*$_3$), 1.33 (d, $J_{P\text{-}H}$ = 13.2 Hz, 9H, C*H*$_3$), 7.84-6.77 (m, 480H, other aromatic protons plus C^{5}*H*, C$^{5'}$*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.22 (s, C^{2}*P*Ph$_3$), 12.26 (s, C$^{8'}$*P*Ph$_2$Me), 5.24 (s, Os*P*Ph$_3$ of **7b**), 3.57 (s, Os*P*Ph$_3$ of **6b**), 3.37 (s, C$^{2'}$*P*Ph$_3$), -0.28 (s, C^{8}*P*Ph$_2$Me). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 333.78 (m, C^{9}, C$^{1'}$), 224.41 (m, C^{1}), 219.56 (m, C$^{9'}$), 164.86 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^{3}), 163.30 (d, $J_{P\text{-}C}$ = 27.2 Hz, C$^{7'}$), 160.55 (d, $J_{P\text{-}C}$ = 21.1 Hz, C$^{3'}$), 160.04 (d, $J_{P\text{-}C}$ = 22.6 Hz, C^{7}), 143.03 (s, C^{5}), 142.86 (s, C$^{5'}$), 119.09 (d, $J_{P\text{-}C}$ = 86.1 Hz, C$^{8'}$), 116.68 (d, $J_{P\text{-}C}$ = 86.0 Hz, C^{2}), 112.86 (s, C^{6}), 112.78 (s, C$^{4'}$), 112.49 (s, C^{4}), 112.13 (s, C$^{6'}$), 99.16 (d, $J_{P\text{-}C}$ =

113.2 Hz, C^{8}), 97.21 (d, $J_{P\text{-}C}$ = 113.2 Hz, $C^{2'}$), 8.12 (d, $J_{P\text{-}C}$ = 58.9 Hz, CH_3), 7.67 (d, $J_{P\text{-}C}$ = 58.9 Hz, $C'H_3$), 136.3-114.1 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{76}H_{62}ClNP_4Os]^{2+}$, 669.6563; Found: 669.6546. Anal. Calcd. for $C_{124}H_{102}B_2ClNP_4Os$: C, 75.32; H, 5.20; N, 0.71. Found: C, 75.64; H, 5.34; N, 0.96.

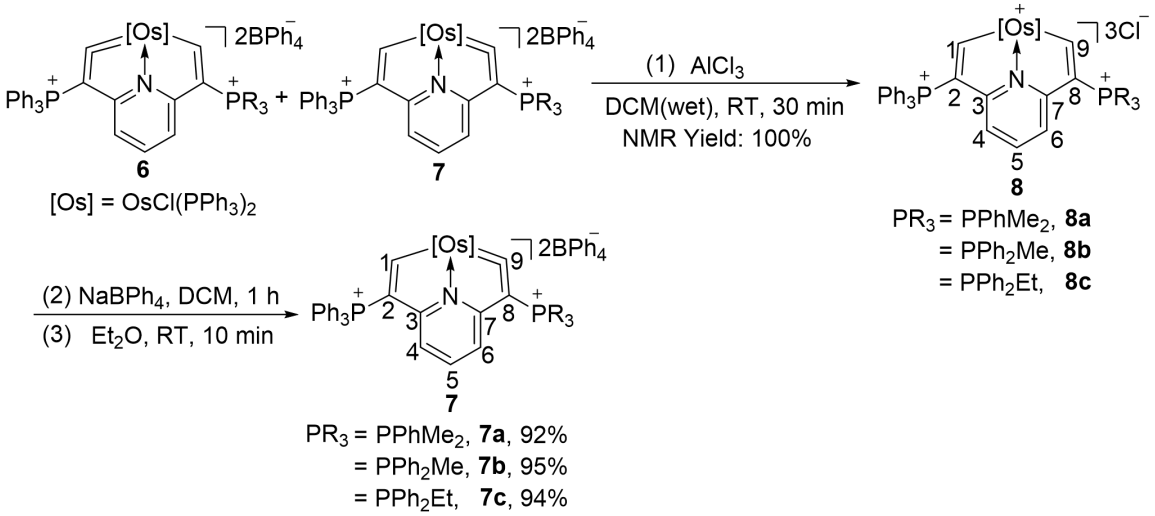
Synthesis and characterization of isomers (6c and 7c)



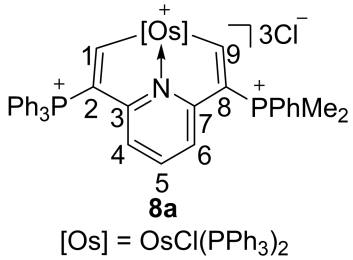
The product was synthesized according to **Procedure 2** with PPh_2Et (86 µL, 0.42 mmol) for 12 h and DDQ (54 mg, 0.24 mmol, 1.7 equiv). The compound **6c** and **7c** was obtained in 83% yield (231 mg). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.33 (d, $J_{P\text{-}H}$ = 18.0 Hz, 2H, $C^{9'}H$), 11.27 (d, $J_{P\text{-}H}$ = 19.2 Hz, 5H, $C^{1}H$), 6.69 (t, $J_{H\text{-}H}$ = 7.8 Hz, 2H, $C^{5'}H$), 6.66 (t, $J_{H\text{-}H}$ = 7.8 Hz, 5H, $C^{5}H$), 6.16 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, $C^{6'}H$), 6.10 (d, $J_{H\text{-}H}$ = 7.8 Hz, 5H, $C^{4}H$), 5.87 (d, $J_{H\text{-}H}$ = 7.8 Hz, 5H, $C^{6}H$), 5.83 (d, $J_{H\text{-}H}$ = 7.8 Hz, 2H, $C^{4'}H$), 2.23-2.12 (m, 14H, CH_2), 0.91-0.83 (m, 21H, CH_3), 7.84-6.31 (m, 672H, other aromatic protons plus $C^{5}H$, $C^{5'}H$). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 16.78 (s, $C^{8'}PPh_2Et$), 14.44 (s, $C^{2}PPh_3$), 7.38 (s, $C^{8}PPh_2Et$), 4.30 (s, $OsPPh_3$ of **7c**), 3.23 (s, $OsPPh_3$ of **6c**+$C^{2'}PPh_3$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 334.09 (m, $C^{1'}$+C^{9}), 223.52 (m, C^{1}), 219.47 (m, $C^{9'}$), 164.68 (d, $J_{P\text{-}C}$ = 24.2 Hz, C^{3}), 163.80 (d, $J_{P\text{-}C}$ = 27.2 Hz, $C^{7'}$), 160.75 (d, $J_{P\text{-}C}$ = 19.6 Hz, $C^{3'}$), 160.04 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^{7}), 143.20 (s, $C^{5'}$), 143.09 (s, C^{5}), 119.31 (d, $J_{P\text{-}C}$ = 92.0 Hz, C^{2}), 118.04 (d, $J_{P\text{-}C}$ = 92.3 Hz, $C^{8'}$), 113.22 (s, C^{6}), 112.98 (s, $C^{4'}$), 112.79 (s, C^{4}), 112.67 (s, $C^{6'}$), 98.25 (d, $J_{P\text{-}C}$ = 108.7 Hz, C^{8}), 97.46 (d, $J_{P\text{-}C}$ = 107.2 Hz, $C^{2'}$), 18.30 (d, $J_{P\text{-}C}$ = 57.3 Hz, CH_2), 17.46 (d, $J_{P\text{-}C}$ = 54.3 Hz, $C'H_2$), 7.54 (d, $J_{P\text{-}C}$ = 4.5 Hz, $C'H_3$), 7.42 (d, $J_{P\text{-}C}$ = 4.5 Hz, CH_3), 140.5-115.7 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{77}H_{64}ClNP_4Os]^{2+}$, 676.6641; Found: 676.6632. Anal. Calcd. for $C_{125}H_{104}B_2ClNP_4Os$: C, 75.39; H, 5.26; N, 0.70. Found: C, 75.58; H, 5.52; N, 0.82.

General procedure for the synthesis of 8 and 7 (Procedure 3)

A mixture of **6** and **7** (150 mg, 1.0 equiv) and $AlCl_3$ (15 equiv) were dissolved in DCM (wet, 2 mL). The reaction mixture was stirred for 30 minutes at room temperature to give an orange suspension, the solid suspension was removed through a filter to give an orange solution of **8** (approximately 100% yield based on ^1H and $^{31}P\{1H\}$ NMR), then added $NaBPh_4$ (15 equiv) to the orange solution and stirred for 1 hour at room temperature to give a brown suspension, the solid suspension was removed through a filter to take excess sodium off. Et_2O (20 mL) was added into the residue and stirred for 10 minutes. The compound **7** was obtained in 92~95% yield as a yellow solid by filtration.

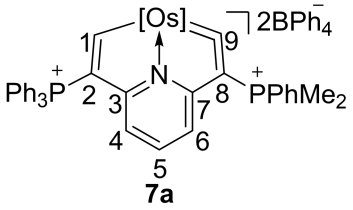


Synthesis and characterization of 8a and 7a



The product **8a** was synthesized according to **Procedure 3** with a mixture of **6a** and **7a** (150 mg, 0.078 mmol) and $AlCl_3$ (156 mg, 1.17 mmol). ^1H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 9.00 (dd, $J_{P\text{-}H}$ = 11.1 Hz, $J_{H\text{-}H}$ = 5.1 Hz, 1H, C^1H), 8.64 (dd, $J_{P\text{-}H}$ = 11.4 Hz, $J_{H\text{-}H}$ = 4.8 Hz, 1H, C^9H), 7.78 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 6.56 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6H), 6.45 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4H), 1.94 (d, $J_{P\text{-}H}$ = 12.6 Hz, 6H, CH_3), 8.11-6.49 (m, other aromatic protons plus C^5H, C^6H, C^4H). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 22.83 (s, Os*P*Ph_3), 12.13 (s, C^2*P*Ph_3), 11.75 (s, C^8*P*$PhMe_2$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 212.76 (td apparent t, $J_{P\text{-}C}$ = 6.1 Hz, C^1),

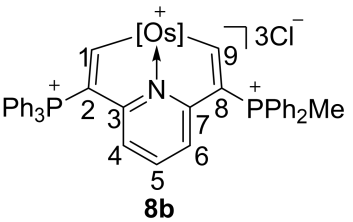
209.49 (td apparent t, $J_{P\text{-}C}$ = 6.8 Hz, C^9), 159.14 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^3), 157.33 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^7), 146.83 (s, C^5), 124.28 (d, $J_{P\text{-}C}$ = 86.0 Hz, C^8), 121.75 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^2), 118.94 (s, C^4), 117.85 (s, C^6), 8.92 (d, $J_{P\text{-}C}$ = 57.3 Hz, *C*H_3), 146.5-114.2 (m, other aromatic carbons).



7a
[Os] = $OsCl(PPh_3)_2$

The compound **7a** was obtained in 92% yield (137 mg) according to **Procedure 3**. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.31 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1*H*), 7.08 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5*H*), 6.22 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 6.07 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 1.45 (d, $J_{P\text{-}H}$ = 13.2 Hz, 6H, C*H*$_3$), 7.95-6.38 (m, 91 H, other aromatic protons plus C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.19 (s, C^2*P*Ph_3), 6.11 (s, Os*P*Ph_3), -0.80 (s, C^8*P*PhMe). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 332.96 (m, C^9), 224.29 (m, C^1), 164.65 (d, $J_{P\text{-}C}$ = 28.7 Hz, C^3), 159.38 (d, $J_{P\text{-}C}$ = 22.6 Hz, C^7), 143.39 (s, C^5), 116.66 (d, $J_{P\text{-}C}$ = 87.5 Hz, C^2), 112.82 (s, C^6), 112.42 (s, C^4), 101.10 (d, $J_{P\text{-}C}$ = 111.7 Hz, C^8), 9.49 (d, $J_{P\text{-}C}$ = 58.9 Hz, *C*H_3), 136.3-117.5 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{71}H_{60}ClNP_4Os]^{2+}$, 638.6484; Found: 638.6477. Anal. Calcd. for $C_{119}H_{100}B_2ClNP_4Os$: C, 74.63; H, 5.26; N, 0.73. Found: C, 74.48; H, 5.30; N, 0.62.

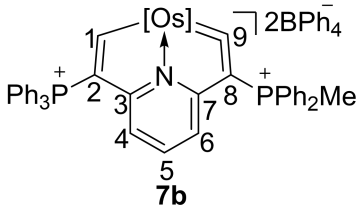
Synthesis and characterization of 8b and 7b



8b
[Os] = $OsCl(PPh_3)_2$

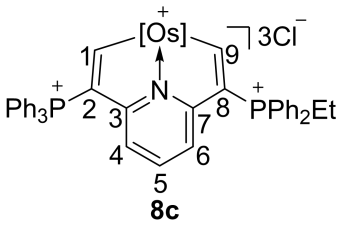
The product **8b** was synthesized according to **Procedure 3** with a mixture of **6b** and **7b** (150 mg, 0.076 mmol) and $AlCl_3$ (152mg, 1.14 mmol). ^{1}H-NMR (400.1 MHz, CD_2Cl_2, δ ppm): 9.08 (dd, $J_{P\text{-}H}$ = 11.2 Hz, $J_{H\text{-}H}$ = 4.8 Hz, 1H, C^1*H*), 8.67 (dd, $J_{P\text{-}H}$ = 11.2 Hz, $J_{H\text{-}H}$ = 4.8 Hz, 1H, C^9*H*), 7.88 (t, $J_{H\text{-}H}$ = 8.0 Hz, 1H, C^5*H*), 6.61 (d, $J_{H\text{-}H}$ = 8.0 Hz, 1H, C^4*H*), 6.57 (d, $J_{H\text{-}H}$ = 8.0 Hz, 1H, C^6*H*), 2.25 (d, $J_{P\text{-}H}$ = 12.8 Hz, 3H, C*H*$_3$), 8.13-6.56 (m, other aromatic protons plus C^5*H*, C^6*H*, C^4*H*). ^{31}P-NMR (161.9 MHz, CD_2Cl_2, δ ppm): 21.99 (s, Os*P*Ph_3), 12.14 (s, C^2*P*Ph_3), 10.75 (s, C^8*P*Ph_2Me). ^{13}C-NMR (100.6 MHz, CD_2Cl_2, δ ppm): 213.34 (td apparent t, $J_{P\text{-}C}$ = 6.4 Hz, C^1), 211.84 (td apparent t, $J_{P\text{-}C}$ =5.6 Hz, C^9), 159.40 (d, $J_{P\text{-}C}$ = 19.1 Hz, C^3), 158.24 (d,

$J_{P\text{-}C}$ = 20.1 Hz, C^7), 147.44 (s, C^5), 123.92 (d, $J_{P\text{-}C}$ = 89.5 Hz, C^8), 122.36 (d, $J_{P\text{-}C}$ = 94.6 Hz, C^2), 119.58 (s, C^4), 119.07 (s, C^6), 8.10 (d, $J_{P\text{-}C}$ = 58.3 Hz, CH_3), 137.7-122.5 (m, other aromatic carbons).



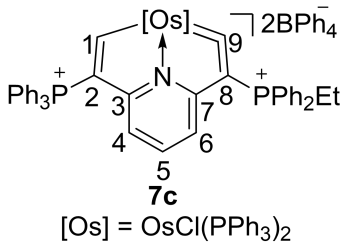
The compound **7b** was obtained in 95% yield (143 mg) according to **Procedure 3**. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.23 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1H), 6.71 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 6.17 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4H), 5.65 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6H), 1.18 (d, $J_{P\text{-}H}$ = 12.6 Hz, 3H, CH_3), 7.83-6.37 (m, 96 H, other aromatic protons plus C^5H). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.22 (s, C^2PPh_3), 5.25 (s, OsPPh_3), -0.29 (s, C^8PPh_2Me). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 333.92 (m, C^9), 224.61 (m, C^1), 164.92 (d, $J_{P\text{-}C}$ = 27.2 Hz, C^3), 160.08 (d, $J_{P\text{-}C}$ = 21.1Hz, C^7), 142.93 (s, C^5), 116.66 (d, $J_{P\text{-}C}$ = 86.0 Hz, C^2), 112.79 (s, C^6), 112.46 (s, C^4), 99.12 (d, $J_{P\text{-}C}$ = 113.2 Hz, C^8), 8.02 (d, $J_{P\text{-}C}$ = 58.9 Hz, CH_3), 136.3-117.4 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{76}H_{62}ClNP_4Os]^{2+}$, 669.6563; Found: 669.6563. Anal. Calcd. for $C_{124}H_{102}B_2ClNP_4Os$: C, 75.32; H, 5.20; N, 0.71. Found: C, 75.45; H, 5.57; N, 0.82.

Synthesis and characterization of 8c and 7c



The product **8c** was synthesized according to **Procedure 3** with a mixture of **6c and 7c** (150 mg, 0.075 mmol) and $AlCl_3$ (151 mg, 1.13 mmol). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 9.03 (dd, $J_{P\text{-}H}$ = 11.1 Hz, $J_{H\text{-}H}$ = 5.4 Hz, 1H, C^1H), 8.89 (dd, $J_{P\text{-}H}$ = 10.8 Hz, $J_{H\text{-}H}$ = 5.4 Hz, 1H, C^9H), 7.82 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 6.64 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6H), 6.49 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4H), 2.52-2.48 (m, 2H, CH_2), 1.20-1.12 (m, 3H, CH_3), 8.06-6.50 (m, other aromatic protons plus C^5H, C^6H, C^4H). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 20.77 (s, OsPPh_3), 16.89 (s, C^8PPh_2Et), 12.04 (s, C^2PPh_3). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 213.26 (td apparent t, $J_{P\text{-}C}$ = 7.5 Hz, C^1), 211.26 (td apparent t, $J_{P\text{-}C}$ = 7.5 Hz, C^9), 159.47 (d, $J_{P\text{-}C}$ = 18.1 Hz, C^3), 158.70 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^7), 147.40 (s, C^5), 123.93 (d, $J_{P\text{-}C}$ = 84.5 Hz, C^8), 122.35 (d, $J_{P\text{-}C}$

= 89.0 Hz, C^2), 119.62 (s, C^4), 119.54 (s, C^6), 17.34 (d, $J_{P\text{-}C}$ = 52.8 Hz, CH_2), 7.54 (d, $J_{P\text{-}C}$ = 4.5 Hz, CH_3), 137.7-112.9 (m, other aromatic carbons).

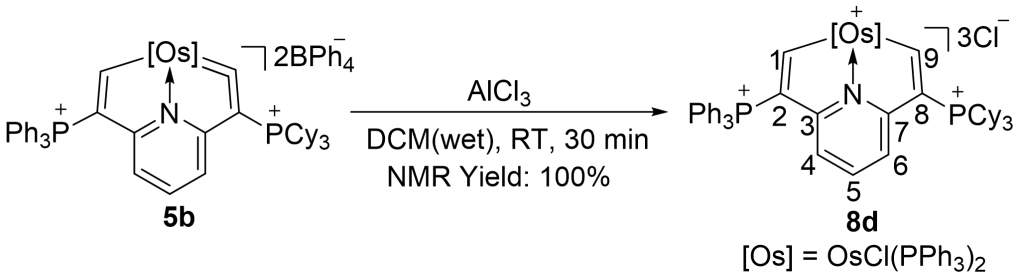


7c

[Os] = $OsCl(PPh_3)_2$

The compound **7c** was obtained in 94% yield (140 mg) according to **Procedure 3**. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.27 (d, $J_{P\text{-}H}$ = 19.2 Hz, 1H, C^1H), 6.63 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 6.09 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4H), 5.85 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6H), 2.20-2.18 (m, 2H, CH_2), 0.88-0.82 (m, 3H, CH_3), 7.84-6.34 (m, 96 H, other aromatic protons plus C^5H). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 14.44 (s, C^2PPh_3), 7.37 (s, C^8PPh_2Et), 4.29 (s, $OsPPh_3$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 334.17 (m, C^9), 223.66 (m, C^1), 164.69 (d, $J_{P\text{-}C}$ = 24.2 Hz, C^3), 160.03 (d, $J_{P\text{-}C}$ = 19.6 Hz, C^7), 142.72 (s, C^5), 119.28 (d, $J_{P\text{-}C}$ = 93.6 Hz, C^2), 112.98 (s, C^6), 112.68 (s, C^4), 98.10 (d, $J_{P\text{-}C}$ = 110.2 Hz, C^8), 18.22 (d, $J_{P\text{-}C}$ = 57.3 Hz, CH_2), 7.27 (d, $J_{P\text{-}C}$ = 6.0 Hz, CH_3), 141.5-115.6 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{77}H_{64}ClNP_4Os]^{2+}$, 676.6641; Found: 676.6639. Anal. Calcd. for $C_{125}H_{104}B_2ClNP_4Os$: C, 75.39; H, 5.26; N, 0.70. Found: C, 75.62; H, 5.54; N, 0.97.

Synthesis and characterization of 8d



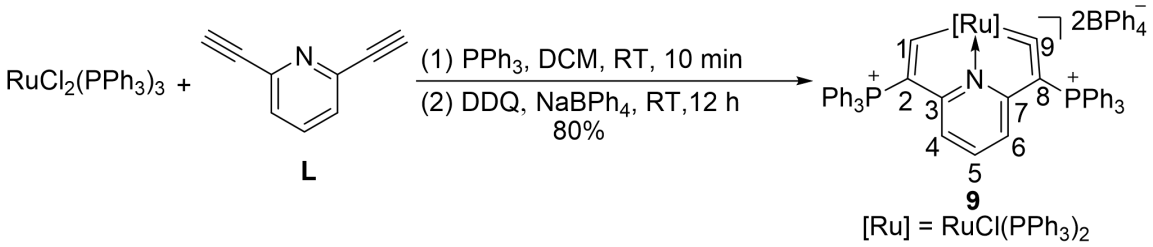
5b **8d**

[Os] = $OsCl(PPh_3)_2$

A mixture of **5b** (150 mg, 1.0 equiv) and $AlCl_3$ (15 equiv) were dissolved in DCM (wet, 2 mL). The reaction mixture was stirred for 30 minutes at room temperature to give an orange suspension, the solid suspension was removed through a filter to give an orange solution of **8d** (approximately 100% yield based on ^{1}H and ^{31}P{1H} NMR). ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 9.25 (dd, $J_{P\text{-}H}$ = 8.4 Hz, $J_{H\text{-}H}$ = 5.1 Hz, 1H, C^9H), 9.14 (dd, $J_{P\text{-}H}$ = 11.4 Hz, $J_{H\text{-}H}$ = 5.1 Hz, 1H, C^1H), 8.11 (t, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^5H), 7.11 (br, C^6H), 6.61 (br, C^4H), 1.85-1.09 (m, 33H, Cy), 8.10-

6.59 (m, other aromatic protons plus C^5*H*, C^6*H*, C^4*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 28.90 (s, C^8*P*Cy$_3$), 17.77 (s, Os*P*Ph$_3$), 12.02 (s, C^2*P*Ph$_3$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 213.22 (td apparent t, $J_{P\text{-}C}$ = 5.8 Hz, C^1), 209.42 (br, C^9), 160.55 (d, $J_{P\text{-}C}$ = 18.1 Hz, C^3), 160.24 (d, $J_{P\text{-}C}$ = 16.6 Hz, C^7), 147.46 (s, C^5), 122.11 (d, $J_{P\text{-}C}$ = 90.5 Hz, C^2), 119.77 (s, C^4), 119.42 (d, $J_{P\text{-}C}$ = 75.5 Hz, C^8), 119.02 (s, C^6), 33.5-25.3 (m, Cy), 147.7-114.8 (m, other aromatic carbons).

Synthesis and characterization of 9



A mixture of $RuCl_2(PPh_3)_3$ (150 mg, 0.16 mmol), PPh_3 (42 mg, 0.16 mmol) and 2,6-diethynylpyridine (20 mg, 0.16 mmol) were dissolved in DCM (5 mL). The reaction mixture was stirred for 10 minutes at room temperature, and DDQ (55 mg, 0.24 mmol) and $NaBPh_4$ (547 mg, 1.6 mmol) were added subsequently. The reaction mixture was stirred for 12 hours at at room temperature to give a brown suspension and the solid suspension was removed through a filter. The filtrate was evaporated to 2 mL recrystallized from CH_2Cl_2/MeOH 1/5 mixture. The compound **9** was obtained in 80% yield (250 mg) as a yellow solid. ^{1}H-NMR (600.1 MHz, CD_2Cl_2, δ ppm): 11.20 (d, $J_{P\text{-}H}$ = 20.4 Hz, 1H, C^1*H*), 6.88 (br, C^5*H*), 6.14 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^4*H*), 5.94 (d, $J_{H\text{-}H}$ = 7.8 Hz, 1H, C^6*H*), 7.81-6.79 (m, 101H, other aromatic protons plus C^5*H*). ^{31}P-NMR (242.9 MHz, CD_2Cl_2, δ ppm): 11.67 (s, C^2*P*Ph$_3$), 3.43 (s, C^8*P*Ph$_3$), 28.60 (s, Ru*P*Ph$_3$). ^{13}C-NMR (150.9 MHz, CD_2Cl_2, δ ppm): 366.80 (m, C^9), 237.88 (m, C^1), 163.61 (d, $J_{P\text{-}C}$ = 28.7 Hz, C^3), 160.55 (d, $J_{P\text{-}C}$ = 18.1 Hz, C^7), 142.34 (s, C^5), 117.41 (s, C^6), 116.82 (d, $J_{P\text{-}C}$ = 80.0 Hz, C^2), 116.22 (s, C^4), 99.11 (d, $J_{P\text{-}C}$ = 110.2 Hz, C^8), 136.3-117.2 (m, other aromatic carbons). HRMS (ESI): m/z calcd for $[C_{81}H_{64}ClNP_4Ru]^{2+}$, 655.6355; Found: 655.6357. Anal. Calcd. for $C_{129}H_{104}B_2ClNP_4Ru$: C, 79.45; H, 5.38; N, 0.72. Found: C, 79.21; H, 5.69; N, 0.97.

3. X-ray Crystallographic Analysis

Single-crystal X-ray diffraction data were collected on a Bruker CMOs area detector with monochromated Cu Kα radiation (λ = 1.54184 Å) for **1**, **P1'**, **2**, **3a**, **4d**, **5a**, **5c**, **7a** and **9**, on a Bruker D8-Venture with Ga generator (λ = 1.34139 Å) for **4a**. With Olex2 (Dolomanov *et al*., 2009), the structure was solved using the SHELXT[3] structure solution program and refined with the SHELXL[4] refinement package using least-squares minimization. Non-hydrogen atoms were refined anisotropically unless otherwise stated. Hydrogen atoms were introduced at their geometric positions and refined as riding atoms unless otherwise stated. Single crystals suitable for X-ray diffraction were grown from a solution of CH_2Cl_2 (**P1'**, **2**, **3a**, **5a**, **5c**, **7a** and **9**), $ClCH_2CH_2Cl$ (**1**, **4a** and **4d**) layered with hexane. X-ray crystal structures have been deposited in the Cambridge Crystallographic Database under the deposition numbers CCDC 2314889 (**1**), CCDC 2314895 (**P1'**), CCDC 2314890 (**2**), CCDC 2314891 (**3a**), CCDC 2314892 (**4a**), CCDC 2314893 (**4d**), CCDC 2314886 (**5a**), CCDC 2314884 (**5c**), CCDC 2314888 (**7a**), CCDC 2314894 (**9**). The data can be obtained free of charge from the CCDC (www.ccdc.cam.ac.uk/data_request/cif).

Crystal data for 1

$[C_{63}H_{49}Cl_2NOsP_3]BF_4 \cdot ClCH_2CH_2Cl$, molecular weight = 1359.80, temperature = 100.0 K, monoclinic, space group $P2_1/n$, a = 22.014(3) Å, b = 21.683(3) Å, c = 12.1814(15) Å, α = 90°, β = 98.337(5)°, γ = 90°, V = 5752.9(12) Å^3, Z = 4, ρ_{calc} = 1.570 g/cm^3, μ = 7.140 mm^{-1}, $F(000)$ = 2720.0, crystal size 0.10×0.10×0.09 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 8.156 to 144.834°, 54624 reflections, 10943 independent reflections (R_{int} = 0.0572, R_σ = 0.0413), data/restraints/parameters : 10943/159/759, GOF = 1.049, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0359/0.0846, R_1/ wR_2 (all data) : 0.0434/0.0896, largest diff. peak/hole : 1.49-1.29 e.Å^{-3}

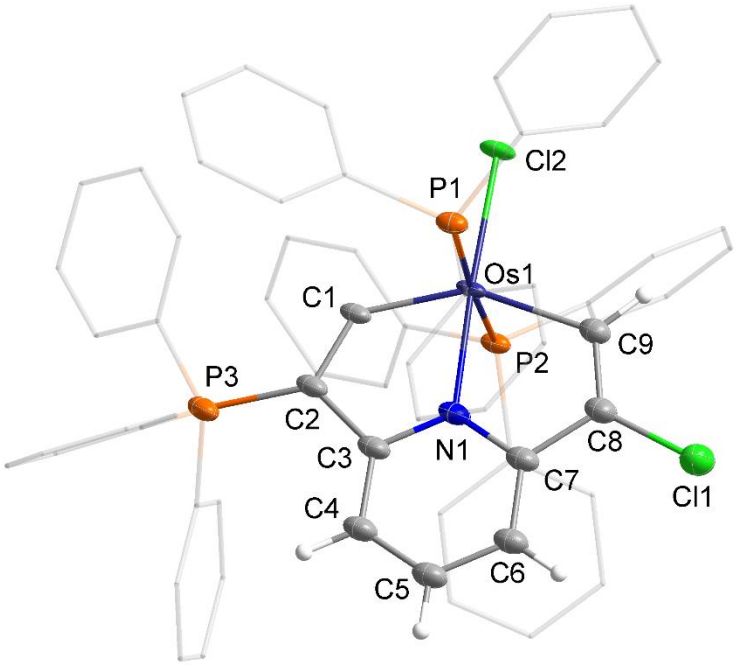


Figure S5. X-ray molecular structure for the cation of complex **1** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 1.841(4), Os1–N1 2.098(3), Os1–C9 2.102(4), C1–C2 1.381(5), C2–C3 1.461(5), C3–C4 1.405(5), C4–C5 1.383(6), C5–C6 1.380(6), C6–C7 1.389(5), C7–C8 1.445(5), C8–C9 1.334(5), C3–N1 1.354(5), C7–N1 1.359(5); C8–Cl1 1.754(4); Os1–C1–C2 129.2(3), C1–C2–C3 107.7(3), C2–C3–N1 111.1(3), C3–N1–Os1 118.4(2), N1–Os1–C1 73.61(13), Os1–N1–C7 120.2(2), N1–C7–C8 110.8(3), C7–C8–C9 117.3(3), C8–C9–Os1 117.4(3), N1–C3–C4 119.5(3), C3–C4–C5 119.1(4), C4–C5–C6 120.7(4), C5–C6–C7 118.8(4), C6–C7–N1 120.5(3), C3–N1–C7 124.4(3).

Crystal data for P1'

$[C_{64}H_{50}ClNOOsP_3]BPh_4 \cdot 3CH_2Cl_2$, molecular weight = 1741.59, temperature = 100.0(2) K, triclinic, space group *P-1*, *a* = 14.0545(4) Å, *b* = 17.0441(5) Å, *c* = 17.7828(6) Å, *α* = 78.0980(10)°, *β* = 81.6520(10)°, *γ* = 70.8870(10)°, *V* = 3924.5(2) Å^3, *Z* = 2, ρ_{calc} = 1.474 g/cm^3, *μ* = 6.221 mm^{-1}, *F*(000) = 1764.0, crystal size 0.2×0.18×0.15 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.568 to 144.292°, 76359 reflections, 15401 independent reflections (R_{int} = 0.0546, R_σ = 0.0359), data/restraints/parameters : 15401/6/946, GOF = 1.070, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0358/0.0958, R_1/ wR_2 (all data) : 0.0359/0.0958, largest diff. peak/hole : 1.93/-1.63 e.Å^{-3}

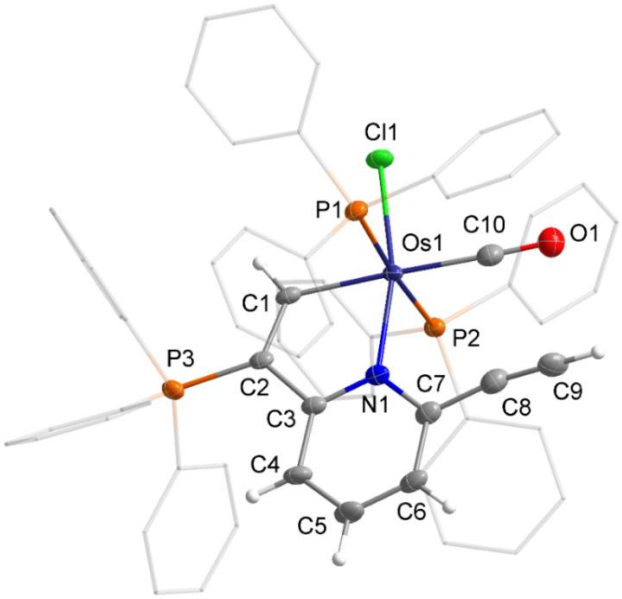


Figure S6. X-ray molecular structure for the cation of complex **P1'** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.061(3), Os1–N1 2.099(2), Os1–C10 1.934(3), C1–C2 1.350(4), C2–C3 1.467(4), C3–C4 1.385(4), C4–C5 1.383(4), C5–C6 1.382(5), C6–C7 1.392(4), C7–C8 1.423(4), C8–C9 1.217(6), C3–N1 1.382(3), C7–N1 1.366(4); Os1–C1–C2 117.6(2), C1–C2–C3 115.7(2), C2–C3–N1 112.9(2), C3–N1–Os1 116.57(18), N1–Os1–C1 76.96(10), Os1–N1–C7 126.57(18), N1–C7–C8 119.9(3), C7–C8–C9 170.1(4), N1–C3–C4 121.7(3), C3–C4–C5 120.8(3), C4–C5–C6 118.1(3), C5–C6–C7 119.9(3), C6–C7–N1 122.6(3), C3–N1–C7 116.9(2).

Crystal data for 2

$[C_{63}H_{50}Cl_2NOsP_3]Cl_2$, molecular weight = 1245.95, temperature = 100.0 K, monoclinic, space group $P2_1/n$, a = 12.5847(5) Å, b = 20.8470(8) Å, c = 21.1394(8) Å, α = 90°, β = 93.8120(10)°, γ = 90°, V = 5533.7(4) Å^3, Z = 4, ρ_{calc} = 1.496 g/cm^3, μ = 7.262 mm^{-1}, F(000) = 2496.0, crystal size 0.15×0.13×0.12 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.96 to 144.644°, 95746 reflections, 10922 independent reflections (R_{int} = 0.0378, R_σ = 0.0183), data/restraints/parameters : 10922/0/658, GOF = 1.054, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0316/0.0823, R_1/ wR_2 (all data) : 0.0324/0.0830, largest diff. peak/hole : 1.64/-1.74 e.Å^{-3}

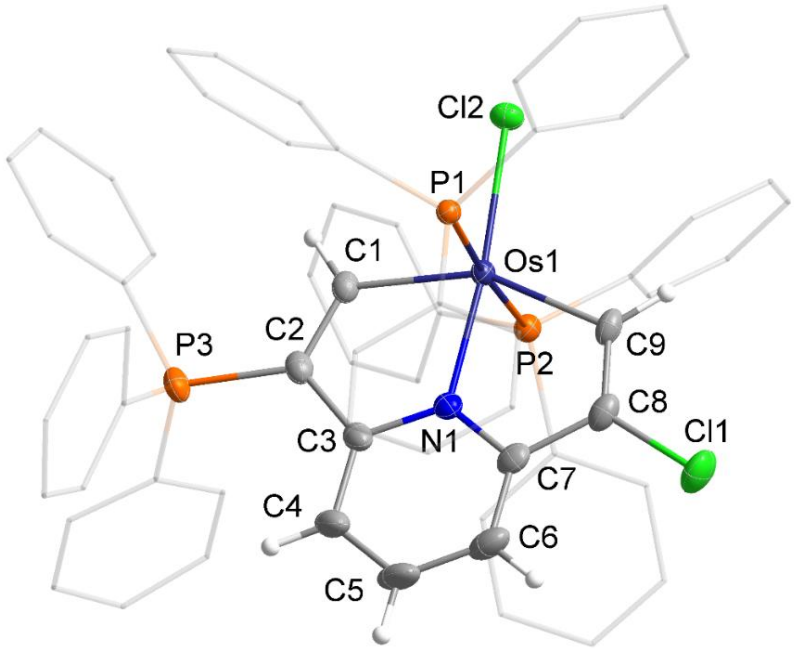


Figure S7. X-ray molecular structure for the cation of complex **2** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.025(3), Os1–N1 2.078(3), Os1–C9 2.096(3), C1–C2 1.367(5), C2–C3 1.458(5), C3–C4 1.384(5), C4–C5 1.396(6), C5–C6 1.382(6), C6–C7 1.382(5), C7–C8 1.449(5), C8–C9 1.345(5), C3–N1 1.365(4), C7–N1 1.359(4); Os1–C1–C2 120.1(2), C1–C2–C3 113.7(3), C2–C3–N1 111.3(3), C3–N1–Os1 119.6(2), N1–Os1–C1 75.21(12), Os1–N1–C7 119.6(2), N1–C7–C8 110.9(3), C7–C8–C9 117.83), C8–C9–Os1 115.7(2), N1–C3–C4 120.4(3), C3–C4–C5 119.0(4), C4–C5–C6 119.8(4), C5–C6–C7 119.6(4), C6–C7–N1 120.5(3), C3–N1–C7 120.6(3).

Crystal data for 3a

$[C_{63}H_{49}Cl_2NOsP_3S]PF_6$, molecular weight = 1351.07, temperature = 100.00 K, triclinic, space group *P-1*, *a* = 14.1630(7) Å, *b* = 14.2184(7) Å, *c* = 15.9648(8) Å, α = 98.109(2)°, β = 106.294(2)°, γ = 101.236(2)°, *V* = 2960.5(3) Å^3, *Z* = 2, ρ_{calc} = 1.516 g/cm^3, μ = 6.744 mm^{-1}, *F*(000) = 1348.0, crystal size 0.11×0.10×0.10 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.896 to 144.51°, 79552 reflections, 11652 independent reflections (R_{int} = 0.0526, R_σ = 0.0287), data/restraints/parameters : 11652/0/703, GOF = 1.036, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0311/0.0778, R_1/ wR_2 (all data) : 0.0337/0.0792, largest diff. peak/hole : 1.69/-1.61 e.Å^{-3}

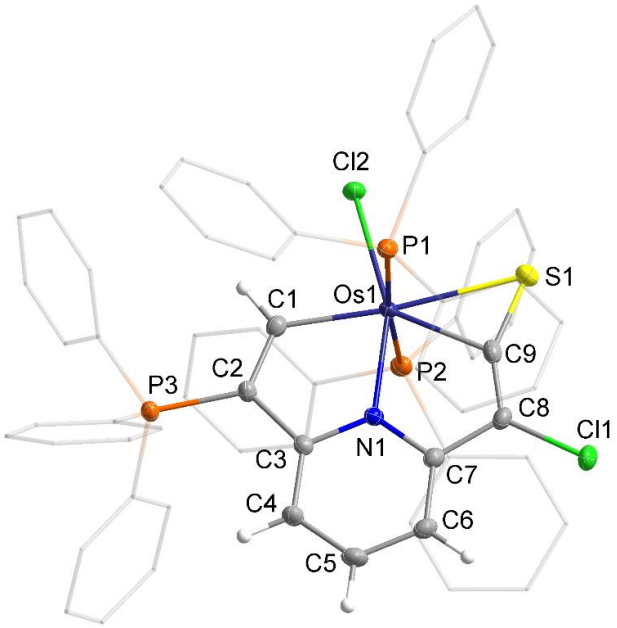


Figure S8. X-ray molecular structure for the cation of complex **3a** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.027(3), Os1–N1 2.103(2), Os1–C9 2.055(3), Os1–S1 2.5588(8), C1–C2 1.363(4), C2–C3 1.456(4), C3–C4 1.390(4), C4–C5 1.392(5), C5–C6 1.375(5), C6–C7 1.396(4), C7–C8 1.425(4), C8–C9 1.335(5), S1–C9 1.624(3), C3–N1 1.367(4), C7–N1 1.365(4); Os1–C1–C2 121.2(2), C1–C2–C3 113.8(3), C2–C3–N1 110.8(3), C3–N1–Os1 119.9(2), N1–Os1–C1 74.20(11), Os1–N1–C7 120.7(2), N1–C7–C8 111.3(3), C7–C8–C9 113.3(3), C8–C9–Os1 122.6(2), S1–Os1–C9 39.35(9), Os1–S1–C9 53.34(11), Os1–C9–S1 87.31(15), N1–C3–C4 120.7(3), C3–C4–C5 119.6(3), C4–C5–C6 119.9(3), C5–C6–C7 119.0(3), C6–C7–N1 121.4(3), C3–N1–C7 119.4(3).

Crystal data for 4a

$[C_{69}H_{53}Cl_2NOsP_3S]BF_4 \cdot 2ClCH_2CH_2Cl$, molecular weight = 1566.90, temperature = 100.00 K, triclinic, space group *P-1*, *a* = 9.9632(9) Å, *b* = 11.5217(10) Å, *c* = 29.202(3) Å, α = 78.917(3)°, β = 82.668(3)°, γ = 88.004(3)°, *V* = 3262.6(3) Å^3, *Z* = 2, ρ_{calc} = 1.595 g/cm^3, μ = 4.957 mm^{-1}, *F*(000) = 1572.0, crystal size 0.1×0.1×0.08 mm^3, $\lambda(Ga_{K\alpha})$ = 1.34139, $2\theta_{range}$ = 6.826 to 111.99°, 60506 reflections, 12772 independent reflections (R_{int} = 0.0686, R_σ = 0.0489), data/restraints/parameters : 12772/99/839, GOF = 1.044, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0486/0.1176, R_1/ wR_2 (all data) : 0.0516/0.1193, largest diff. peak/hole : 1.95/-2.01 e.Å^{-3}

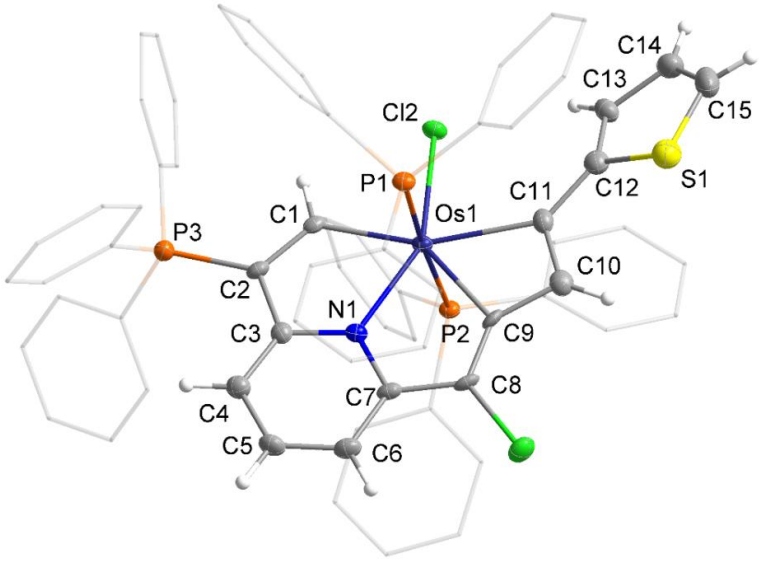


Figure S9. X-ray molecular structure for the cation of complex **4a** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.071(5), Os1–N1 2.135(4), Os1–C9 2.098(4), C1–C2 1.358(7), C2–C3 1.458(6), C3–C4 1.380(7), C4–C5 1.397(7), C5–C6 1.375(7), C6–C7 1.390(7), C7–C8 1.415(7), C8–C9 1.333(7), C3–N1 1.366(6), C7–N1 1.382(6), C9–C10 1.414(7), C10–C11 1.340(7); Os1–C1–C2 122.9(3), C1–C2–C3 122.9(4), C2–C3–N1 110.5(4), C3–N1–Os1 121.6(3), N1–Os1–C1 71.80(16), Os1–N1–C7 119.8(3), N1–C7–C8 111.4(4), C7–C8–C9 115.4(4), C8–C9–Os1 120.9(3), N1–Os1–C9 72.20(17), C9–Os1–C11 58.24(19), Os1–C9–C10 102.9(3), C9–C10–C11 100.6(4), N1–C3–C4 121.5(4), C3–C4–C5 119.4(5), C4–C5–C6 119.7(4), C5–C6–C7 119.3(5), C6–C7–N1 121.2(4), C3–N1–C7 118.6(4).

Crystal data for 4d

$[C_{69}H_{52}BrCl_2NOsP_3S]BF_4 \cdot ClCH_2CH_2Cl$, molecular weight = 1546.90, temperature = 100.00 K, triclinic, space group *P-1*, *a* = 10.0004(13) Å, *b* = 11.4627(15) Å, *c* = 27.876(4) Å, α = 101.832(5)°, β= 93.282(5)°, γ = 91.924(5)°, *V* = 3119.1(7) Å^3, *Z* = 2, ρ_{calc} = 1.647 g/cm^3, μ = 7.694 mm^{-1}, *F*(000) = 1540.0, crystal size 0.12×0.10×0.10 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 6.492 to 144.782°, 61603 reflections, 11830 independent reflections (R_{int} = 0.0566, R_σ = 0.0378), data/restraints/parameters : 11830/152/831, GOF = 1.047, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0356/0.0935, R_1/ wR_2 (all data) : 0.0367/0.0943, largest diff. peak/hole : 1.54/-1.72 eÅ^{-3}

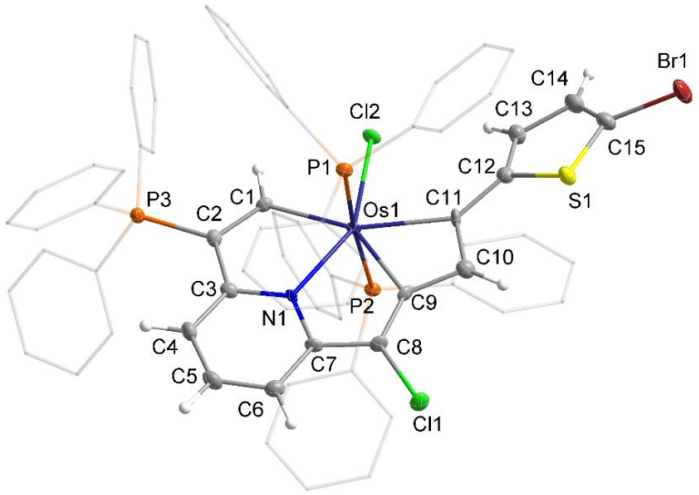


Figure S10. X-ray molecular structure for the cation of complex **4d** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.090(3), Os1–N1 2.147(3), Os1–C9 2.087(3), Os1–C11 2.231(3), C1–C2 1.359(5), C2–C3 1.451(5), C3–C4 1.392(5), C4–C5 1.386(5), C5–C6 1.368(5), C6–C7 1.394(5), C7–C8 1.409(5), C8–C9 1.338(5), C3–N1 1.367(5), C7–N1 1.368(4), C9–C10 1.414(5), C10–C11 1.347(5); Os1–C1–C2 122.0(3), C1–C2–C3 113.6(3), C2–C3–N1 111.3(3), C3–N1–Os1 120.8(2), N1–Os1–C1 72.07(12), Os1–N1–C7 120.5(2), N1–C7–C8 111.0(3), C7–C8–C9 115.3(3), C8–C9–Os1 121.4(3), N1–Os1–C9 71.48(12), C9–Os1–C11 58.85(13), Os1–C9–C10 102.5(2), C9–C10–C11 100.7(3), N1–C3–C4 120.3(3), C3–C4–C5 120.1(3), C4–C5–C6 120.0(3), C5–C6–C7 118.5(3), C6–C7–N1 122.2(3), C3–N1–C7 118.7(3).

Crystal data for 5a

$[C_{66}H_{58}ClNOsP_4]2BPh_4 \cdot 5CH_2Cl_2$, molecular weight = 2277.71, temperature = 100.0(2) K, triclinic, space group *P-1*, *a* = 15.7974(5) Å, *b* = 17.7933(5) Å, *c* = 20.4463(6) Å, α = 75.9630(10)°, β = 89.7200(10)°, γ = 73.0860(10)°, *V* = 5321.0(3) Å^3, *Z* = 2, ρ_{calc} = 1.422 g/cm^3, μ = 5.758 mm^{-1}, *F*(000) = 2324.0, crystal size 0.3×0.24×0.15 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.860 to 144.30°, 50036 reflections, 19988 independent reflections (R_{int} = 0.0516, R_σ = 0.0507), data/restraints/parameters : 19988/0/1246, GOF = 1.046, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0507/0.1336, R_1/ wR_2 (all data) : 0.0516/0.1345, largest diff. peak/hole : 3.48/-2.52 e.Å^{-3}

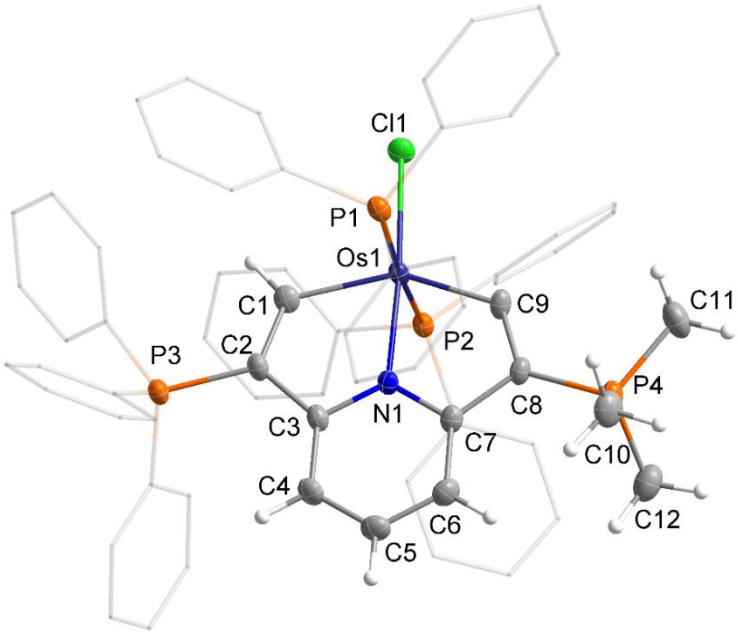


Figure S11. X-ray molecular structure for the cation of complex **5a** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.036(4), Os1–N1 2.083(3), Os1–C9 1.907(4), C1–C2 1.351(5), C2–C3 1.461(5), C3–C4 1.394(5), C4–C5 1.393(6), C5–C6 1.375(5), C6–C7 1.383(5), C7–C8 1.459(5), C8–C9 1.371(5), C3–N1 1.365(5), C7–N1 1.374(5); Os1–C1–C2 121.3(3), C1–C2–C3 113.7(3), C2–C3–N1 110.0(3), C3–N1–Os1 121.1(2), N1–Os1–C1 73.74(13), Os1–N1–C7 119.8(2), N1–C7–C8 110.0(3), C7–C8–C9 109.7(3), C8–C9–Os1 126.9(3), N1–C3–C4 121.0(3), C3–C4–C5 119.3(3), C4–C5–C6 129.4(3), C5–C6–C7 120.1(3), C6–C7–N1 121.0(3), C3–N1–C7 119.1(3).

Crystal data for 5c

$[C_{81}H_{64}ClNOsP_4]2BPh_4$, molecular weight = 2039.28, temperature = 100.0 K, triclinic, space group *P-1*, *a* = 17.3078(18) Å, *b* = 17.5817(18) Å, *c* = 18.5767(19) Å, α = 79.878(4)°, β = 73.879(4)°, γ = 87.864(4)°, *V* = 5345.7(10) Å^3, *Z* = 2, ρ_{calc} = 1.267 g/cm^3, μ = 3.430 mm^{-1}, *F*(000) = 2096.0, crystal size 0.15×0.15×0.12 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.316 to 145.386°, 86820 reflections, 20331 independent reflections (R_{int} = 0.0553, R_σ = 0.0403), data/restraints/parameters : 20331/0/1243, GOF = 1.088, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0366/0.1086, R_1/ wR_2 (all data) : 0.0404/0.1113, largest diff. peak/hole : 0.91/-1.51 e.Å^{-3}

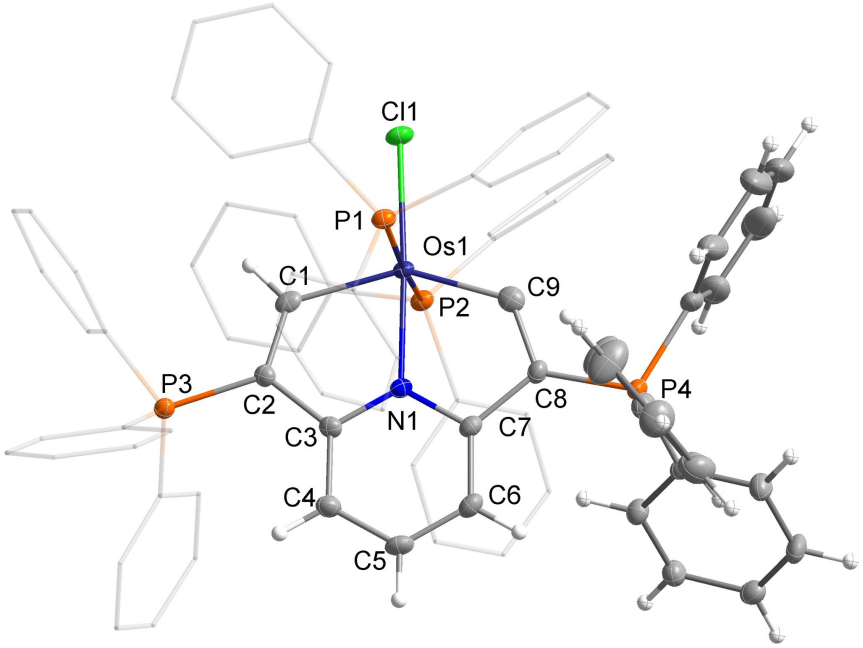


Figure S12. X-ray molecular structure for the cation of complex **5c** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.027(3), Os1–N1 2.093(2), Os1–C9 1.916(3), C1–C2 1.362(4), C2–C3 1.459(4), C3–C4 1.392(4), C4–C5 1.393(4), C5–C6 1.384(5), C6–C7 1.391(4), C7–C8 1.465(4), C8–C9 1.354(4), C3–N1 1.364(4), C7–N1 1.370(4); Os1–C1–C2 121.4(2), C1–C2–C3 113.3(3), C2–C3–N1 110.8(2), C3–N1–Os1 120.36(19), N1–Os1–C1 74.10(11) N1–Os1–C9 73.79(11), Os1–N1–C7 119.15(19), N1–C7–C8 110.1(2), C7–C8–C9 110.5(3), C8–C9–Os1 126.3(2), N1–C3–C4 120.5(3), C3–C4–C5 119.`(3), C4–C5–C6 120.3(3), C5–C6–C7 119.1(3), C6–C7–N1 120.5(3), C3–N1–C7 120.5(2).

Crystal data for 7a

$[C_{71}H_{60}ClNOsP_4]2BPh_4$, molecular weight = 1915.14, temperature = 100.0 K, triclinic, space group *P-1*, *a* = 16.9627(8) Å, *b* = 19.3429(9) Å, *c* = 22.1477(10) Å, α = 110.864(2)°, β = 94.765(2)°, γ = 114.869(2)°, *V* = 5923.8(5) Å^3, *Z* = 2, ρ_{calc} = 1.074 g/cm^3, μ = 3.065 mm^{-1}, *F*(000) = 1968.0, crystal size 0.14×0.12×0.10 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.586 to 145.008°, 113199 reflections, 23065 independent reflections (R_{int} = 0.0600, R_σ = 0.0438), data/restraints/parameters : 23065/36/1143, GOF = 1.026, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0553/0.1635, R_1/ wR_2 (all data) : 0.0584/0.1669, largest diff. peak/hole : 2.15/-2.01 e.Å^{-3}

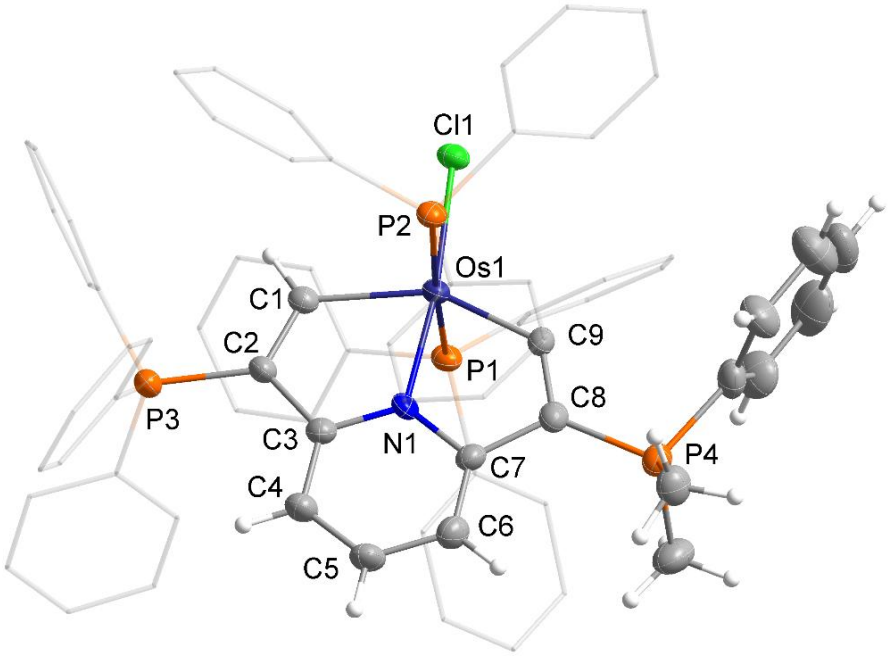


Figure S13. X-ray molecular structure for the cation of complex **7a** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Os1–C1 2.059(4), Os1–N1 2.085(3), Os1–C9 1.874(4), C1–C2 1.367(6), C2–C3 1.463(6), C3–C4 1.399(6), C4–C5 1.381(6), C5–C6 1.388(7), C6–C7 1.373(6), C7–C8 1.463(6), C8–C9 1.356(6), C3–N1 1.364(5), C7–N1 1.382(5); Os1–C1–C2 119.9(3), C1–C2–C3 113.8(4), C2–C3–N1 111.1(4), C3–N1–Os1 120.7(3), N1–Os1–C1 74.42(15), Os1–N1–C7 119.2(3), N1–C7–C8 109.0(4), C7–C8–C9 110.4(4), C8–C9–Os1 127.6(3), N1–C3–C4 120.1(4), C3–C4–C5 119.4(4), C4–C5–C6 120.3(4), C5–C6–C7 119.4(4), C6–C7–N1 120.7(4), C3–N1–C7 120.1(4).

Crystal data for 9

$[C_{81}H_{64}ClNRuP_4]2BPh_4$, molecular weight = 1950.15, temperature = 100.0 K, triclinic, space group *P-1*, *a* = 17.3296(4) Å, *b* = 17.6406(4) Å, *c* = 18.5079(4) Å, α = 79.8370(10)°, β = 73.9580(10)°, γ = 87.9760(10)°, *V* = 5351.8(2) Å^3, *Z* = 2, ρ_{calc} = 1.210 g/cm^3, μ = 2.361 mm^{-1}, *F*(000) = 2032.0, crystal size 0.13×0.11×0.11 mm^3, $\lambda(Cu_{K\alpha})$ = 1.54178, $2\theta_{range}$ = 5.044 to 144.864°, 56038 reflections, 20270 independent reflections (R_{int} = 0.0360, R_σ = 0.0426), data/restraints/parameters : 20270/0/1243, GOF = 1.038, R_1/ wR_2 (I ≥ 2σ(I)) : 0.0415/0.1064, R_1/ wR_2 (all data) : 0.0448/0.1084, largest diff. peak/hole: 0.94/-1.00 e.Å^{-3}

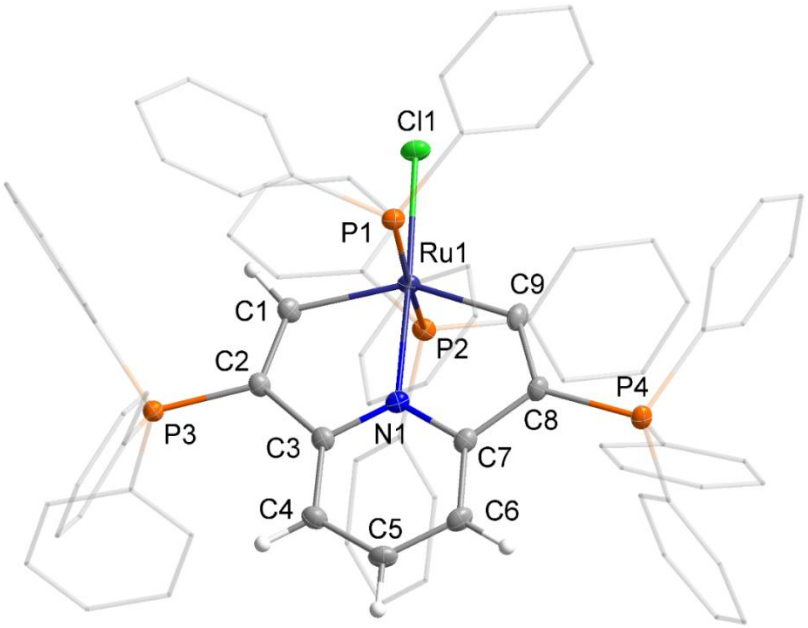


Figure S14. X-ray molecular structure for the cation of complex **9** drawn with 50% probability level. The hydrogen atoms at Ph groups were omitted for clarity. Selected bond lengths (Å) and angles (°): Ru1–C1 1.998(2), Ru1–N1 2.0864(16), Ru1–C9 1.916(2), C1–C2 1.361(3), C2–C3 1.463(3), C3–C4 1.396(3), C4–C5 1.385(3), C5–C6 1.389(3), C6–C7 1.396(3), C7–C8 1.464(3), C8–C9 1.353(3), C3–N1 1.357(3), C7–N1 1.362(3); Ru1–C1–C2 121.89(16), C1–C2–C3 112.74(18), C2–C3–N1 110.89(17), C3–N1–Ru1 119.90(13), N1–Ru1–C1 74.48(8), Ru1–N1–C7 119.26(14), N1–C7–C8 110.00(17), C7–C8–C9 111.04(19), C8–C9–Ru1 125.49(17), N1–C3–C4 120.44(19), C3–C4–C5 119.0(2), C4–C5–C6 120.42(19), C5–C6–C7 118.77(19), C6–C7–N1 120.48(19), C3–N1–C7 120.83(17).

4. NMR and HRMS Spectra

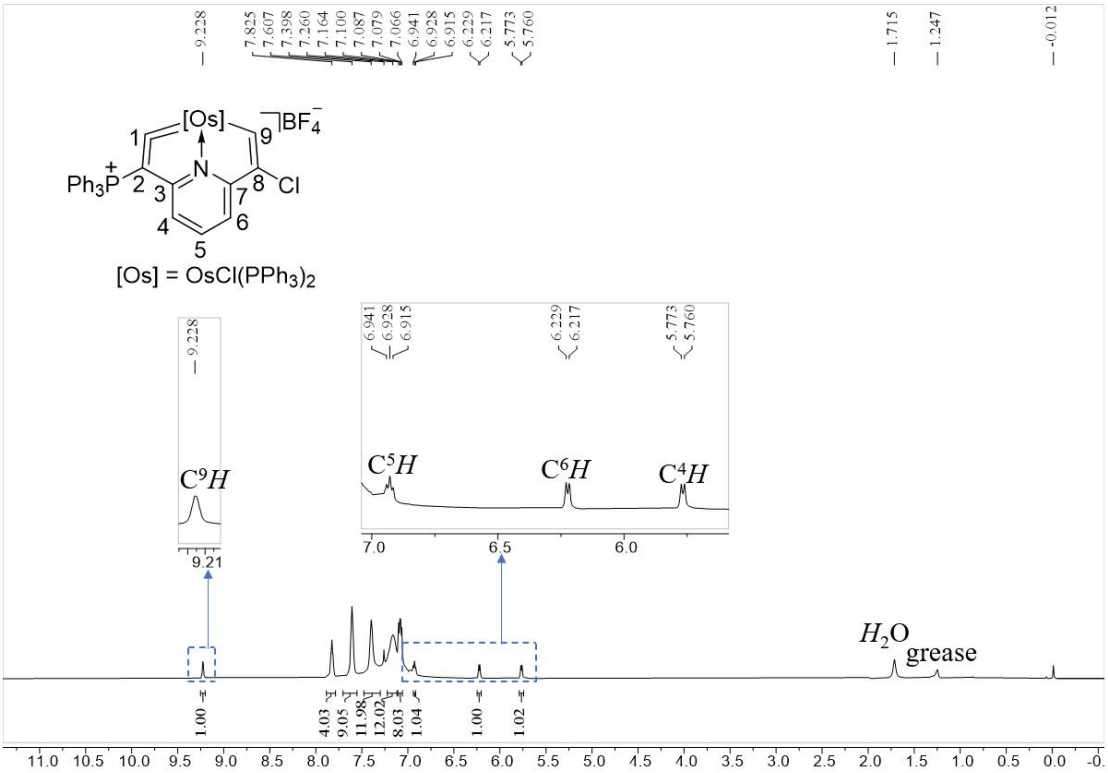


Figure S15. The ^{1}H NMR (600.1 MHz, $CDCl_3$) spectrum for complex **1**.

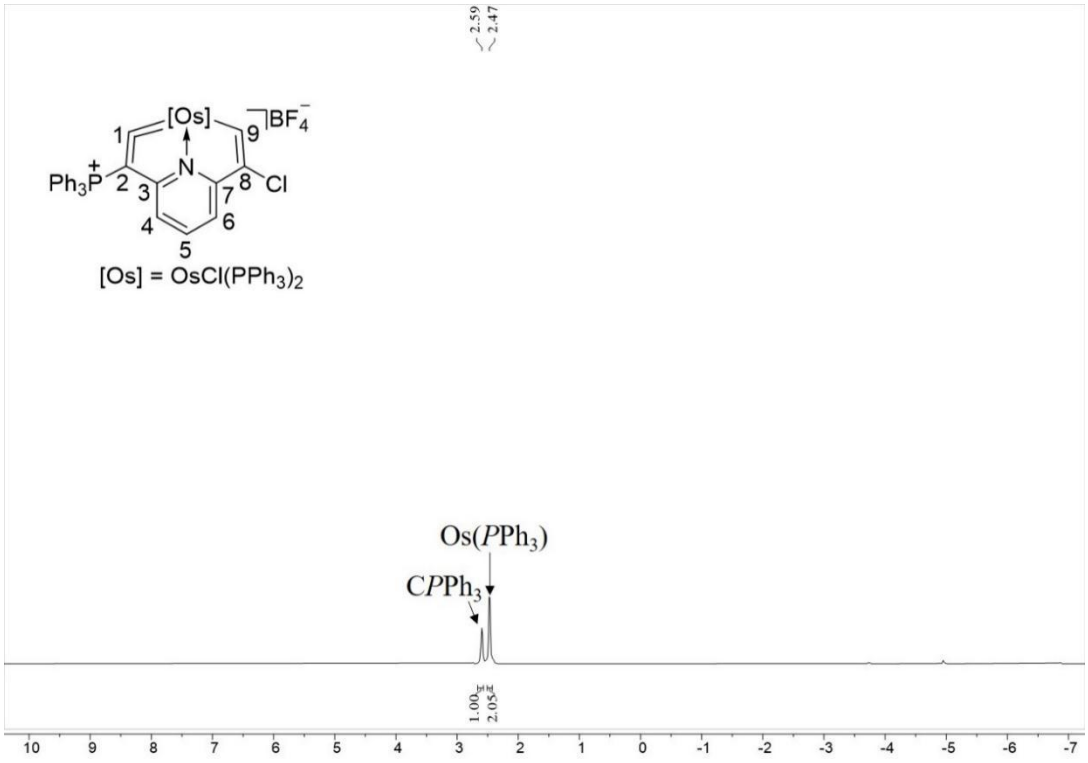


Figure S16. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, $CDCl_3$) spectrum for complex **1**.

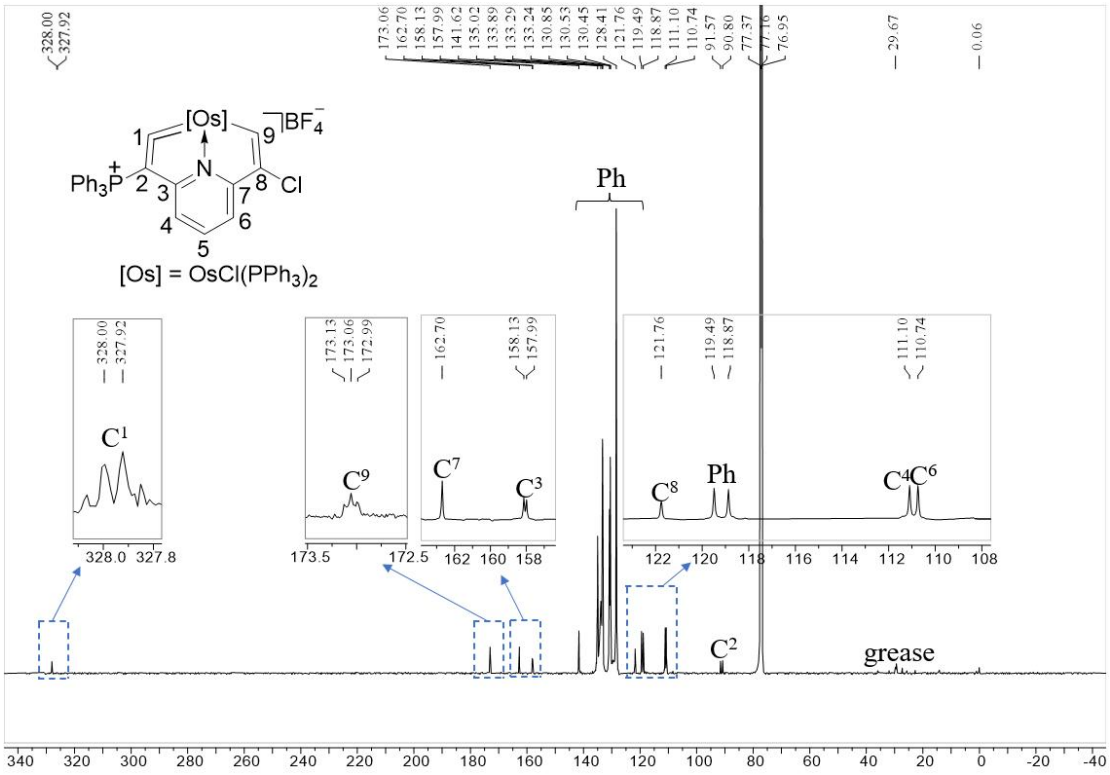


Figure S17. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, $CDCl_3$) spectrum for complex **1**.

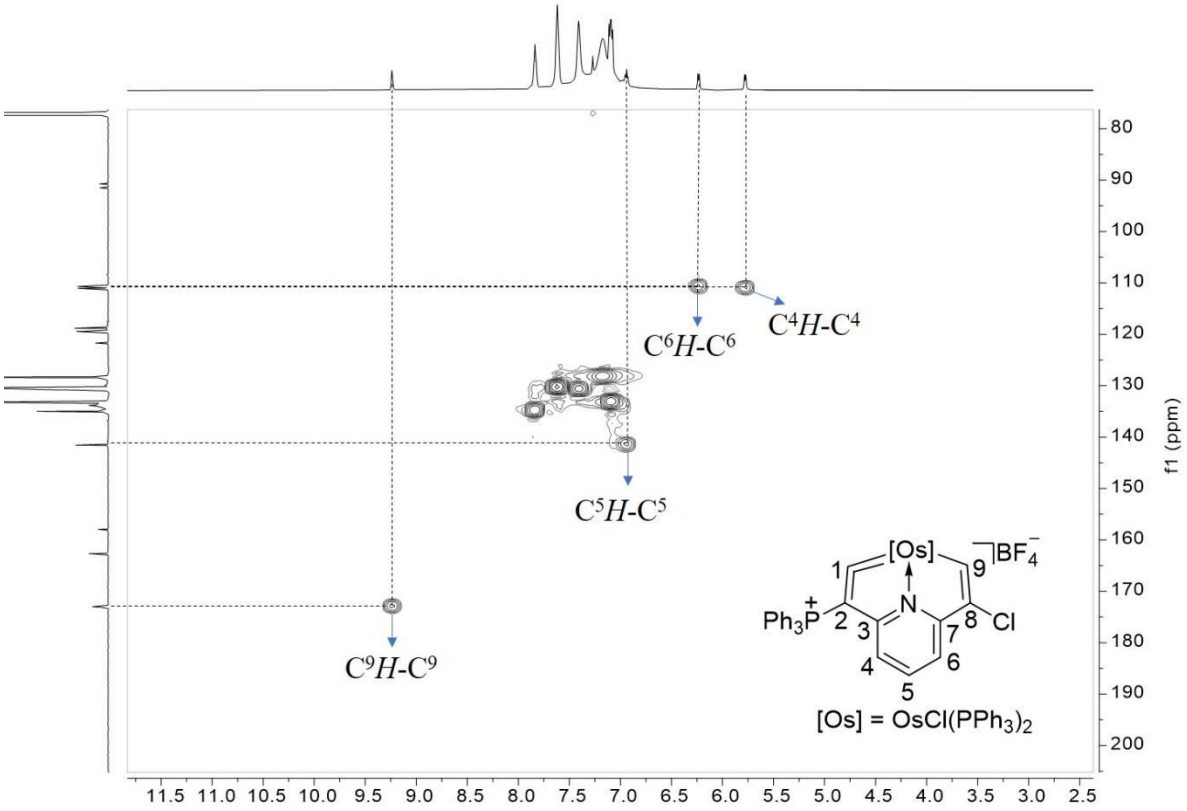


Figure S18. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **1**.

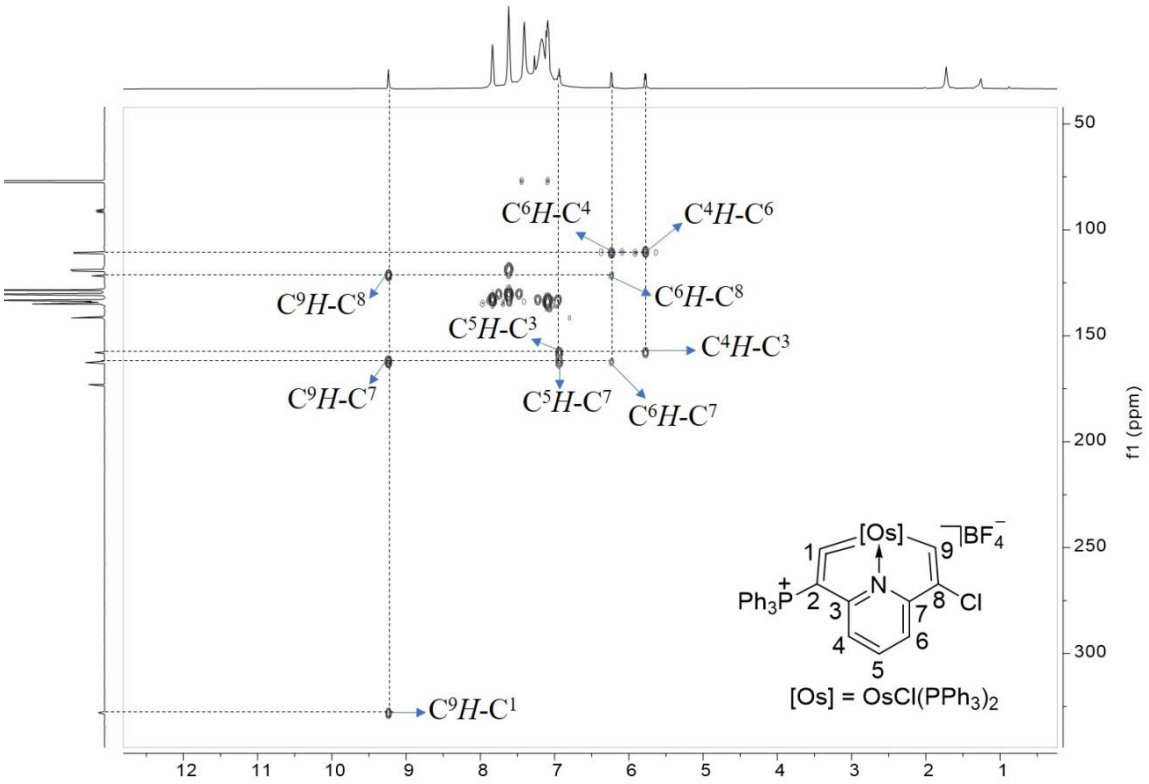


Figure S19. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **1**.

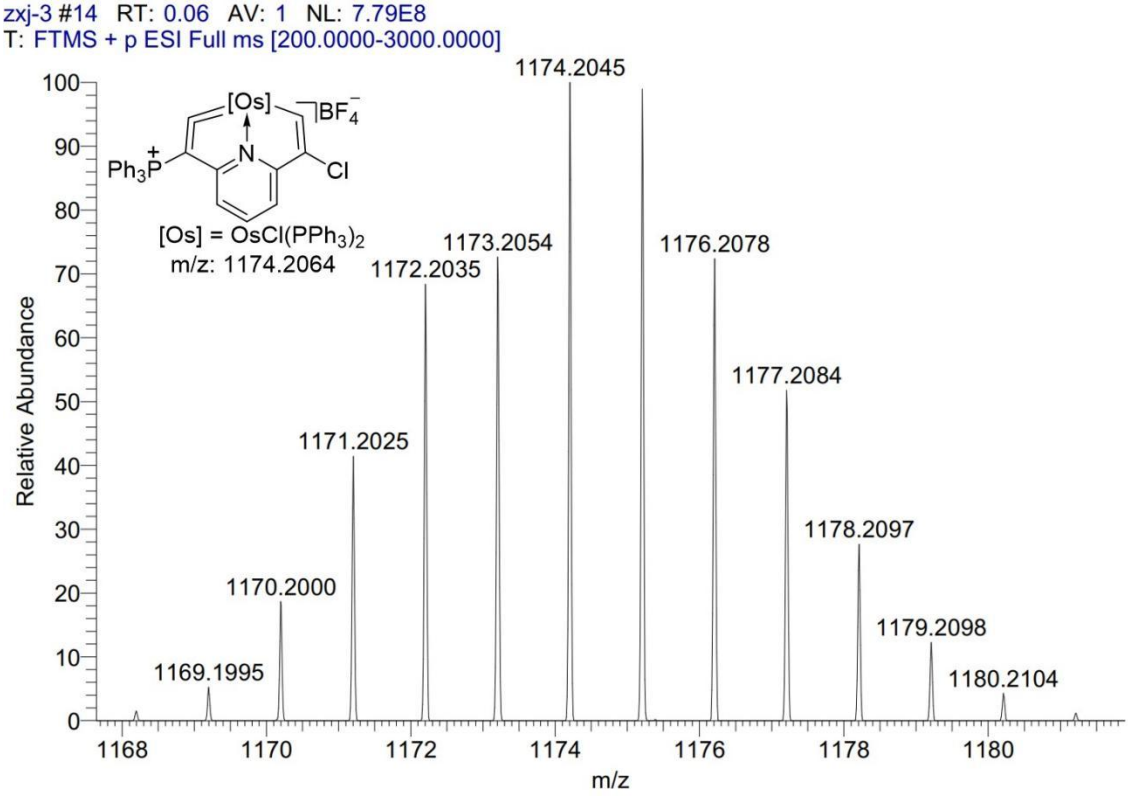


Figure S20. Positive-ion ESI-MS spectrum of [**1**]$^+$ measured in methanol.

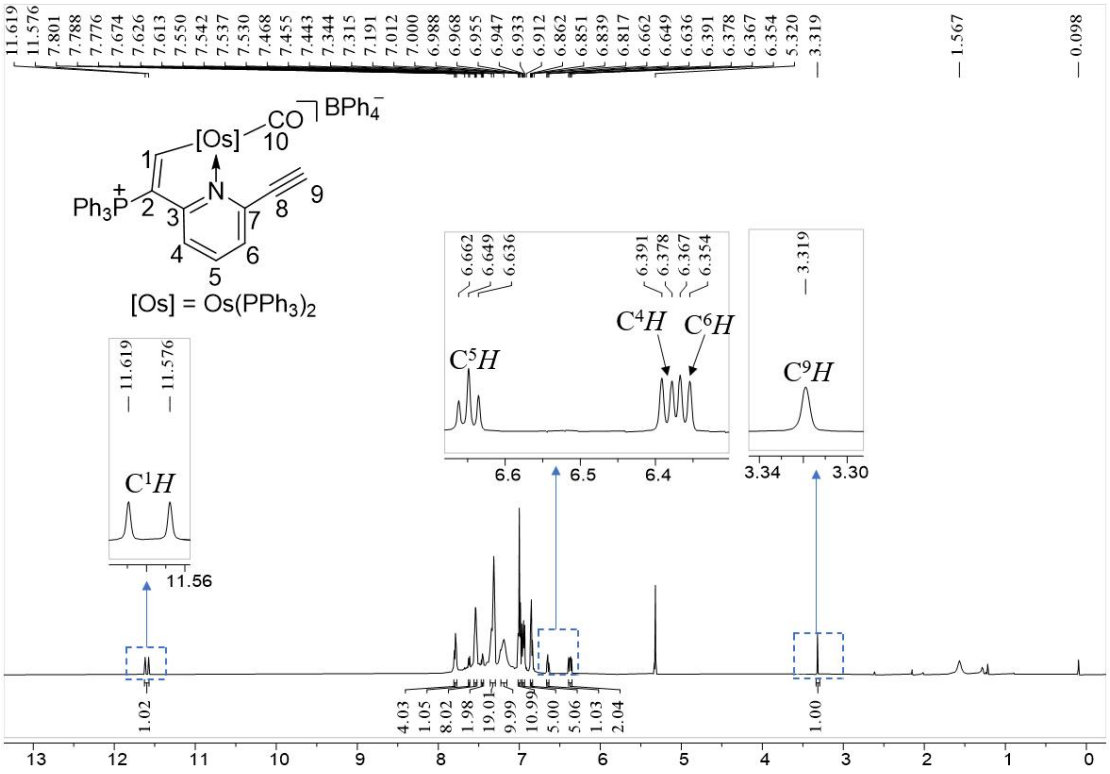


Figure S21. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **P1'**.

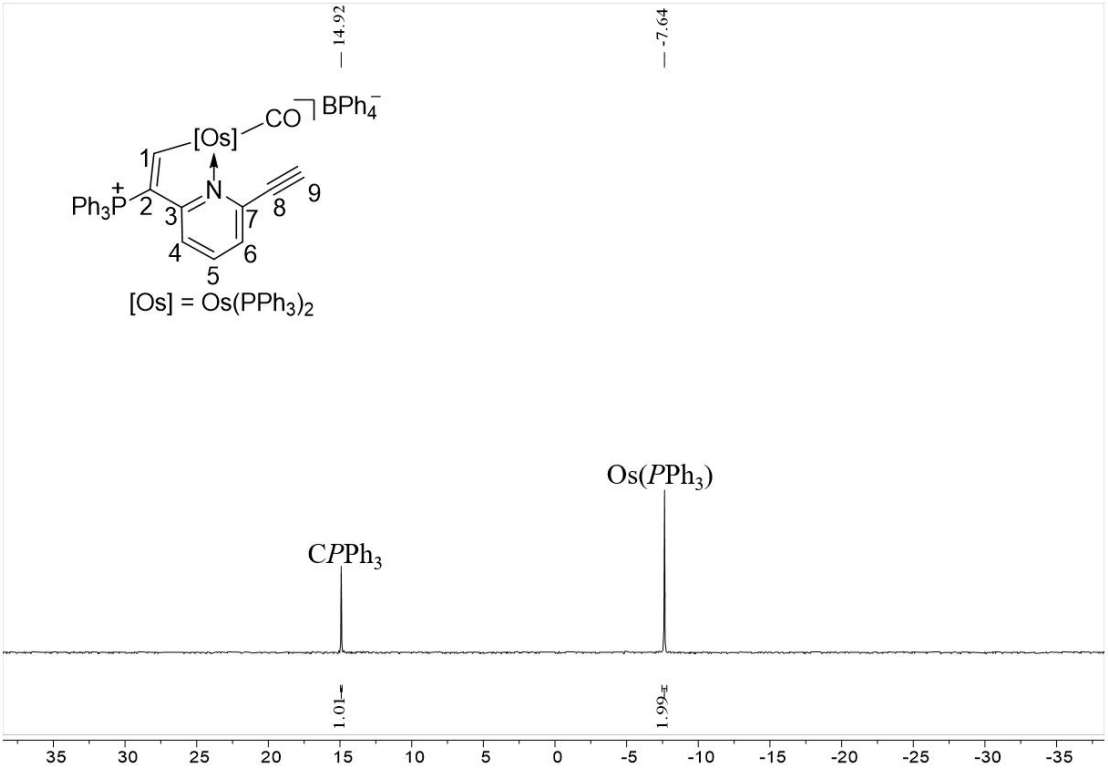


Figure S22. The $^{31}P\{^1H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **P1'**.

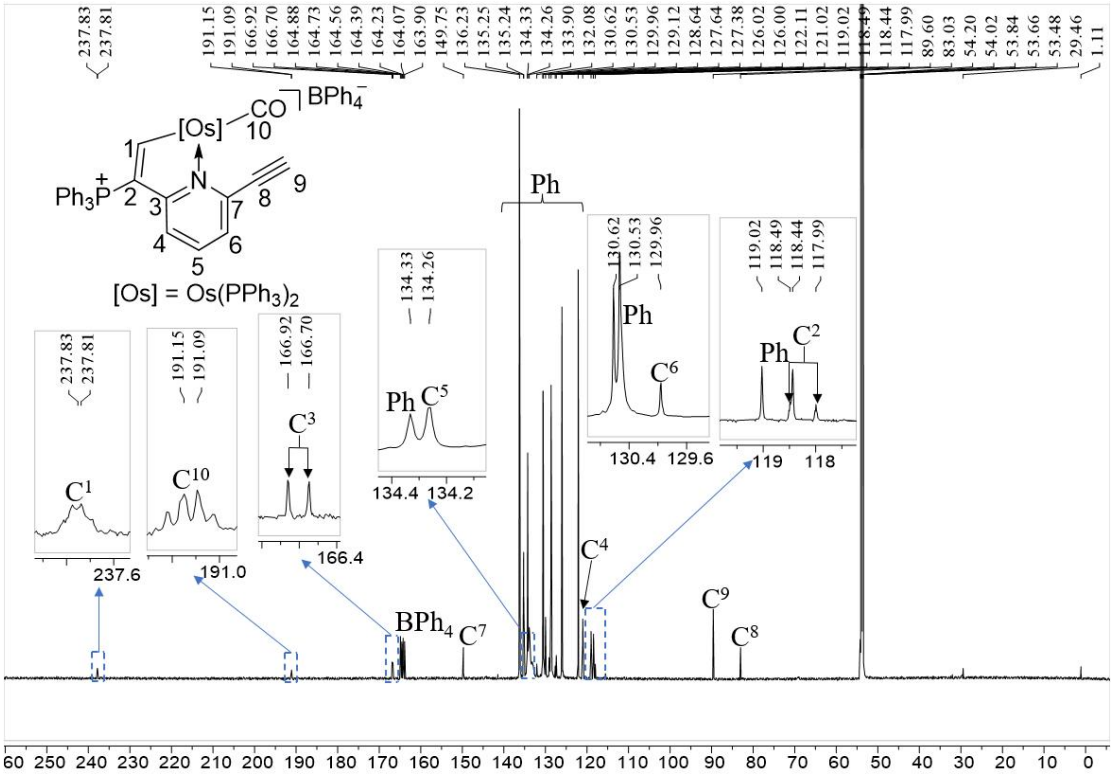


Figure S23. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **P1'**.

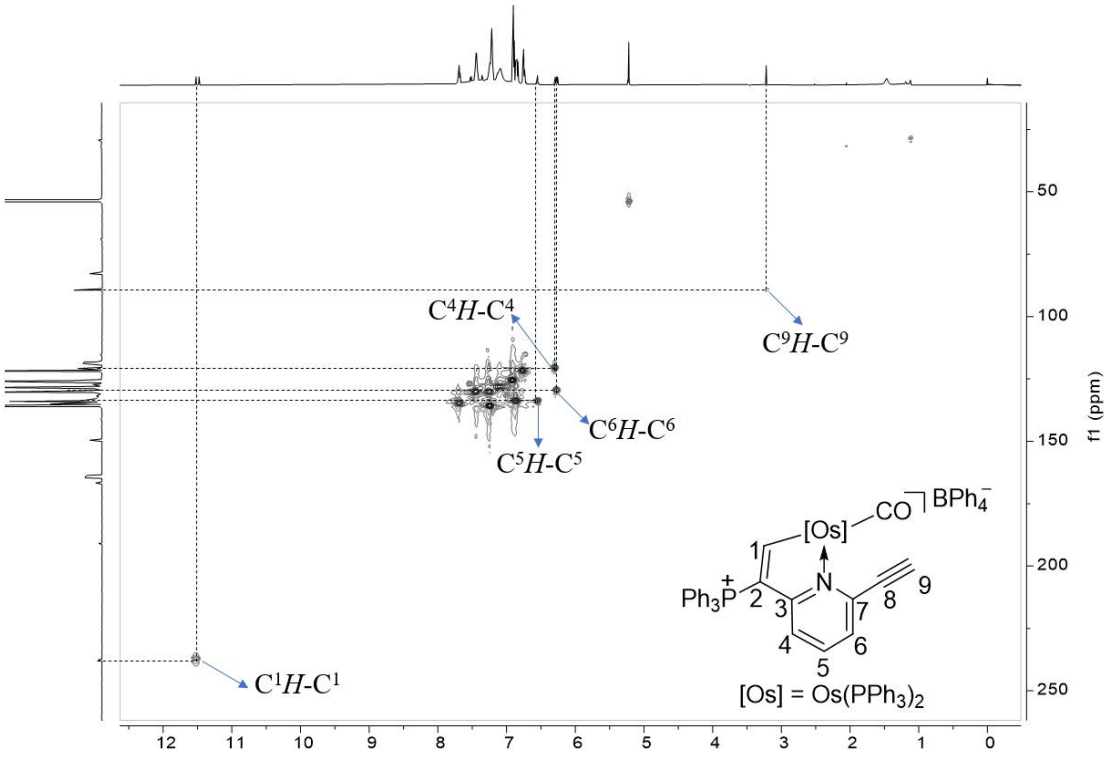


Figure S24. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **P1'**.

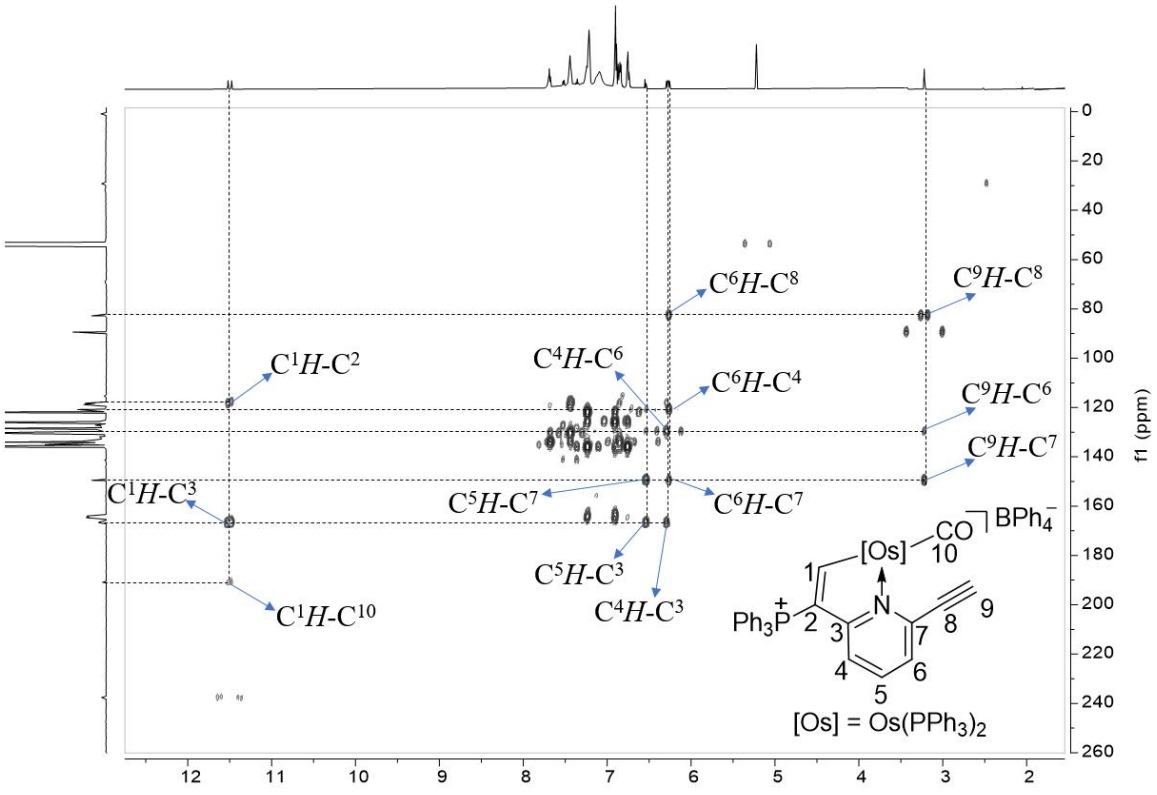


Figure S25. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **P1'**.

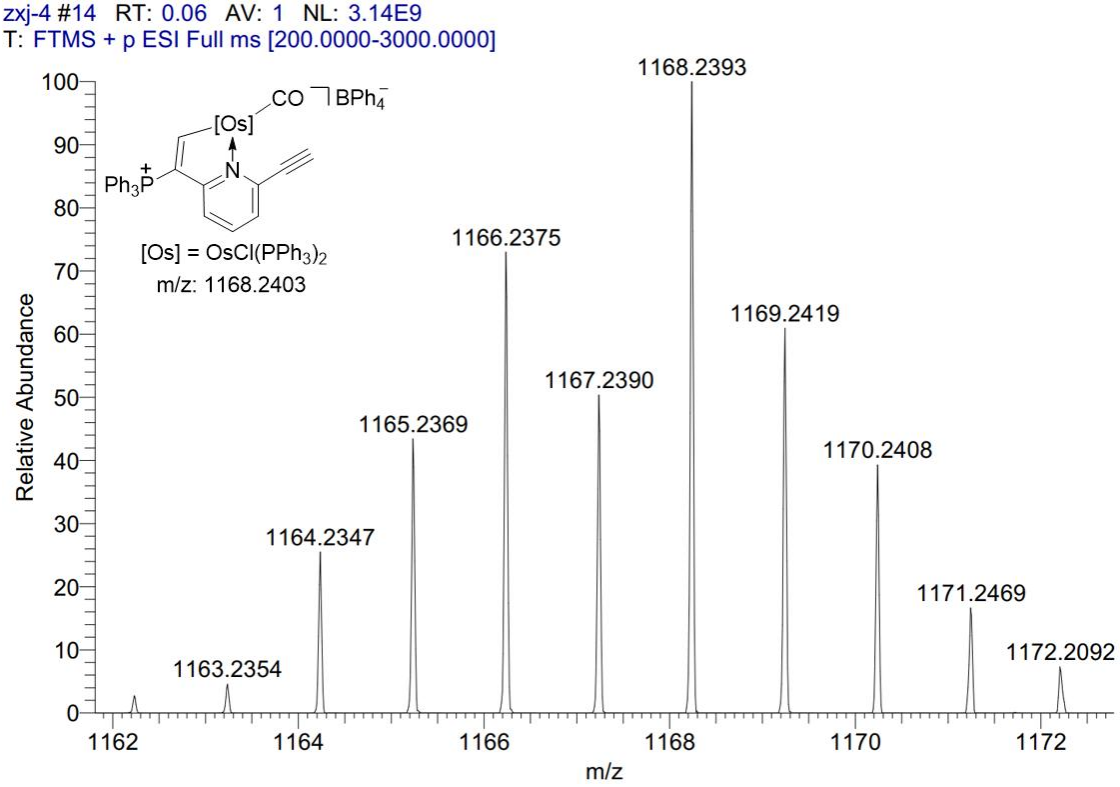


Figure S26. Positive-ion ESI-MS spectrum of [**P1'**]$^{+}$ measured in methanol.

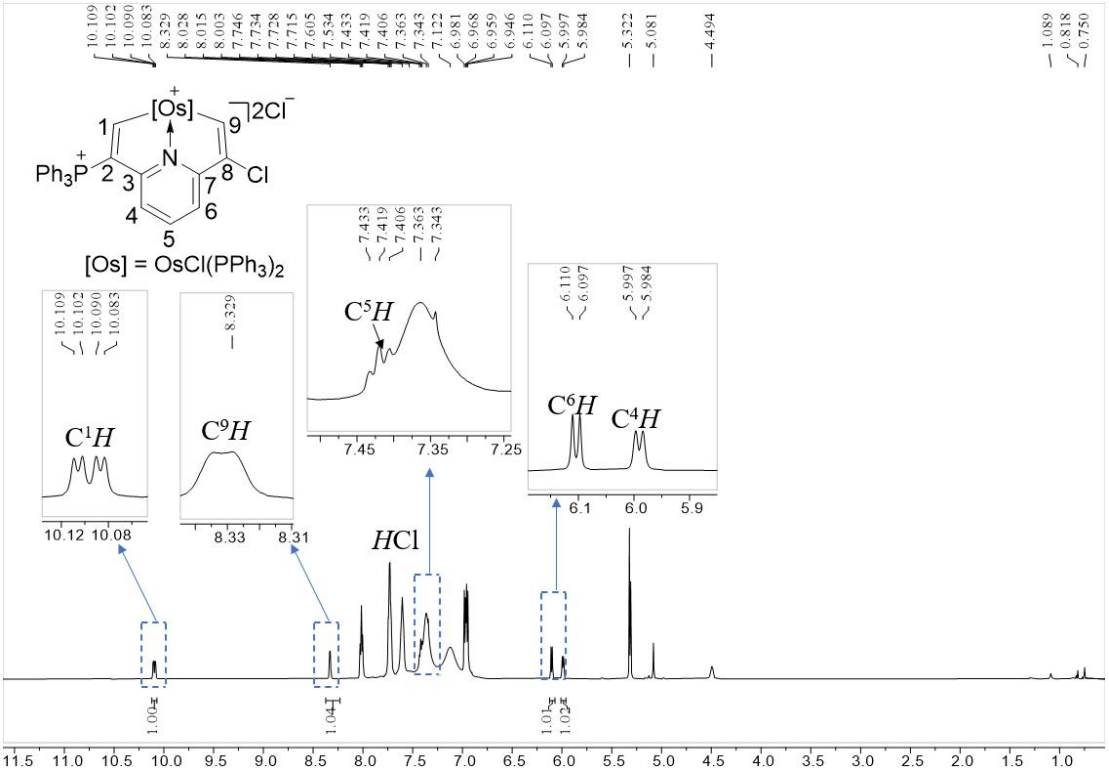


Figure S27. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **2**.

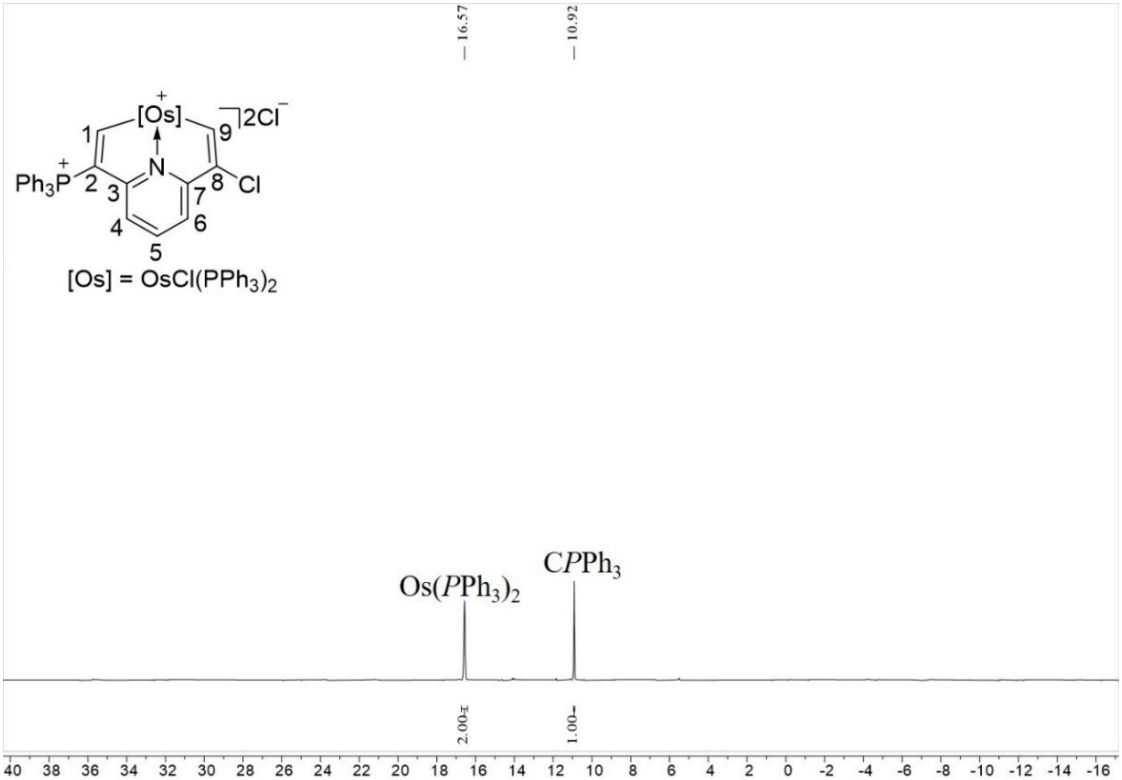


Figure S28. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **2**.

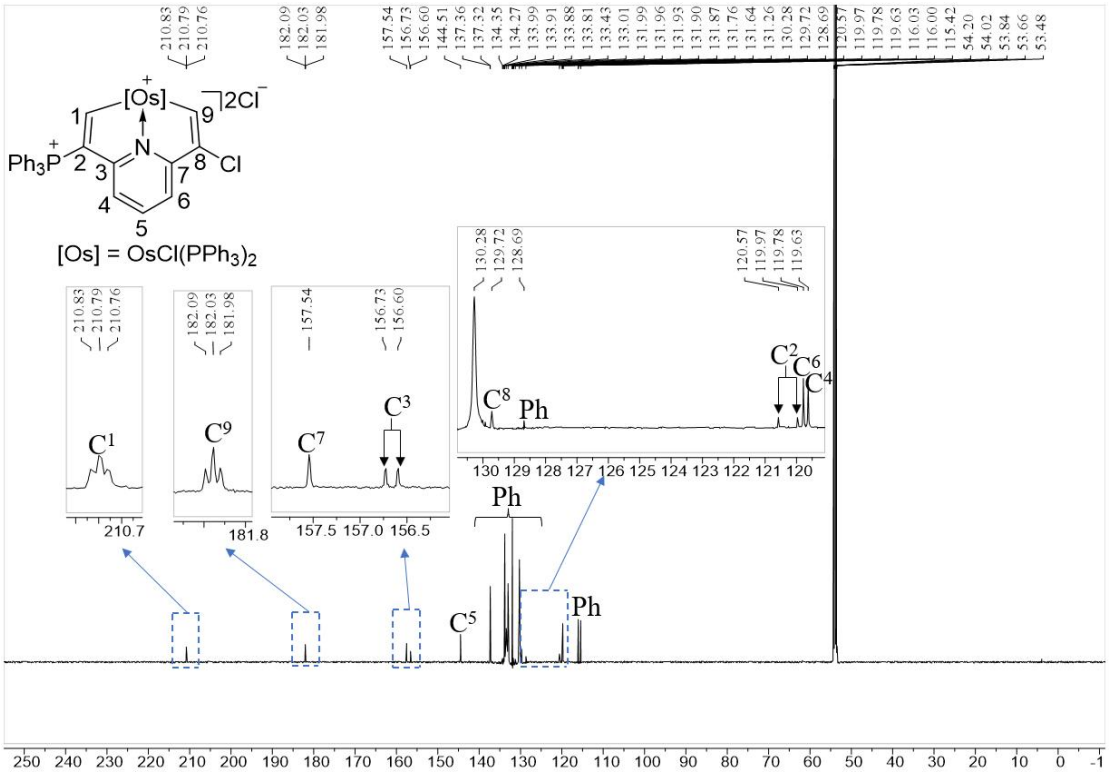


Figure S29. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **2**.

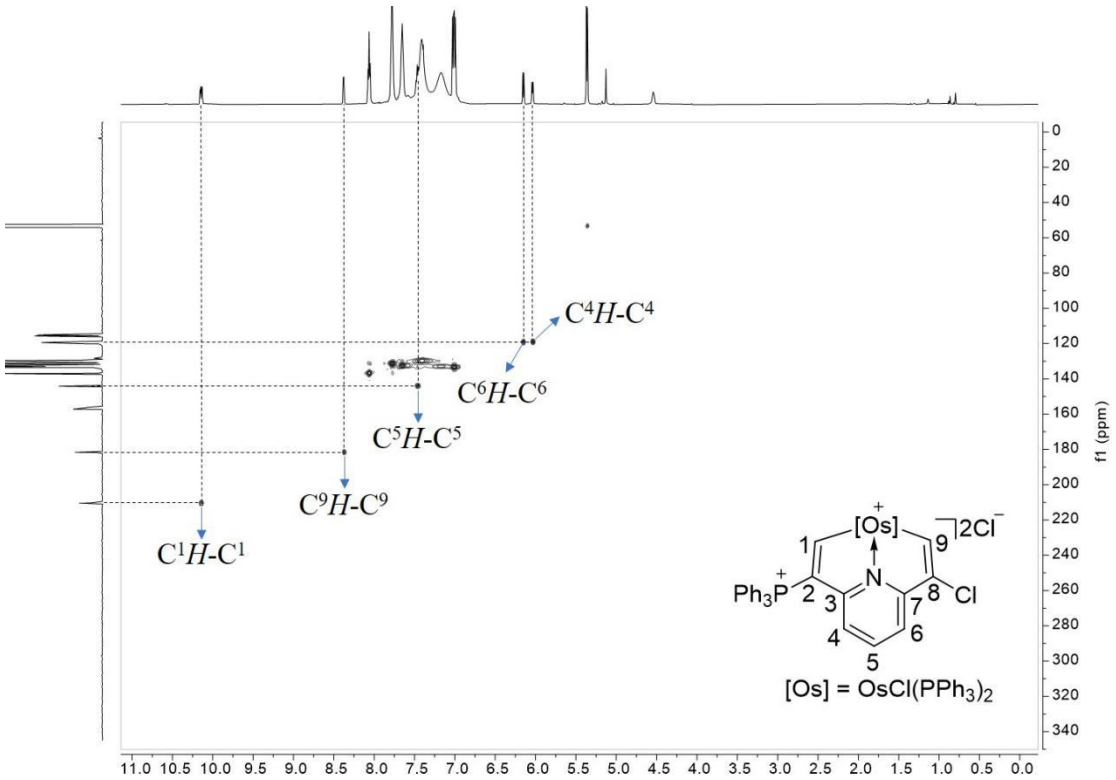


Figure S30. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **2**.

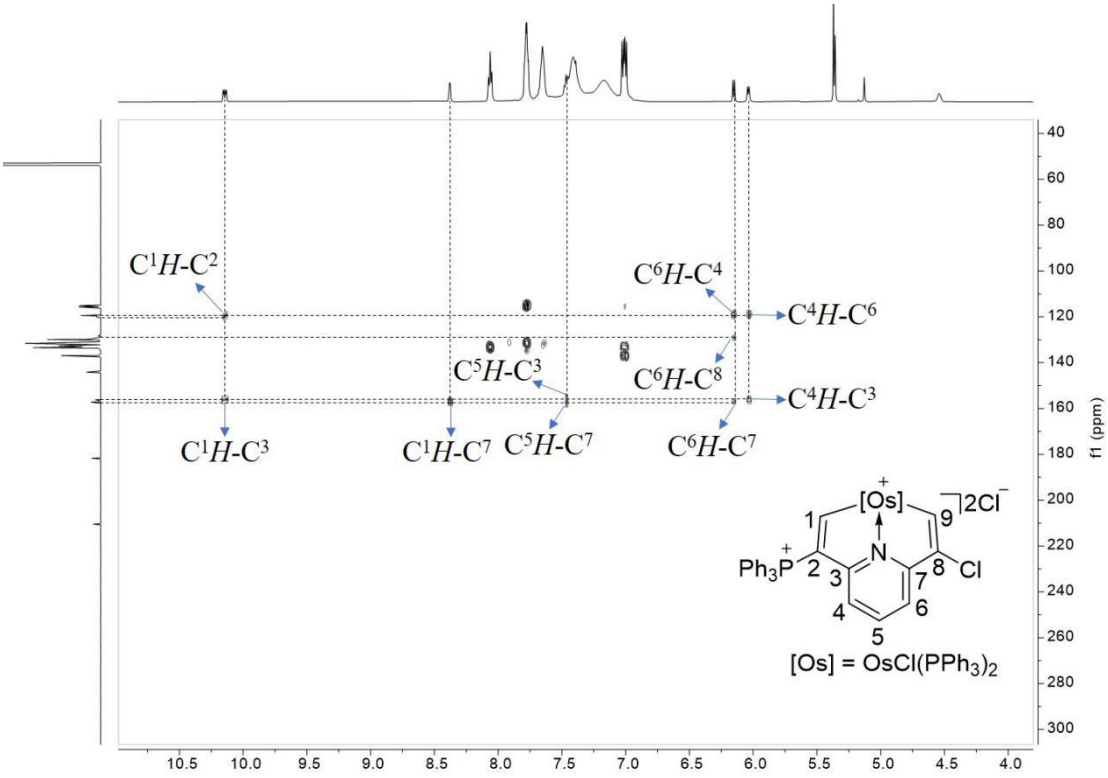


Figure S31. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **2**.

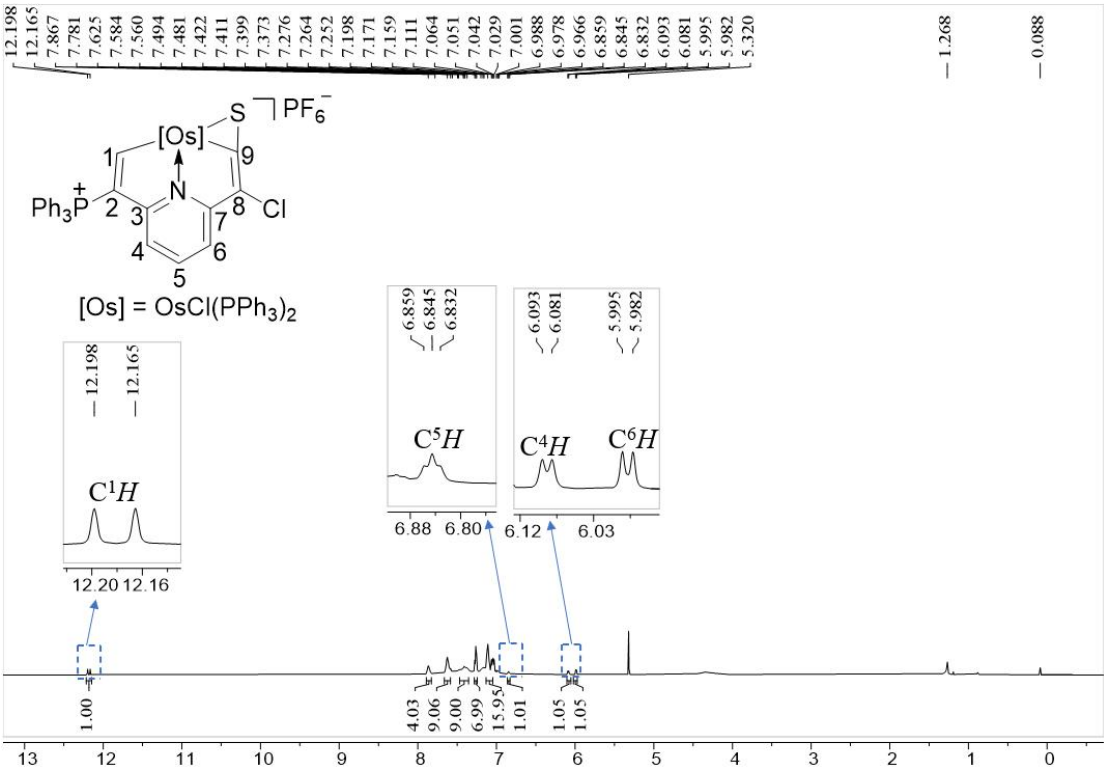


Figure S32. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **3a**.

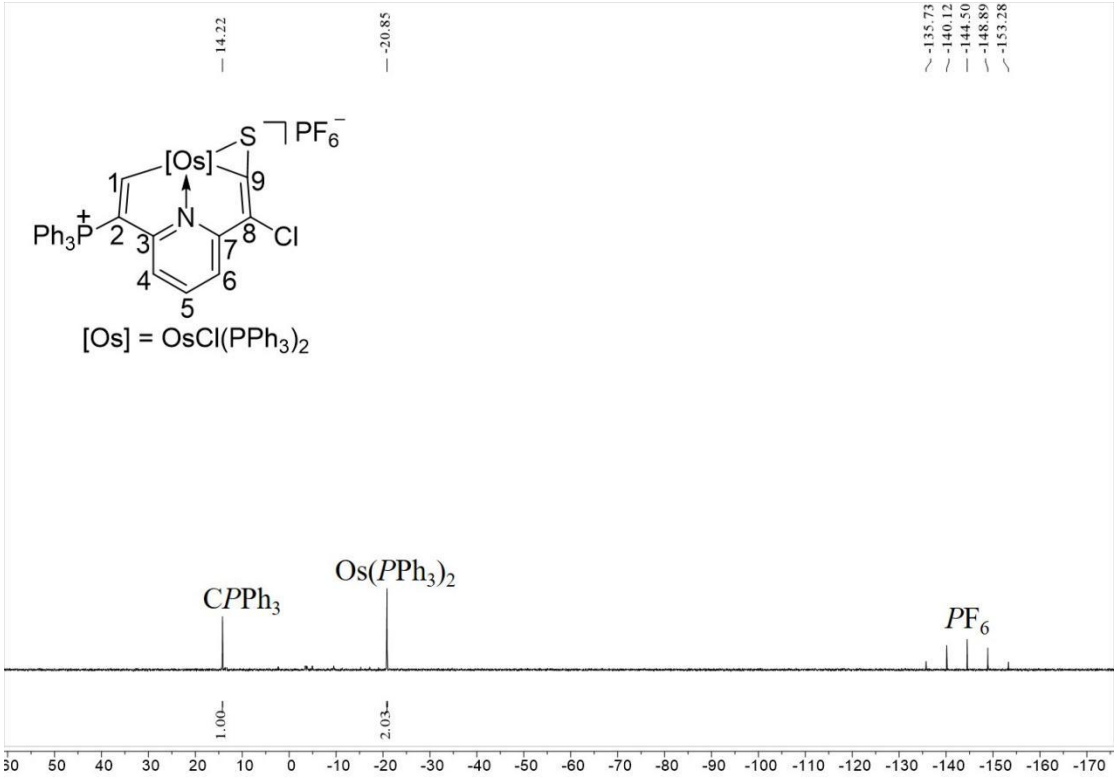


Figure S33. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **3a**.

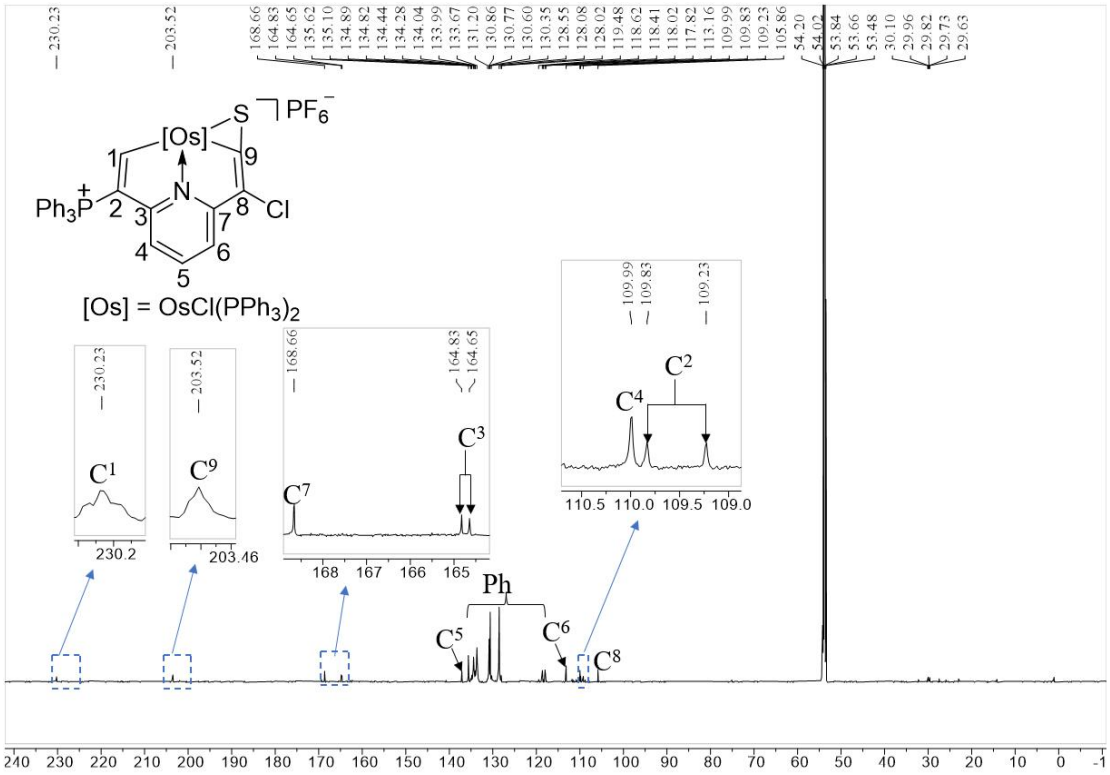


Figure S34. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **3a**.

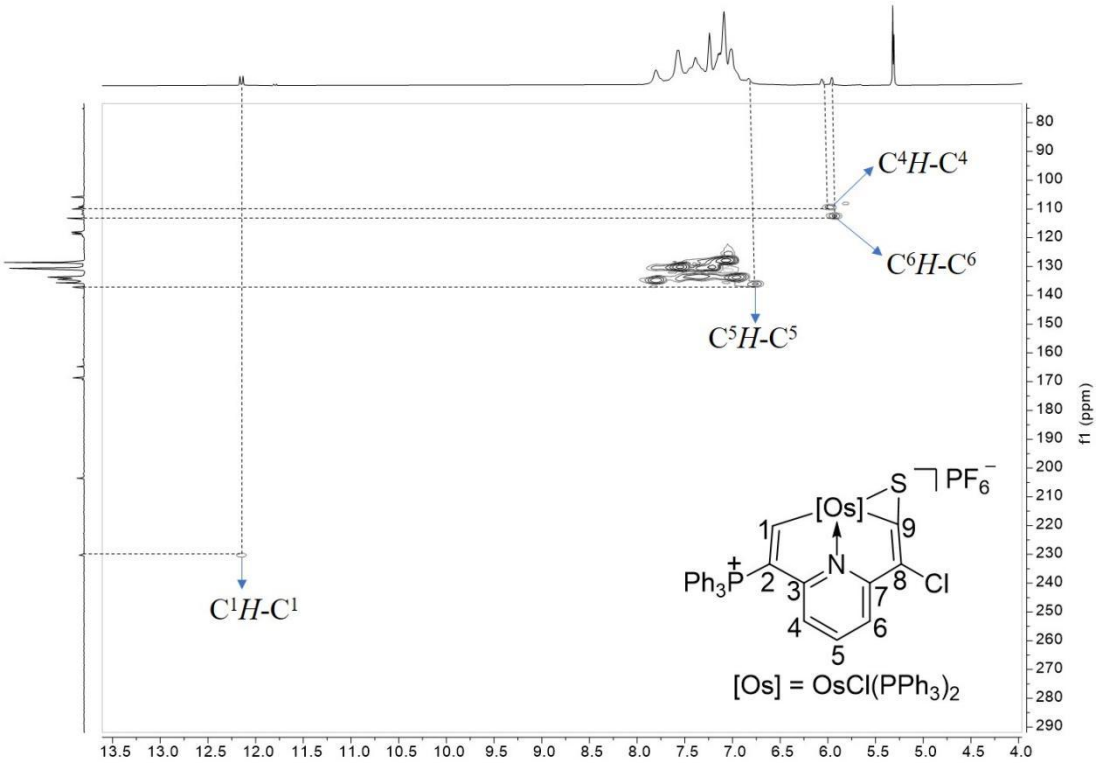


Figure S35. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **3a**.

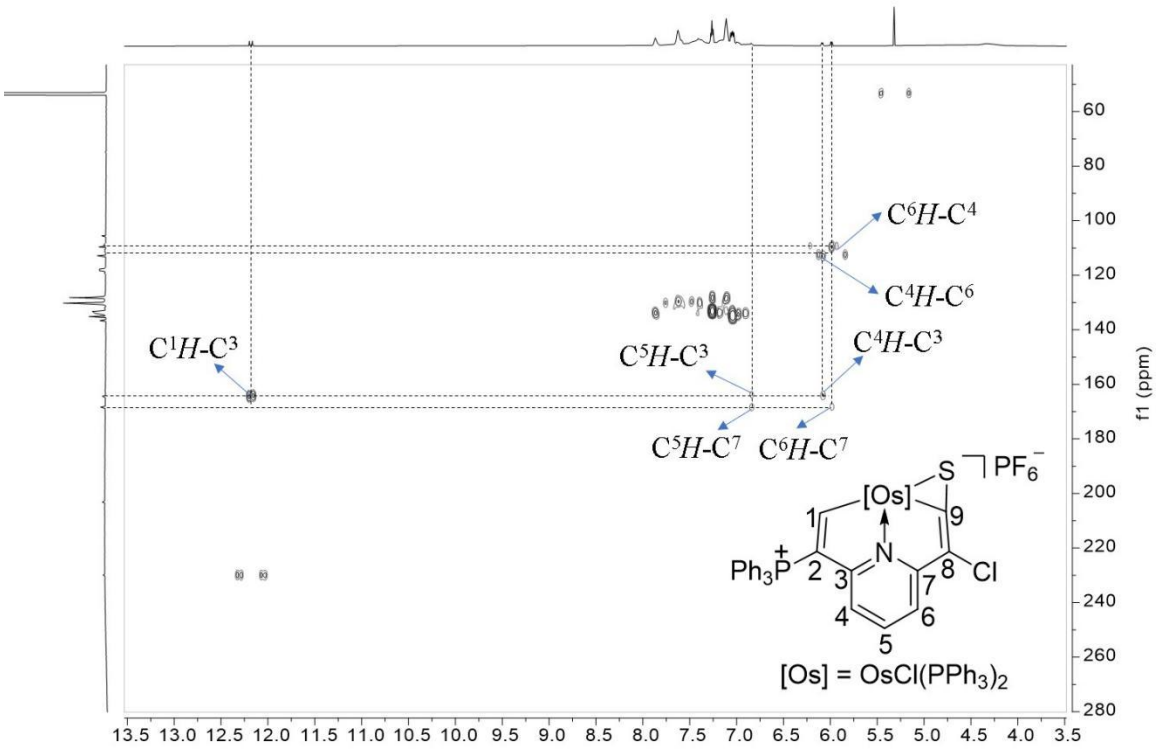


Figure S36. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **3a**.

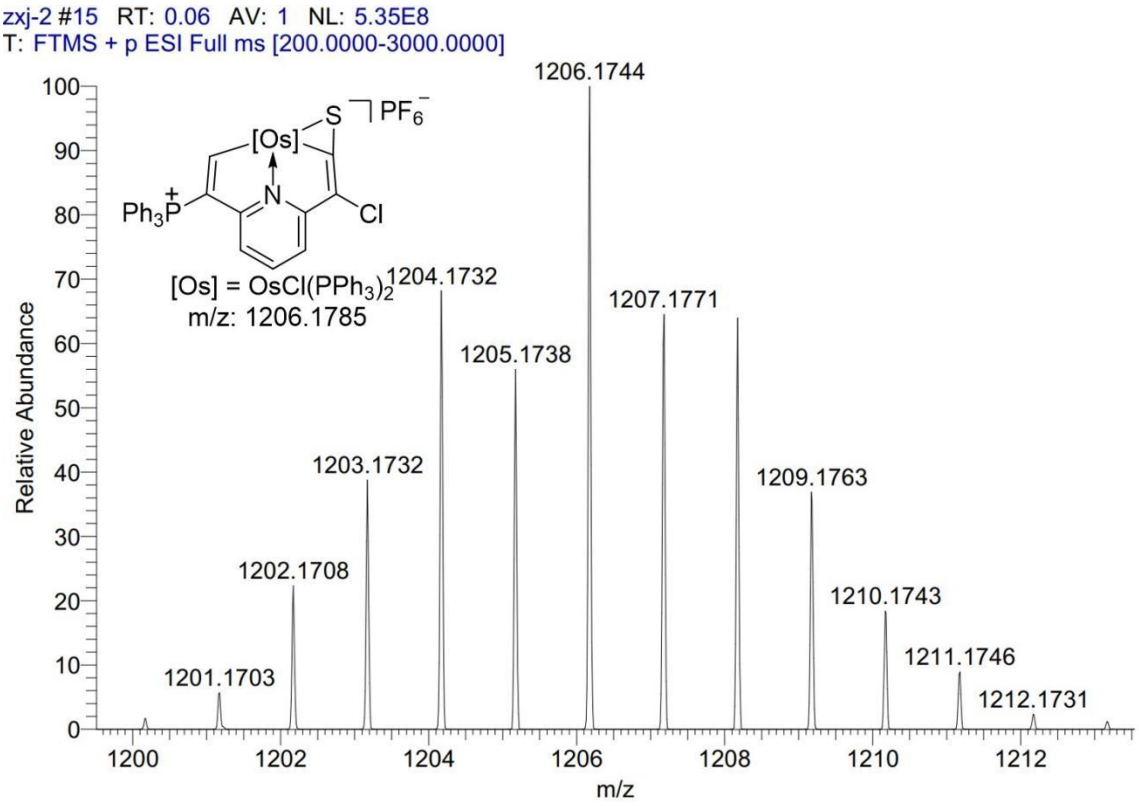


Figure S37. Positive-ion ESI-MS spectrum of [**3a**]$^{+}$ measured in methanol.

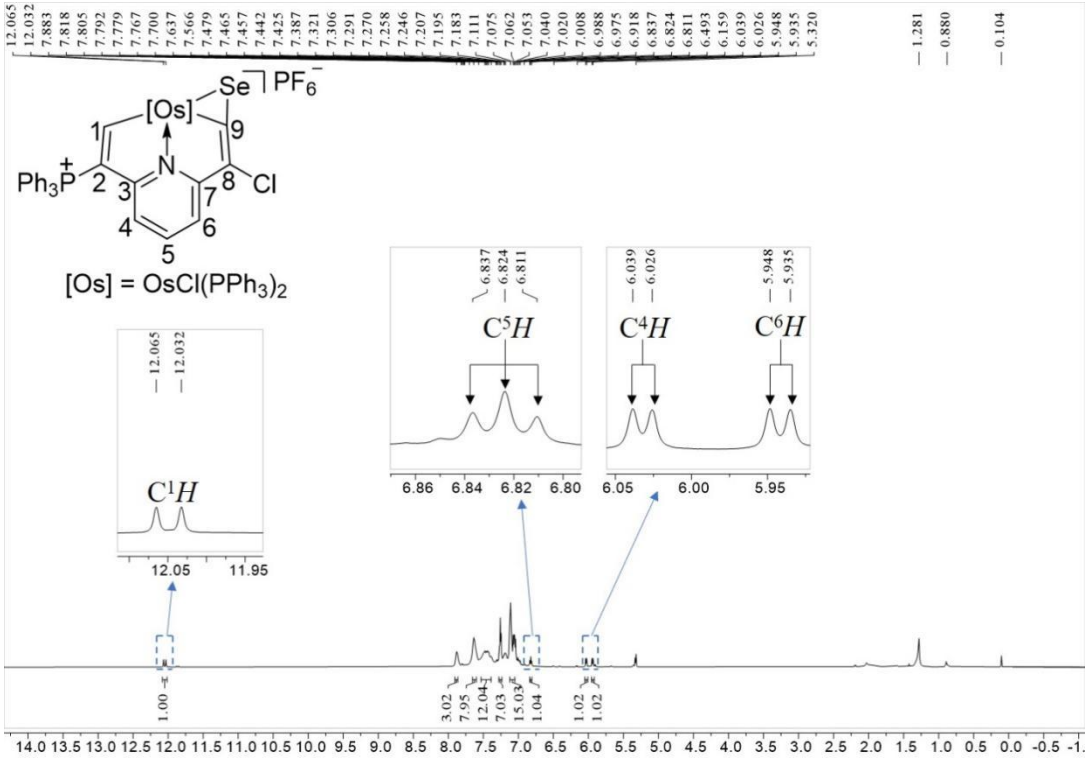


Figure S38. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **3b**.

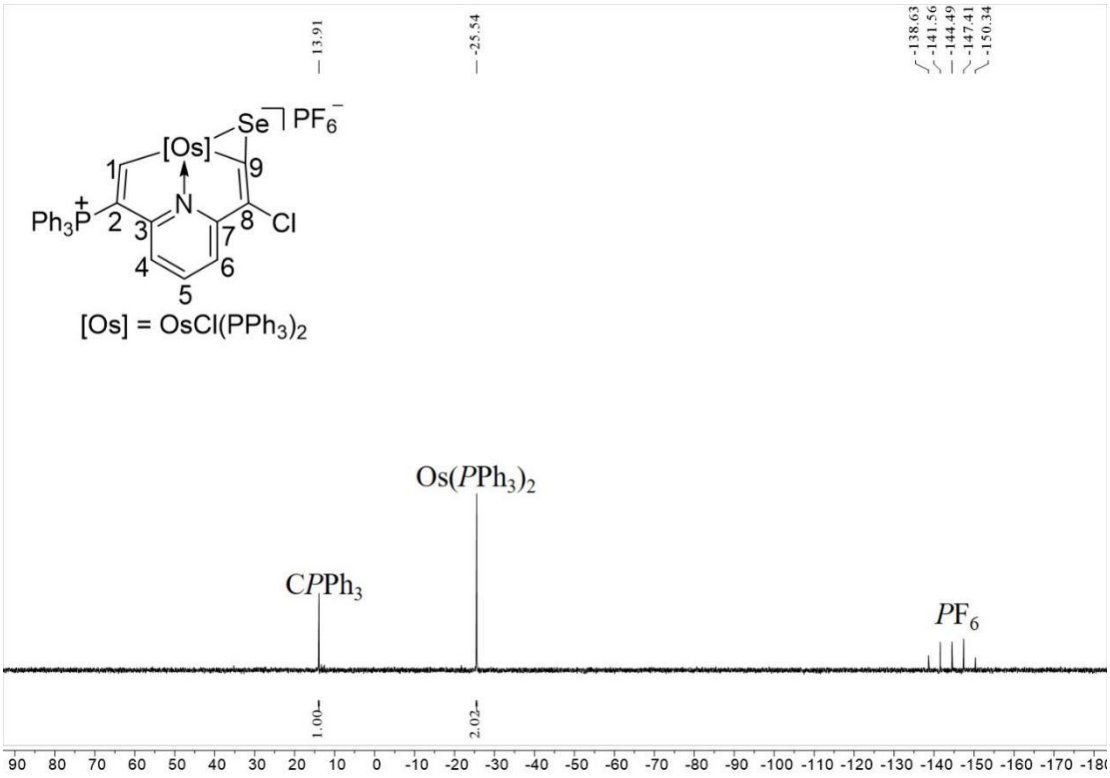


Figure S39. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **3b**.

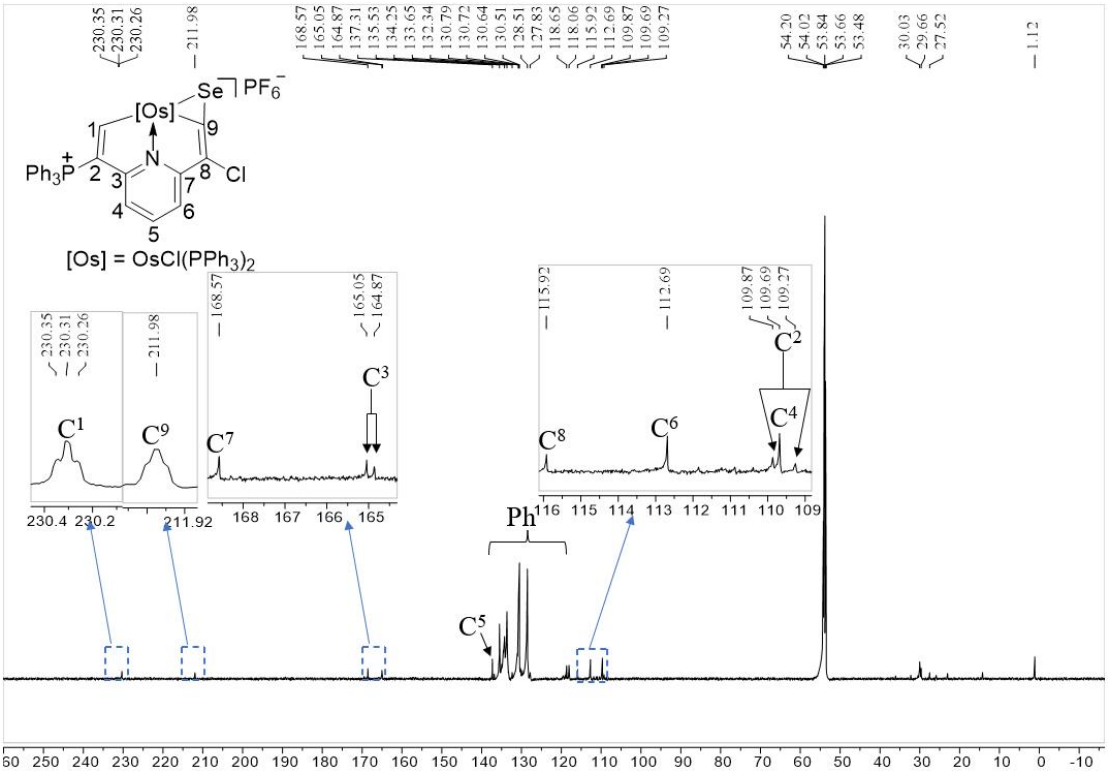


Figure S40. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **3b**.

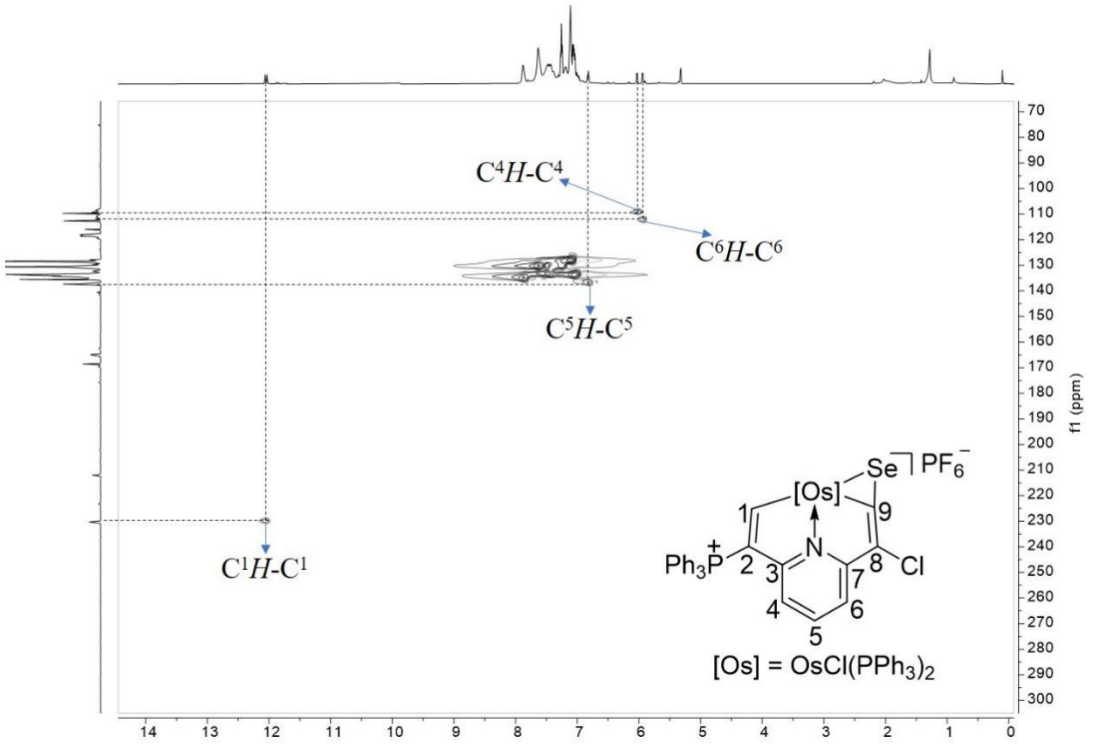


Figure S41. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **3b**.

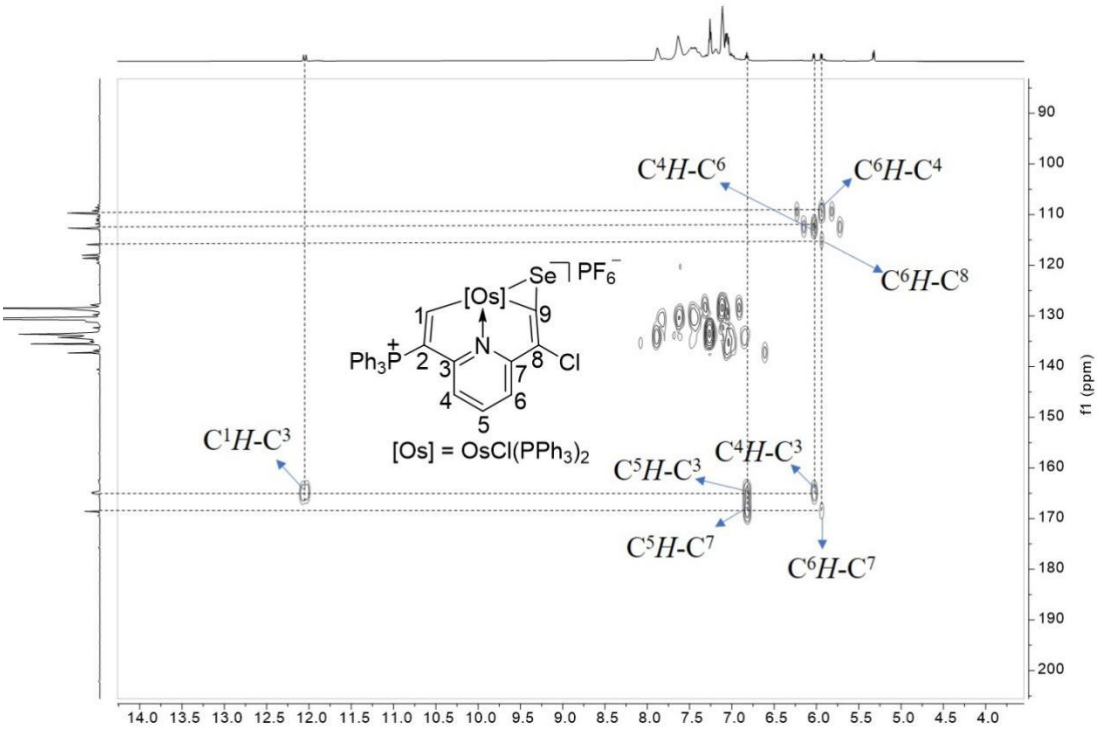


Figure S42. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **3b**.

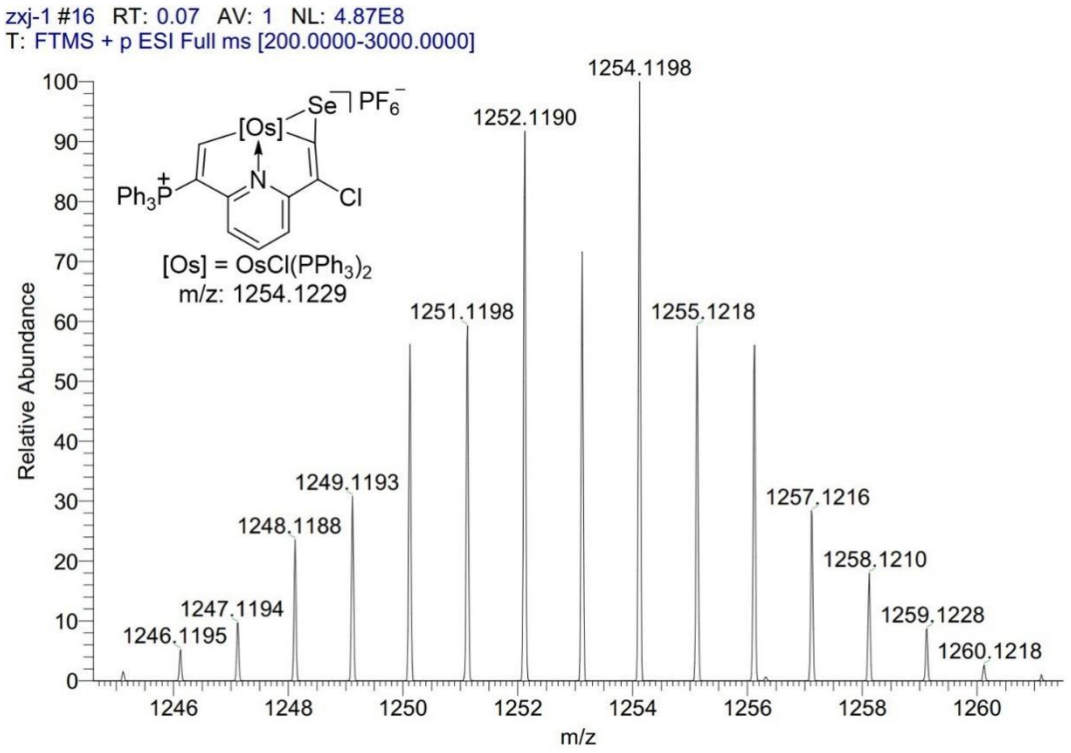


Figure 43. Positive-ion ESI-MS spectrum of [**3b**]$^{+}$ measured in methanol.

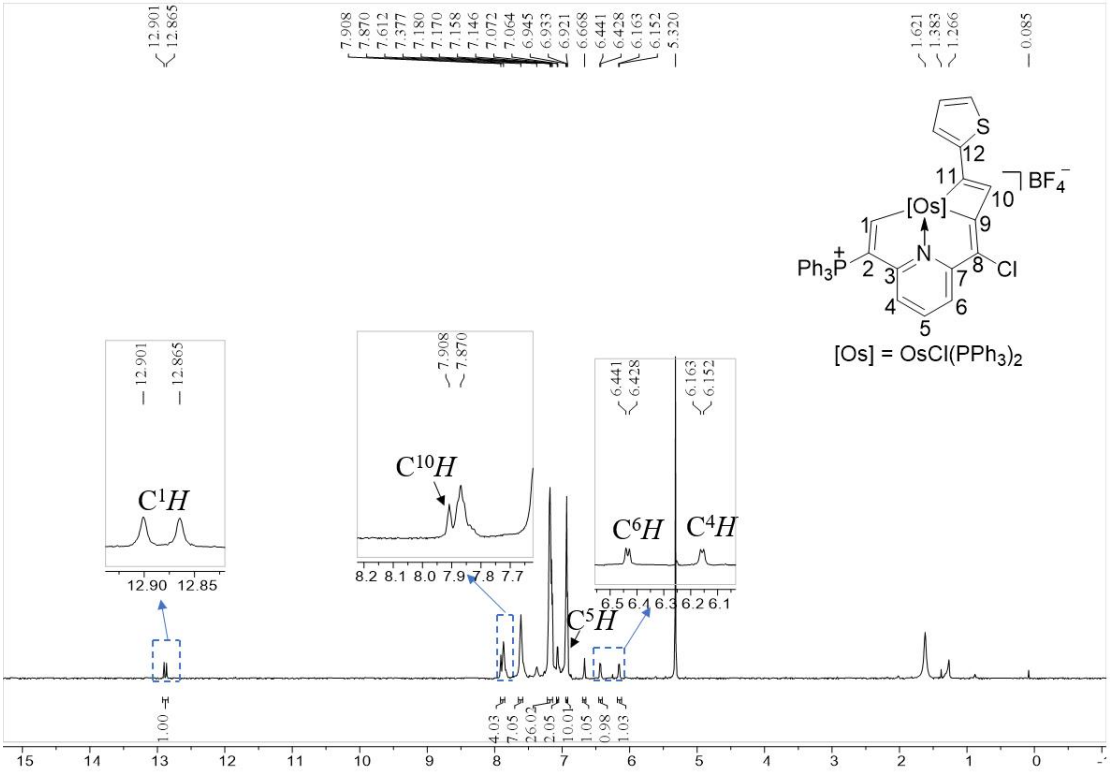


Figure S44. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **4a**.

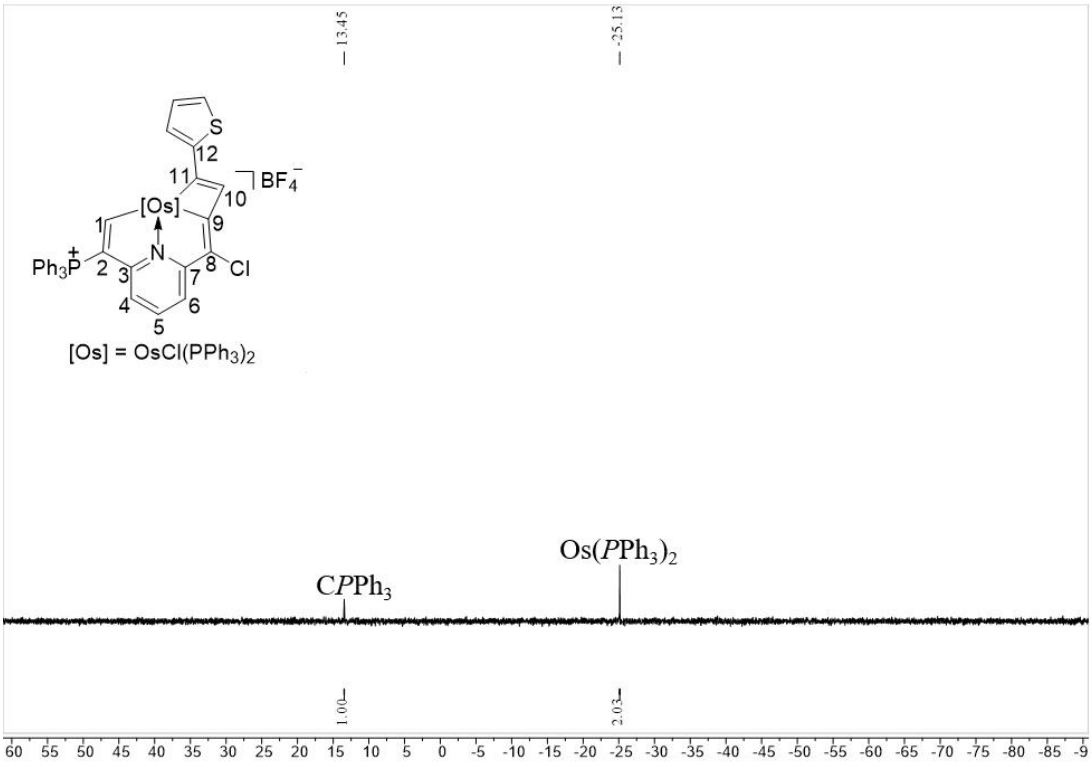


Figure S45. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **4a**.

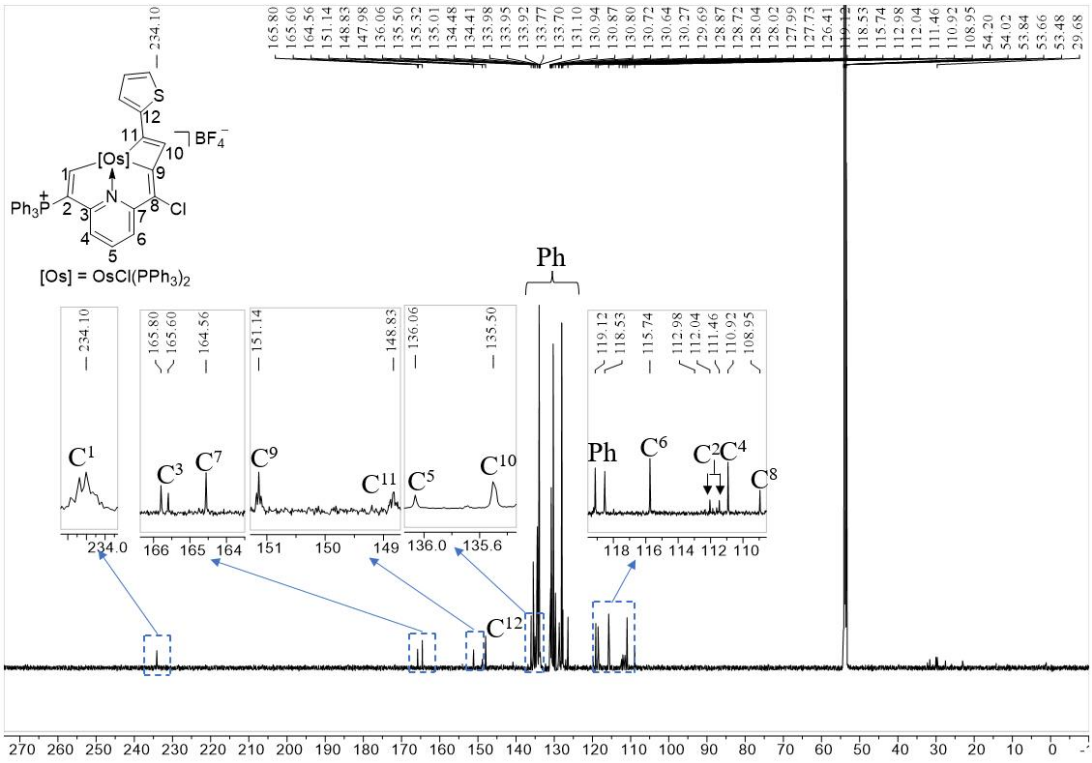


Figure S46. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **4a**.

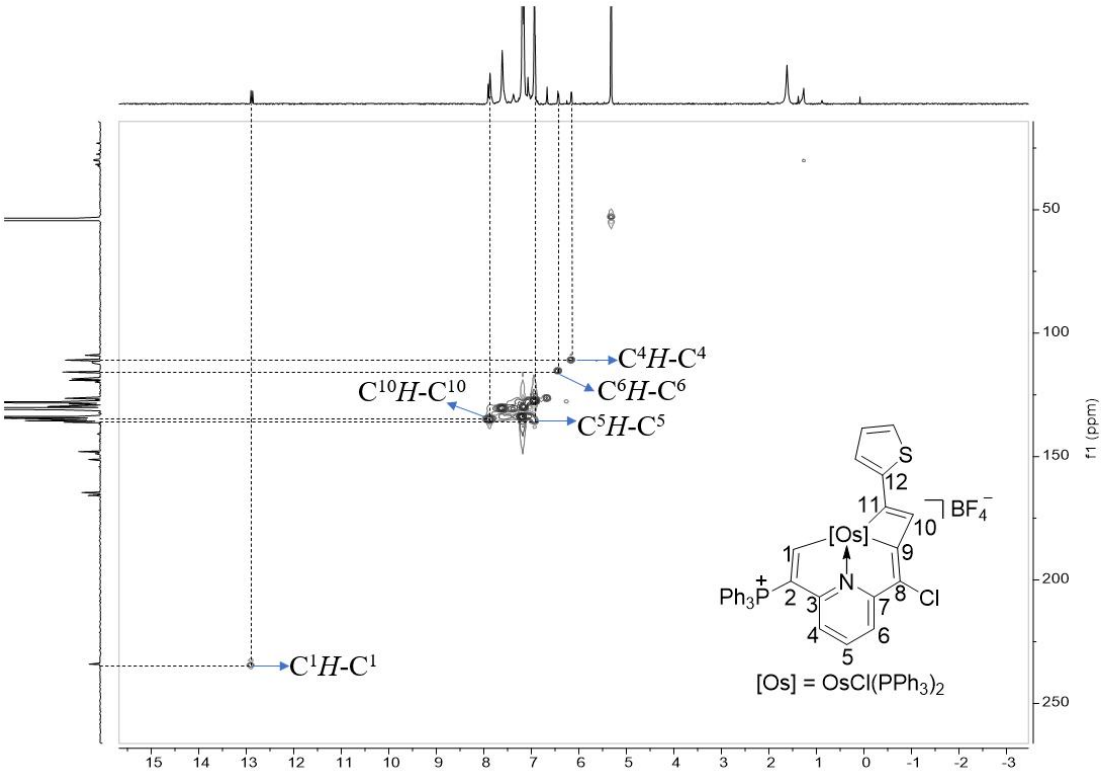


Figure S47. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **4a**.

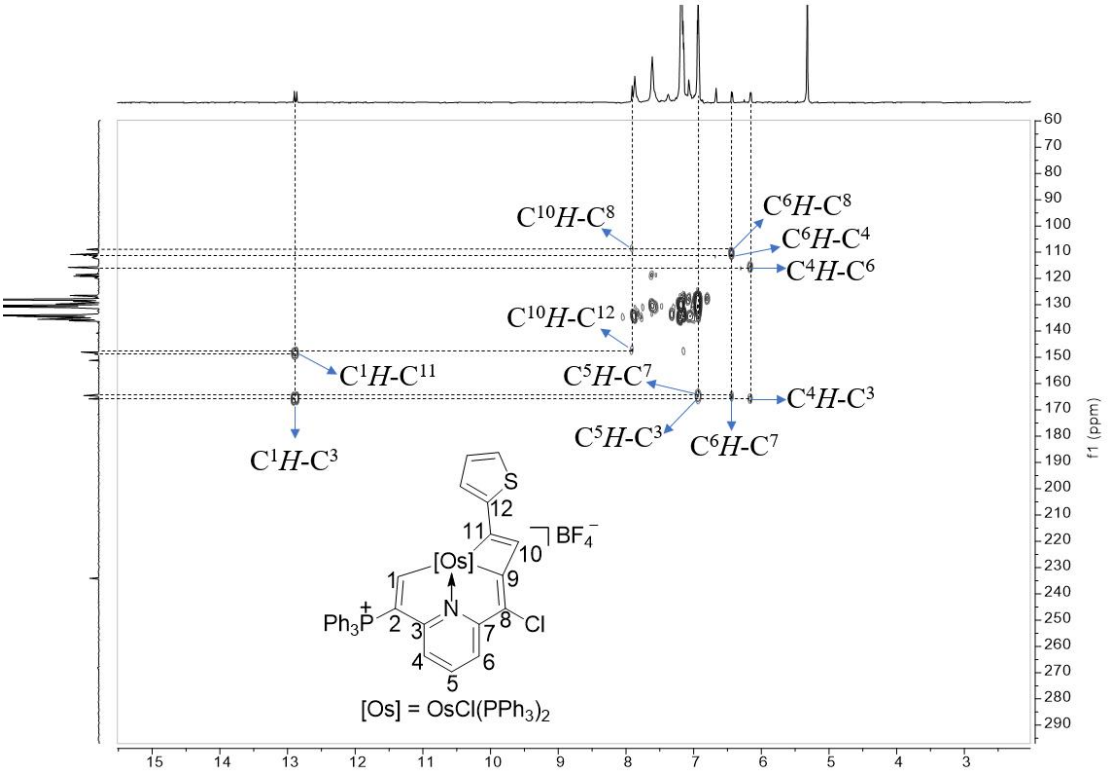


Figure S48. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **4a**.

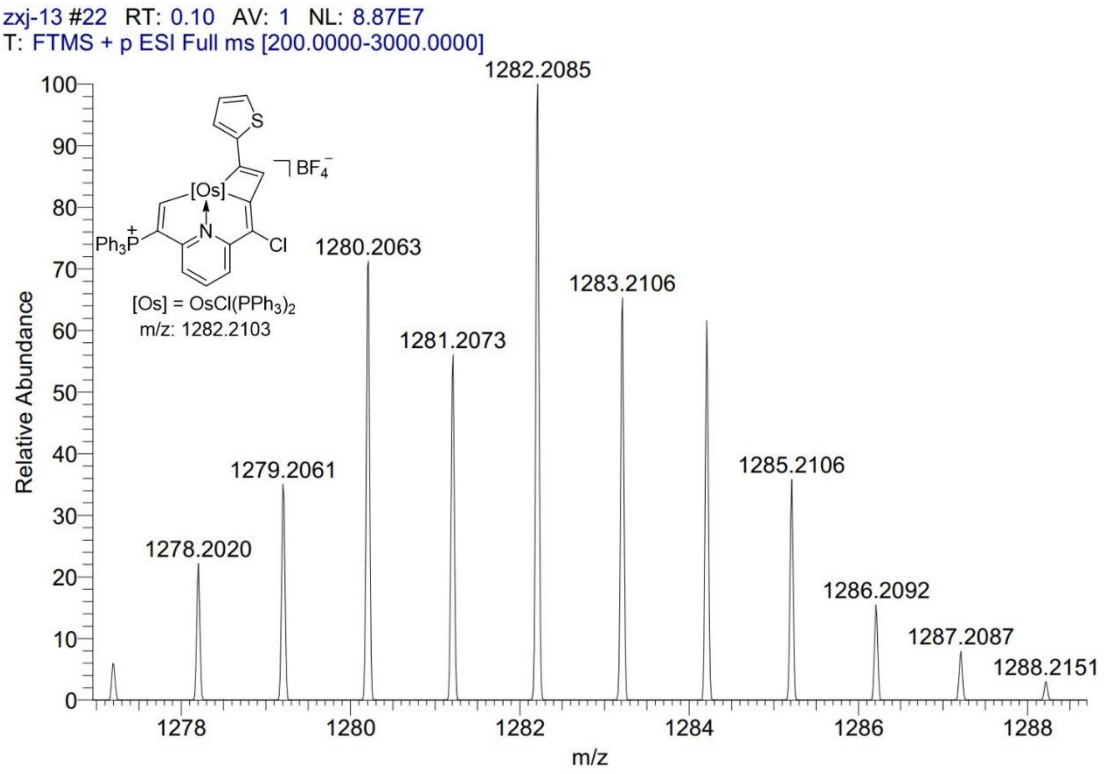


Figure S49. Positive-ion ESI-MS spectrum of [**4a**]$^{+}$ measured in methanol.

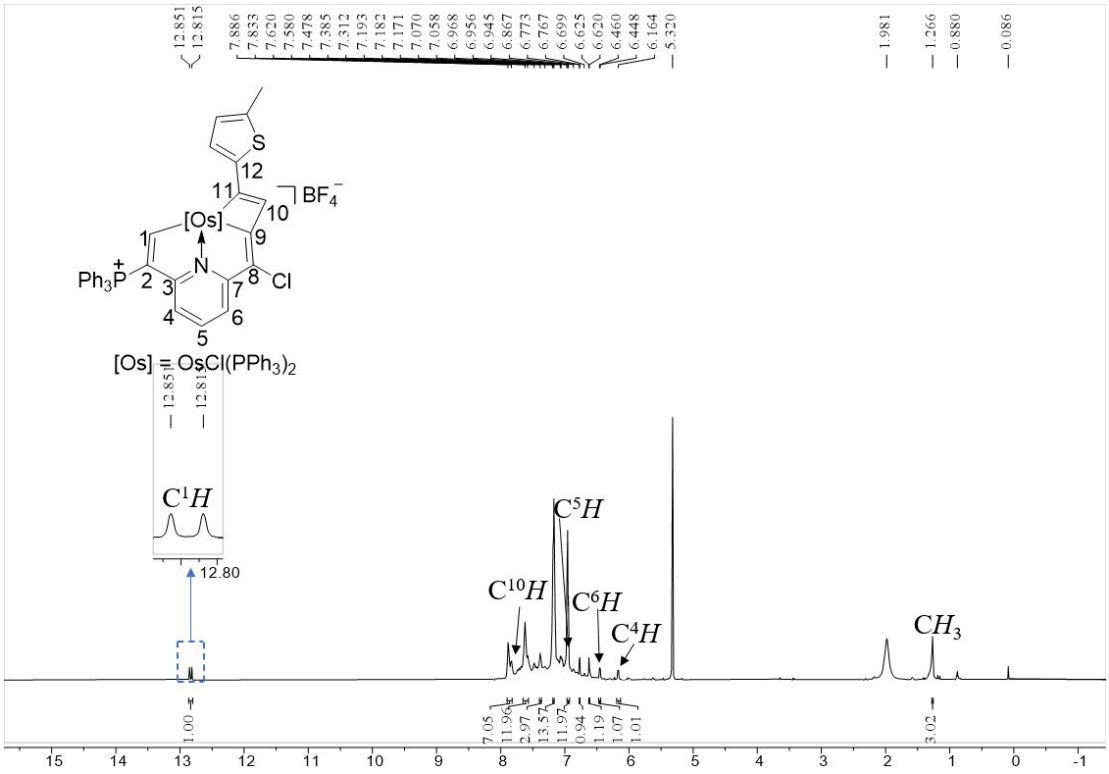


Figure S50. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **4b**.

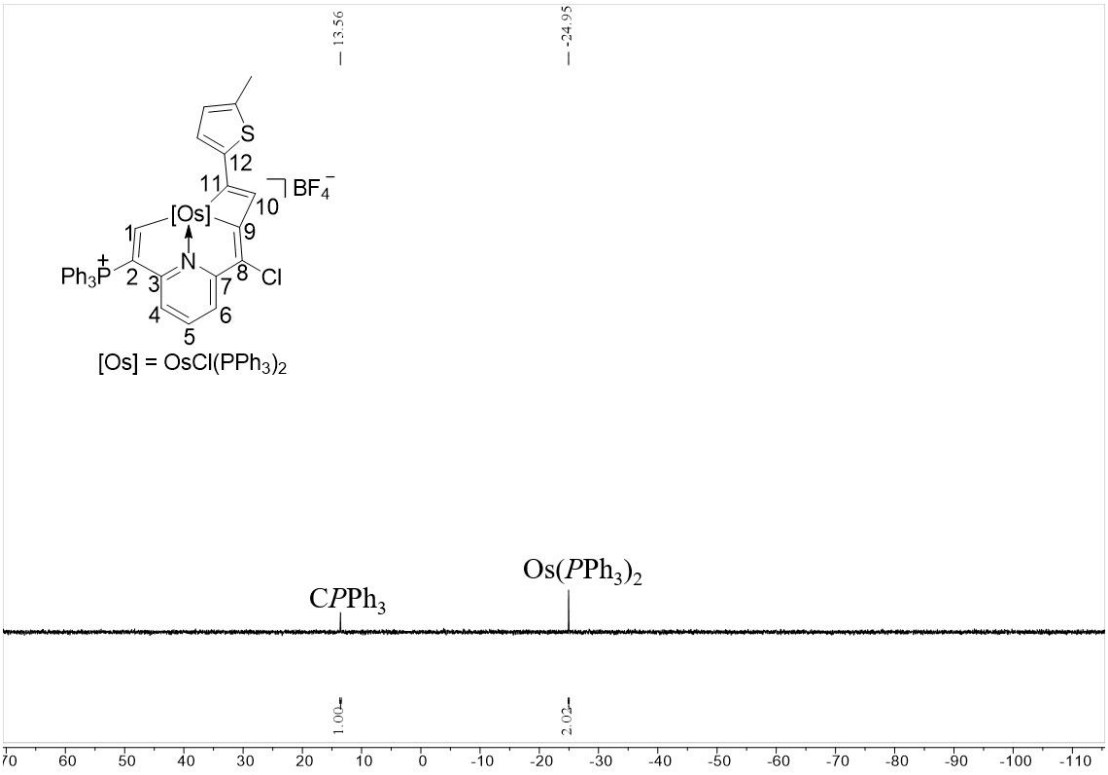


Figure S51. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **4b**.

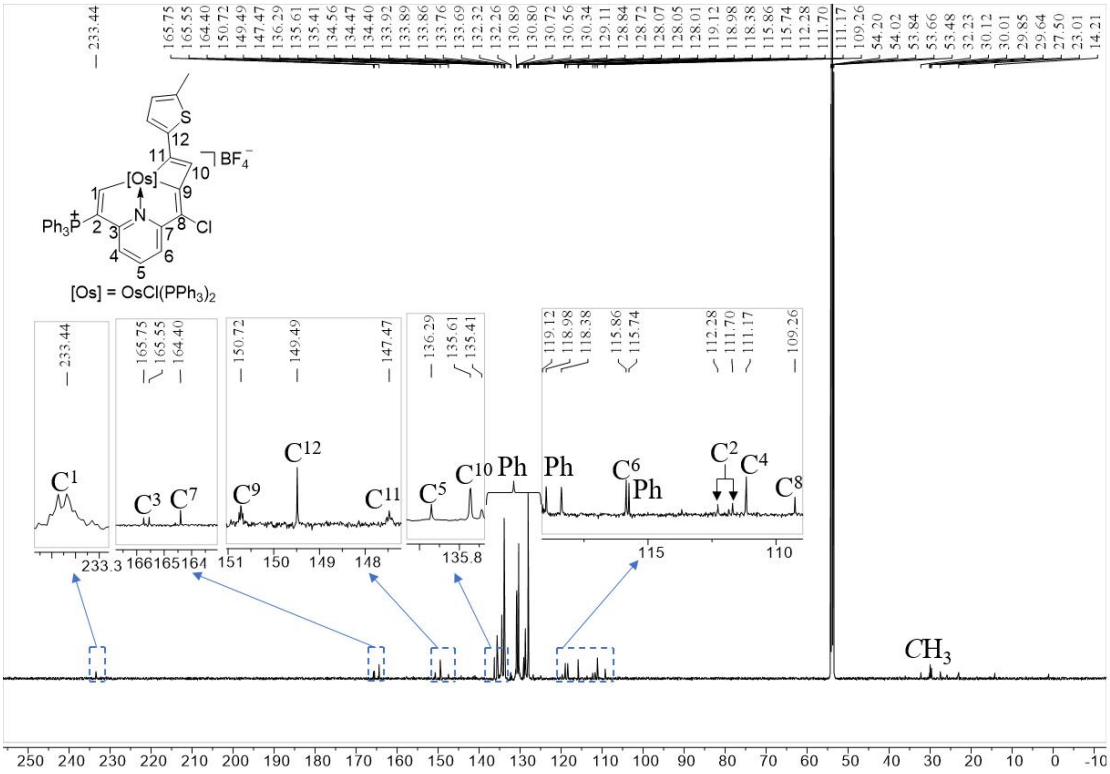


Figure S52. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **4b**.

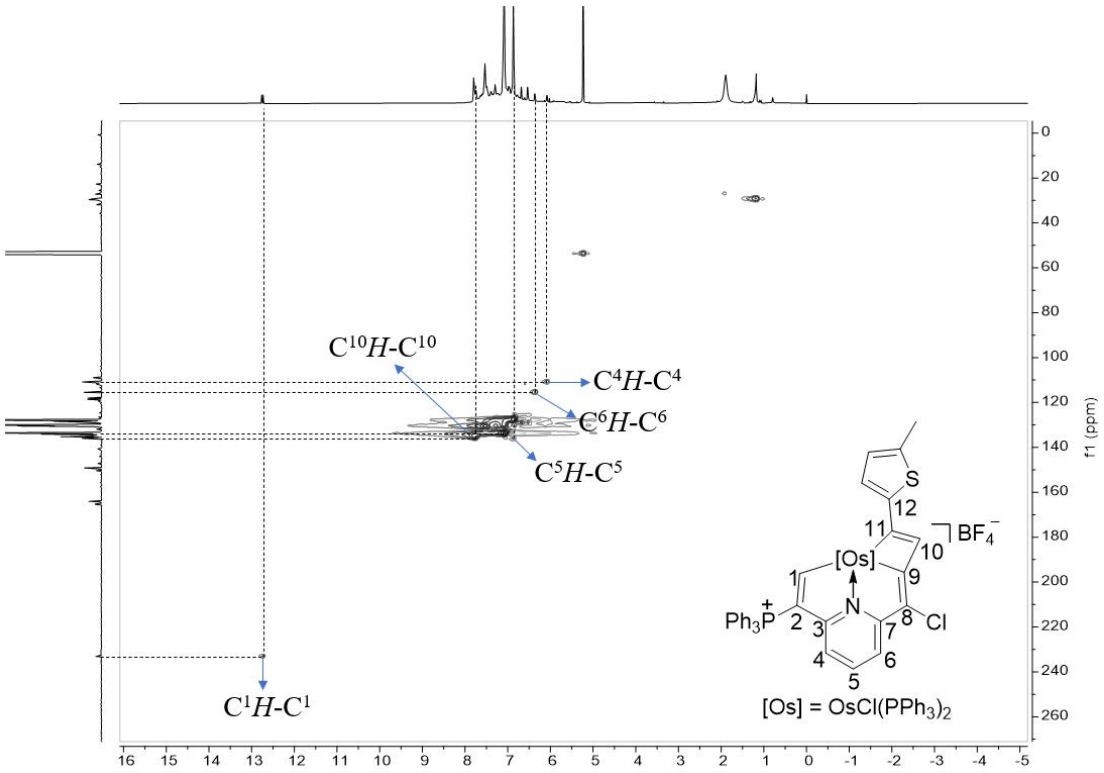


Figure S53. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **4b**.

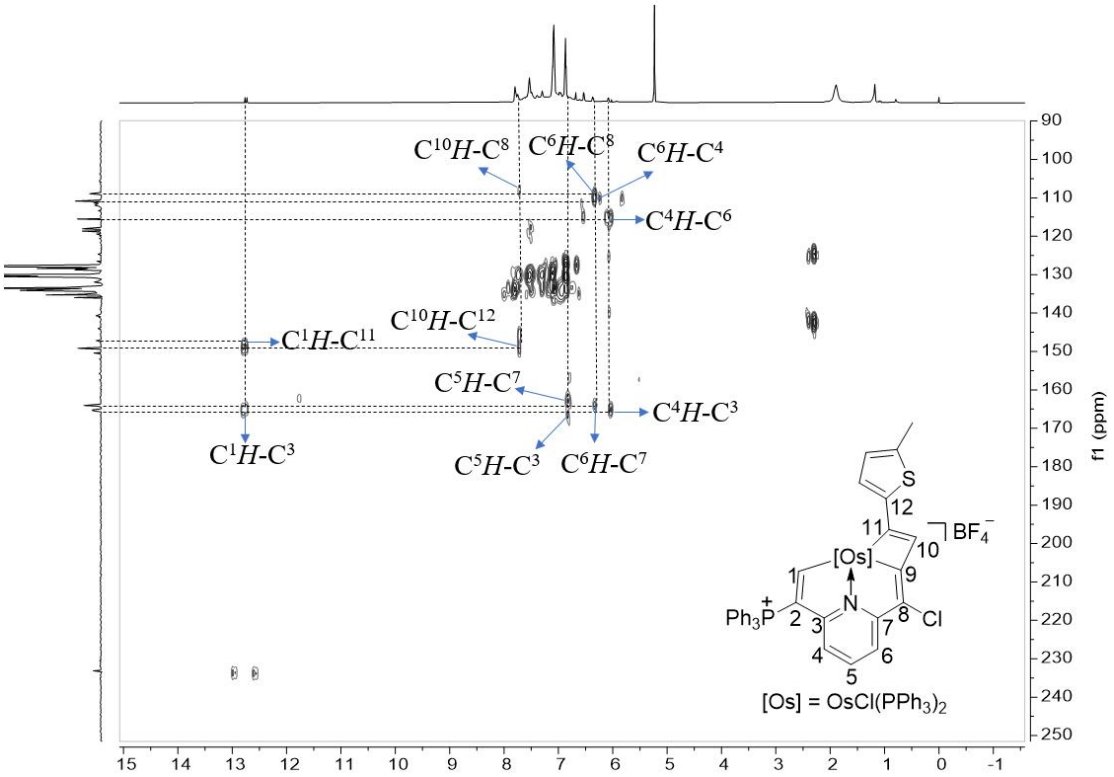


Figure S54. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **4b**.

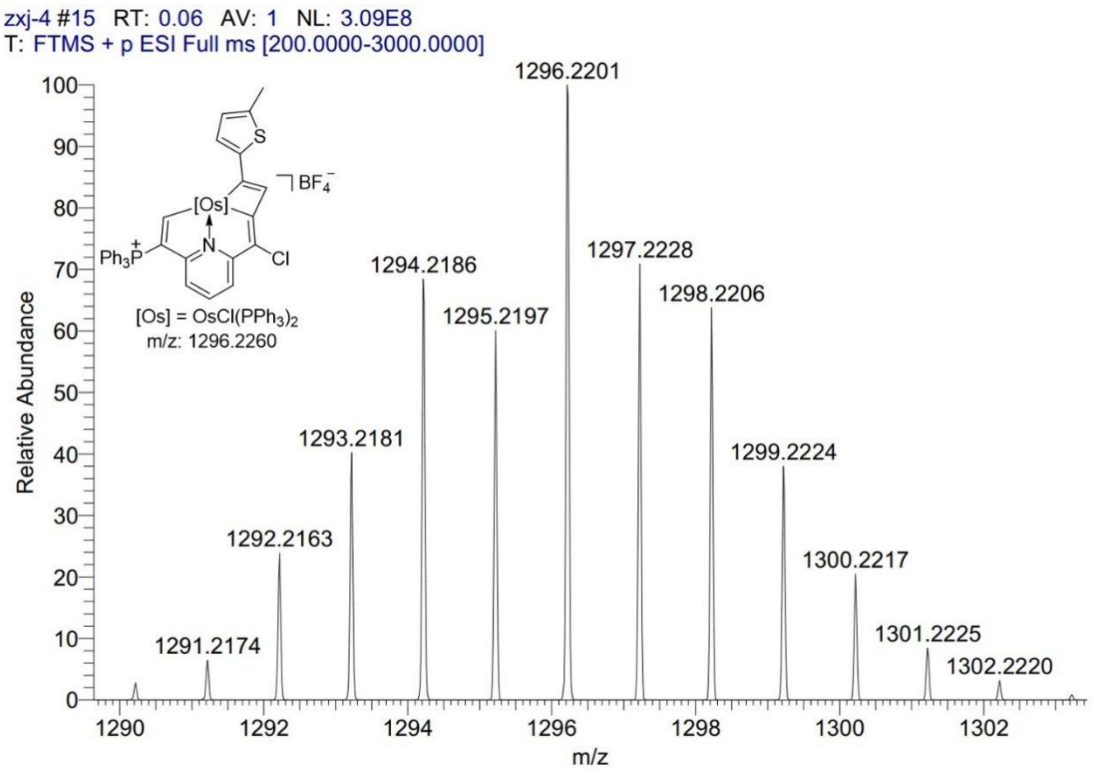


Figure 55. Positive-ion ESI-MS spectrum of [**4b**]$^{+}$ measured in methanol.

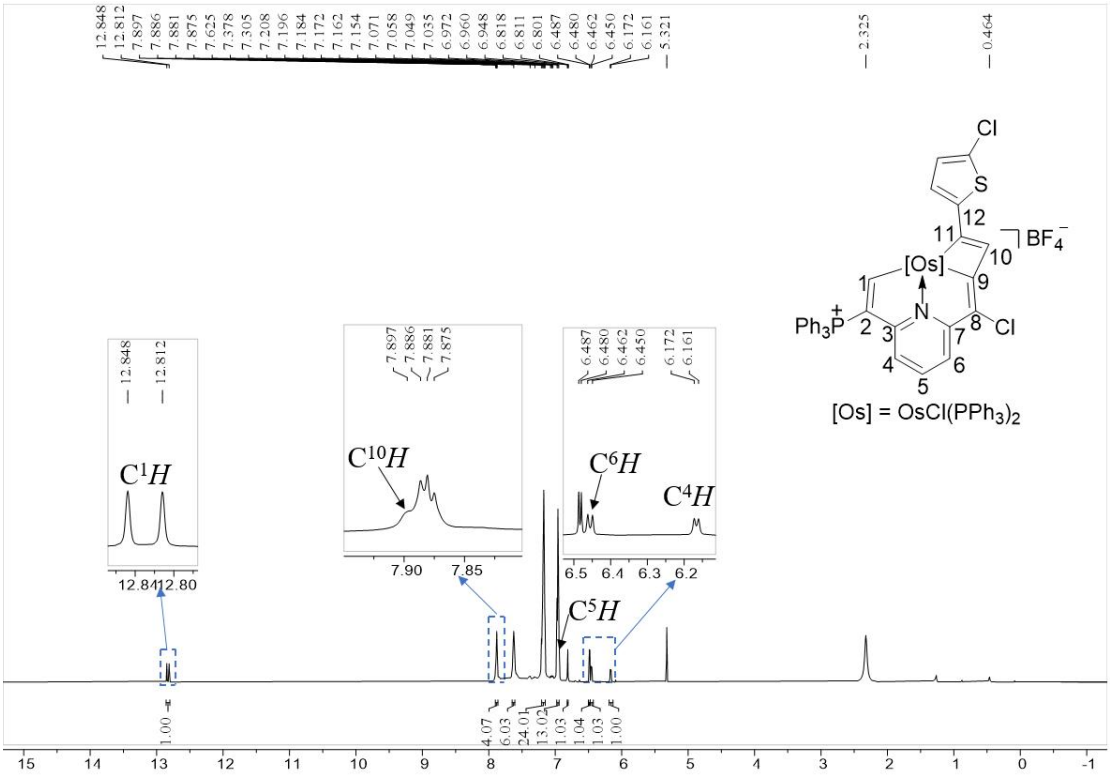


Figure S56. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **4c**.

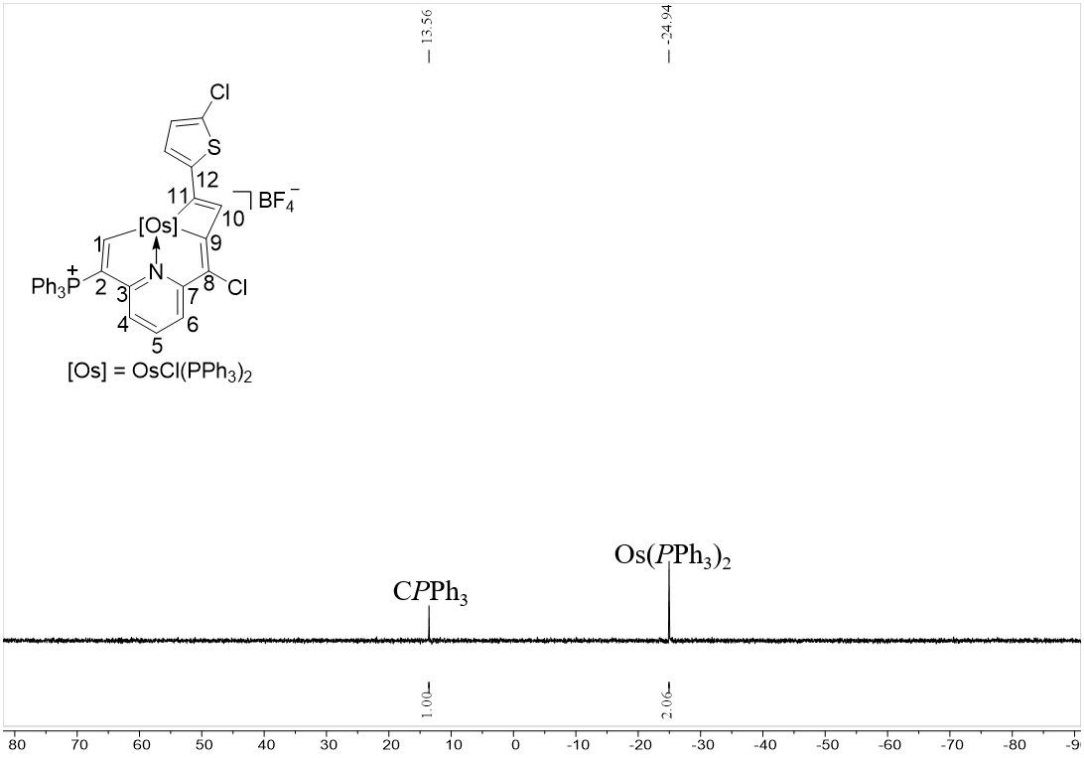


Figure S57. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **4c**.

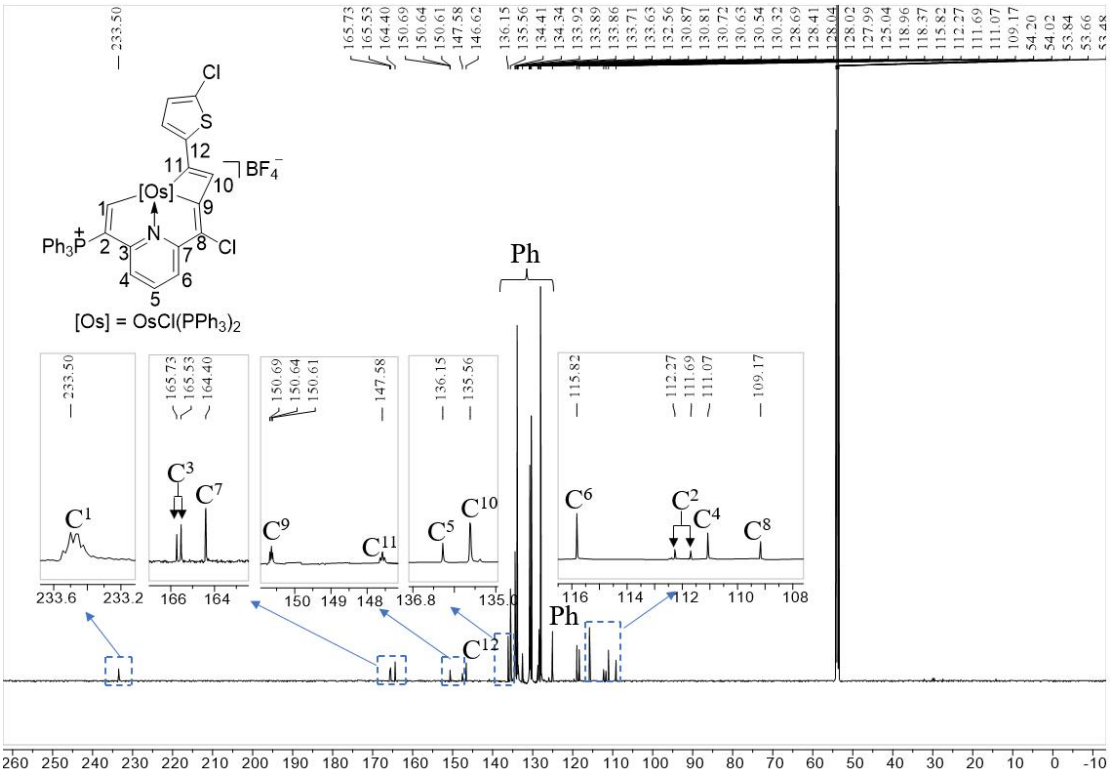


Figure S58. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **4c**.

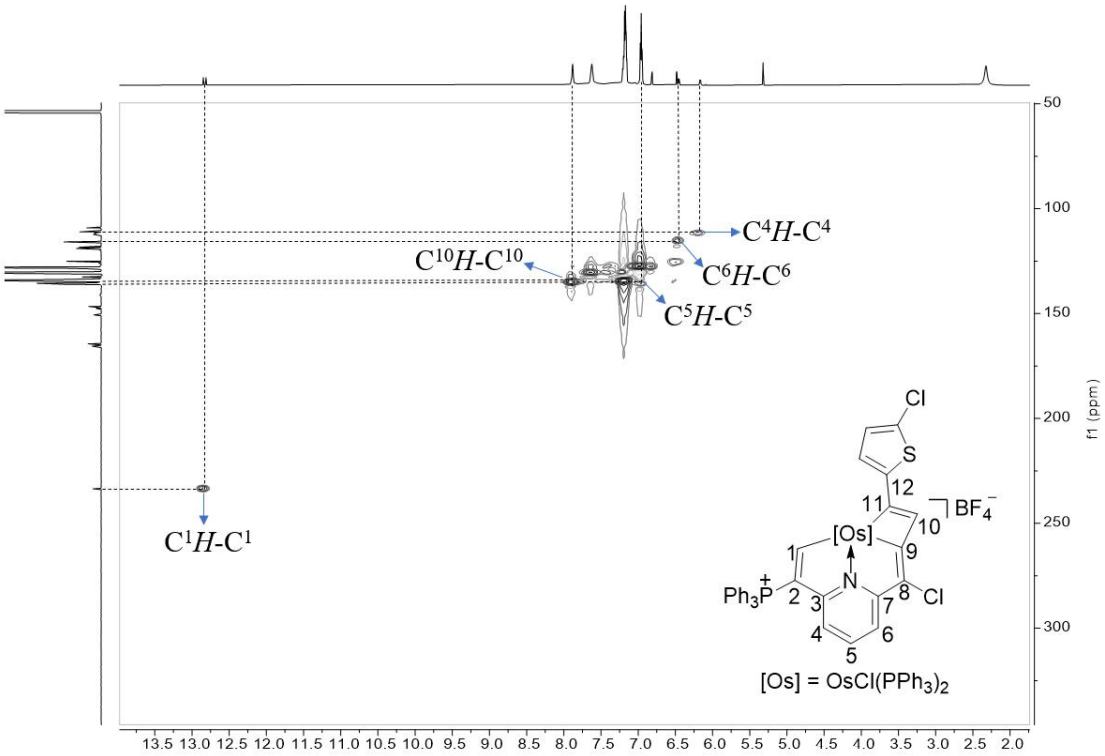


Figure S59. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **4c**.

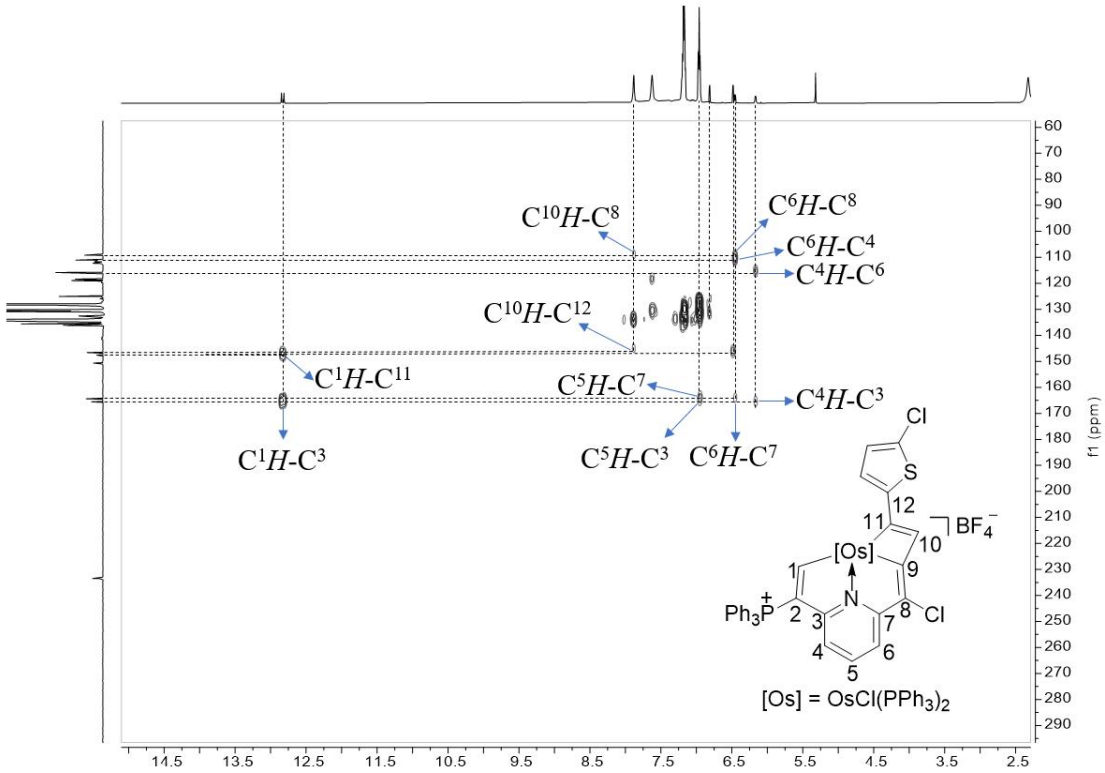


Figure S60. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **4c**.

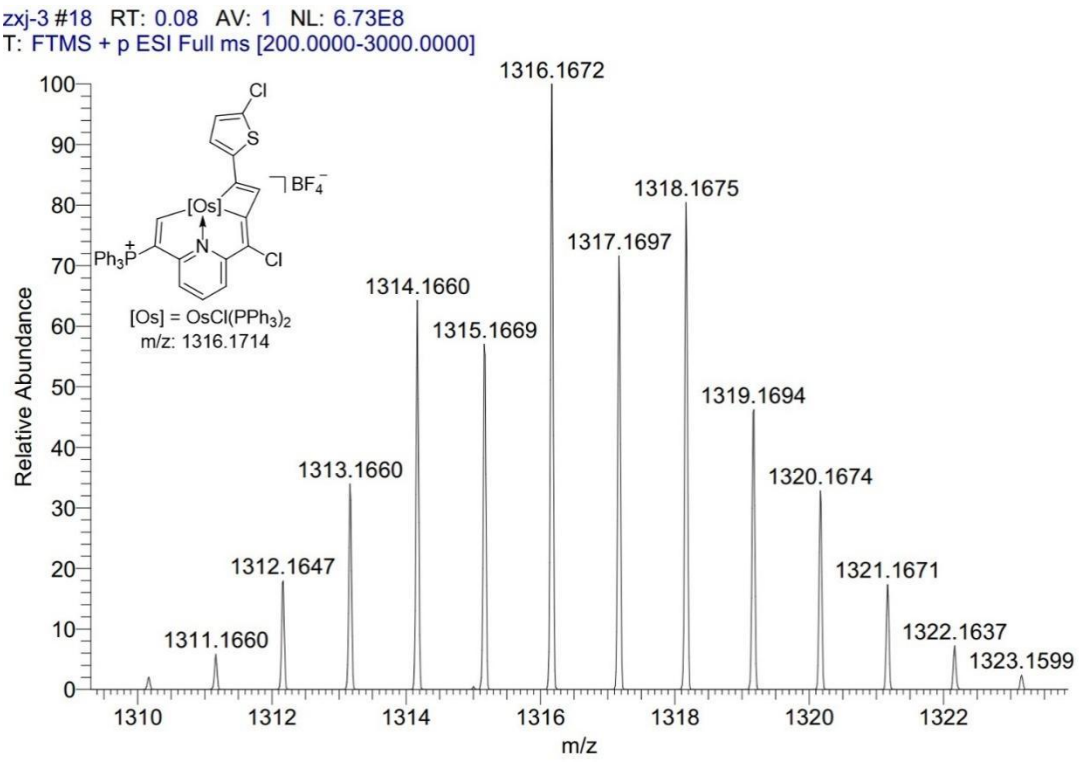


Figure S61. Positive-ion ESI-MS spectrum of [**4c**]$^+$ measured in methanol.

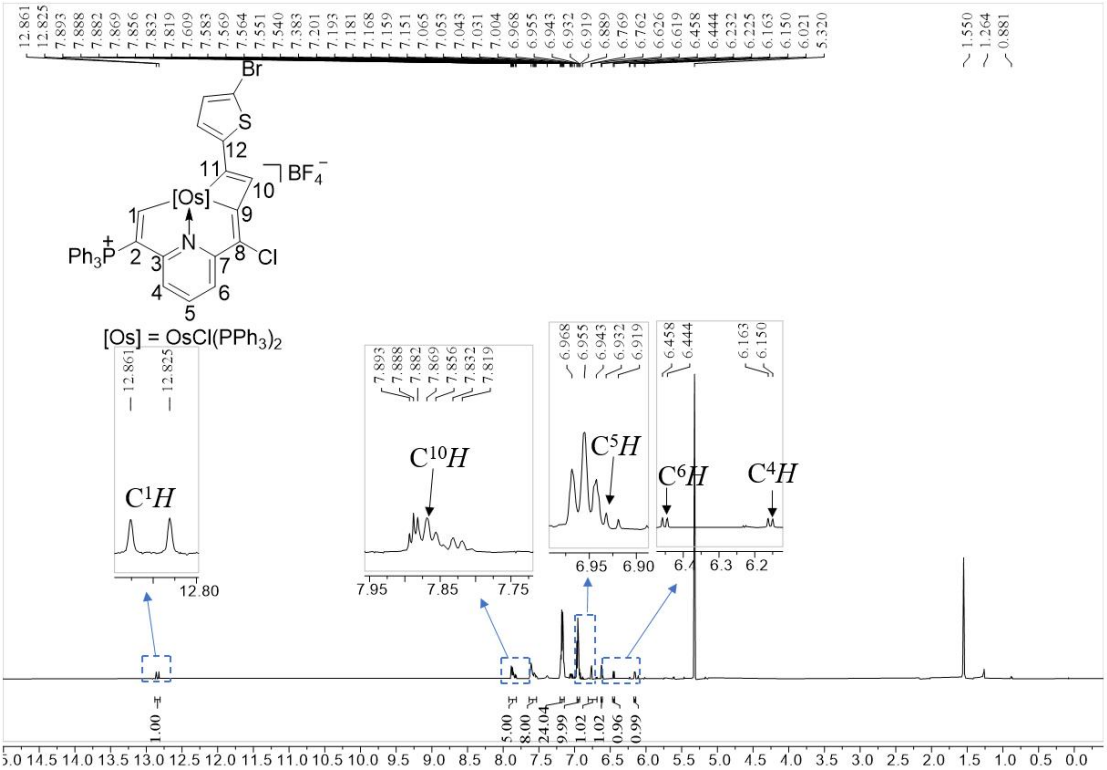


Figure S62. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **4d**.

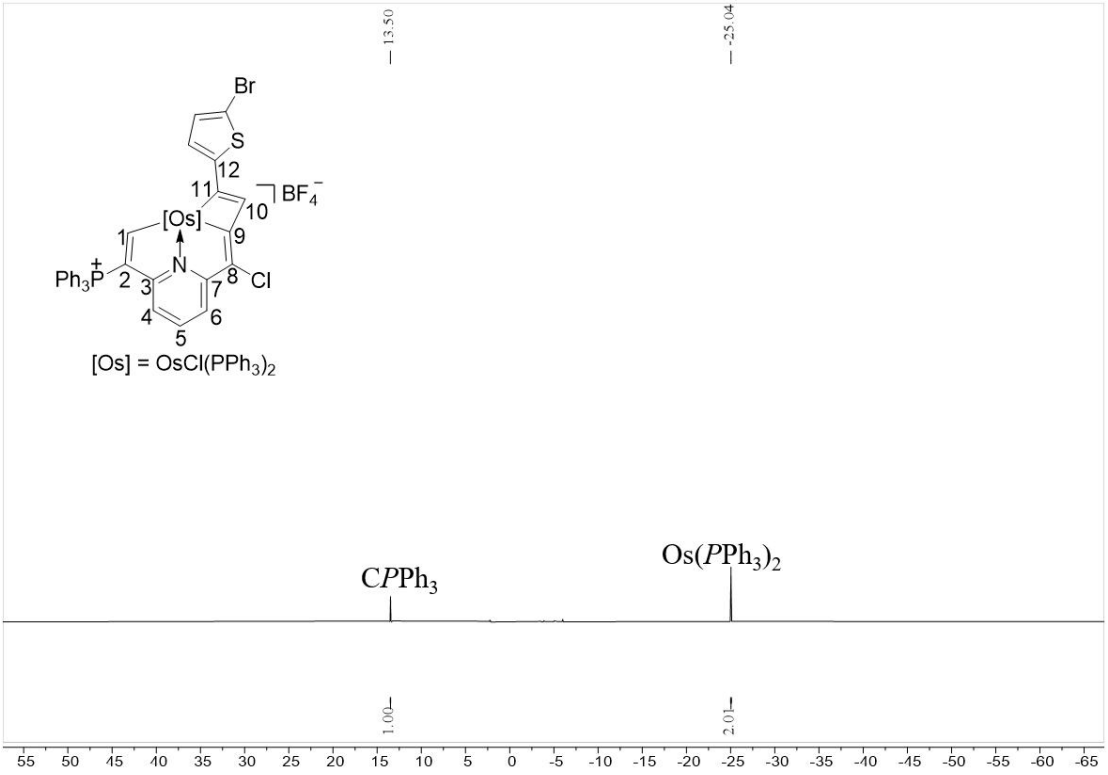


Figure S63. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **4d**.

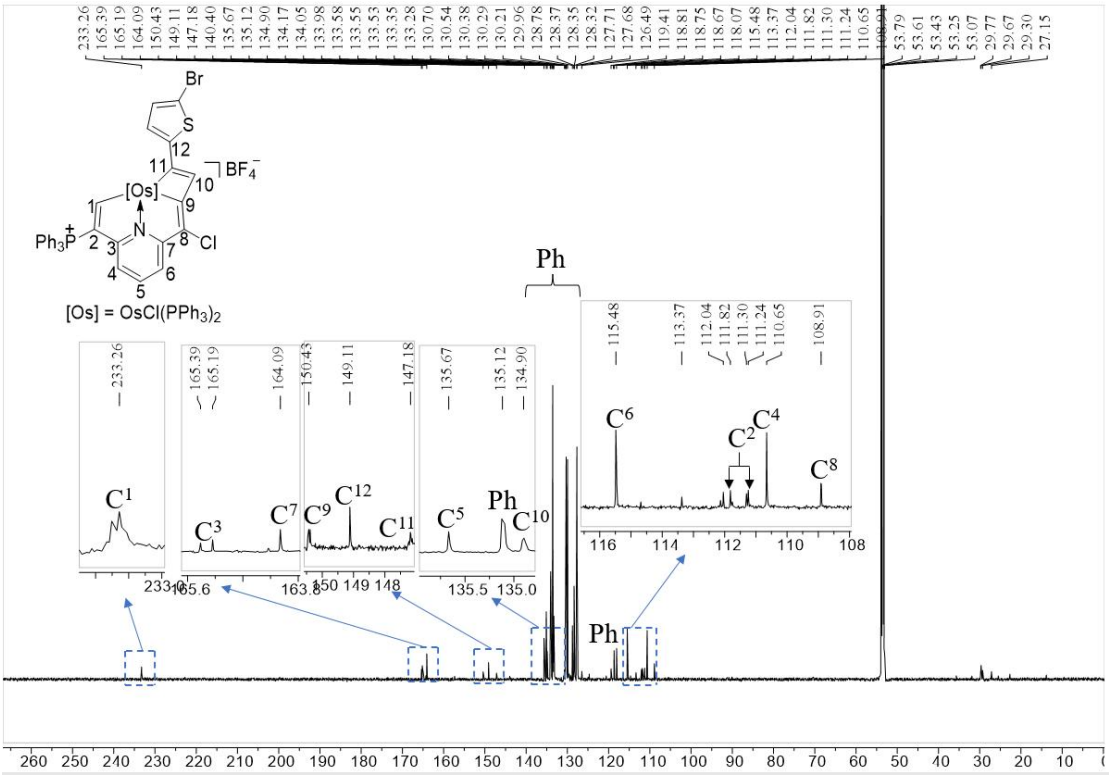


Figure S64. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **4d**.

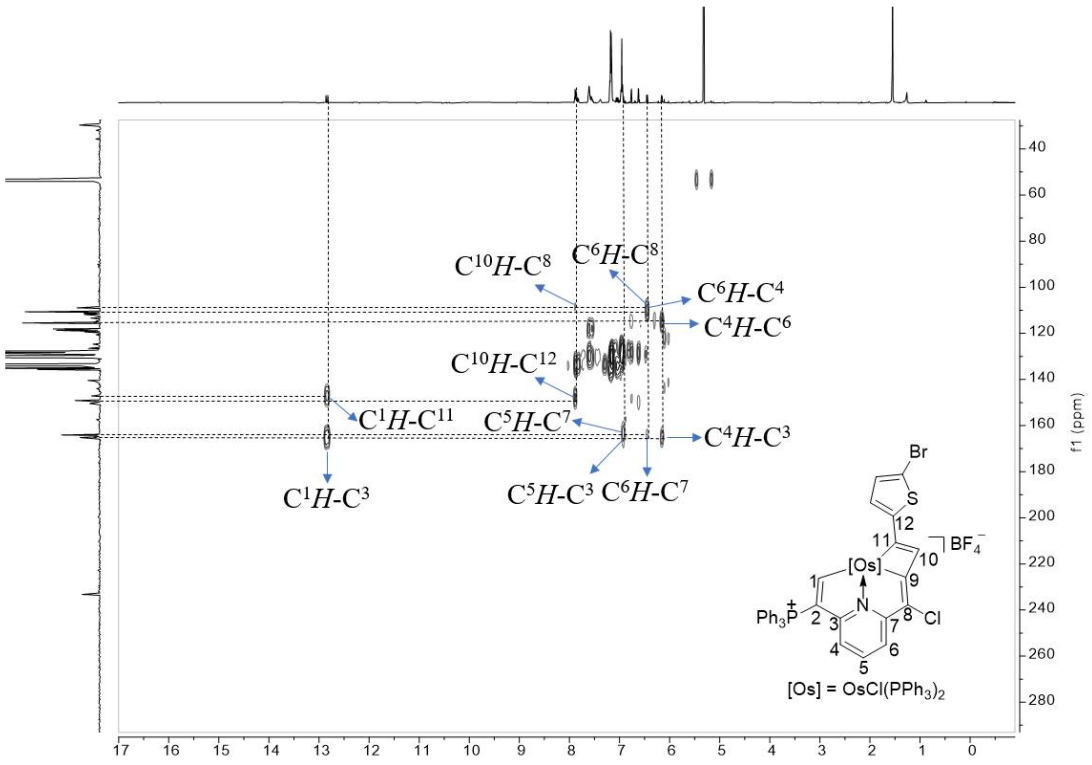


Figure S65. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **4d**.

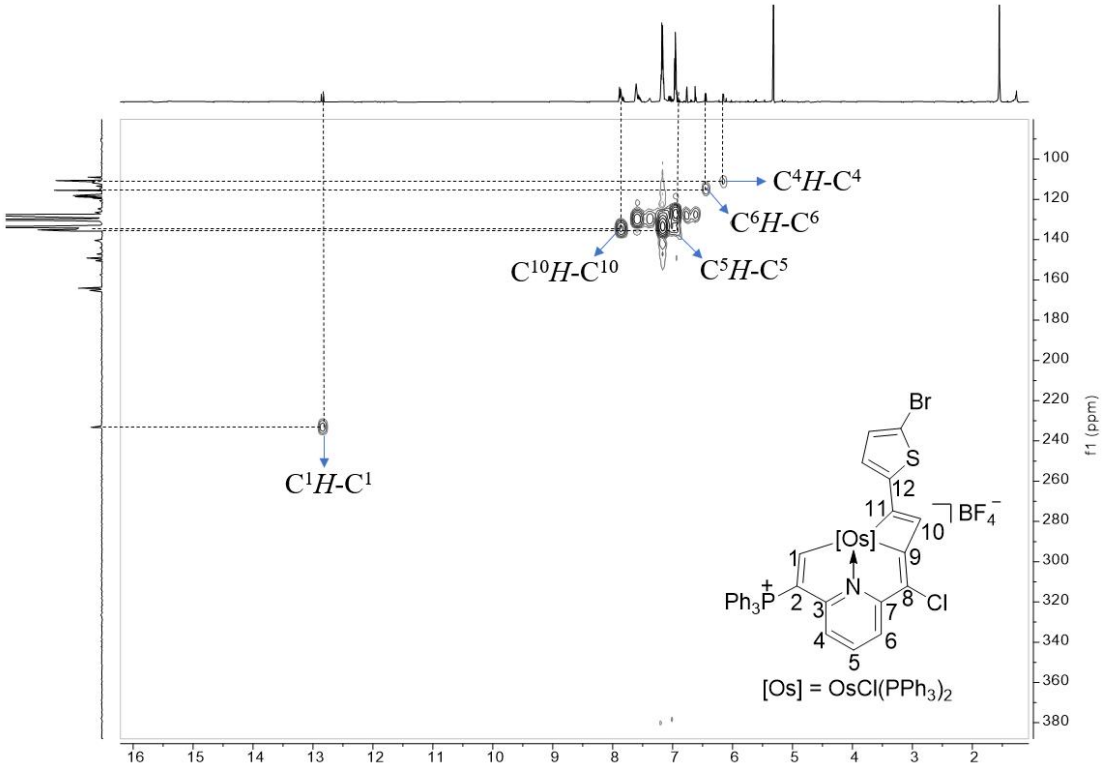


Figure S66. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **4d**.

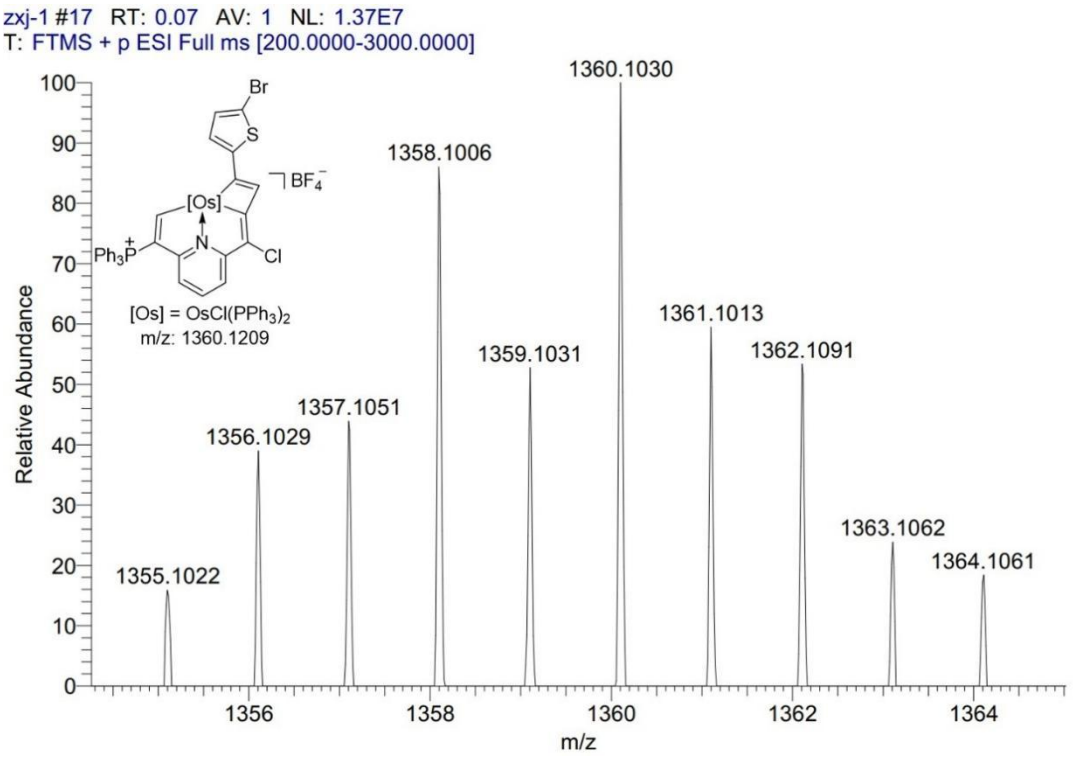


Figure 67. Positive-ion ESI-MS spectrum of [**4d**]$^{+}$ measured in methanol.

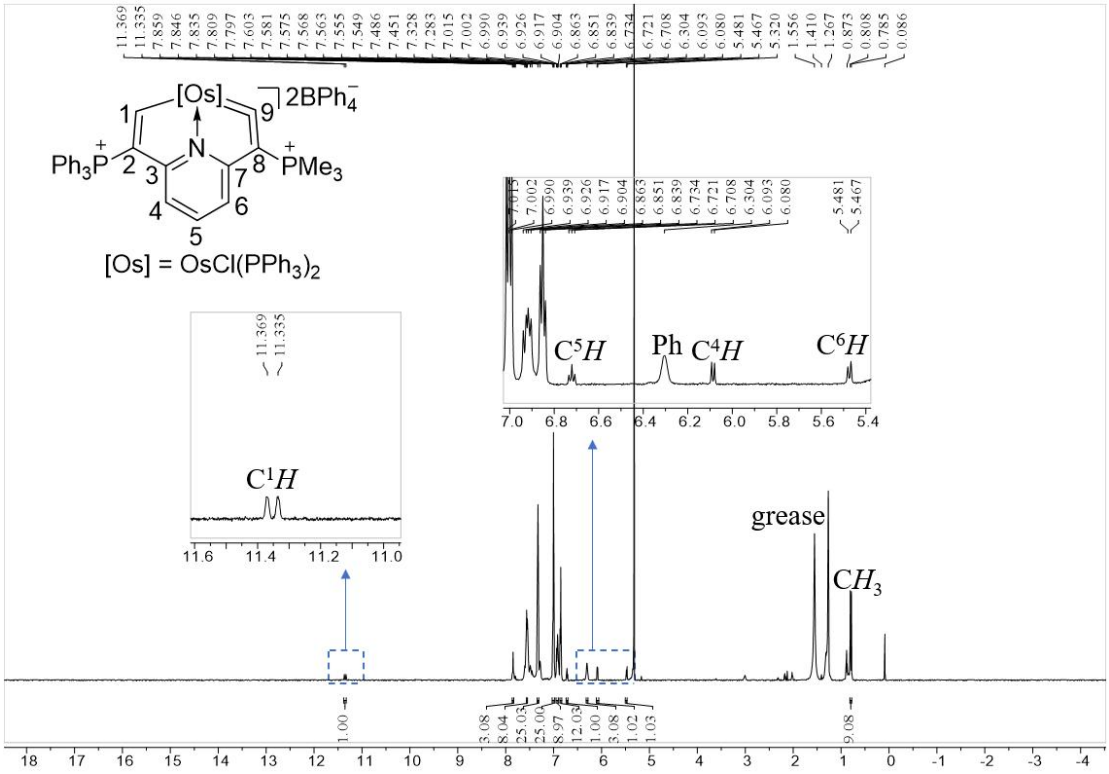


Figure S68. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **5a**.

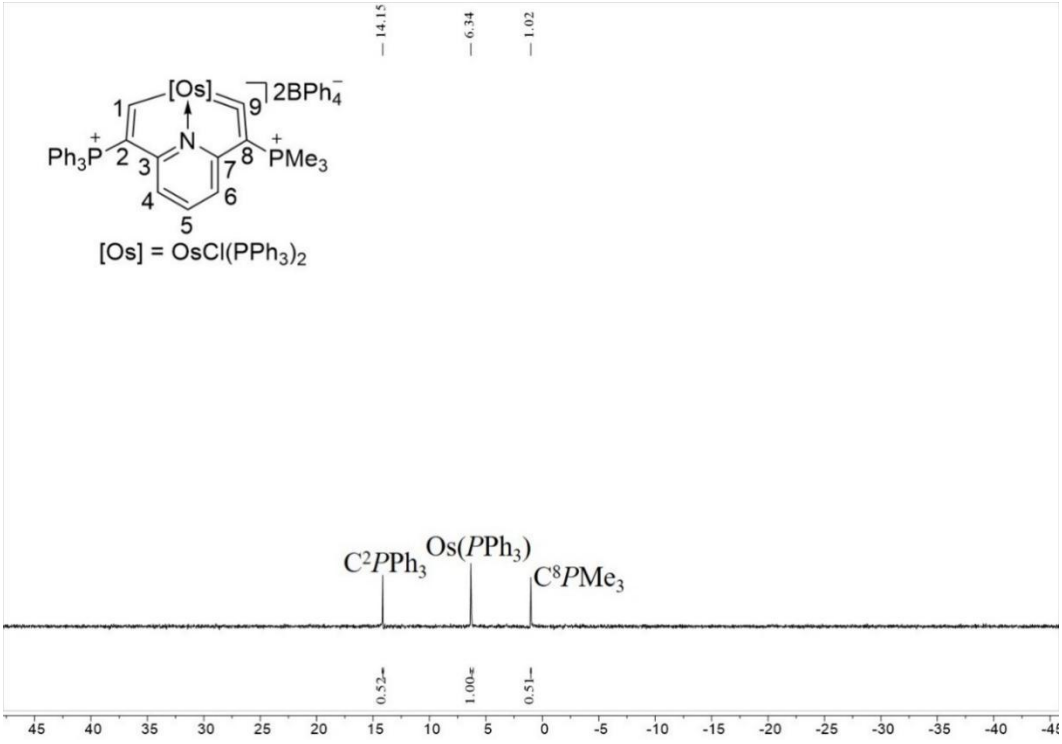


Figure S69. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **5a**.

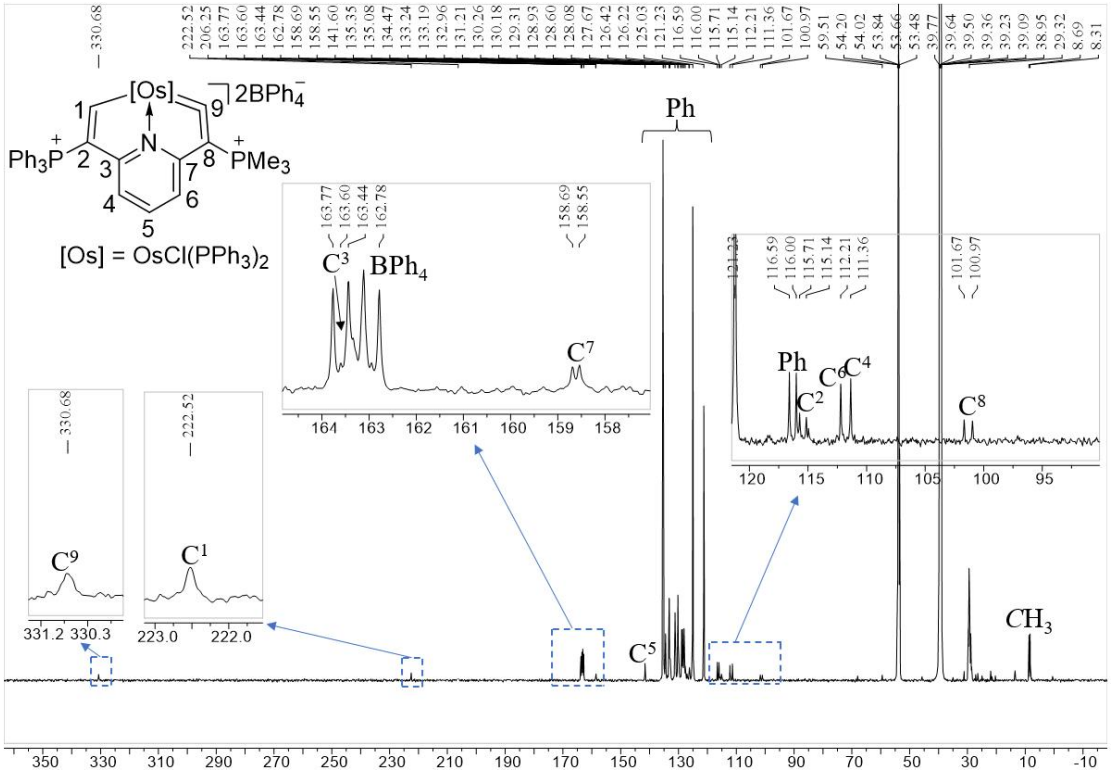


Figure S70. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, $CD_2Cl_2/(CD_3)_2SO$ = 1/1) spectrum for complex **5a**.

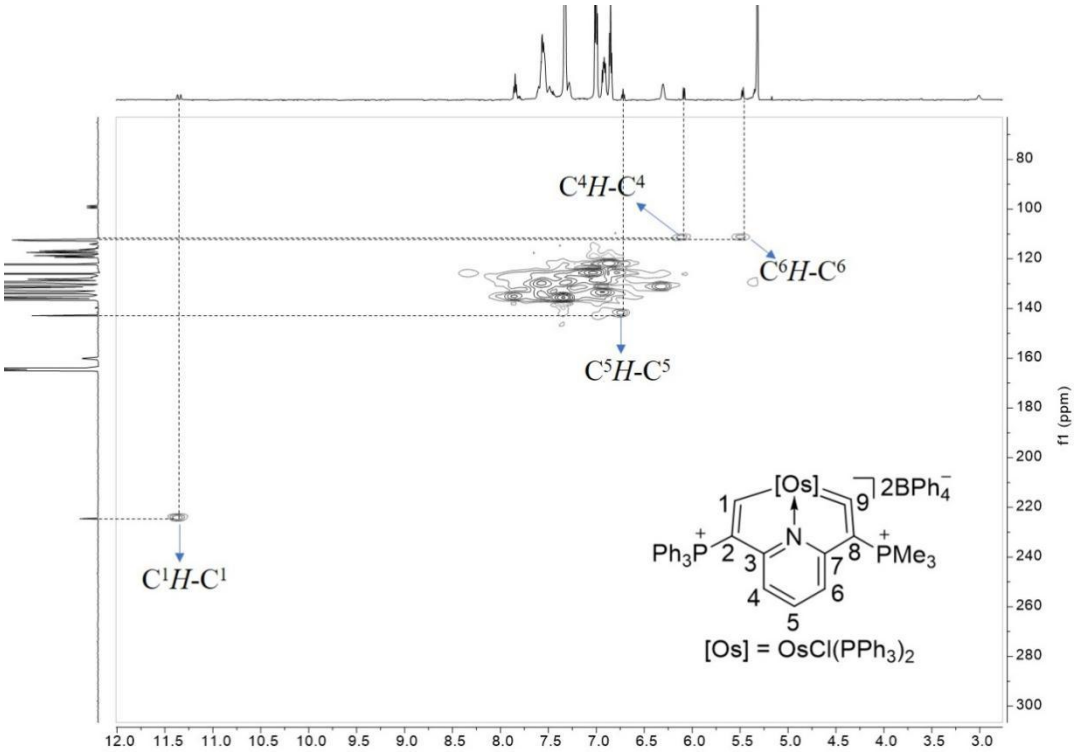


Figure S71. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **5a**.

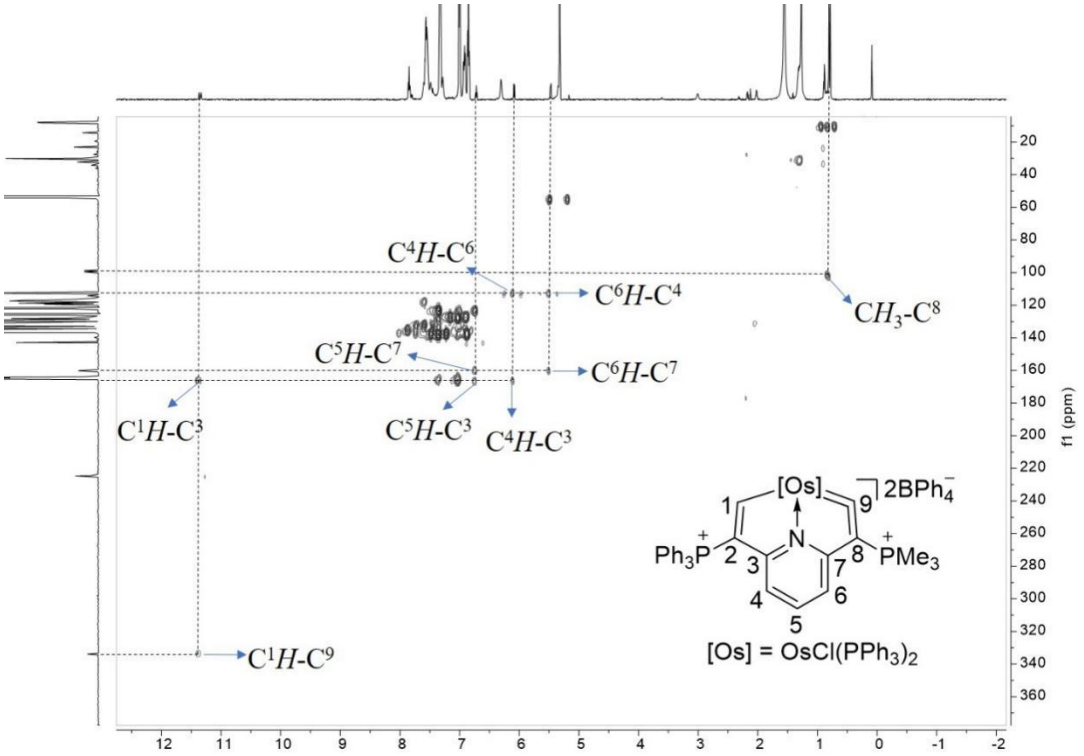


Figure S72. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **5a**.

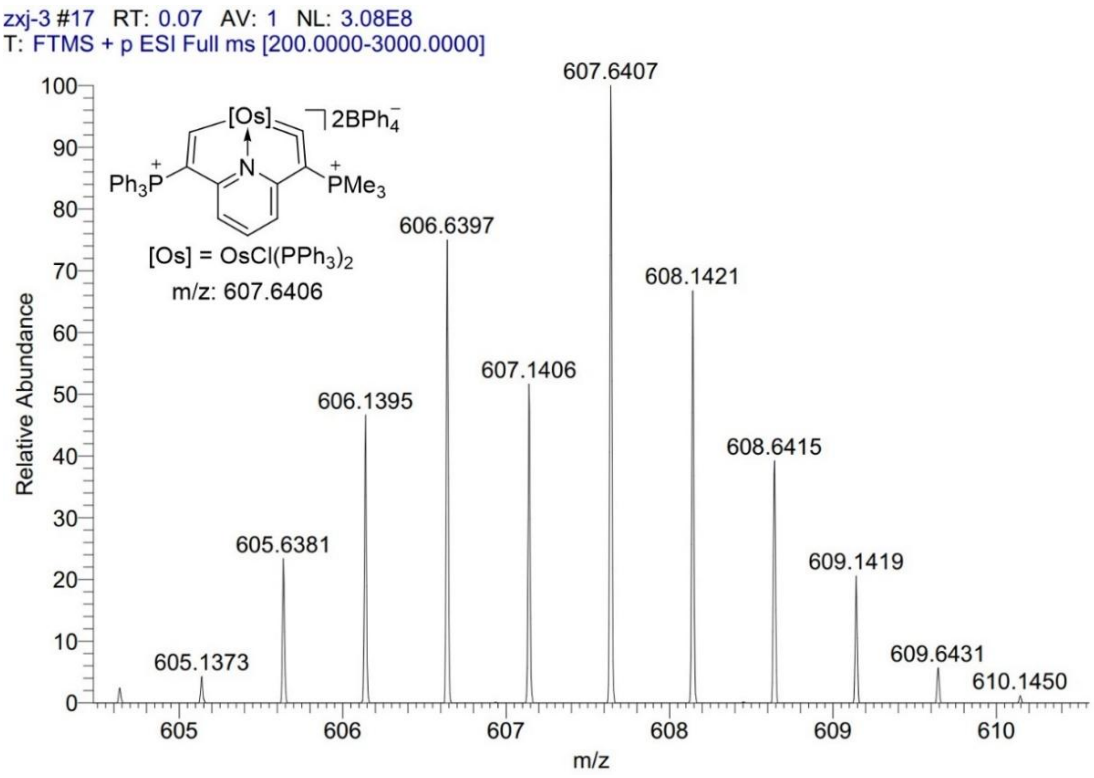


Figure S73. Positive-ion ESI-MS spectrum of [**5a**]$^+$ measured in methanol.

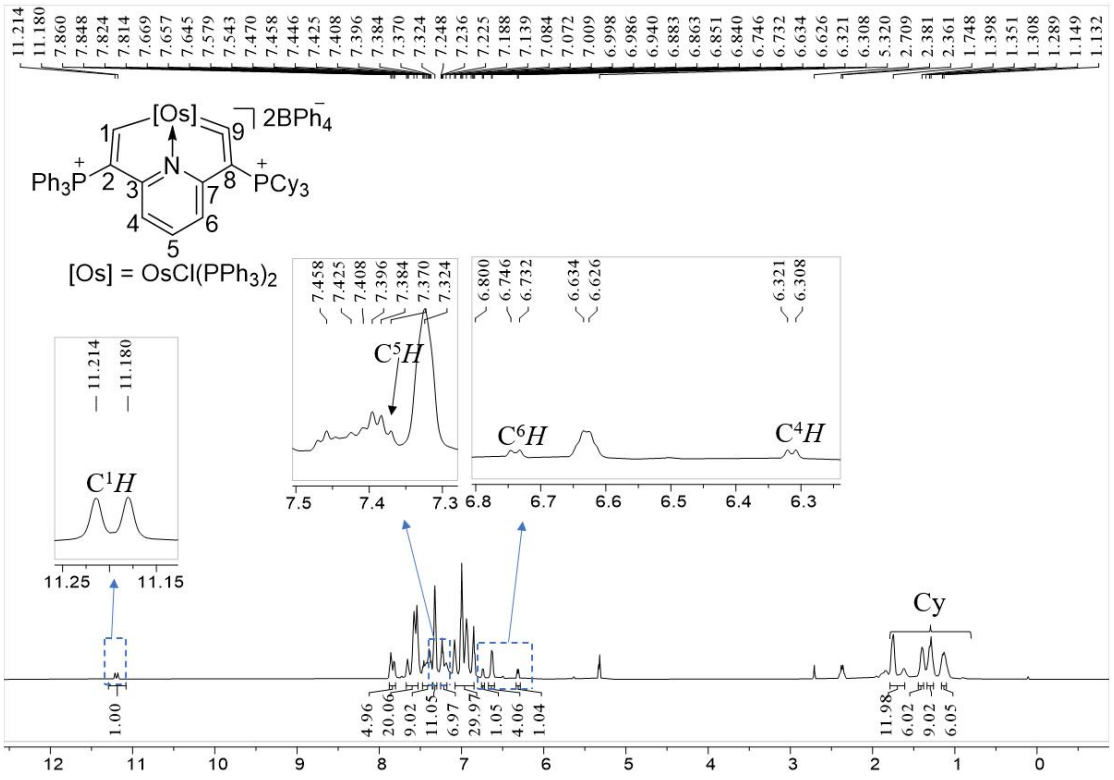


Figure S74. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **5b**.

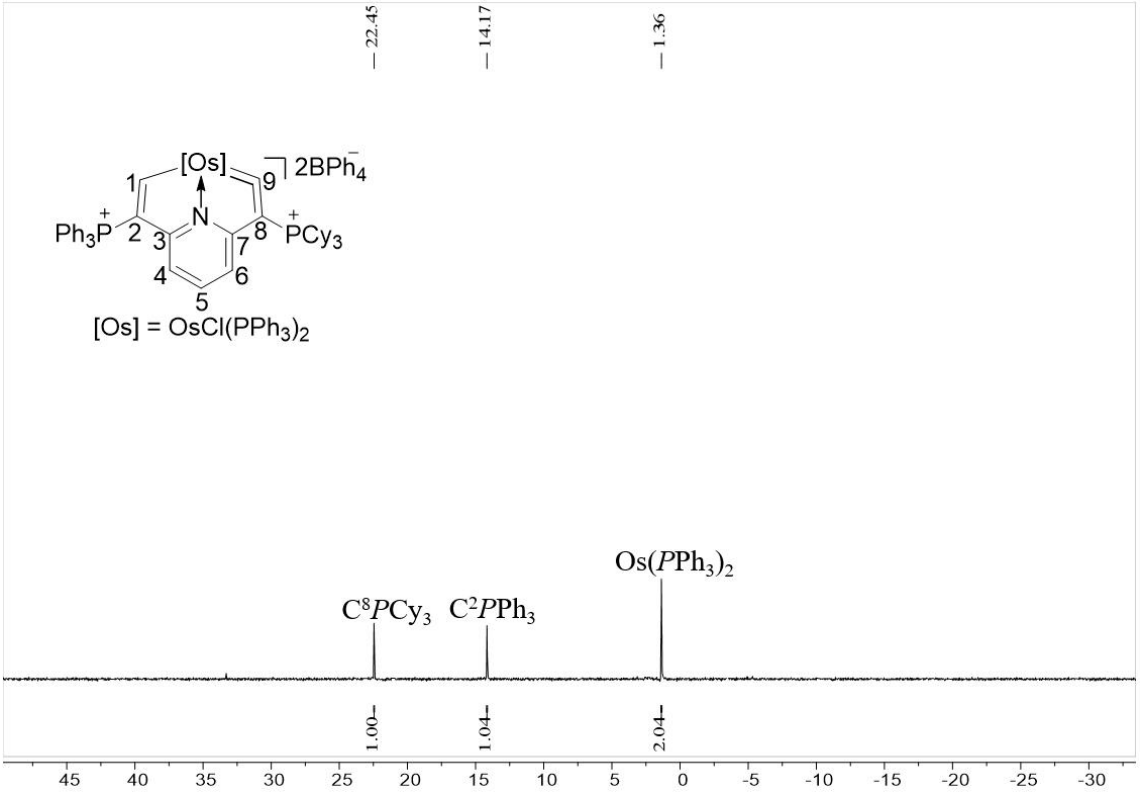


Figure S75. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **5b**.

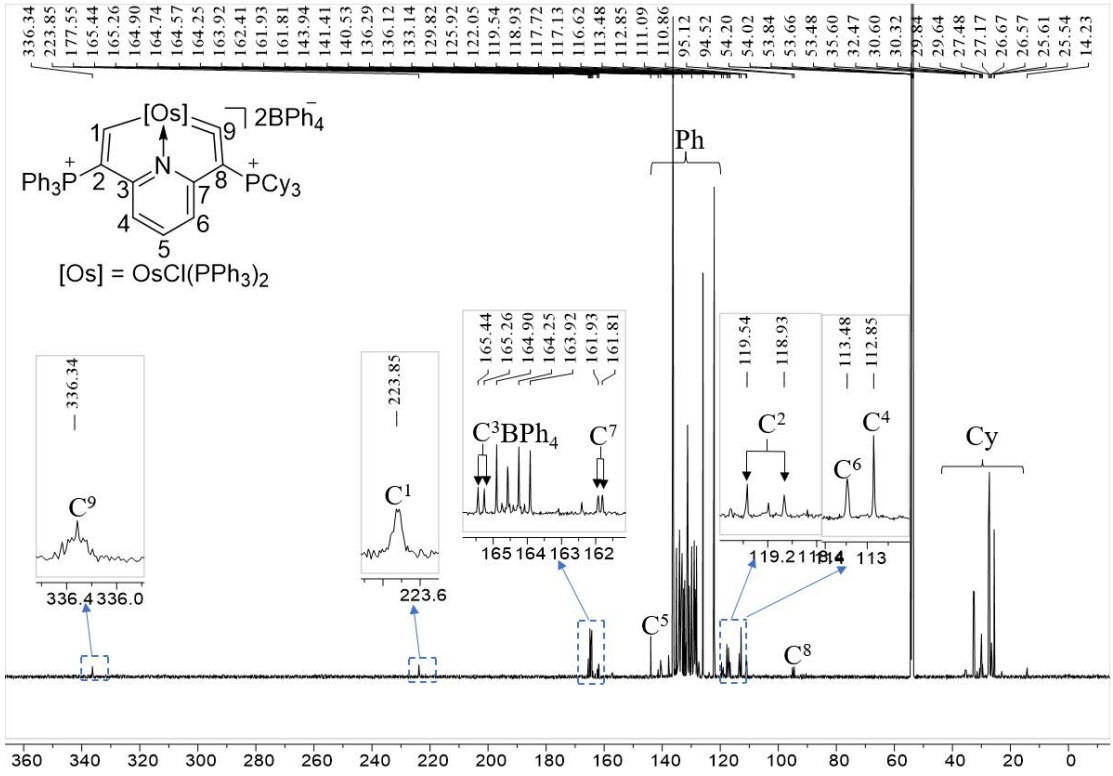


Figure S76. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **5b**.

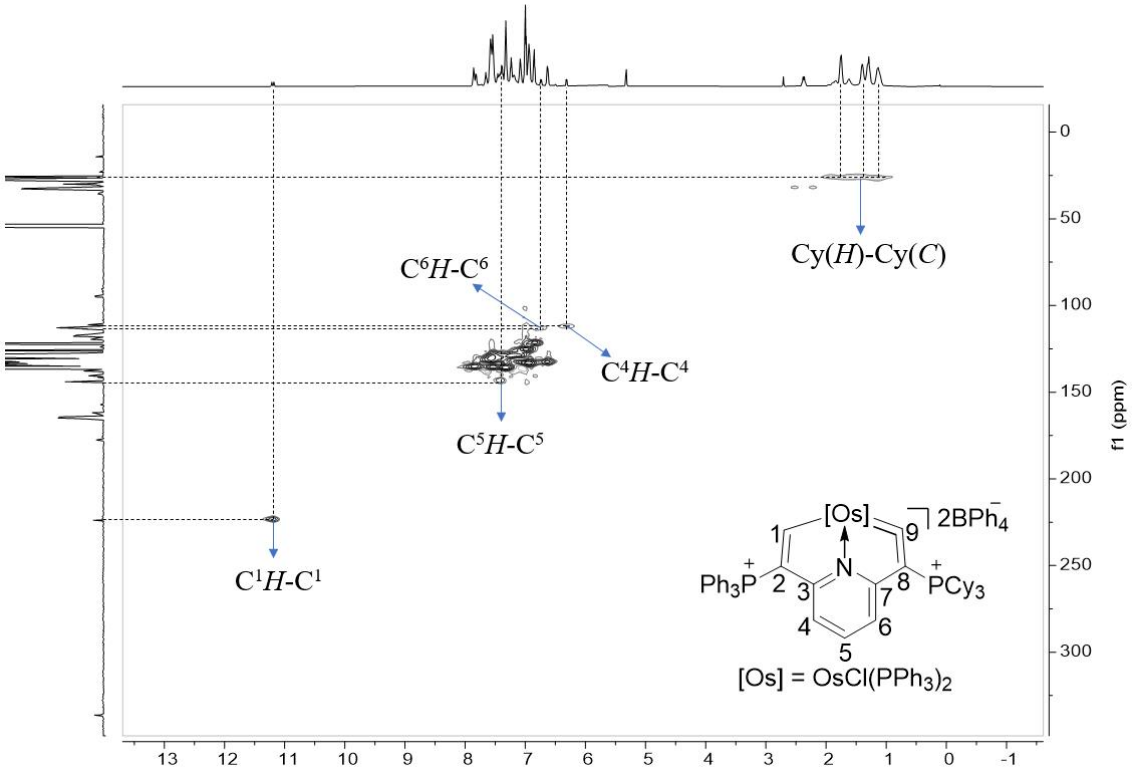


Figure S77. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **5b**.

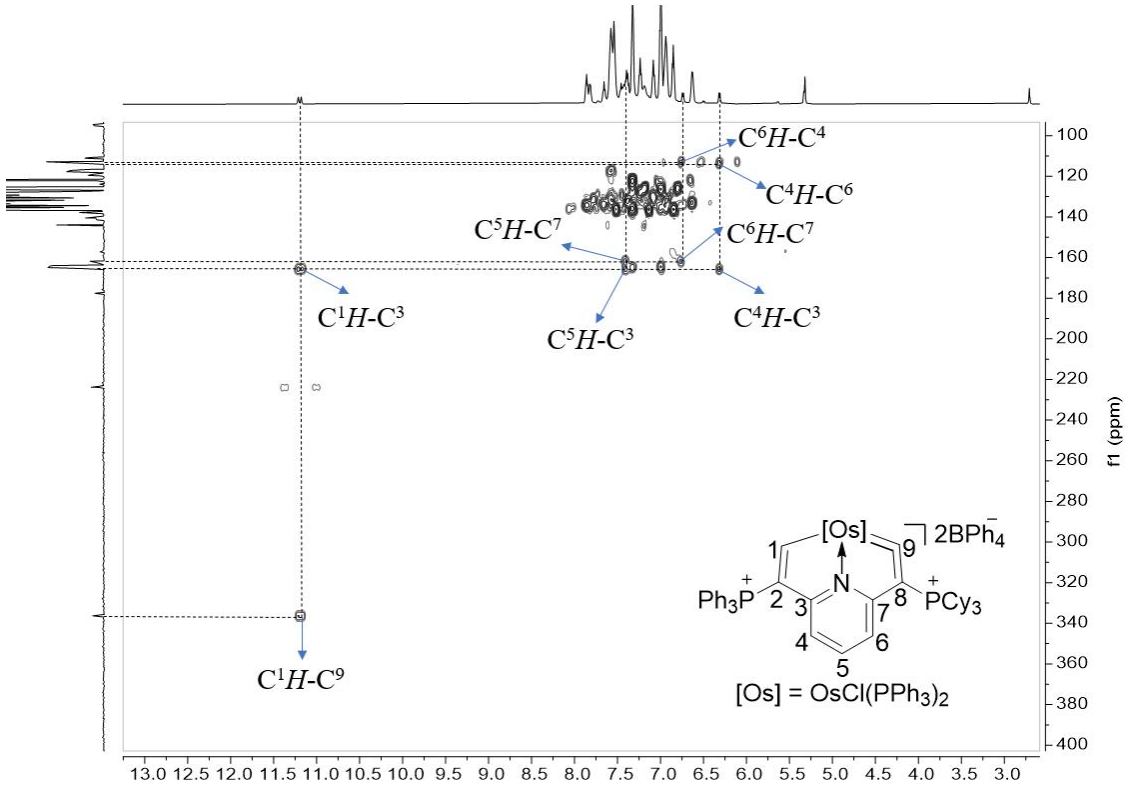


Figure S78. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **5b**.

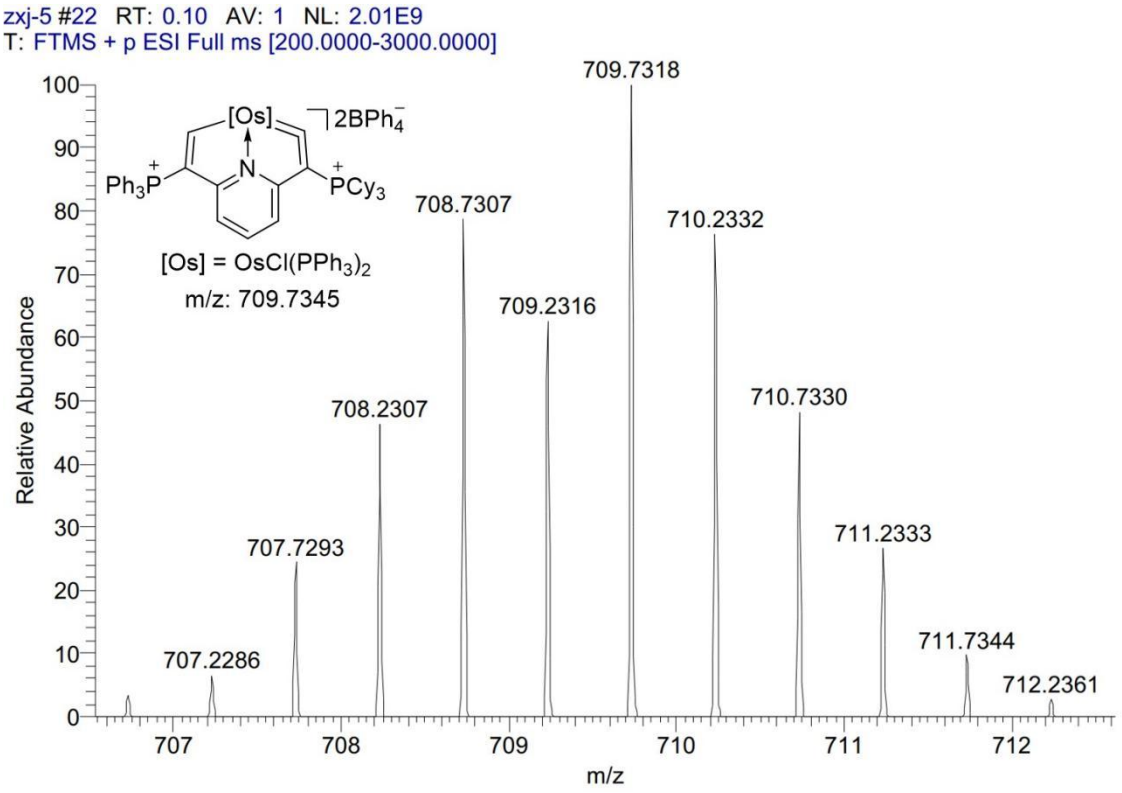


Figure 79. Positive-ion ESI-MS spectrum of [**5b**]$^{+}$ measured in methanol.

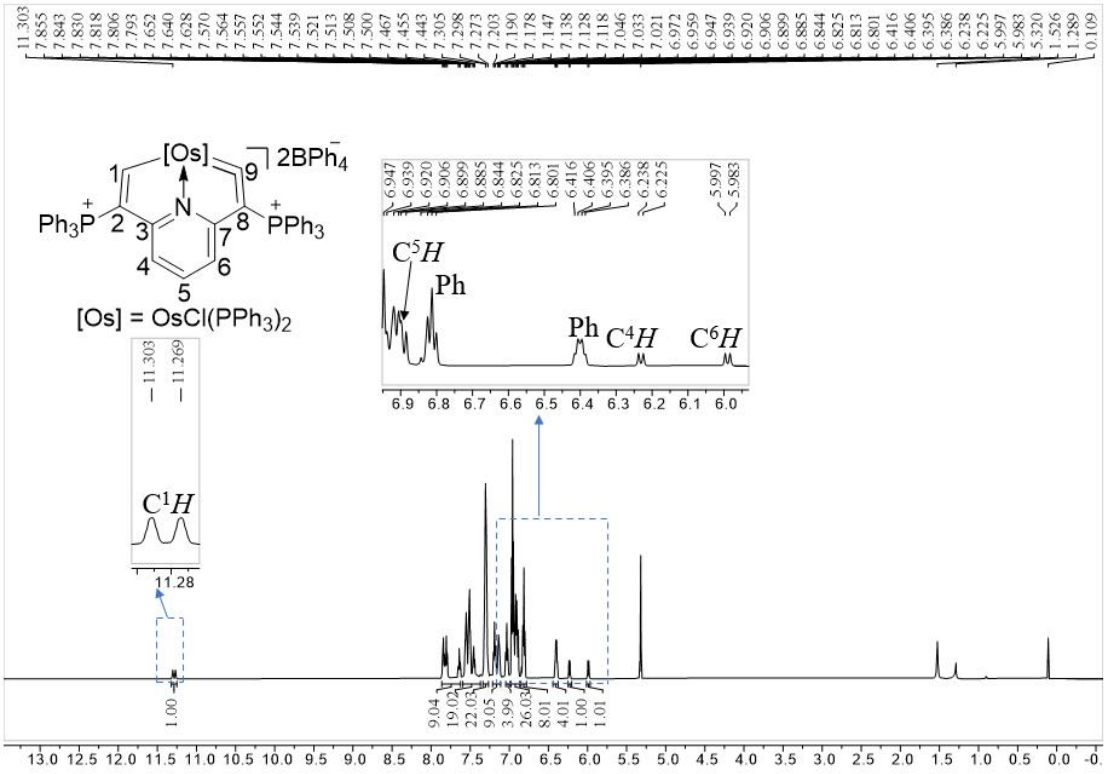


Figure S80. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **5c**.

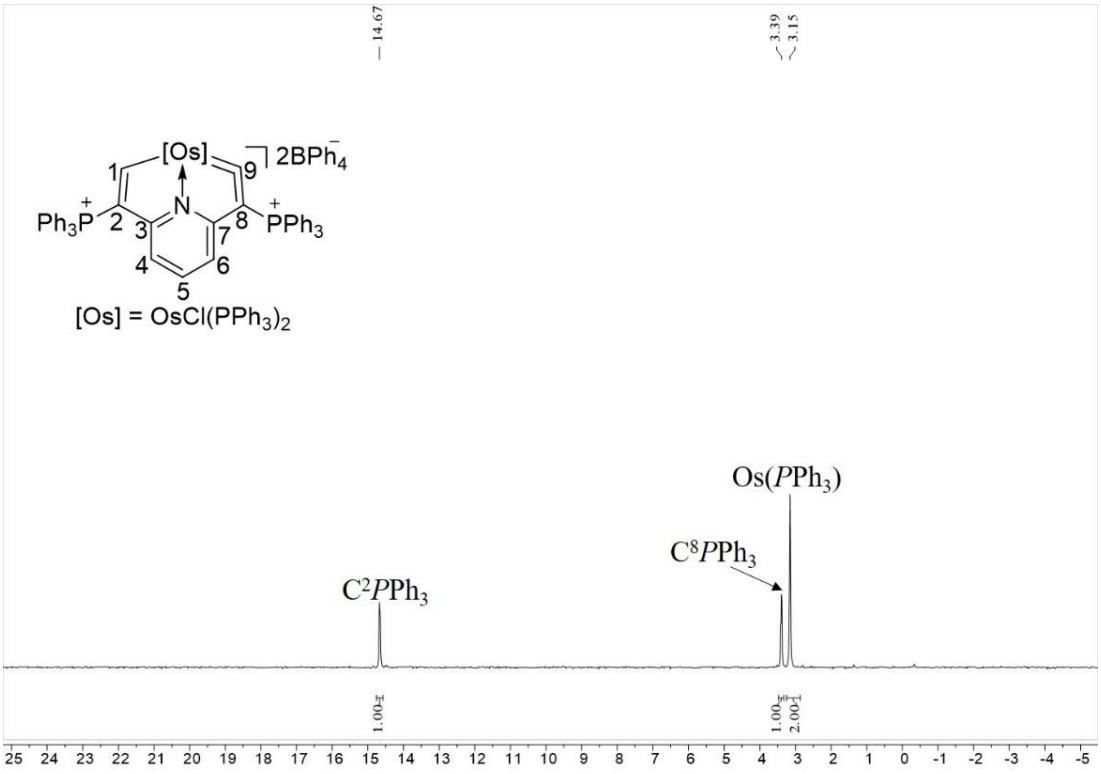


Figure S81. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **5c**.

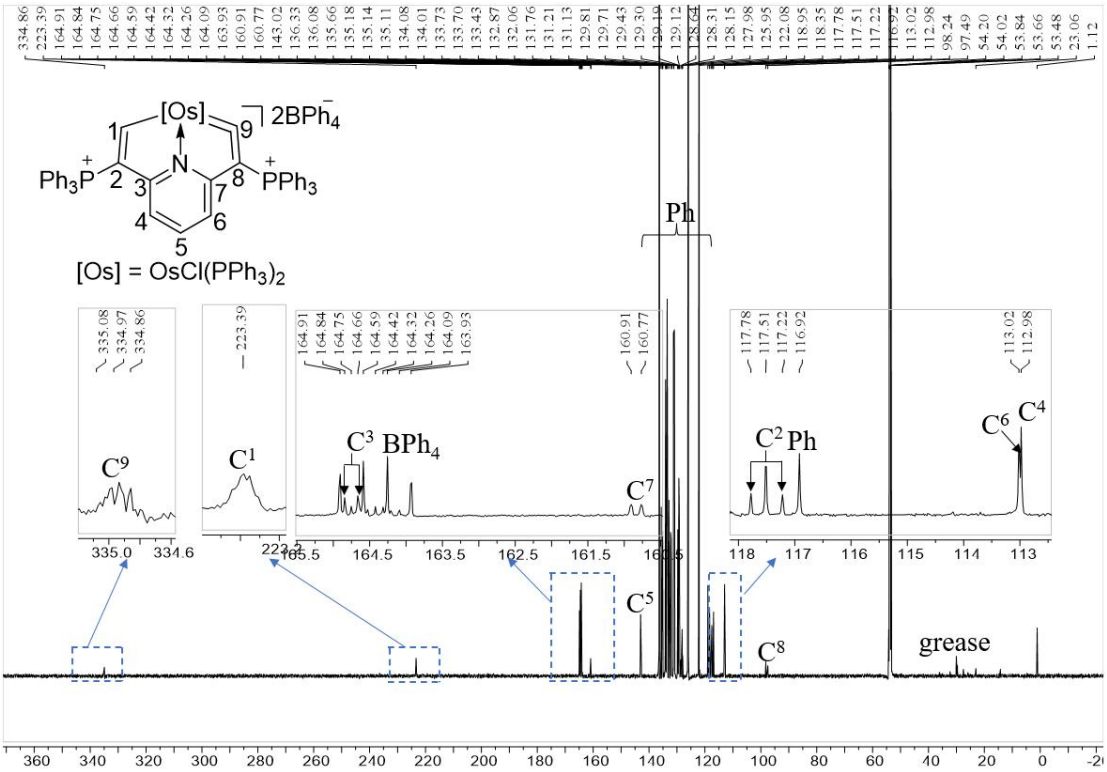


Figure S82. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **5c**.

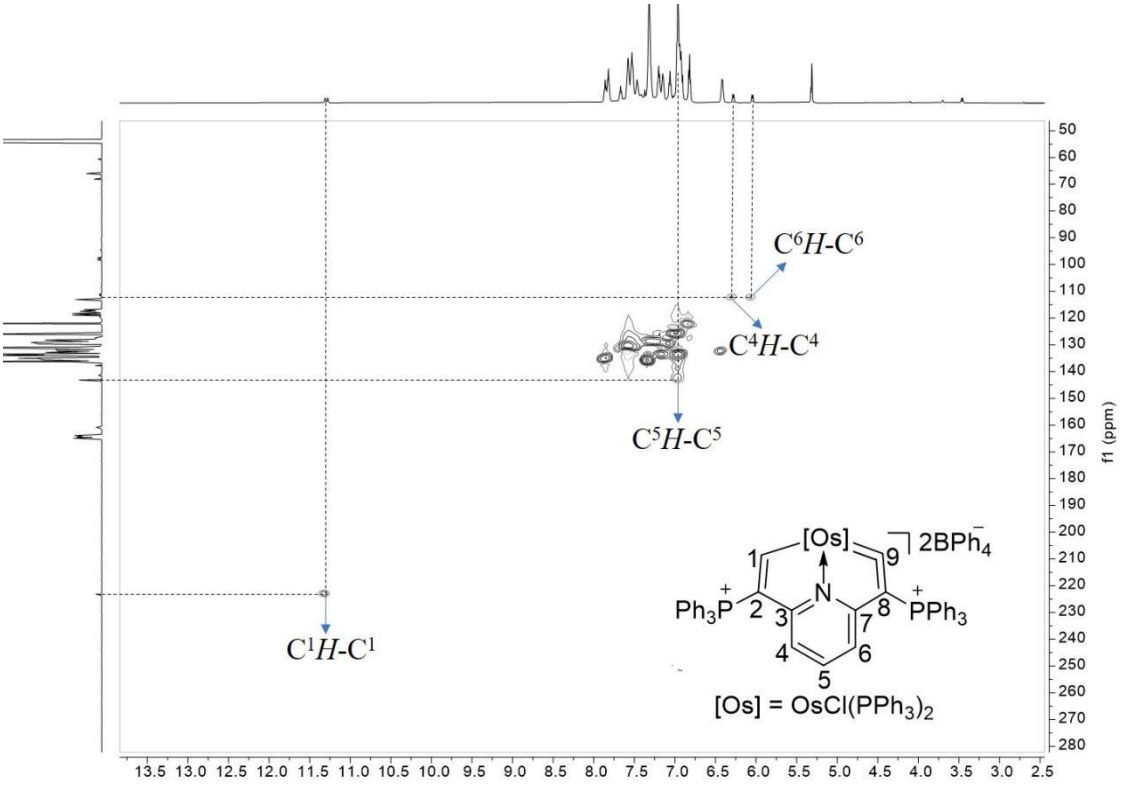


Figure S83. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **5c**.

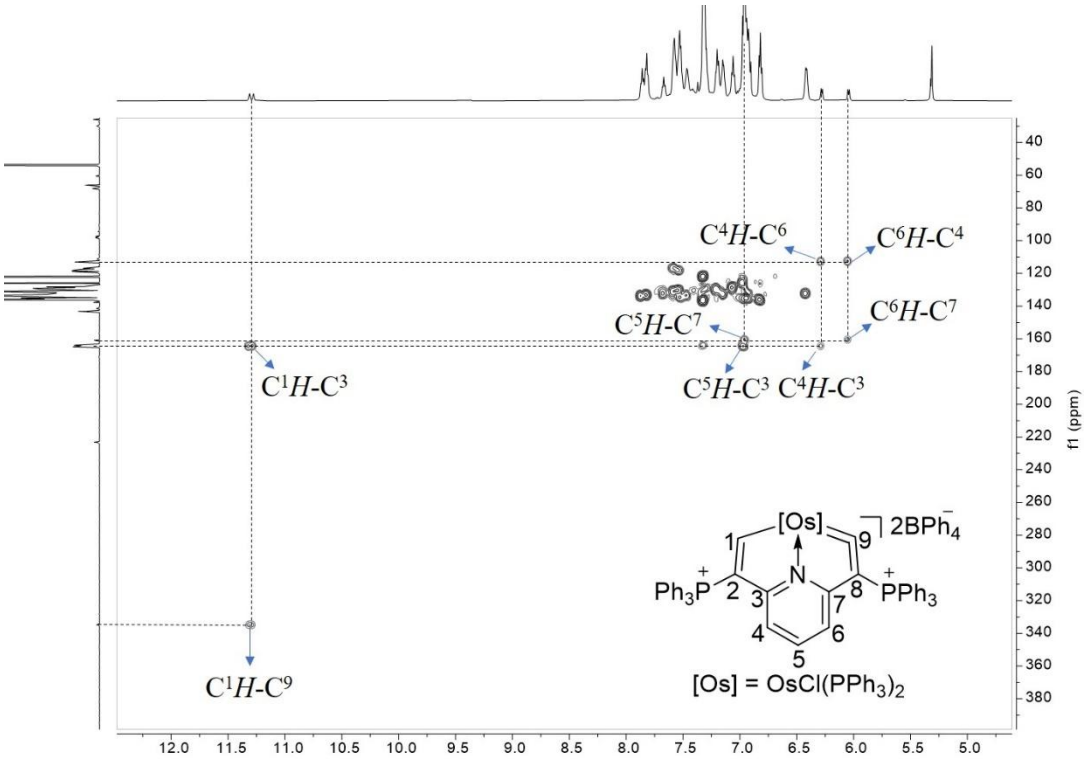


Figure S84. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **5c**.

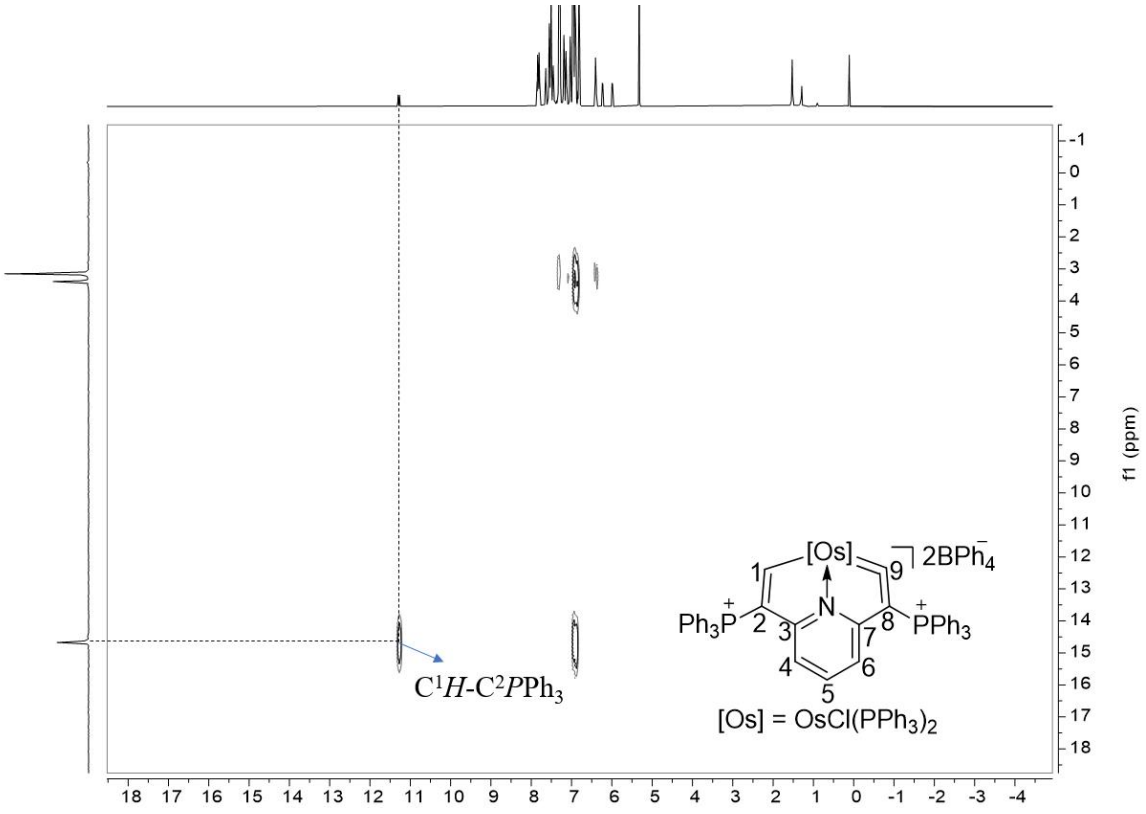


Figure S85. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complex **5c**.

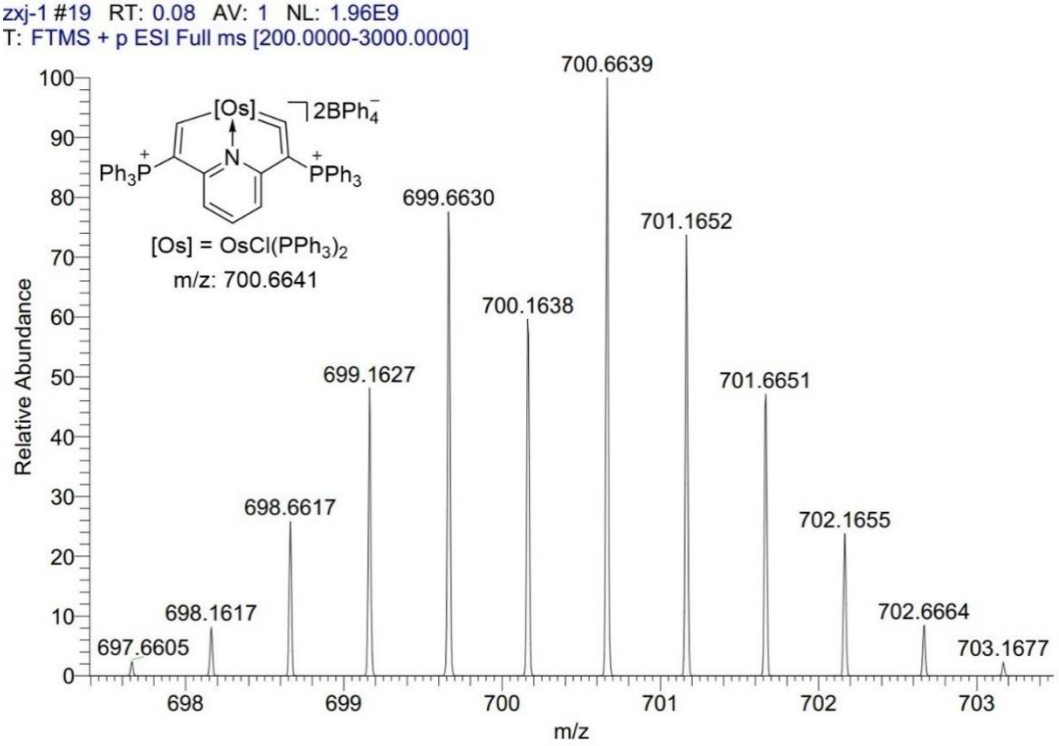


Figure S86. Positive-ion ESI-MS spectrum of [**5c**]$^{+}$ measured in methanol.

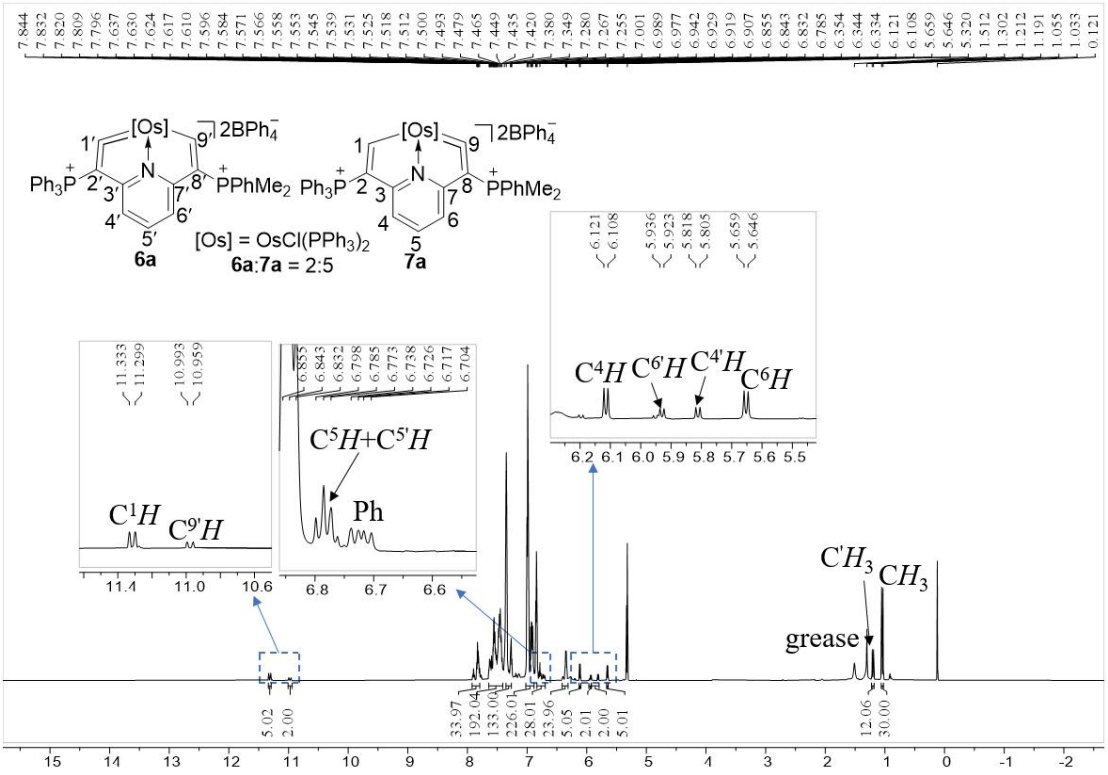


Figure S87. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

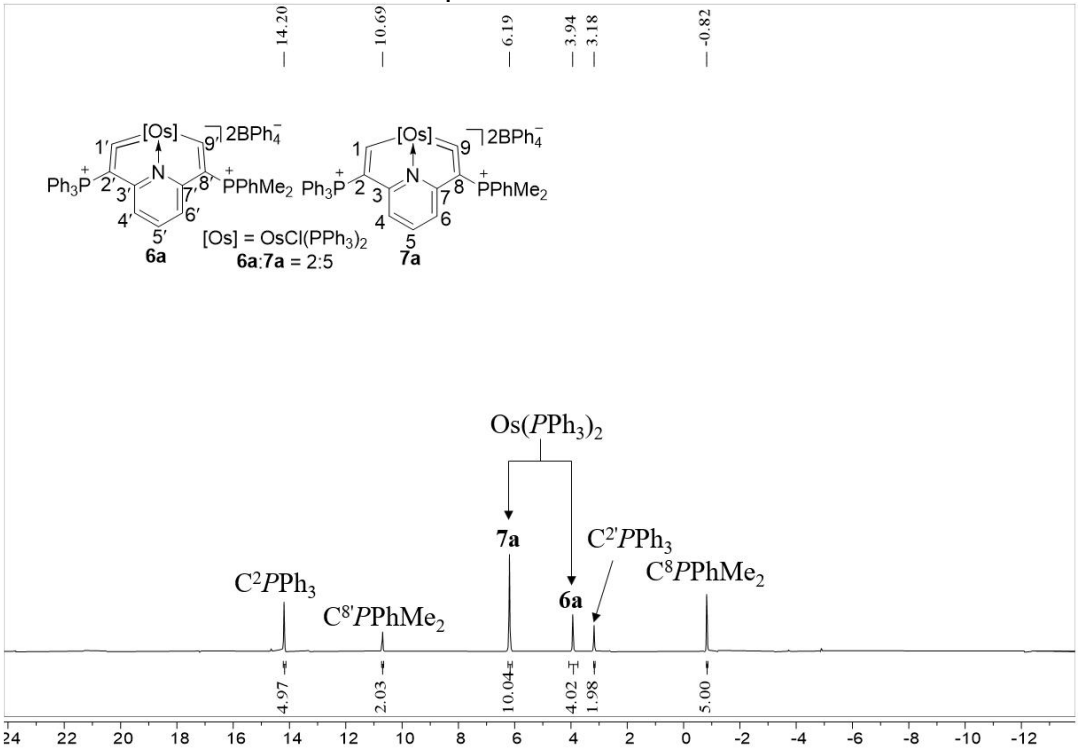


Figure S88. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

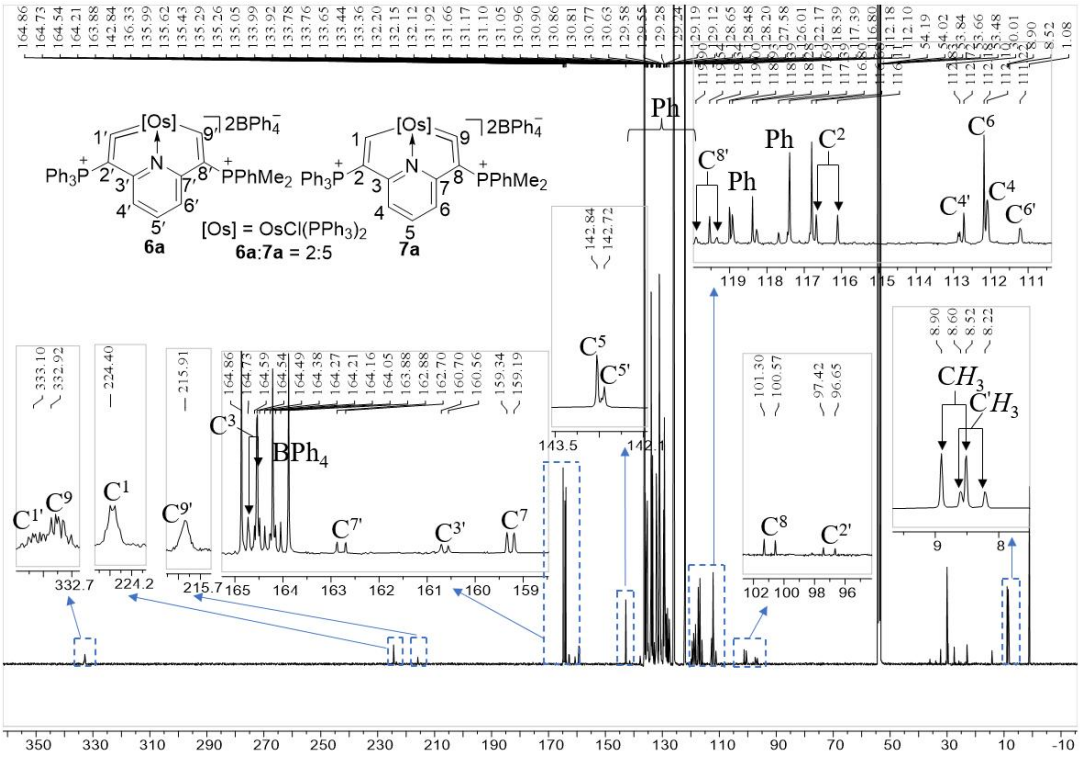


Figure S89. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

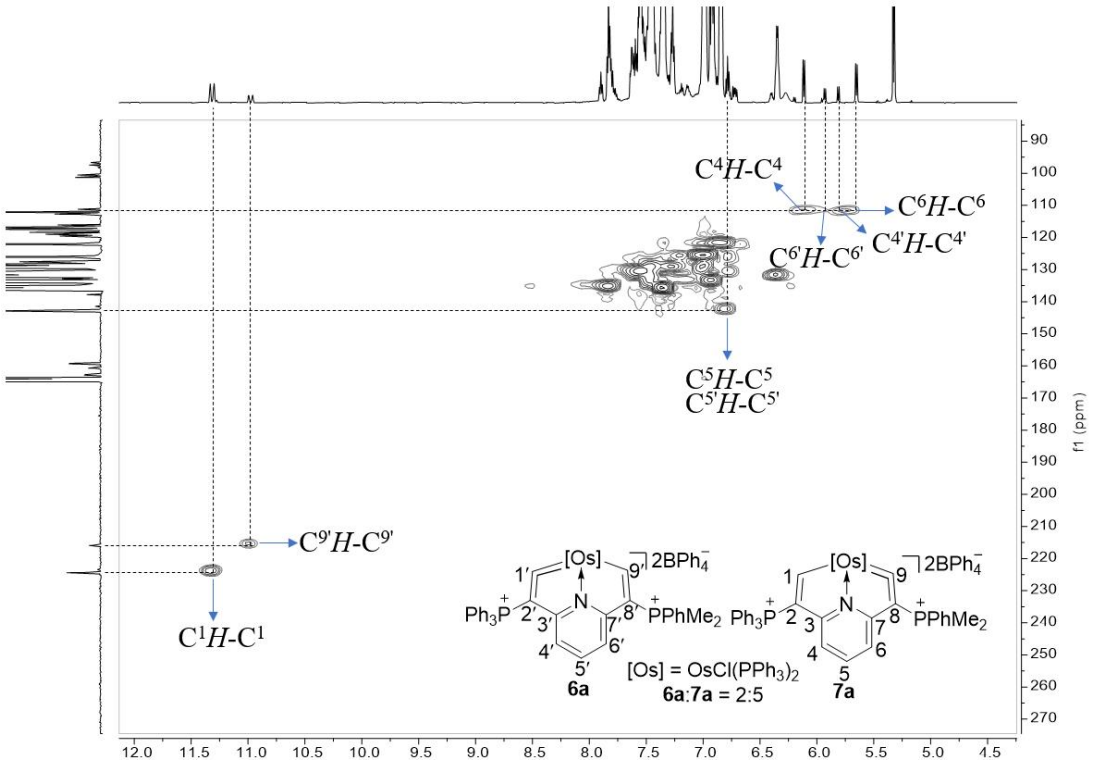


Figure S90. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

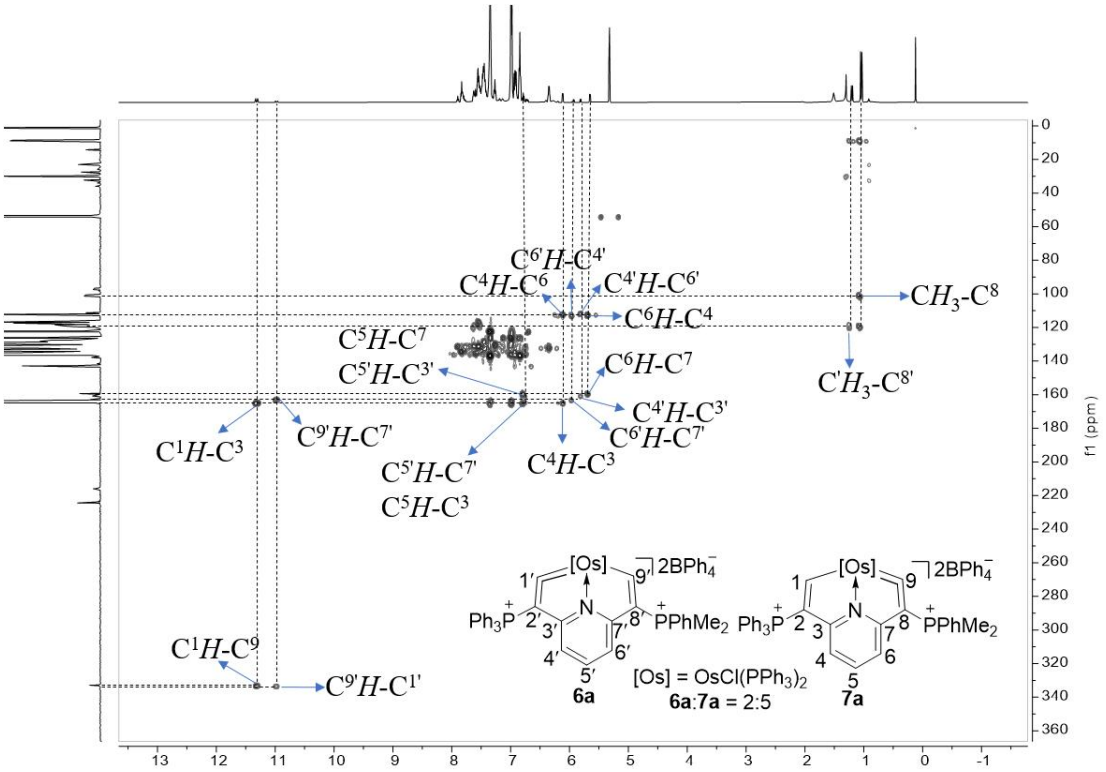


Figure S91. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

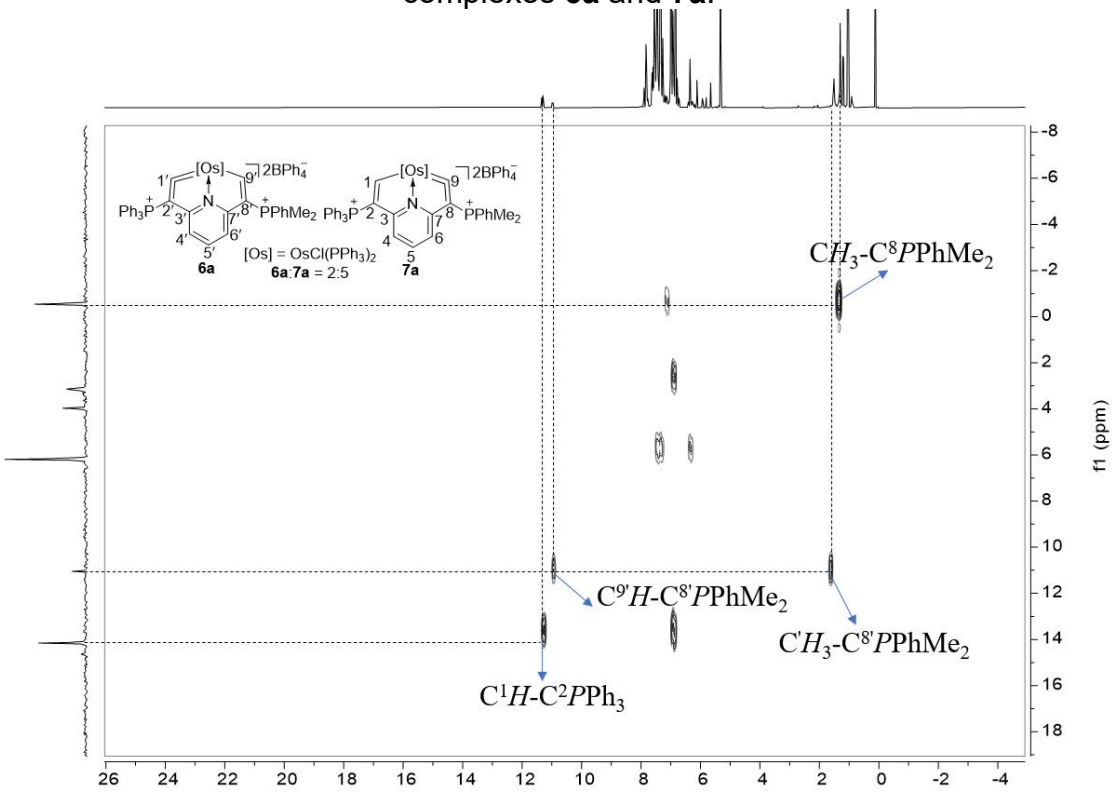


Figure S92. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complexes **6a** and **7a**.

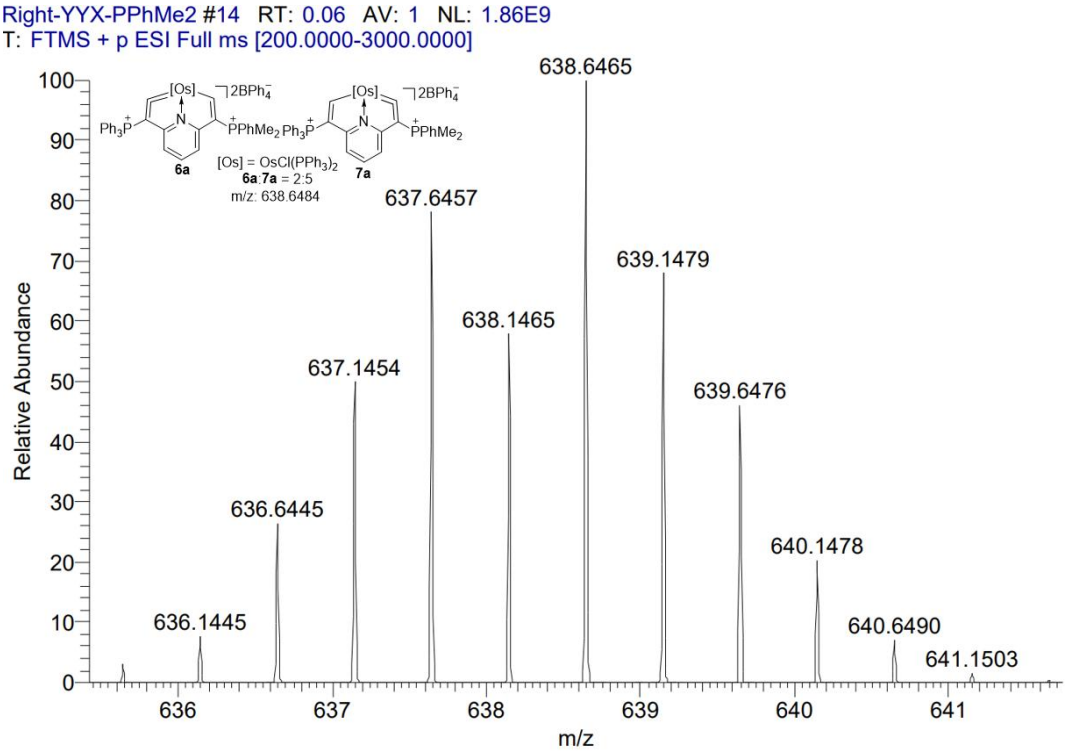


Figure S93. Positive-ion ESI-MS spectrum of [**6a** and **7a**]$^{+}$ measured in methanol.

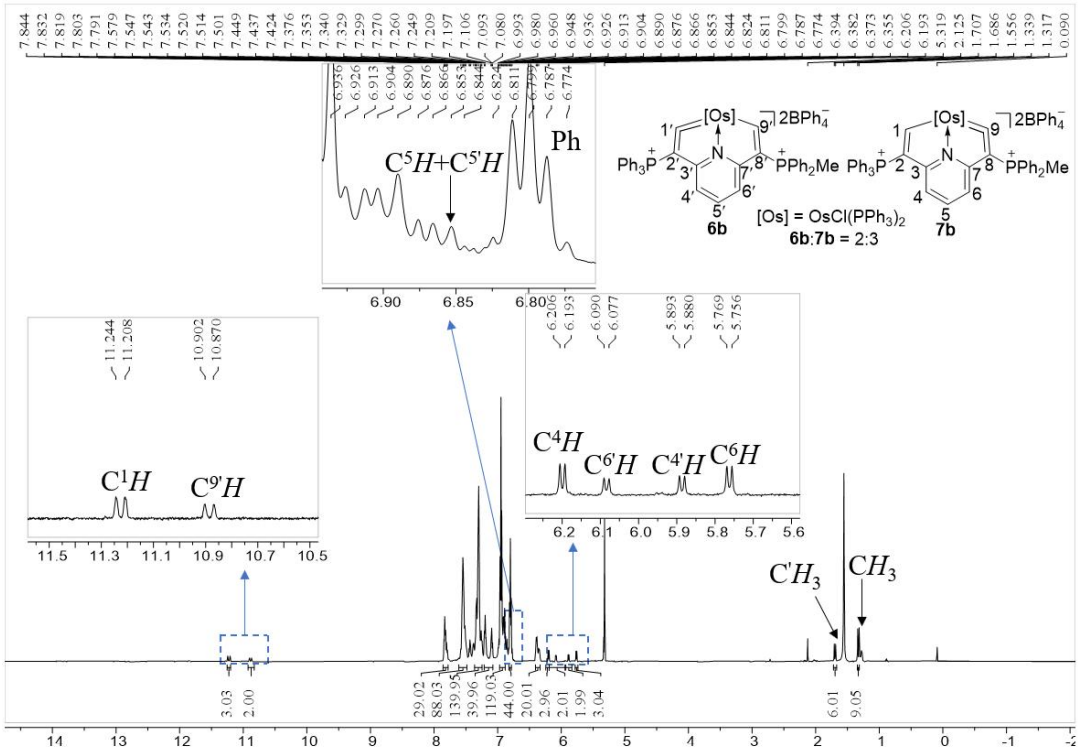


Figure S94. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

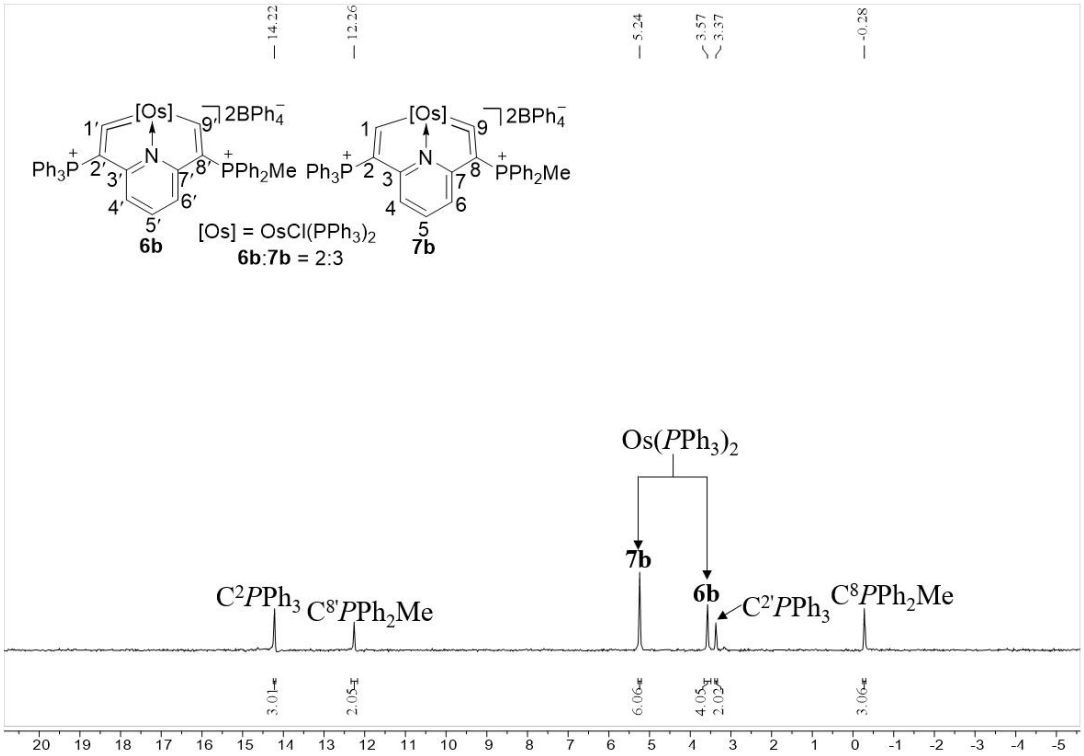


Figure S95. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

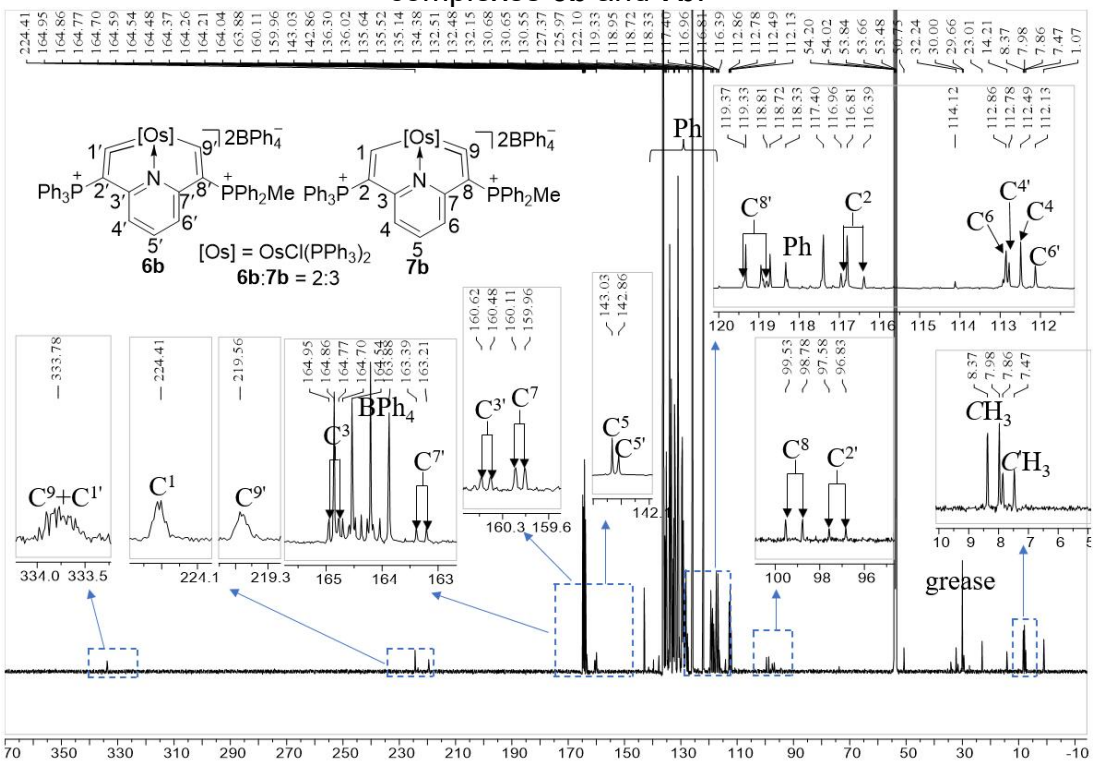


Figure S96. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

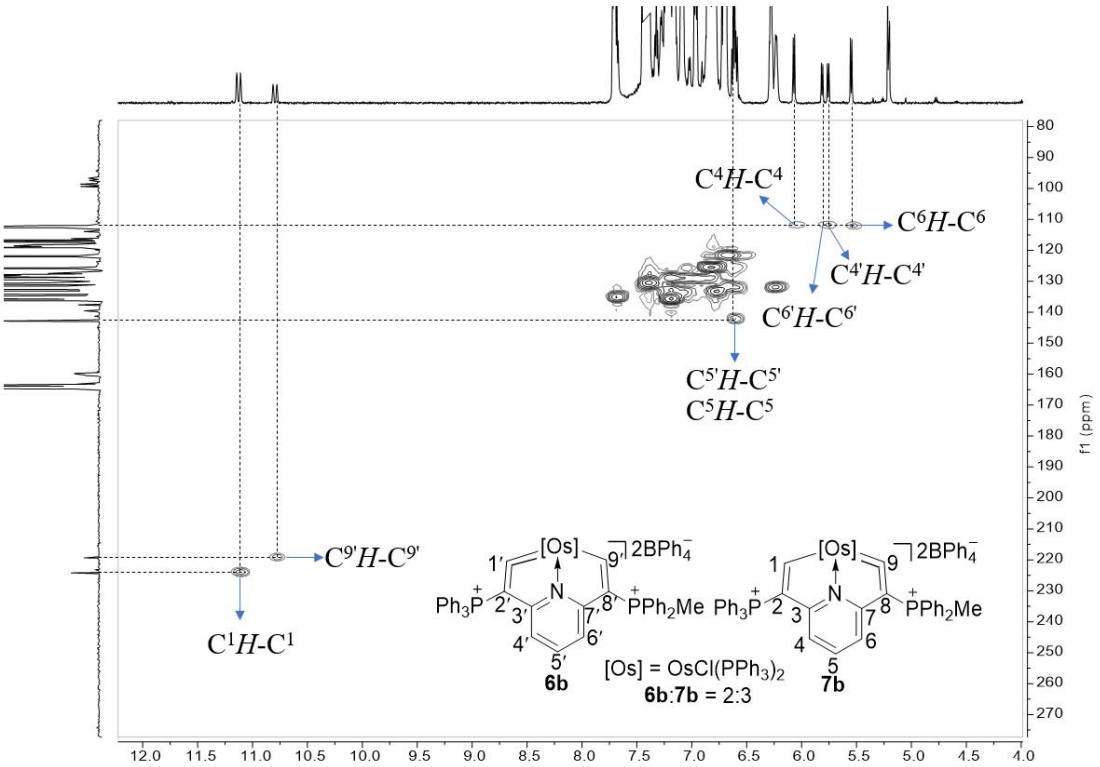


Figure S97. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

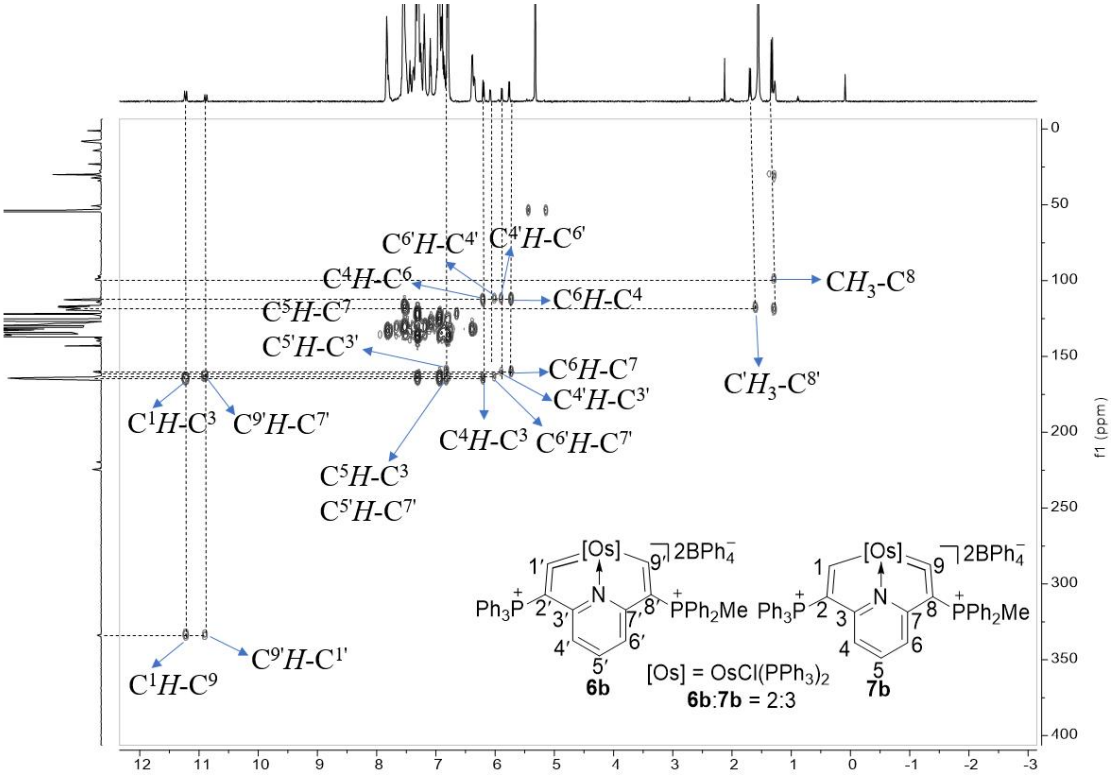


Figure S98. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

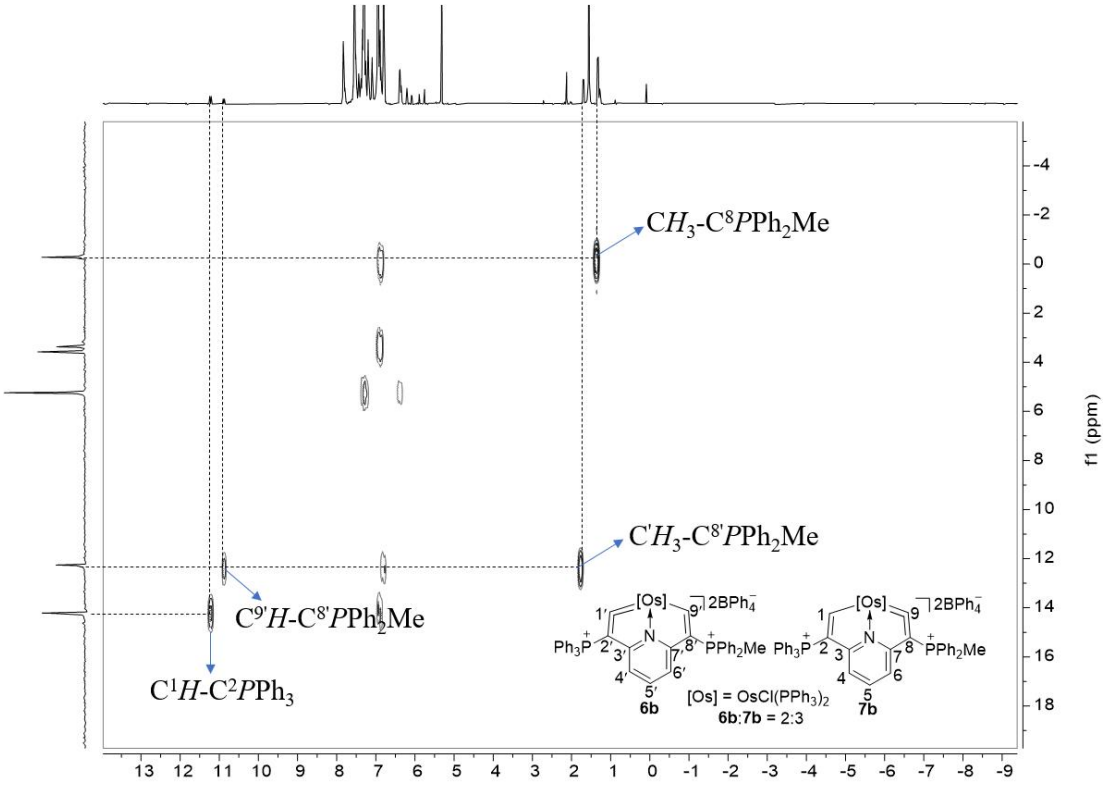


Figure S99. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complexes **6b** and **7b**.

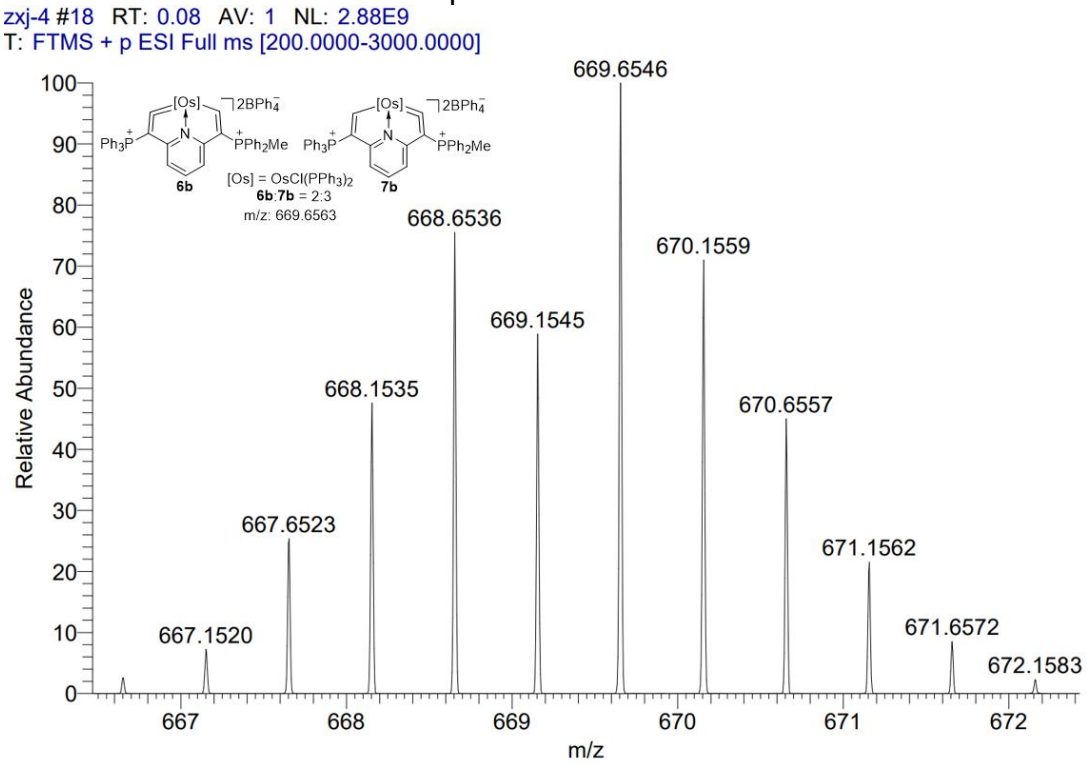


Figure S100. Positive-ion ESI-MS spectrum of [**6b** and **7b**]$^{+}$ measured in methanol.

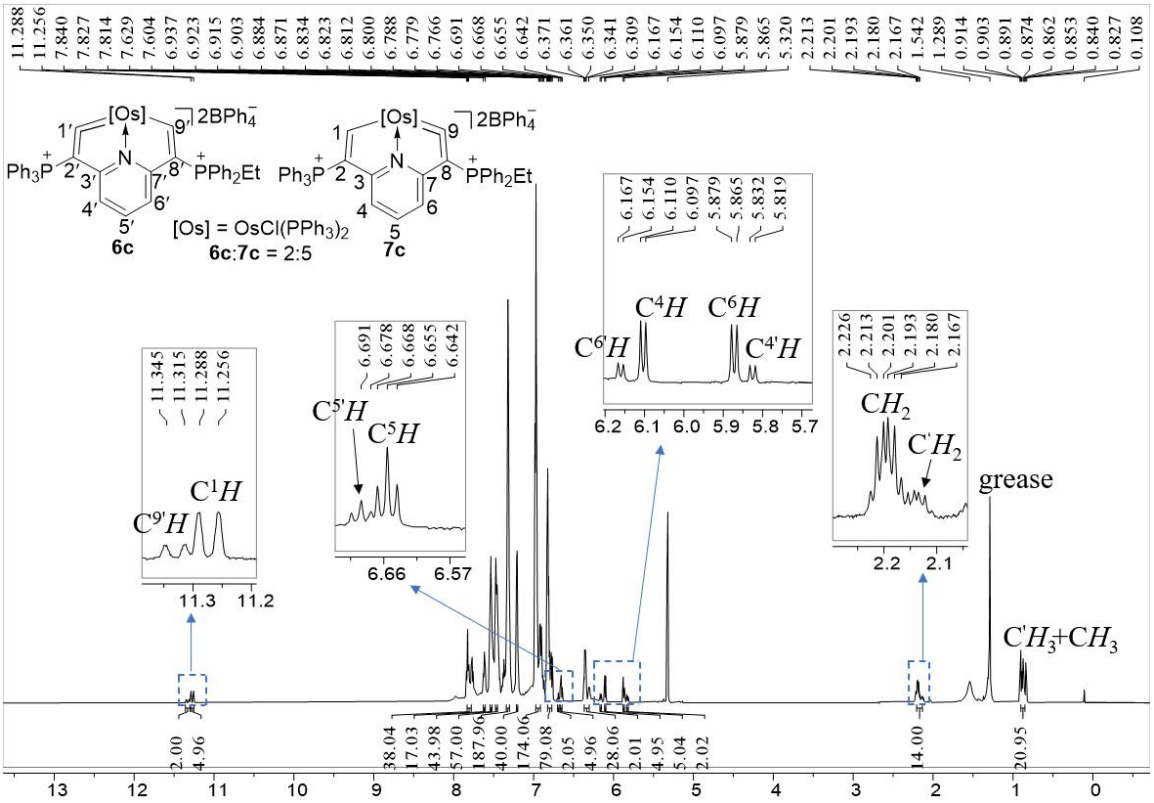


Figure S101. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

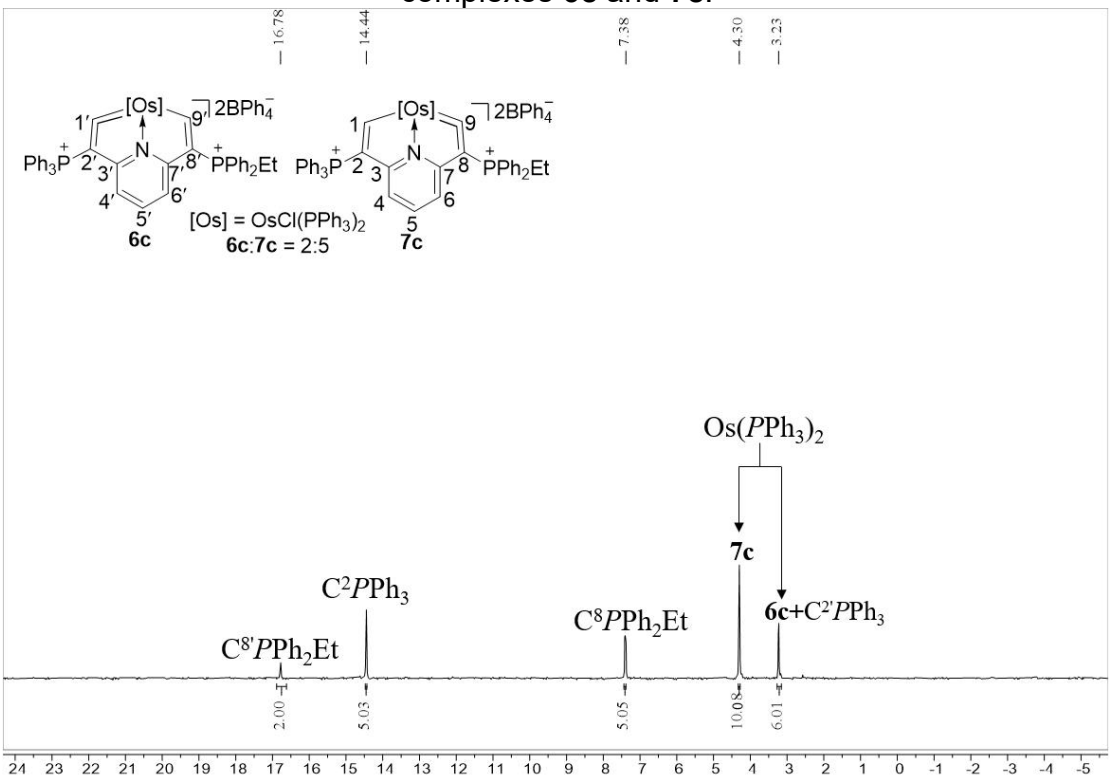


Figure S102. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

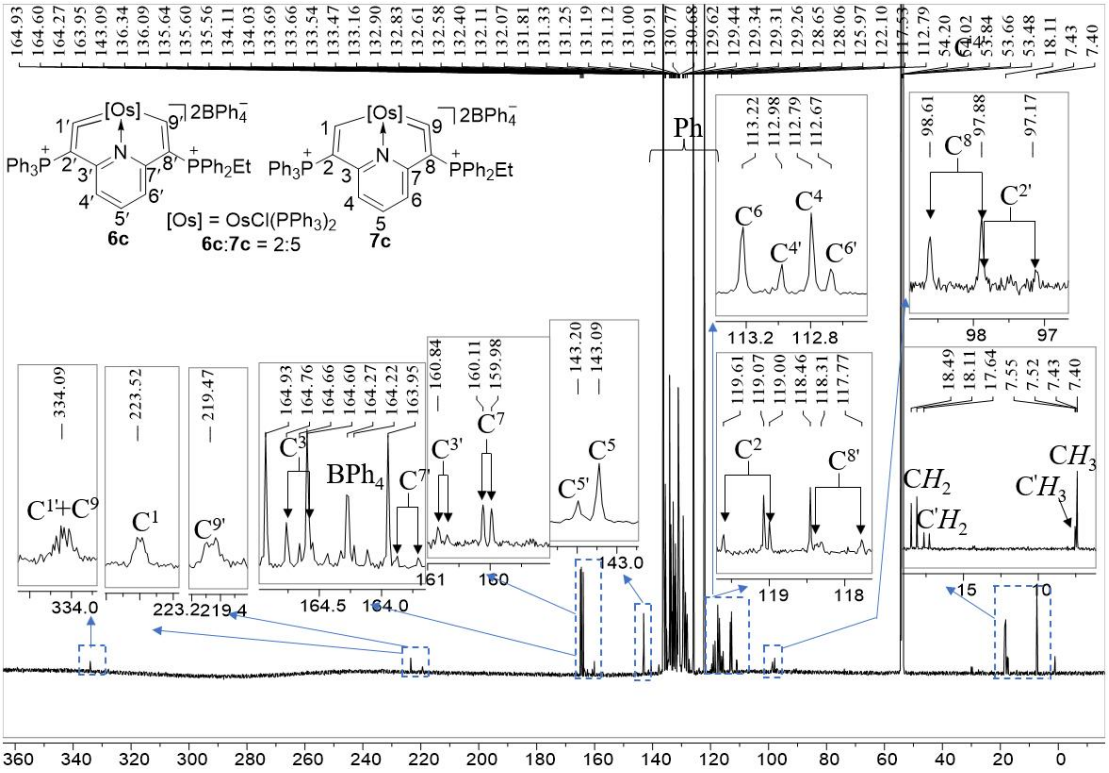


Figure S103. The $^{13}C\{^1H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

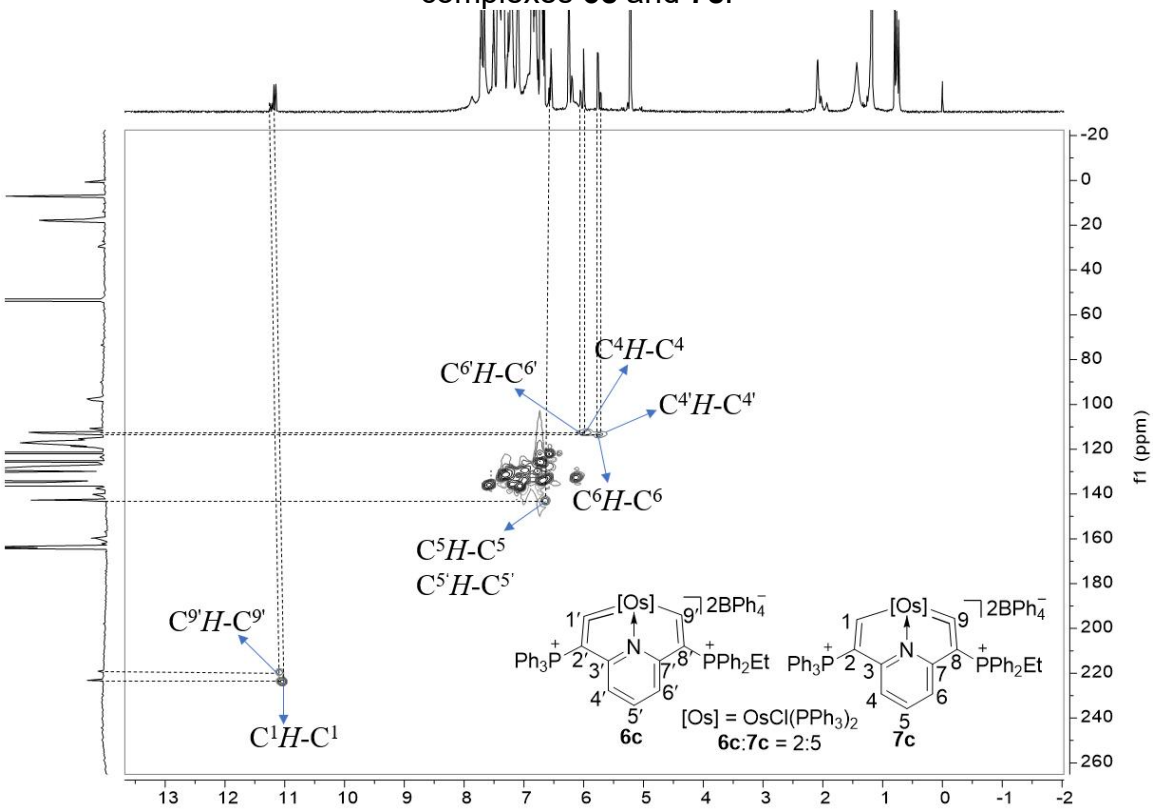


Figure S104. The ^1H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

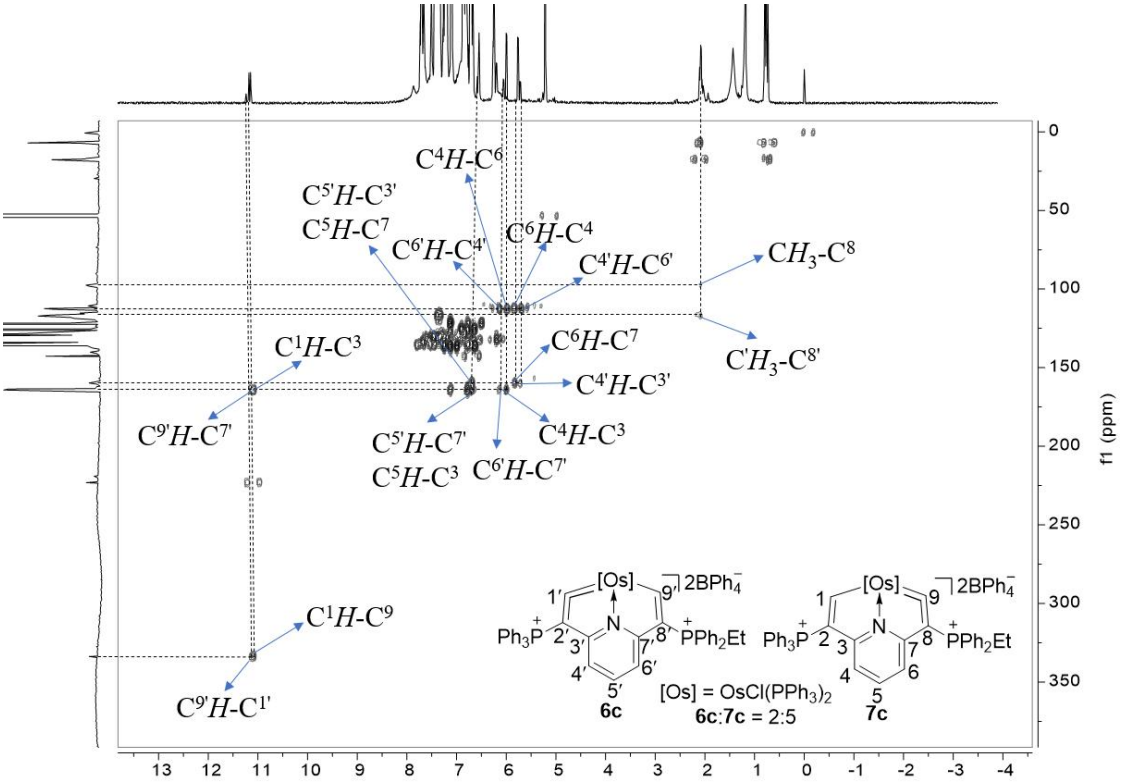


Figure S105. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

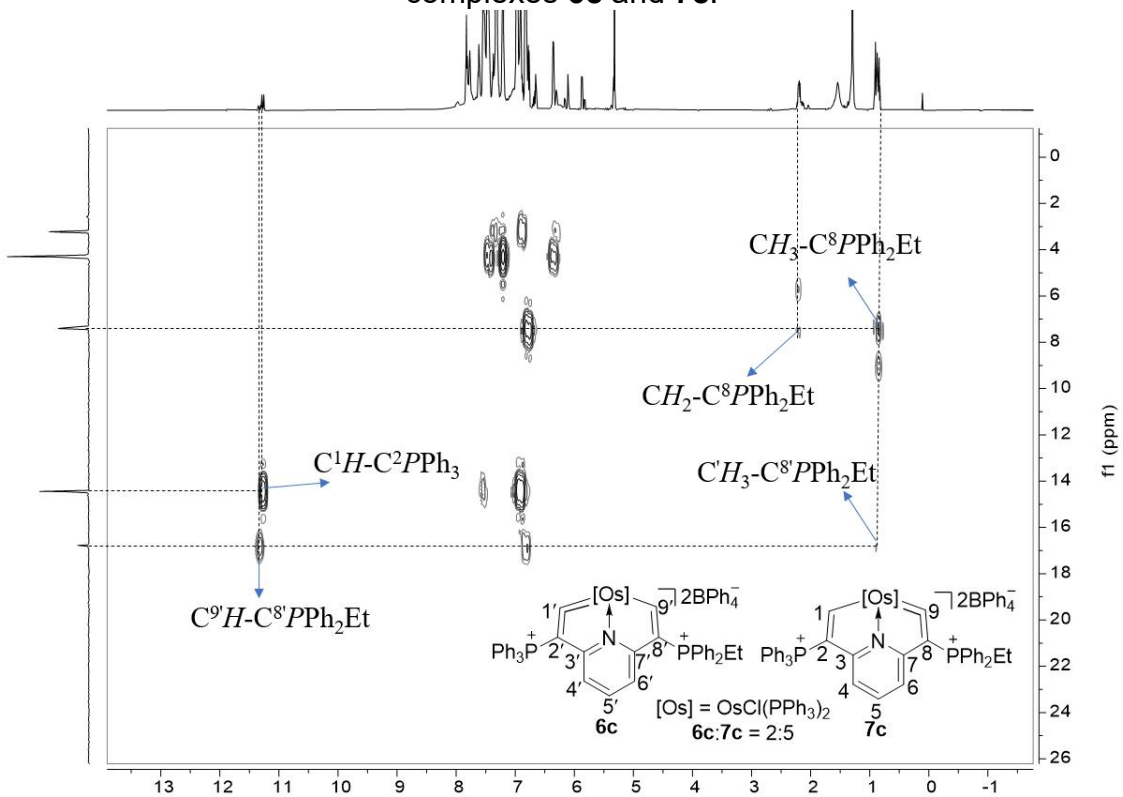


Figure S106. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complexes **6c** and **7c**.

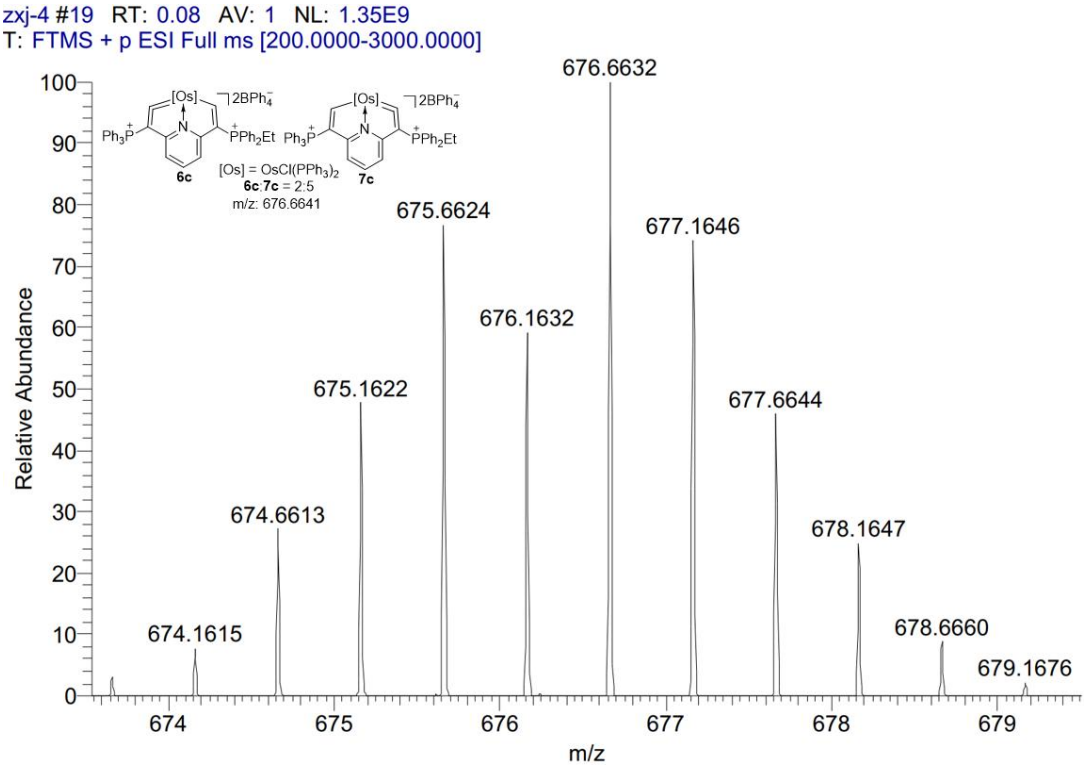


Figure S107. Positive-ion ESI-MS spectrum of [**6c** and **7c**]$^+$ measured in methanol.

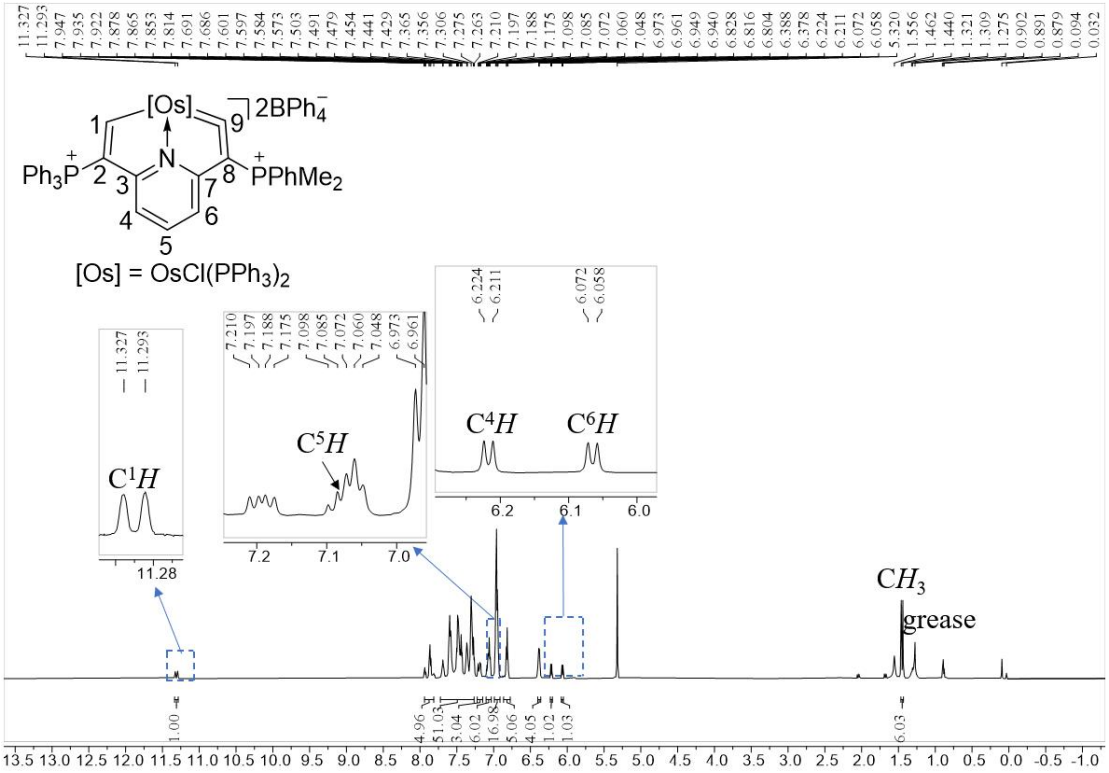


Figure S108. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **7a**.

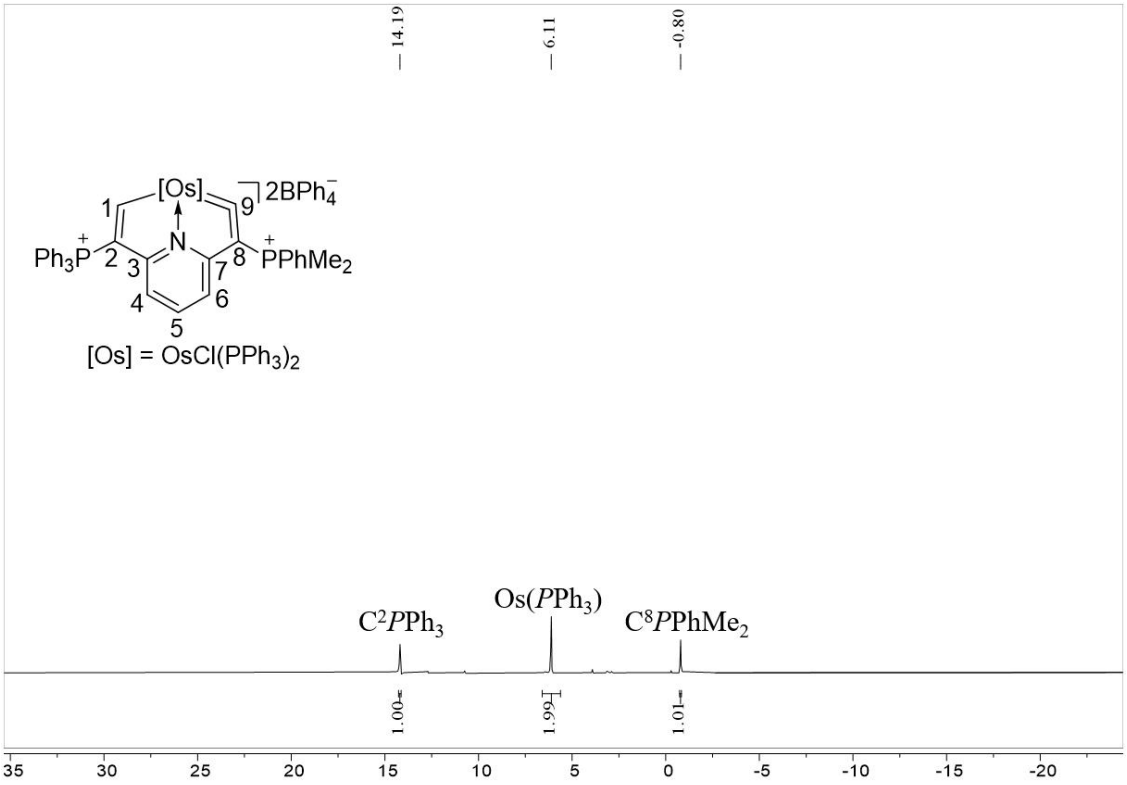


Figure S109. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **7a**.

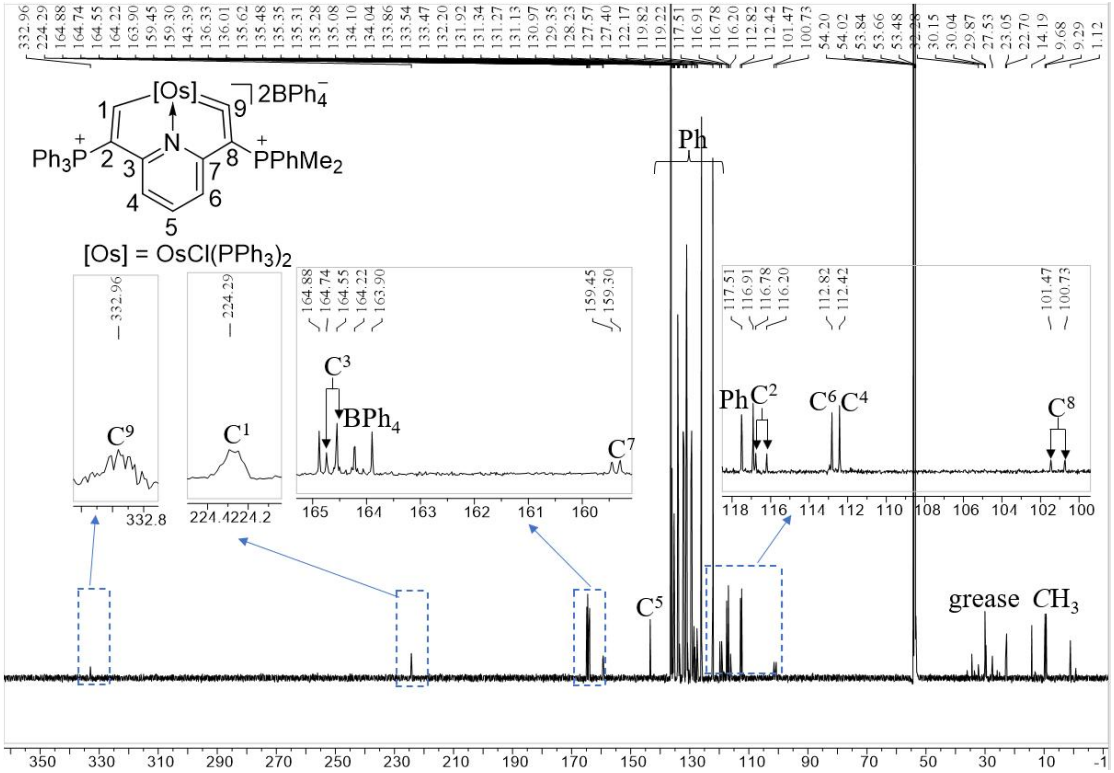


Figure S110. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **7a**.

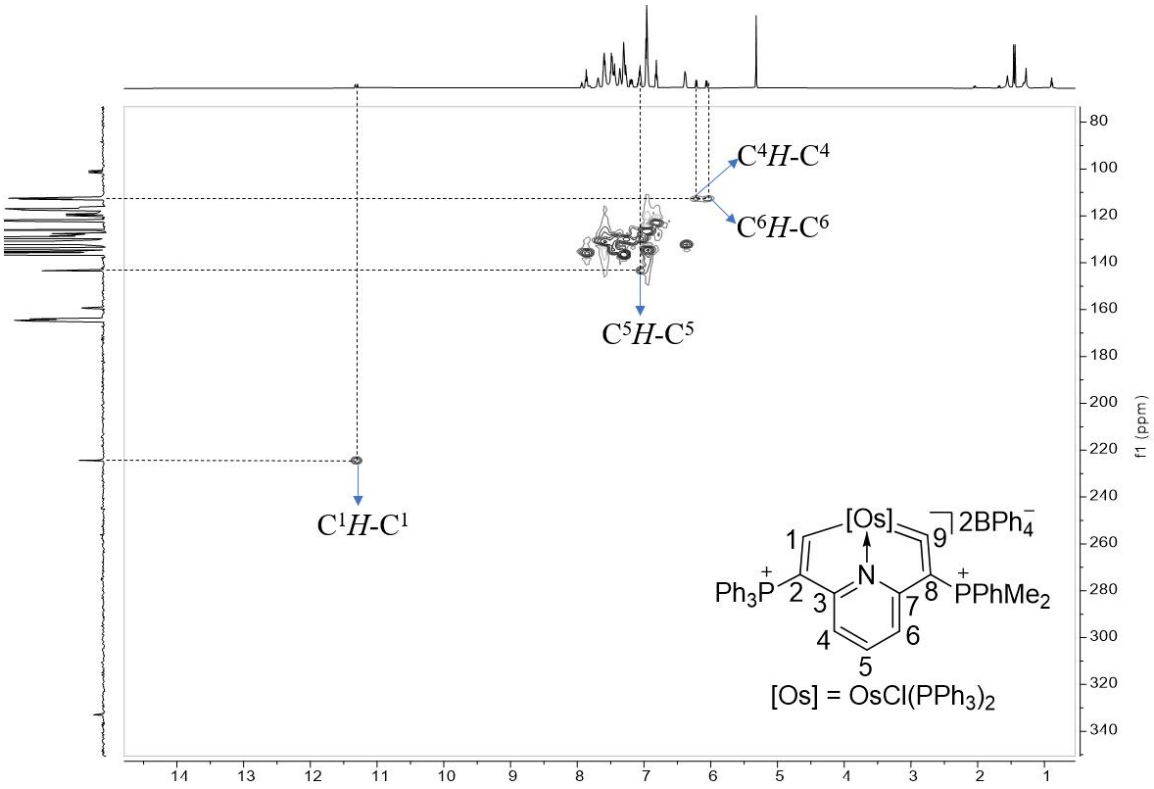


Figure S111. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **7a**.

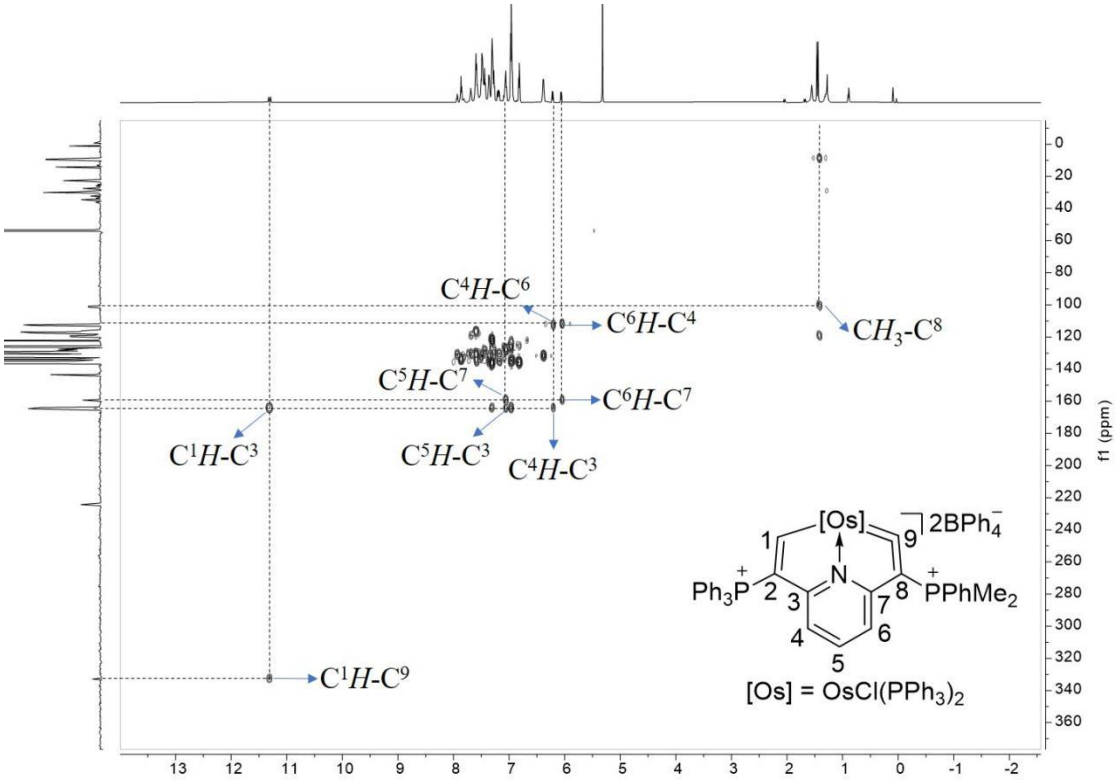


Figure S112. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **7a**.

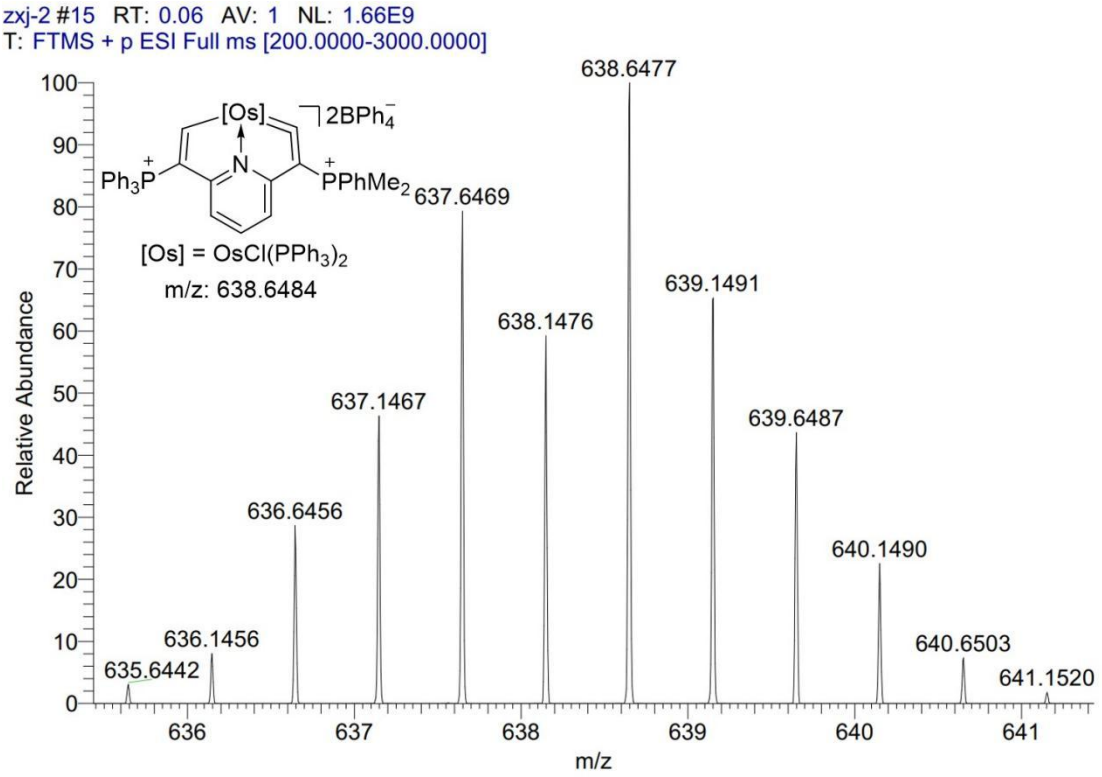


Figure S113. Positive-ion ESI-MS spectrum of [**7a**]$^+$ measured in methanol.

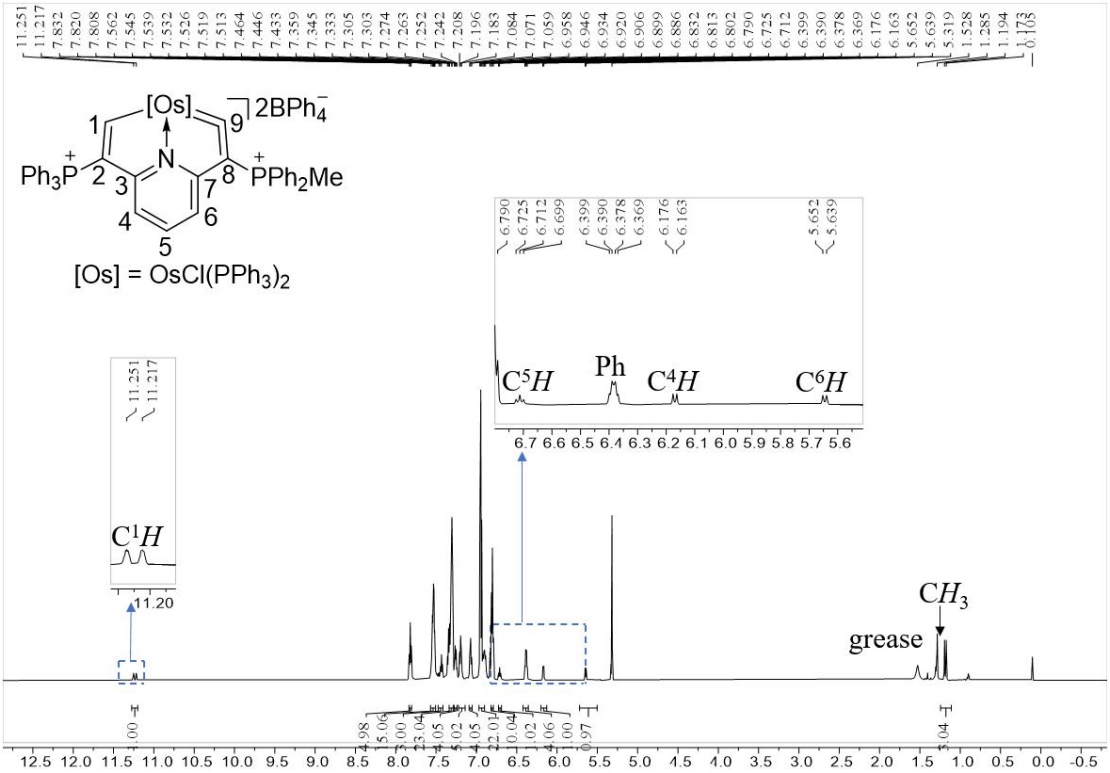


Figure S114. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **7b**.

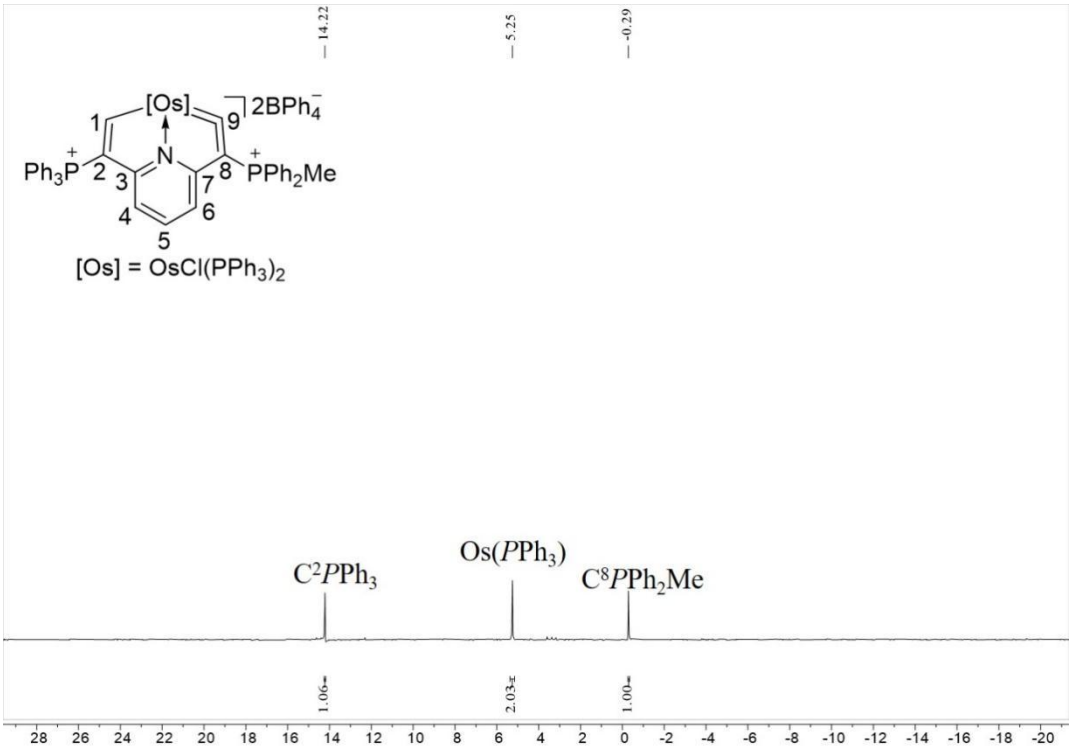


Figure S115. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **7b**.

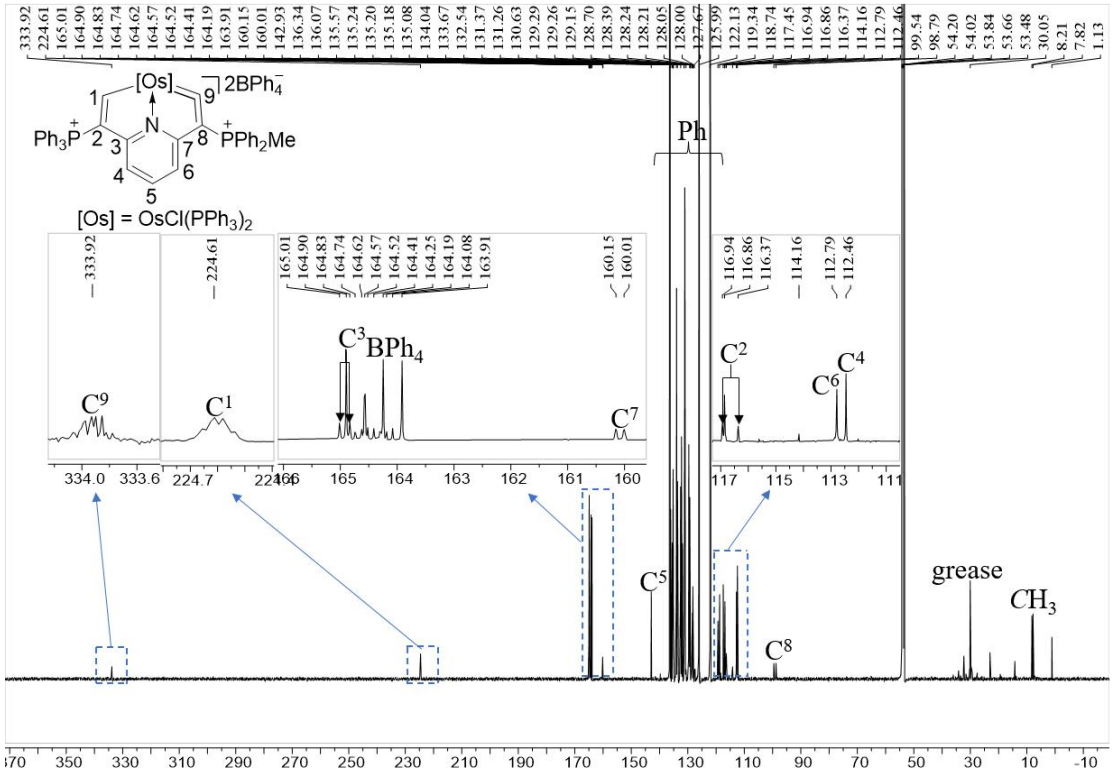


Figure S116. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **7b**.

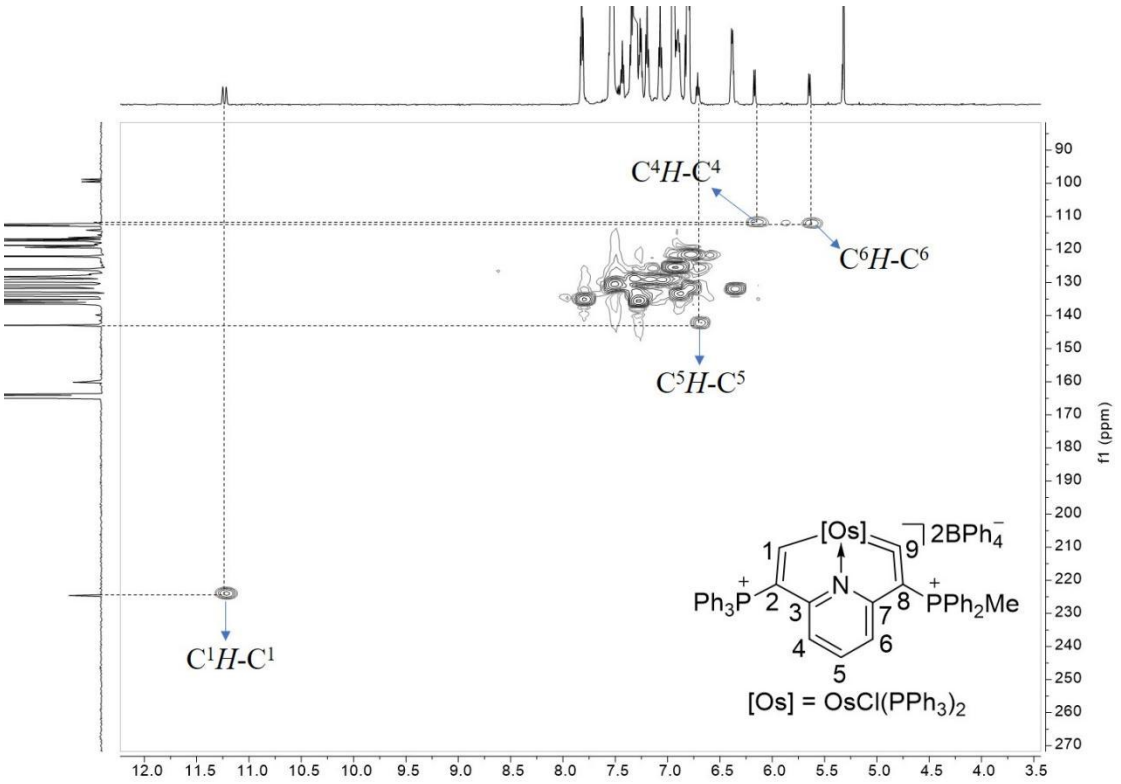


Figure S117. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **7b**.

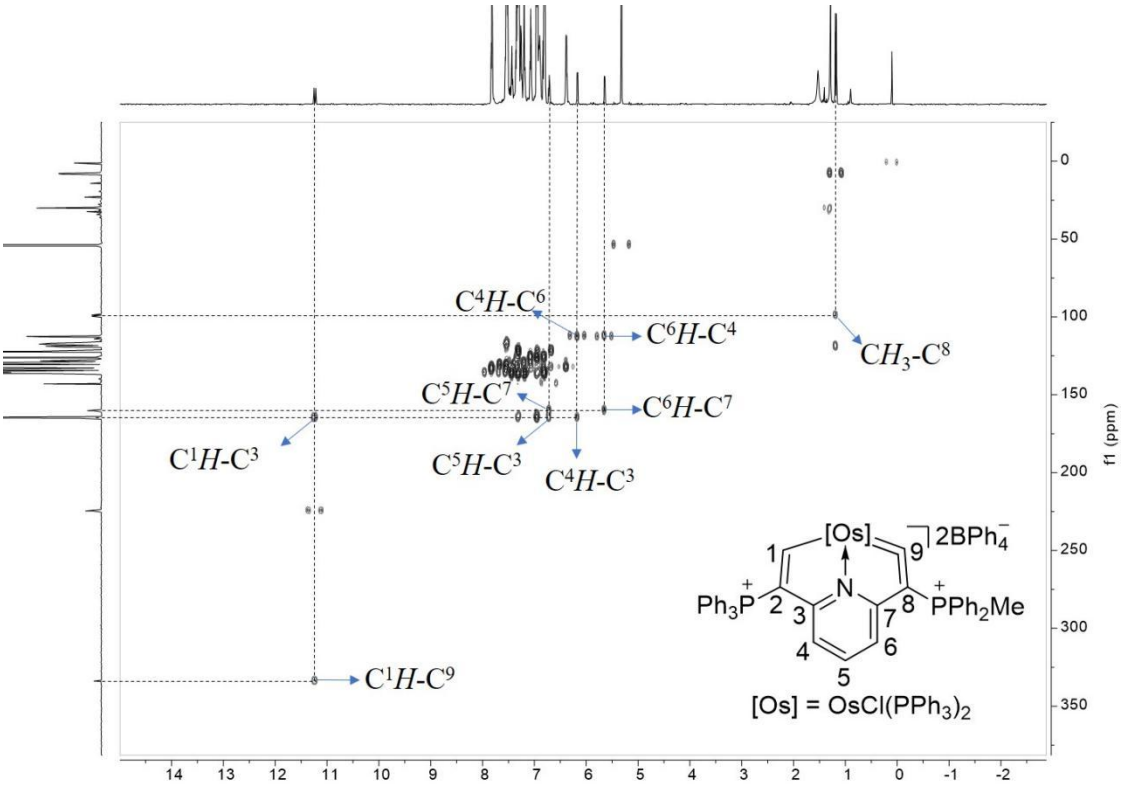


Figure S118. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **7b**.

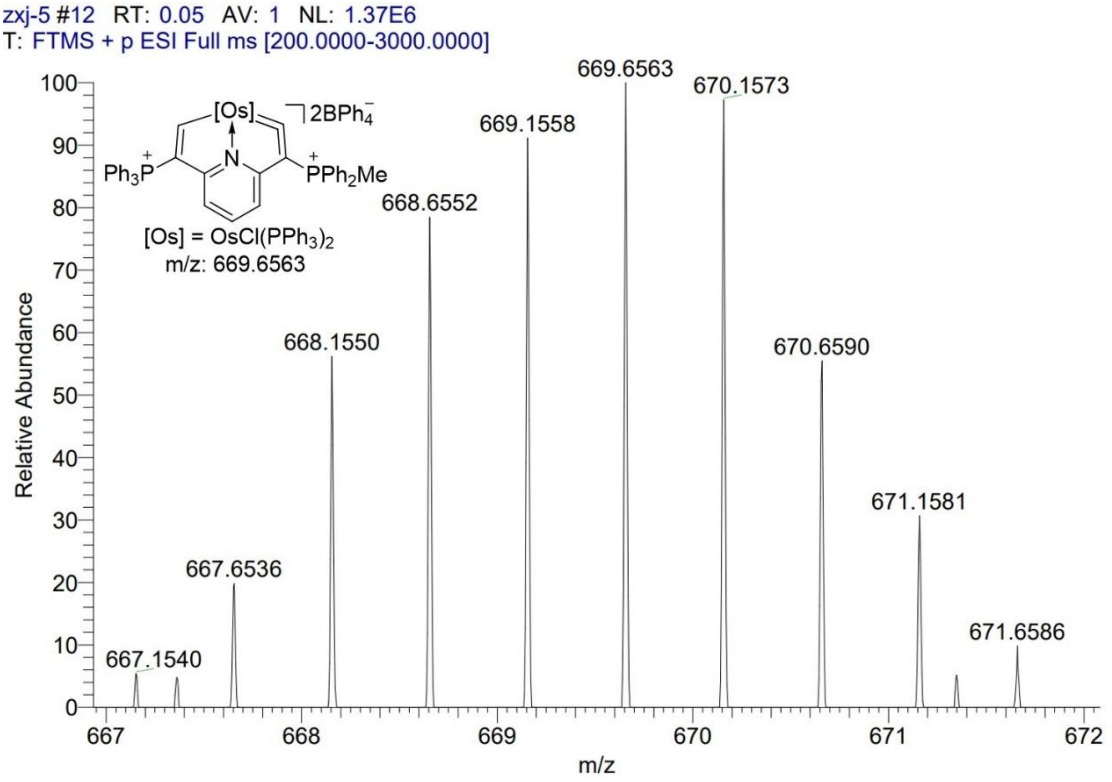


Figure S119. Positive-ion ESI-MS spectrum of [**7b**]$^{+}$ measured in methanol.

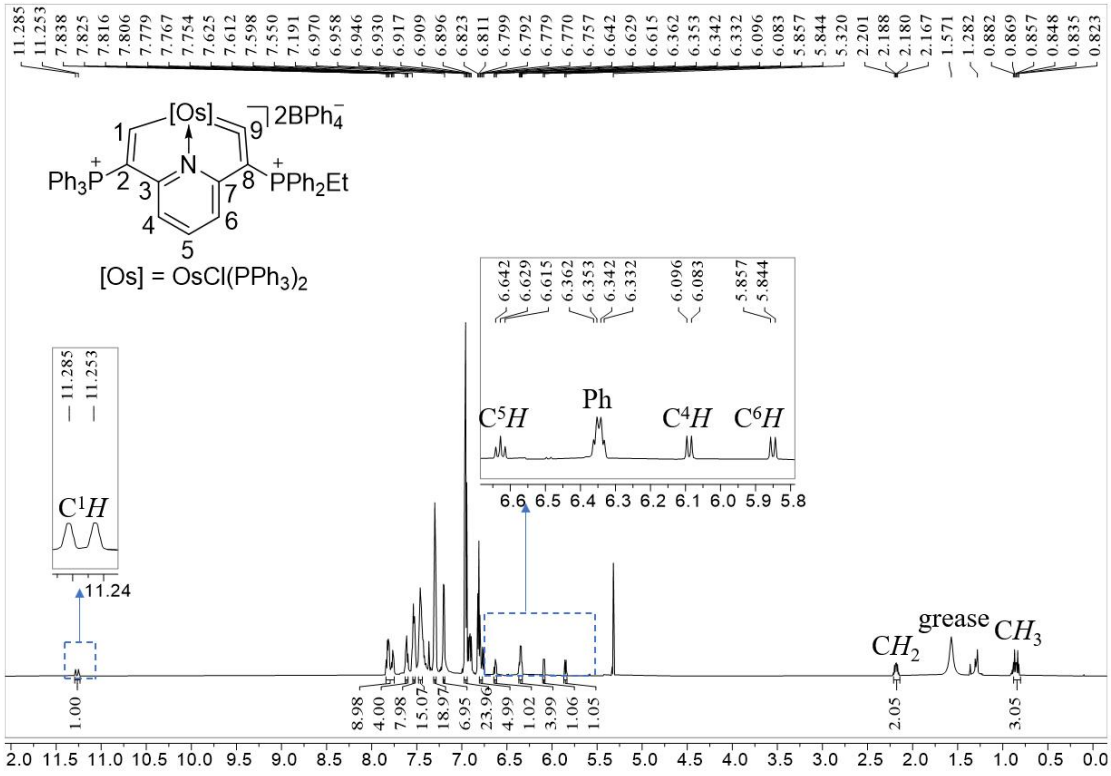


Figure S120. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **7c**.

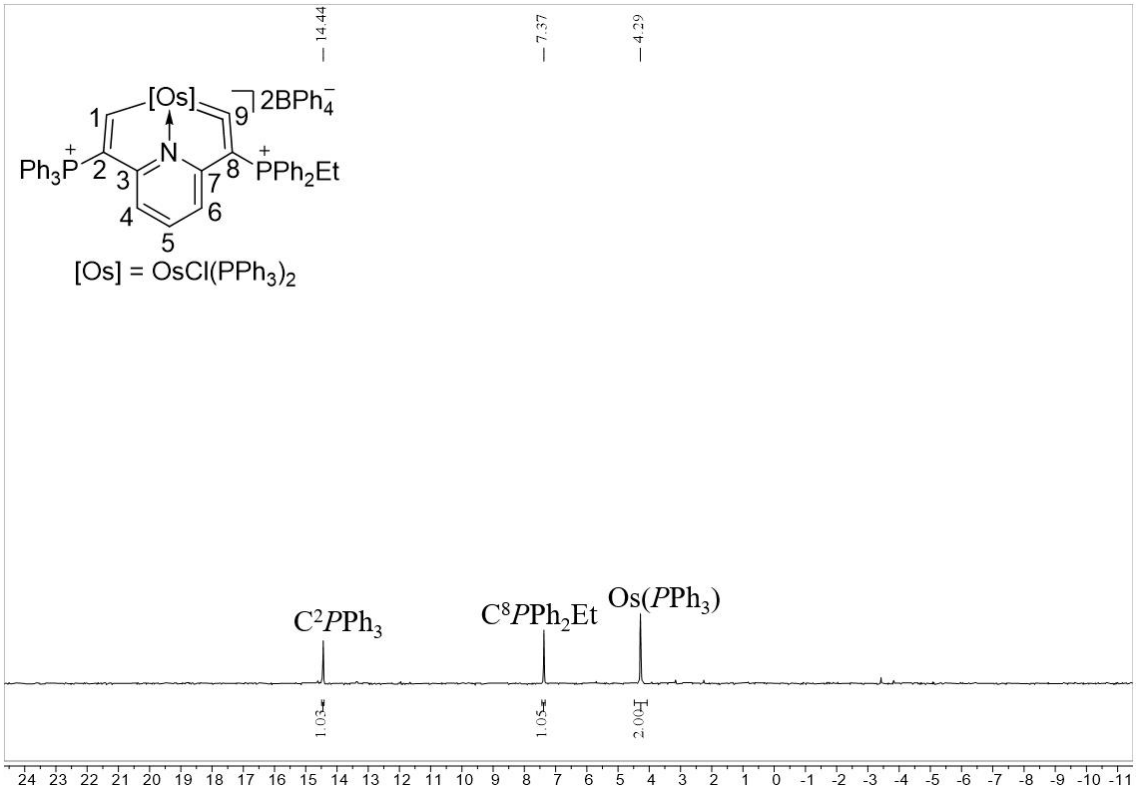


Figure S121. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **7c**.

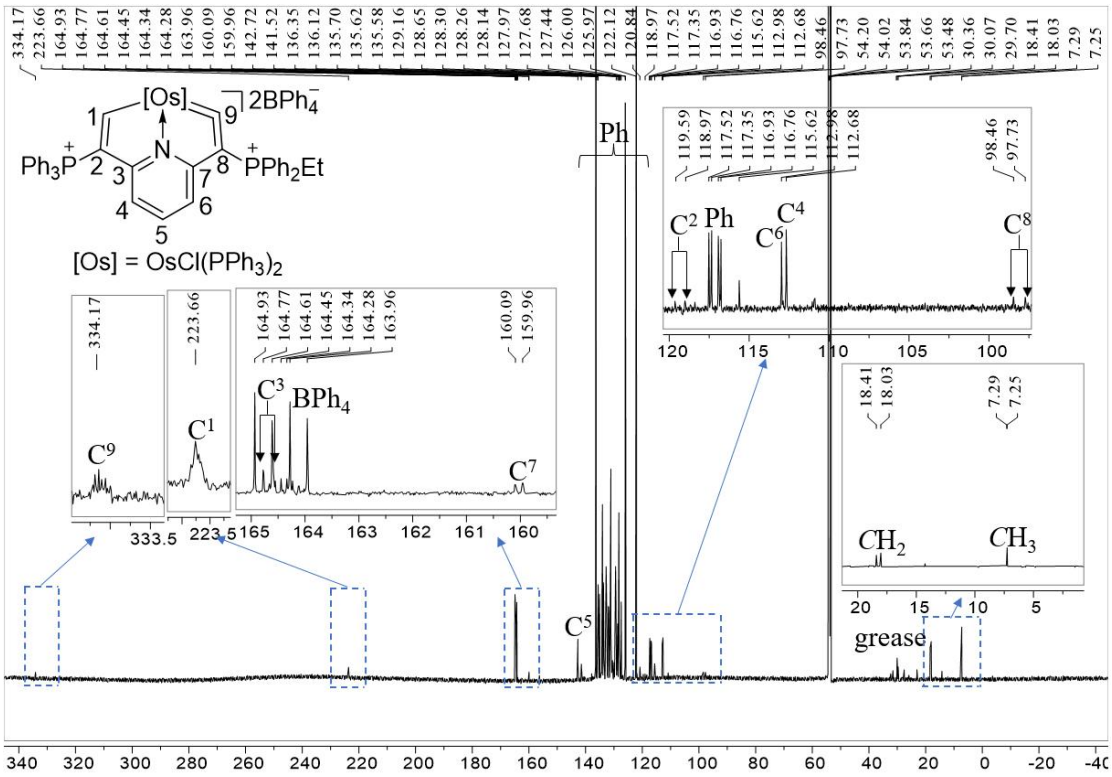


Figure S122. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **7c**.

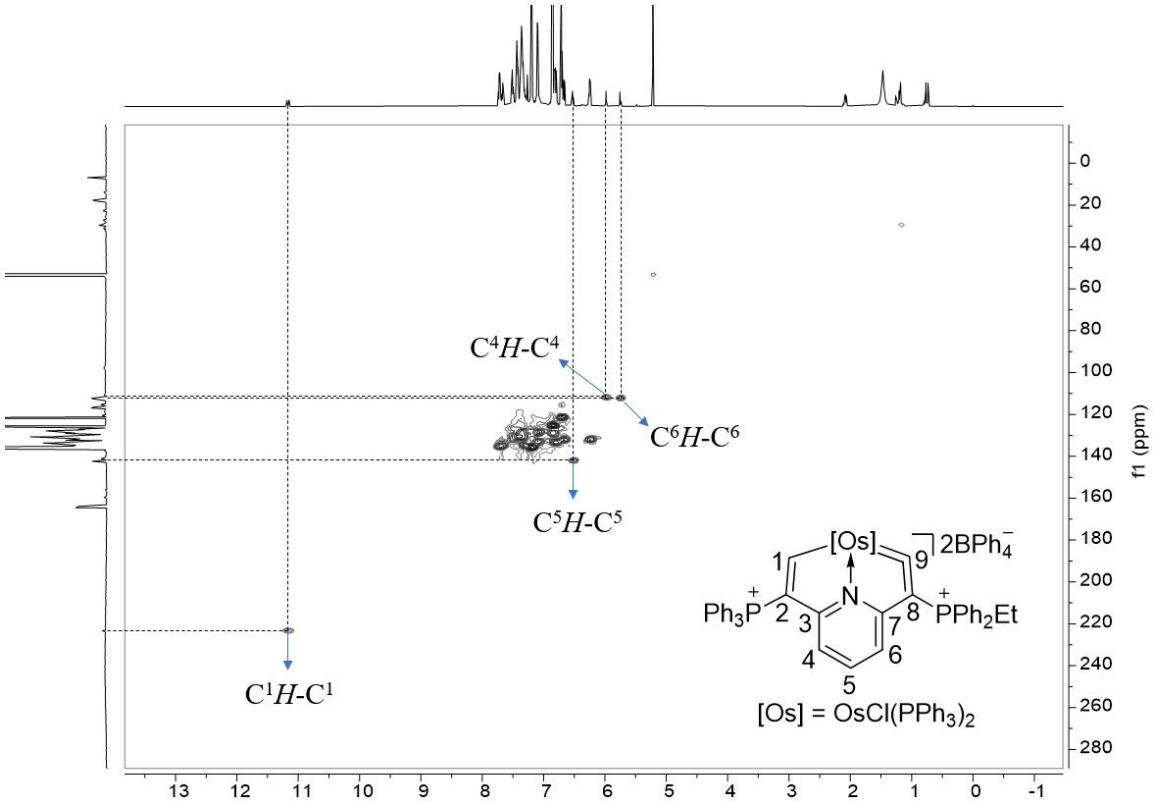


Figure S123. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **7c**.

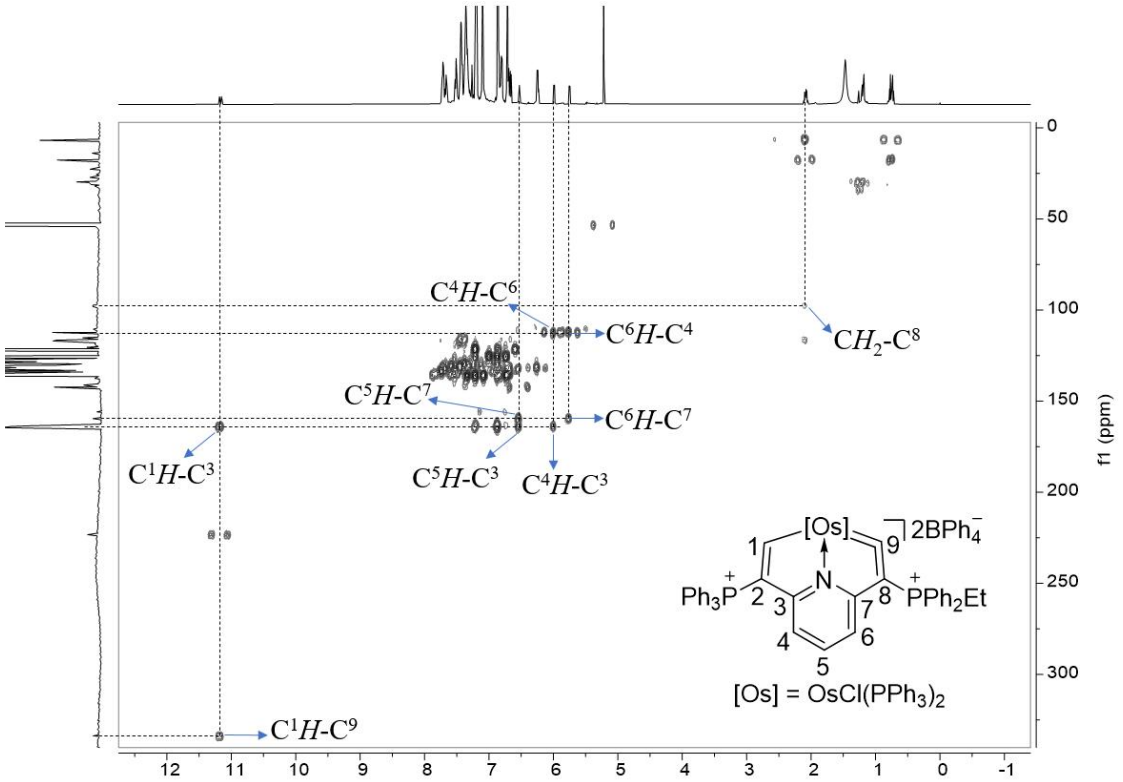


Figure S124. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **7c**.

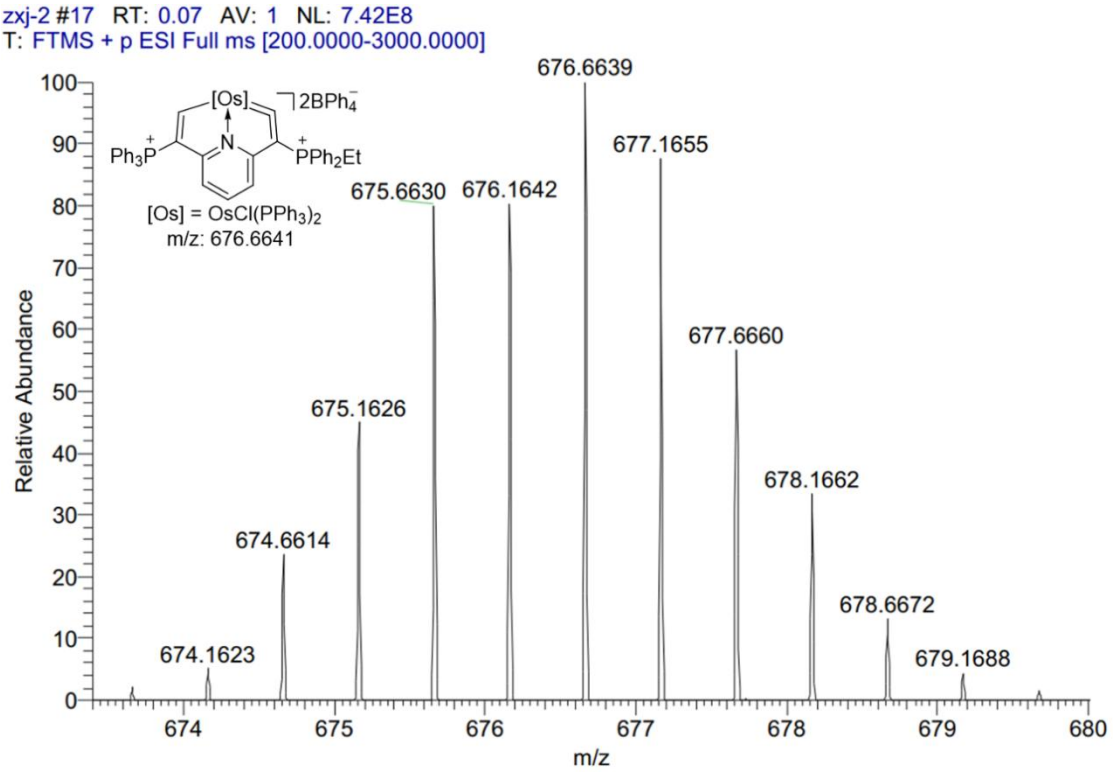


Figure S125. Positive-ion ESI-MS spectrum of [**7c**]$^{+}$ measured in methanol.

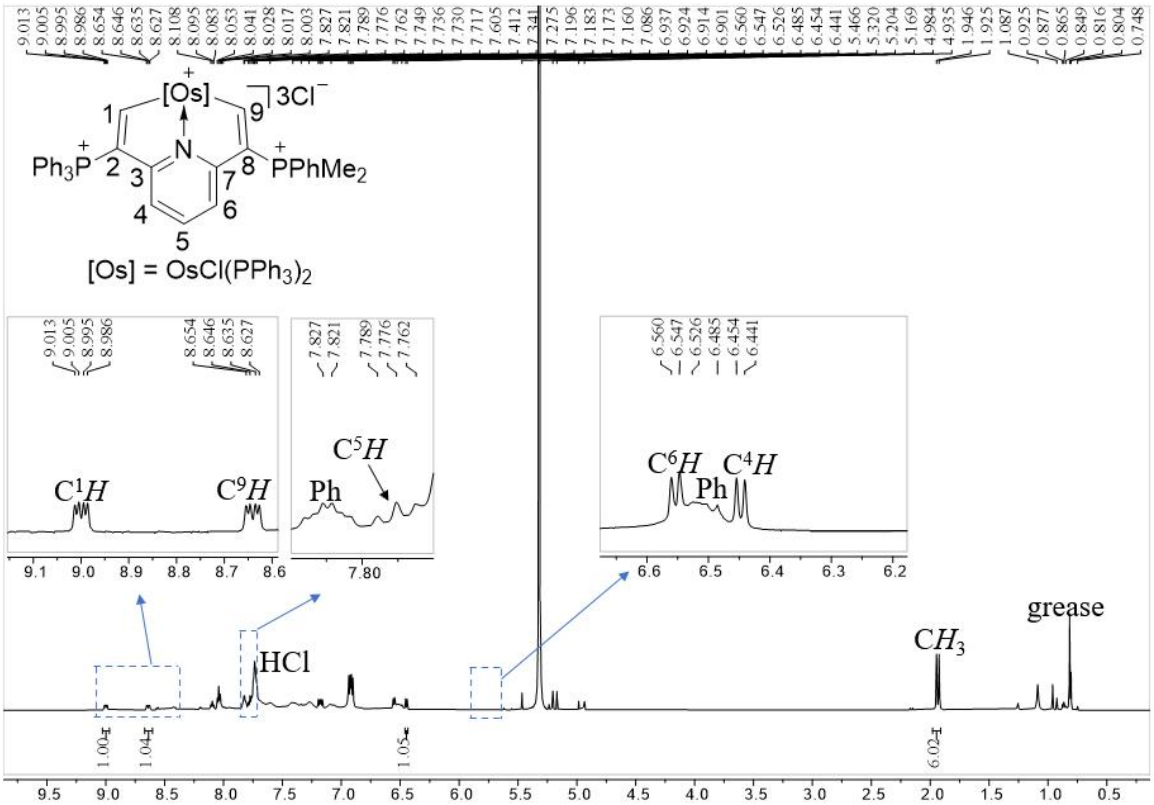


Figure S126. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **8a**.

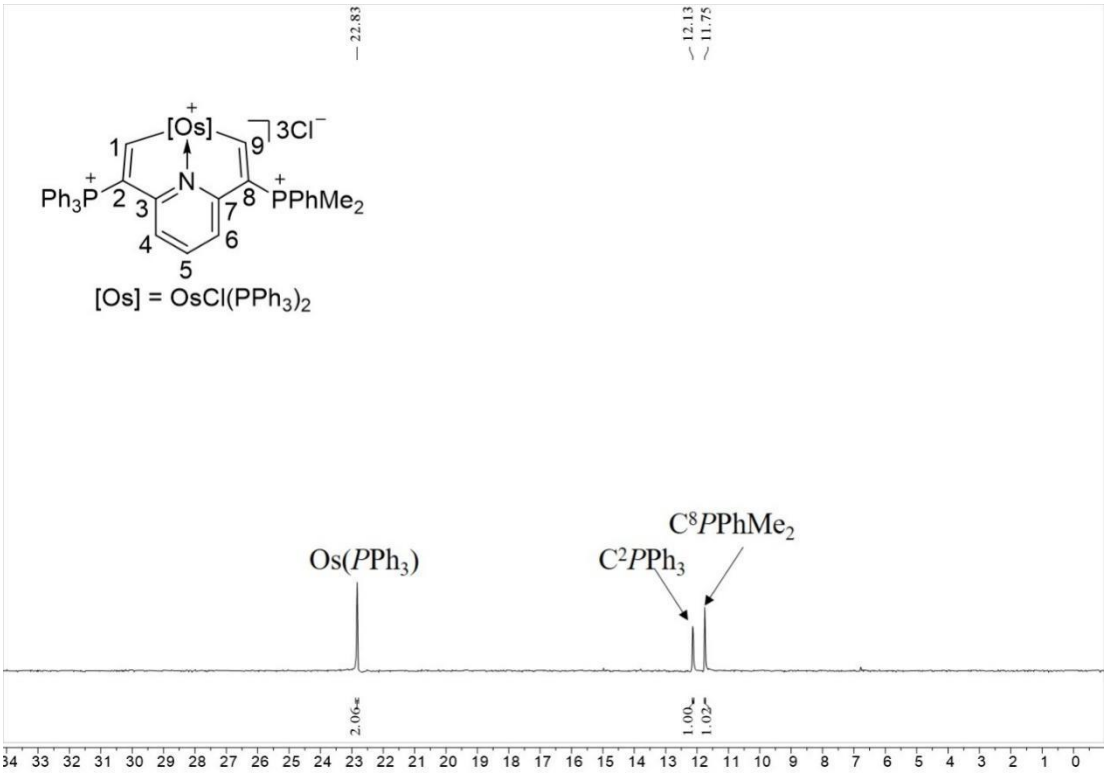


Figure S127. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **8a**.

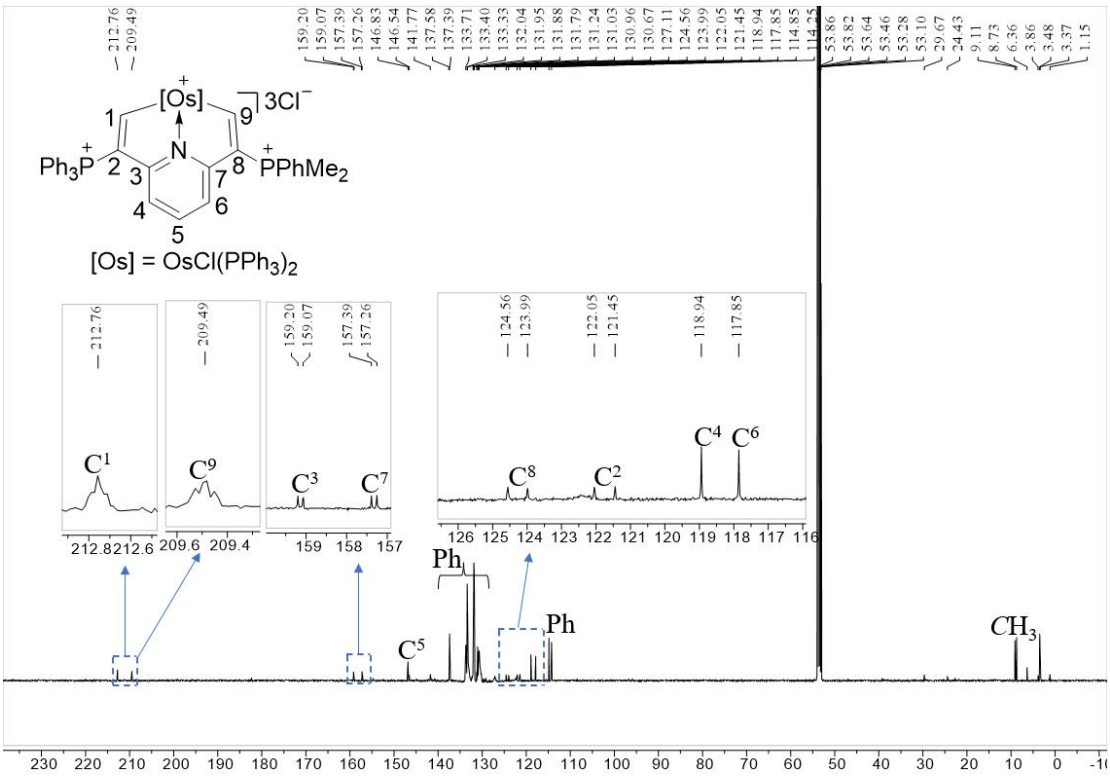


Figure S128. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **8a**.

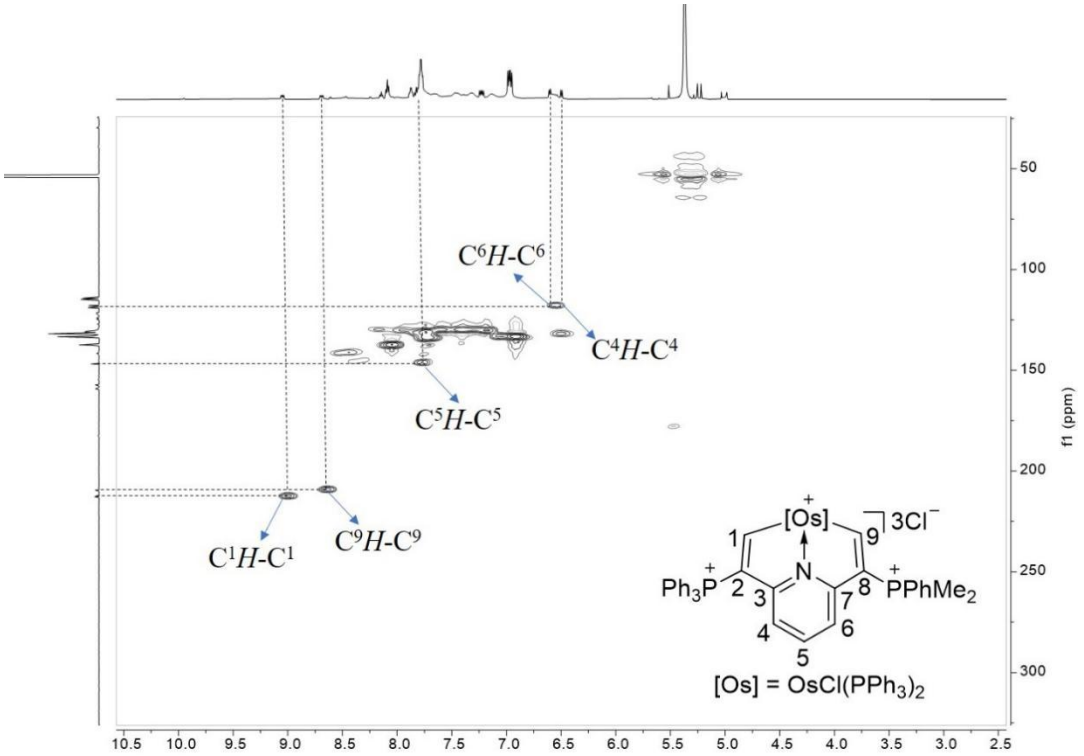


Figure S129. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **8a**.

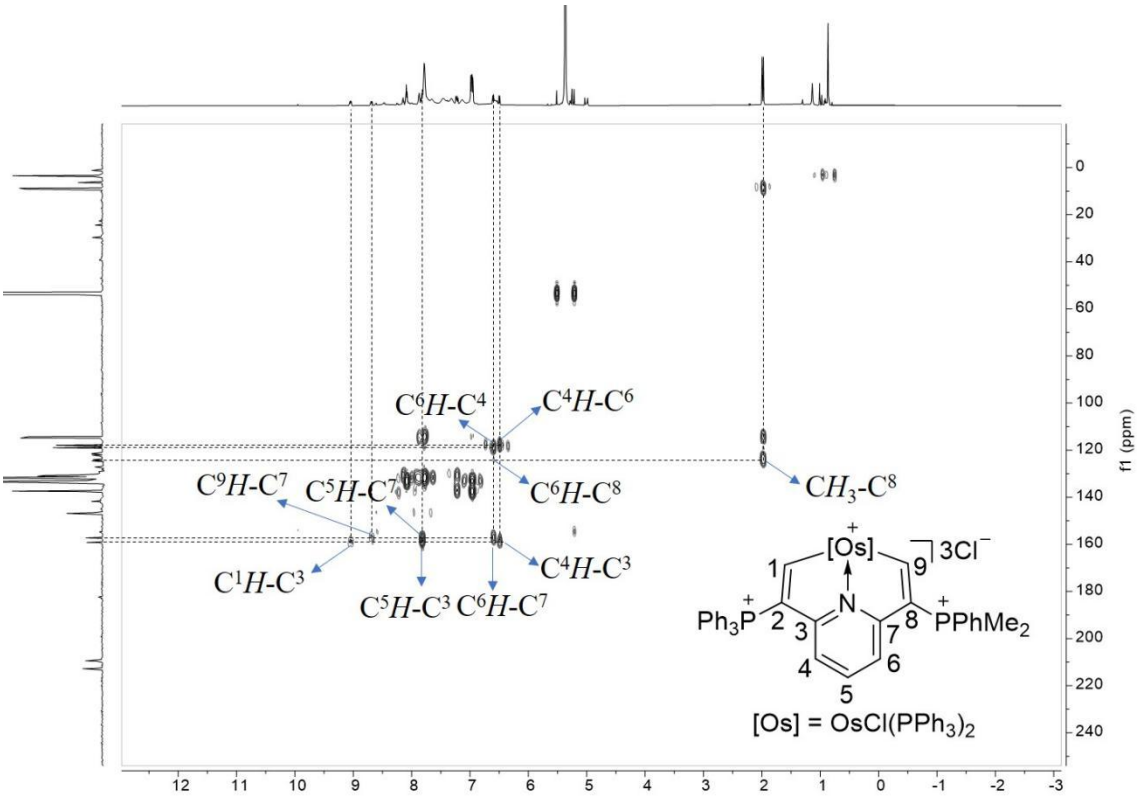


Figure S130. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **8a**.

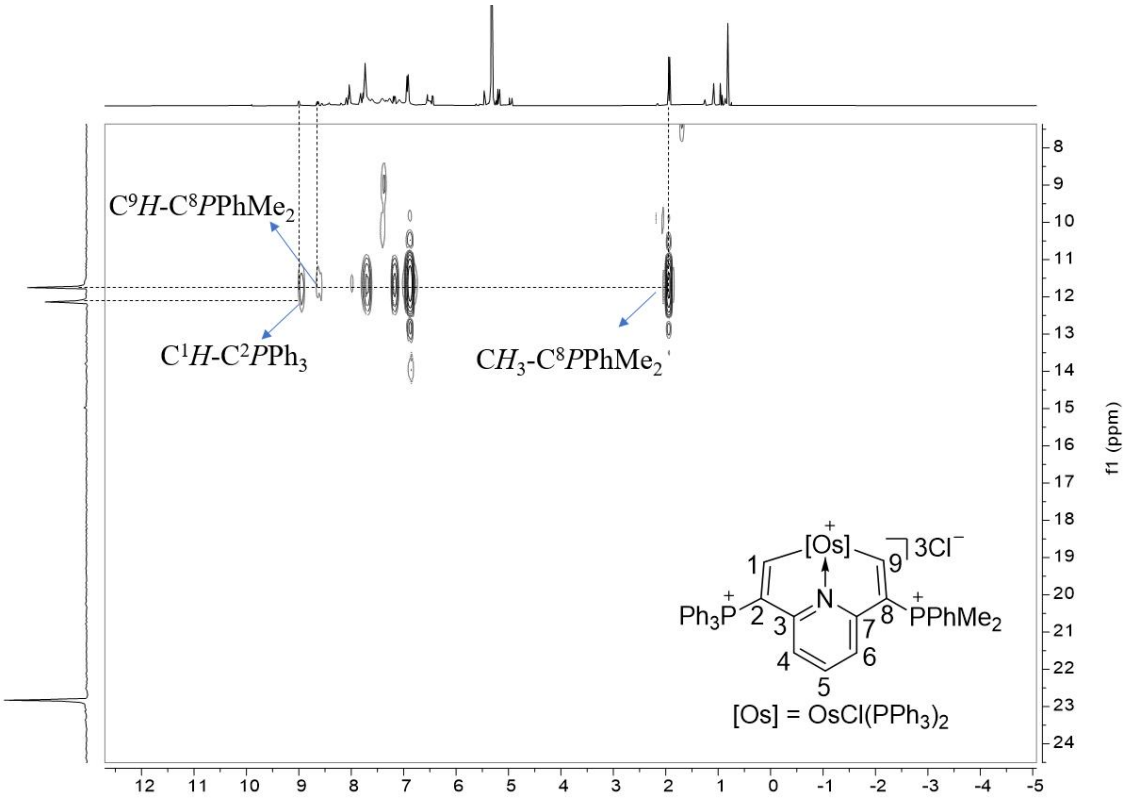


Figure S131. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complex **8a**.

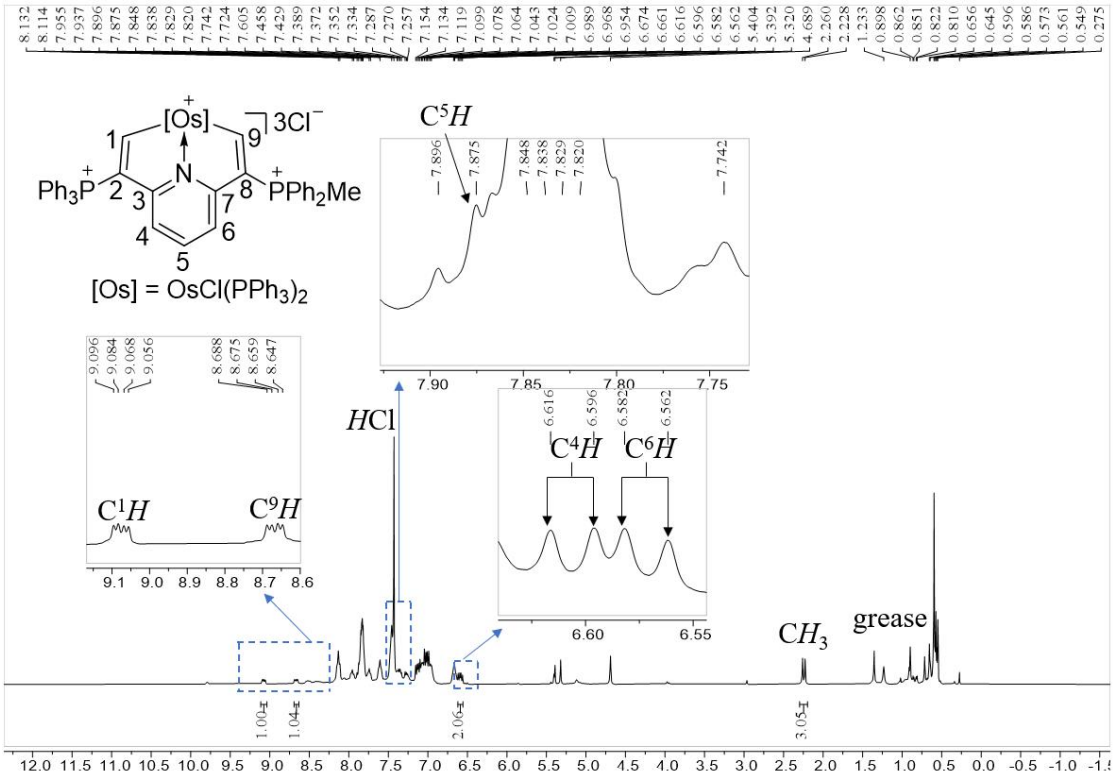


Figure S132. The ^{1}H NMR (400.1 MHz, CD_2Cl_2) spectrum for complex **8b**.

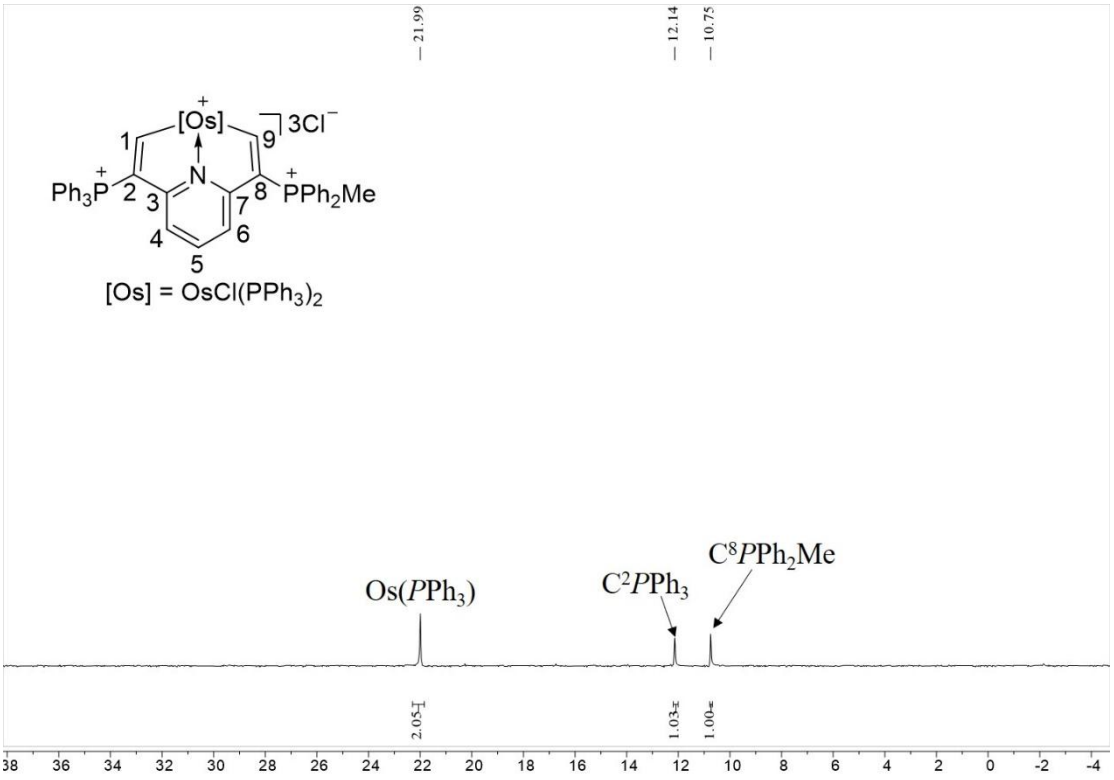


Figure S133. The $^{31}P\{^{1}H\}$ NMR (161.9 MHz, CD_2Cl_2) spectrum for complex **8b**.

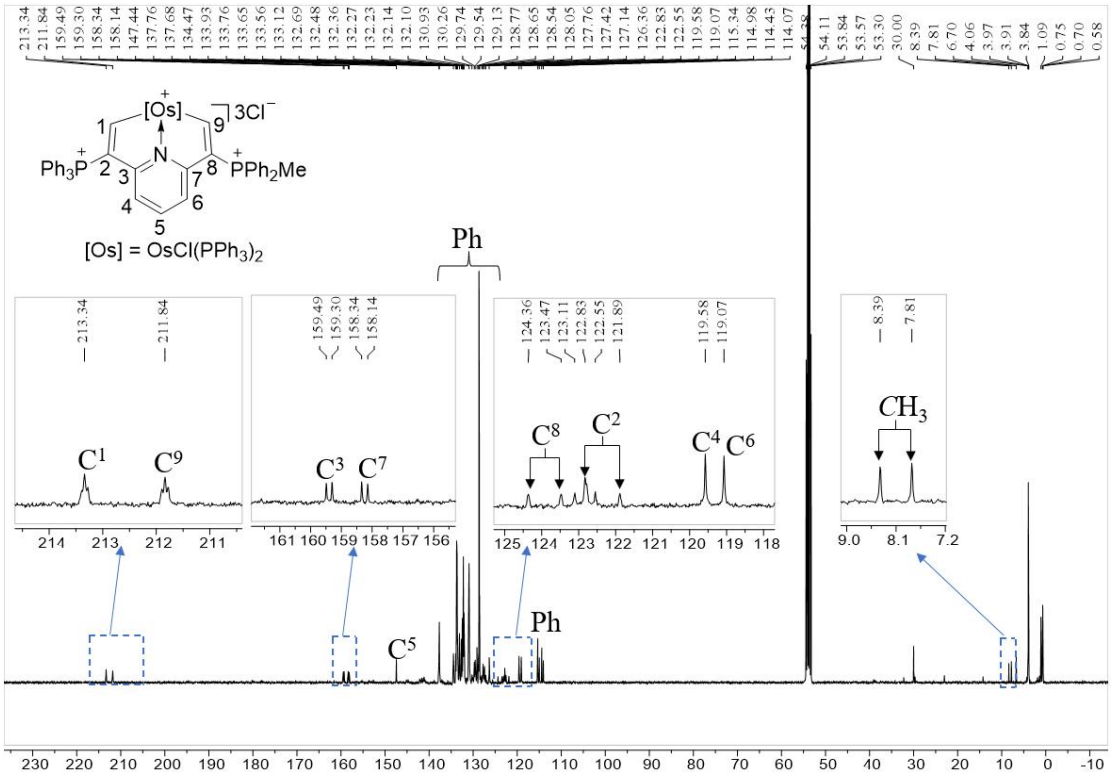


Figure S134. The $^{13}C\{^{1}H\}$ NMR (100.6 MHz, CD_2Cl_2) spectrum for complex **8b**.

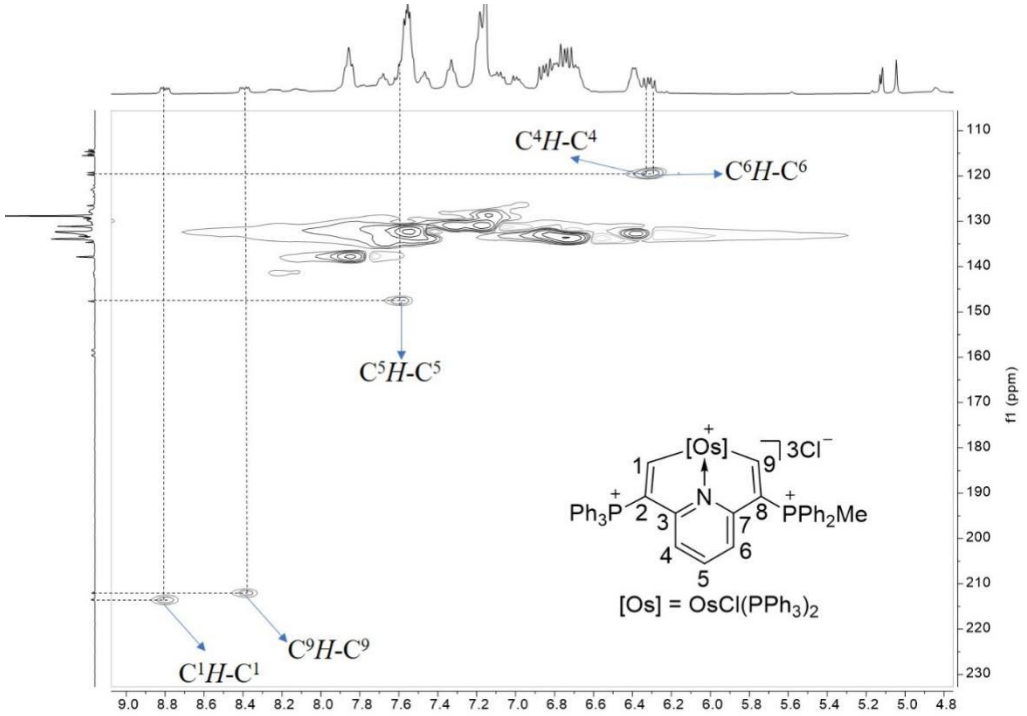


Figure S135. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **8b**.

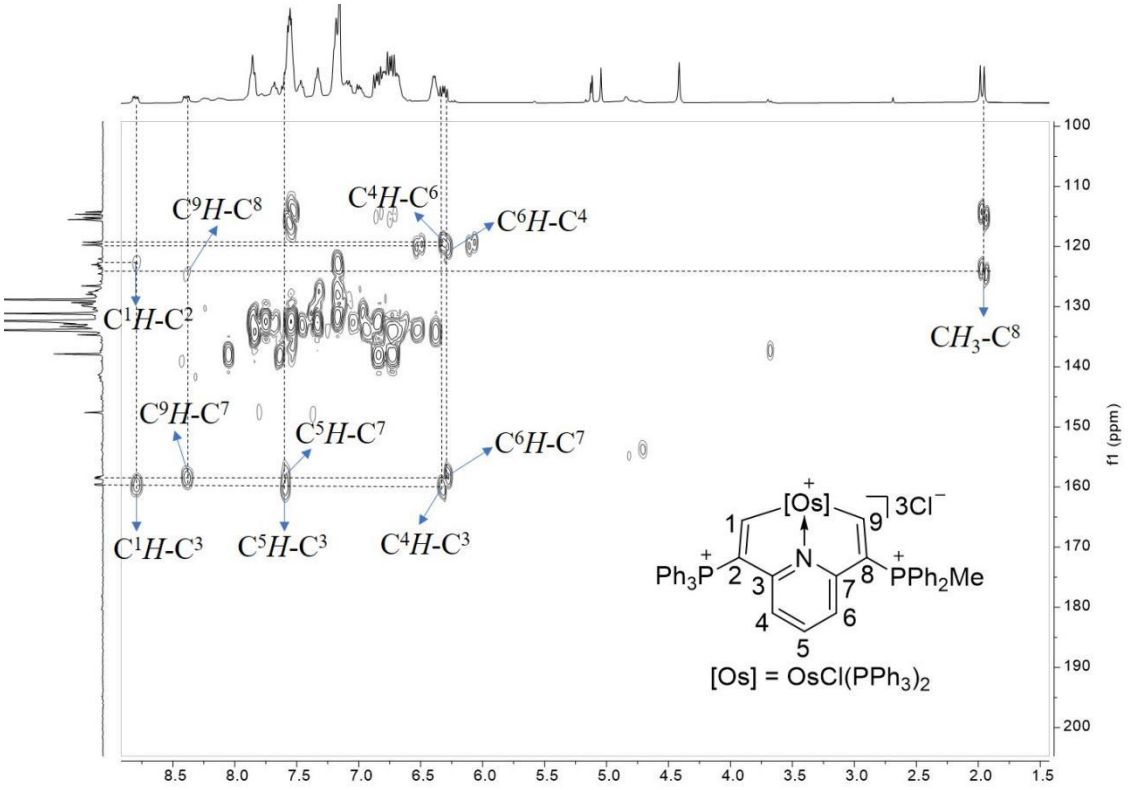


Figure S136. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **8b**.

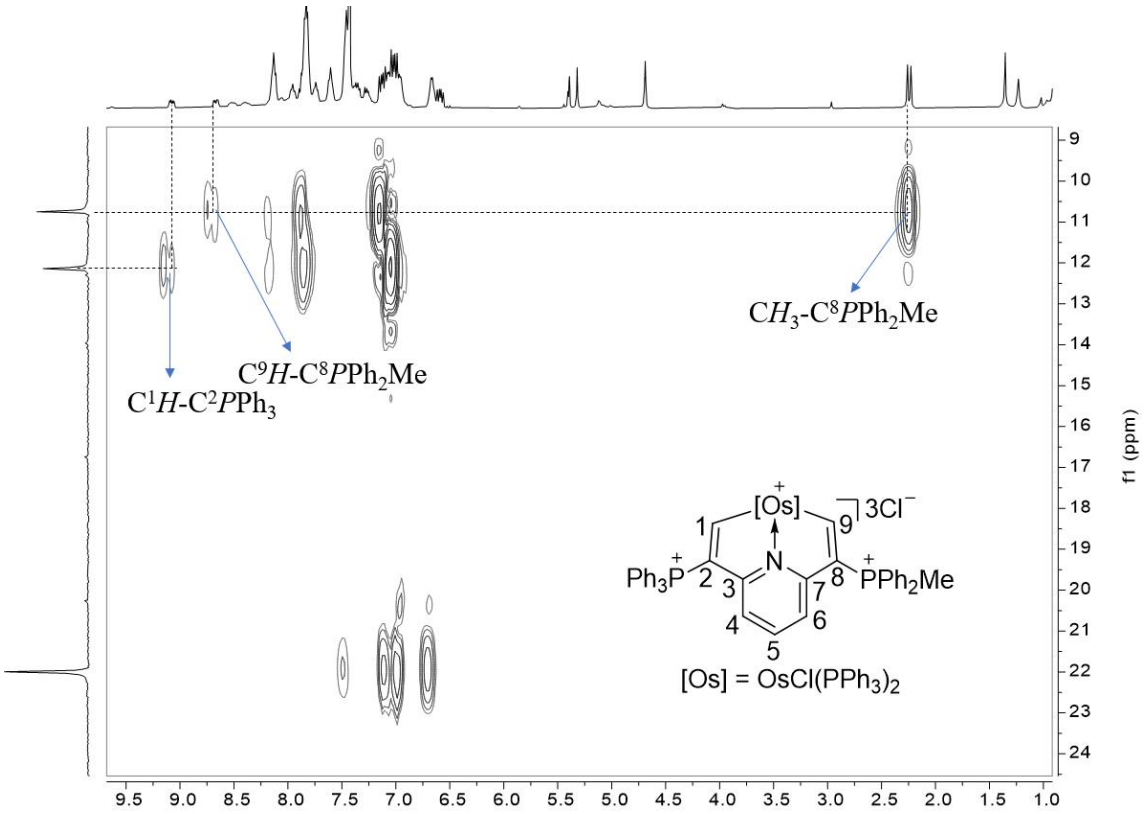


Figure S137. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complex **8b**.

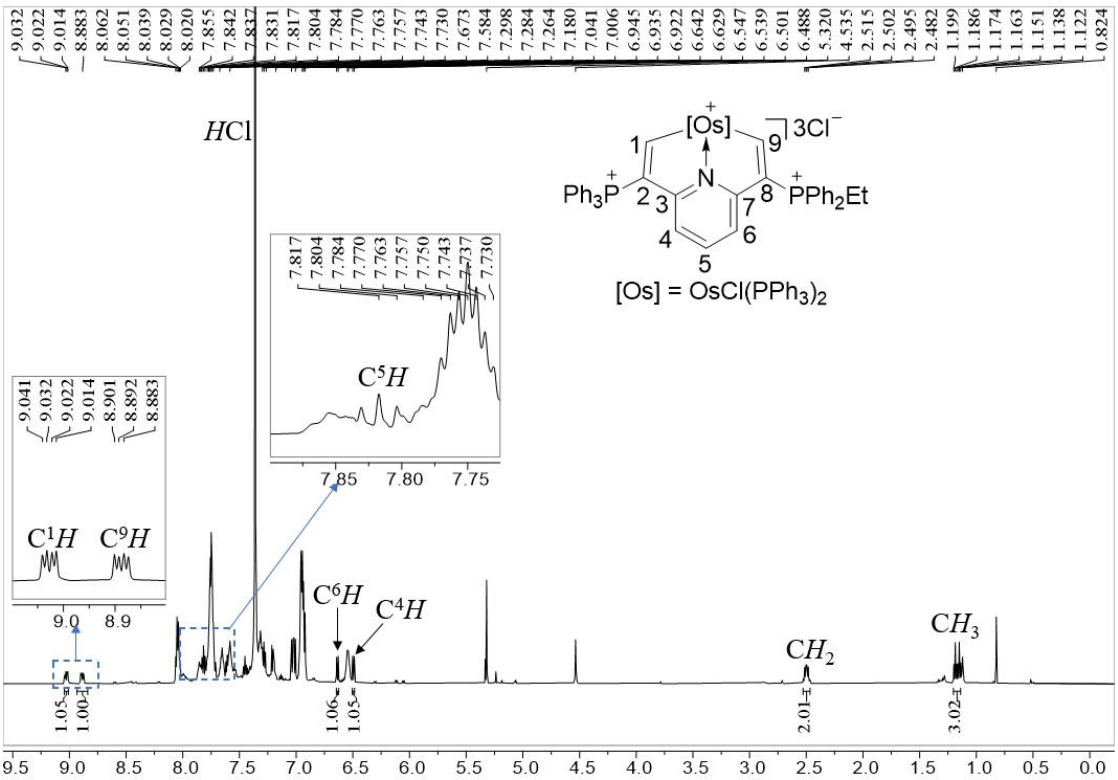


Figure S138. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **8c**.

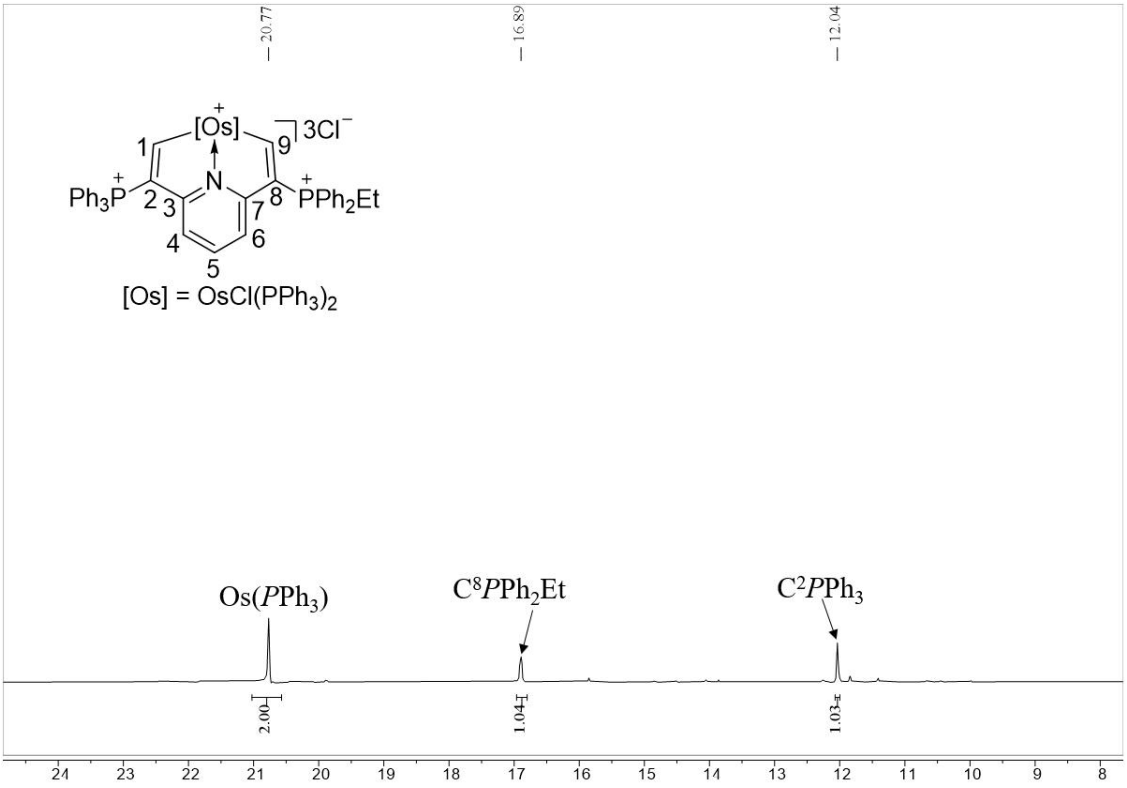


Figure S139. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **8c**.

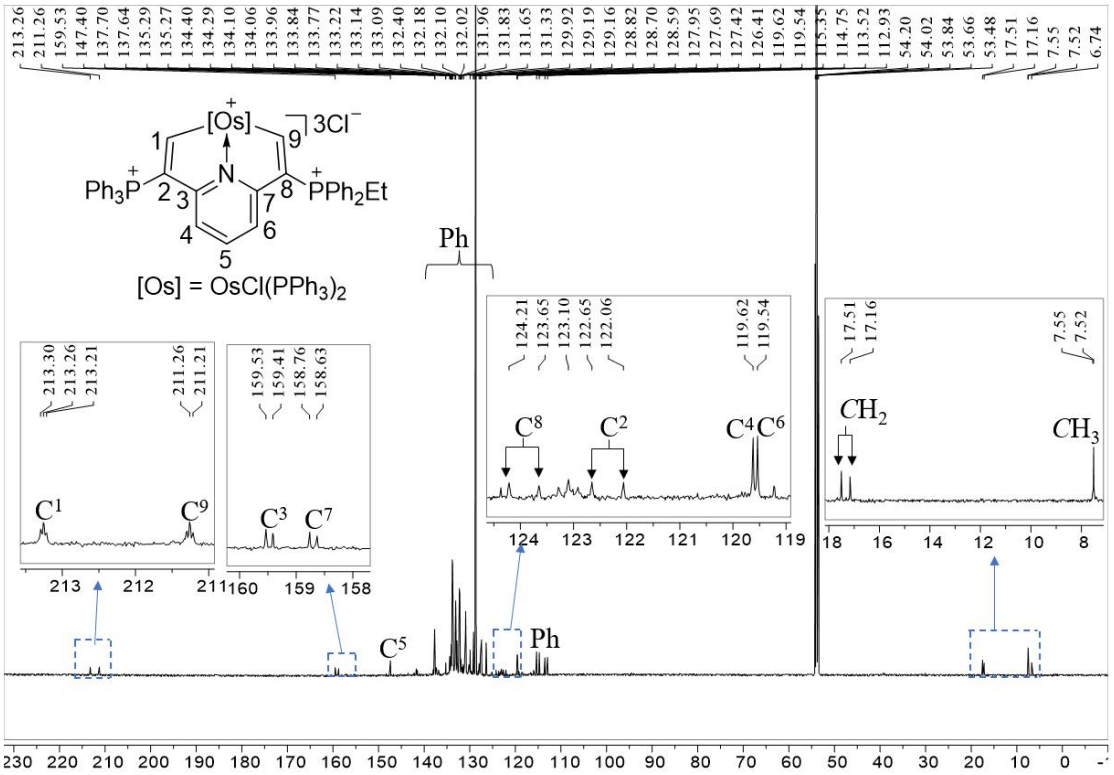


Figure S140. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **8c**.

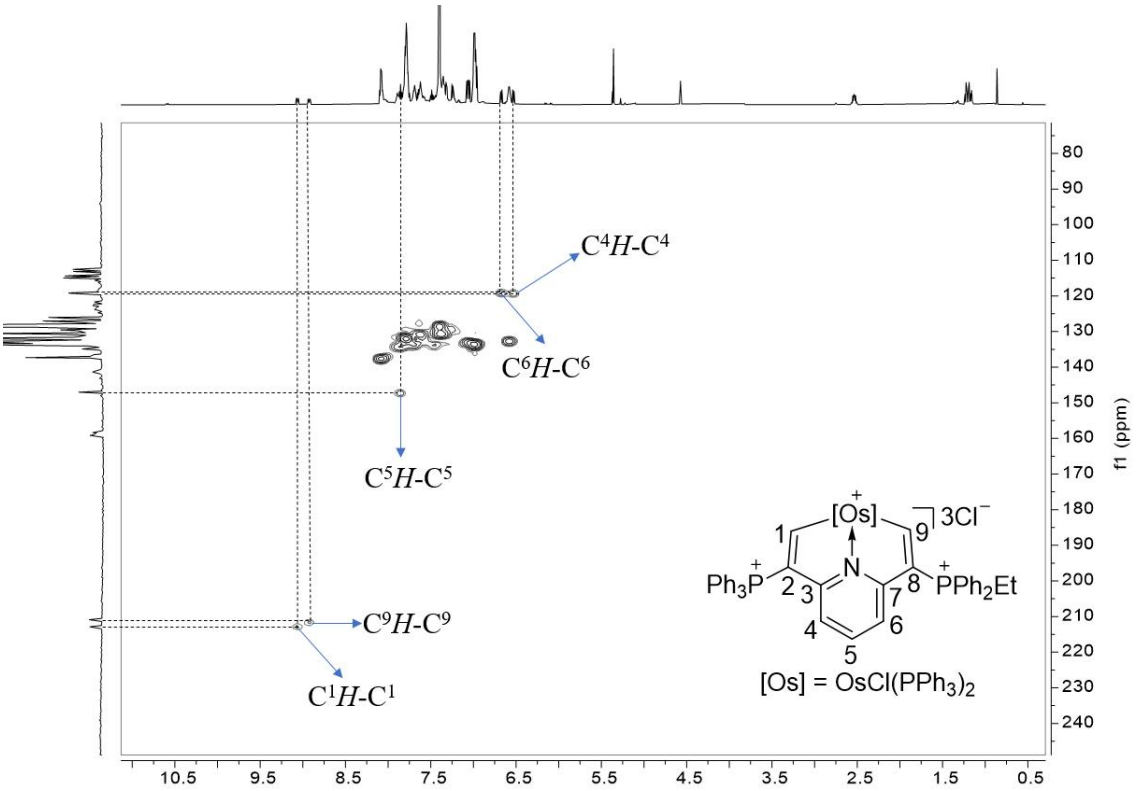


Figure S141. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **8c**.

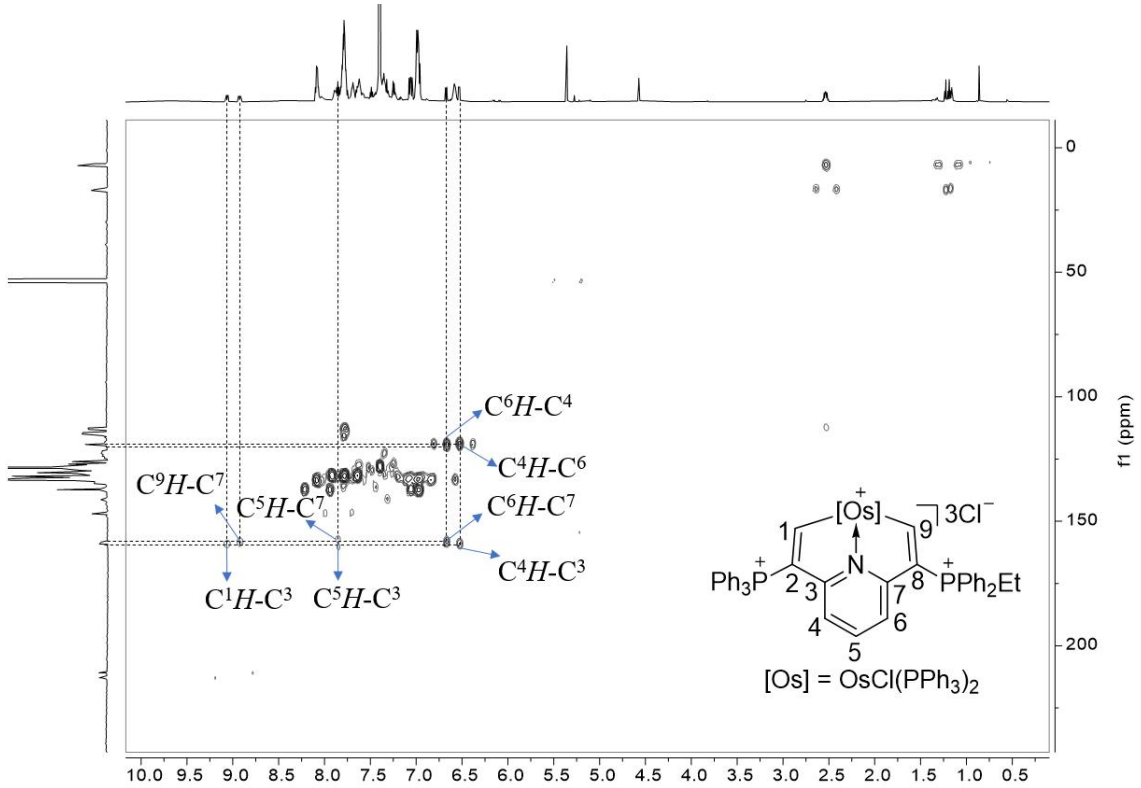


Figure S142. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **8c**.

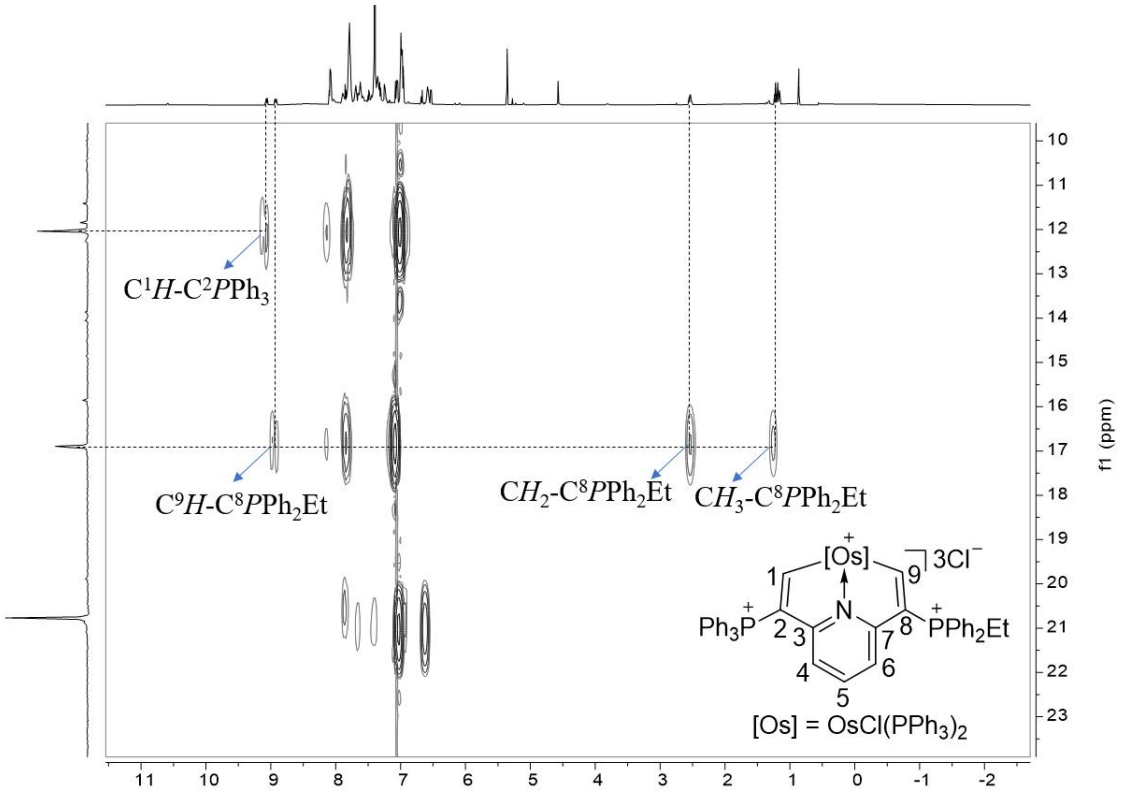


Figure S143. The ^{1}H-^{31}P HMBC (242.9 MHz, CD_2Cl_2) spectrum for complex **8c**.

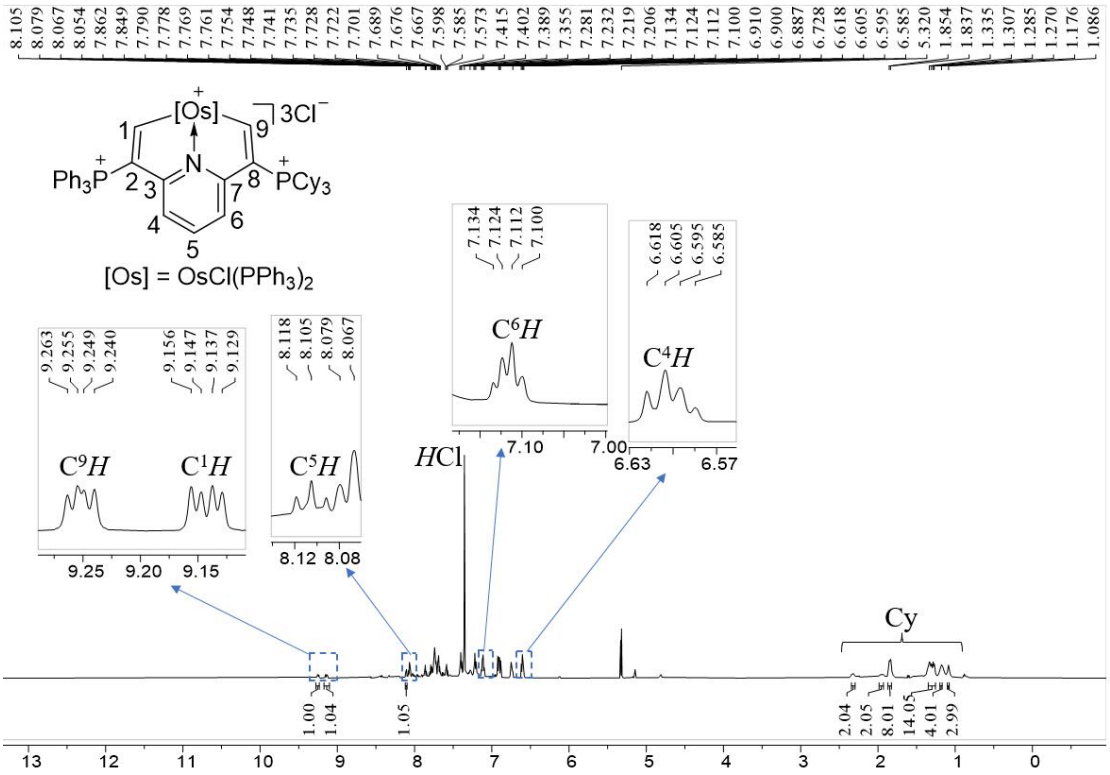


Figure S144. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **8d**.

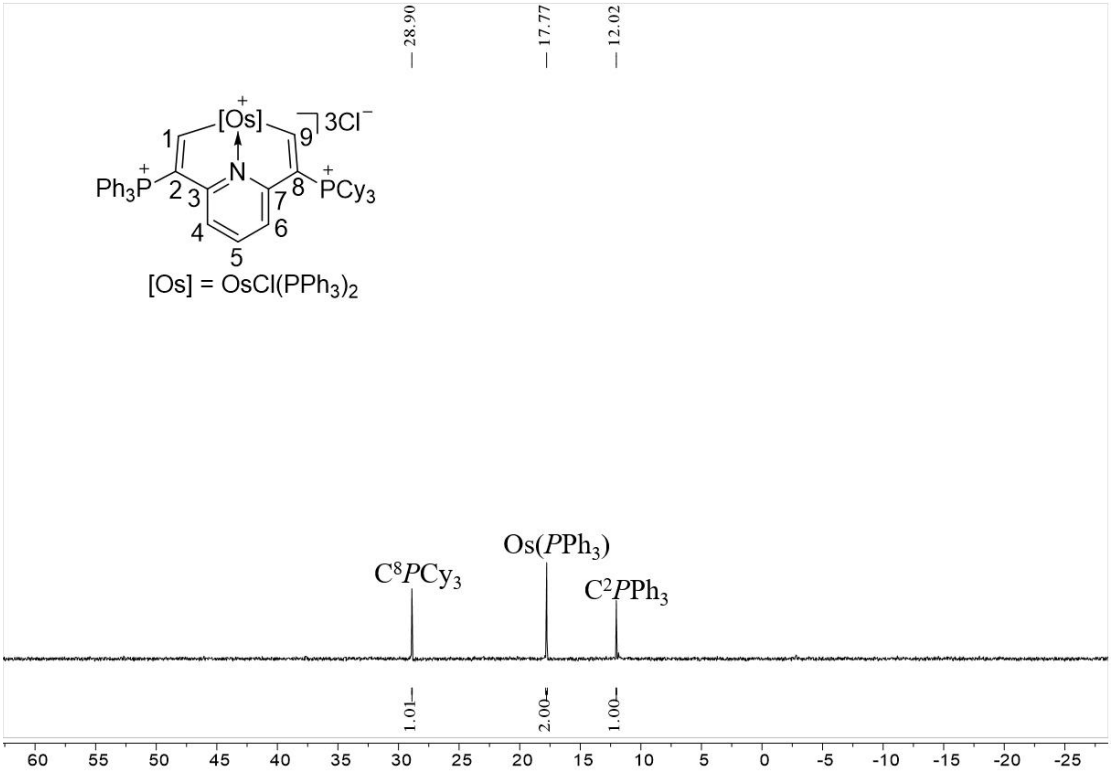


Figure S145. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **8d**.

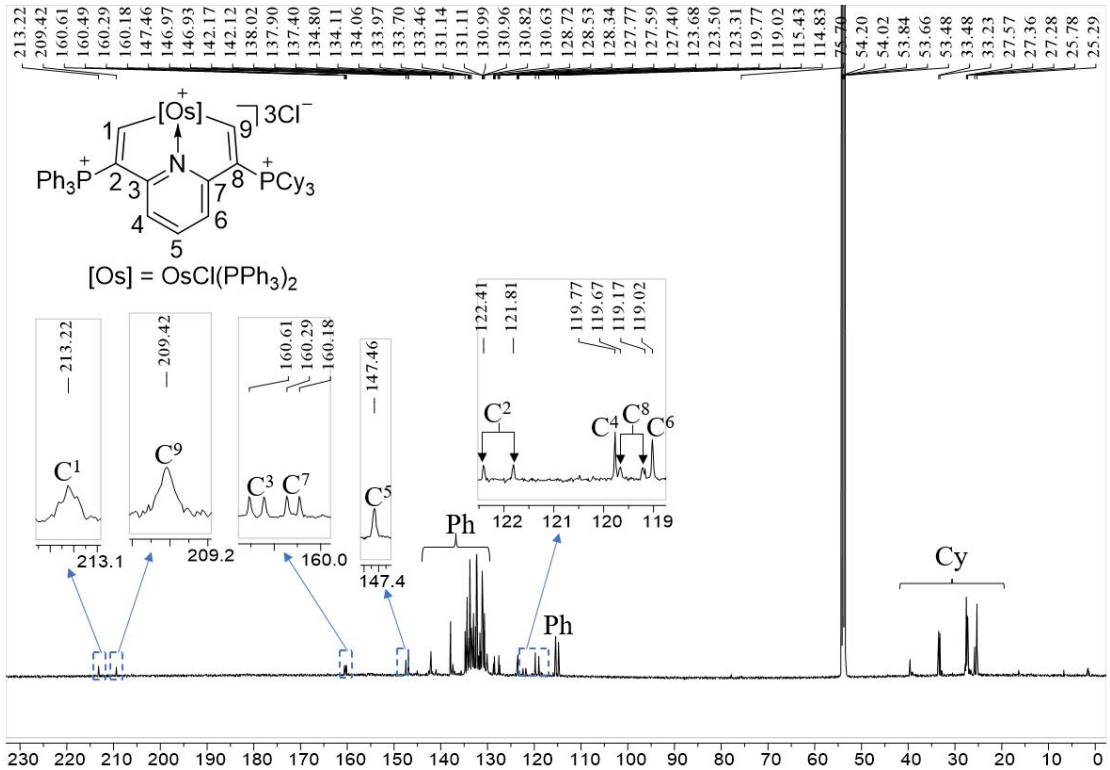


Figure S146. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **8d**.

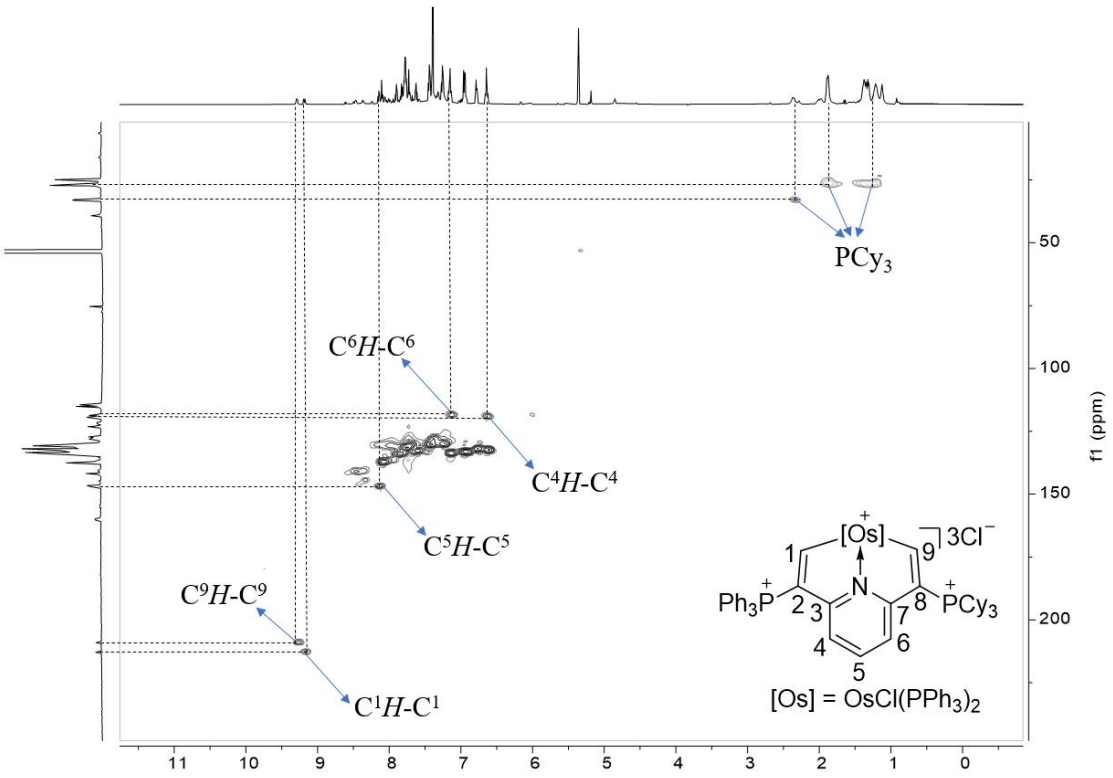


Figure S147. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **8d**.

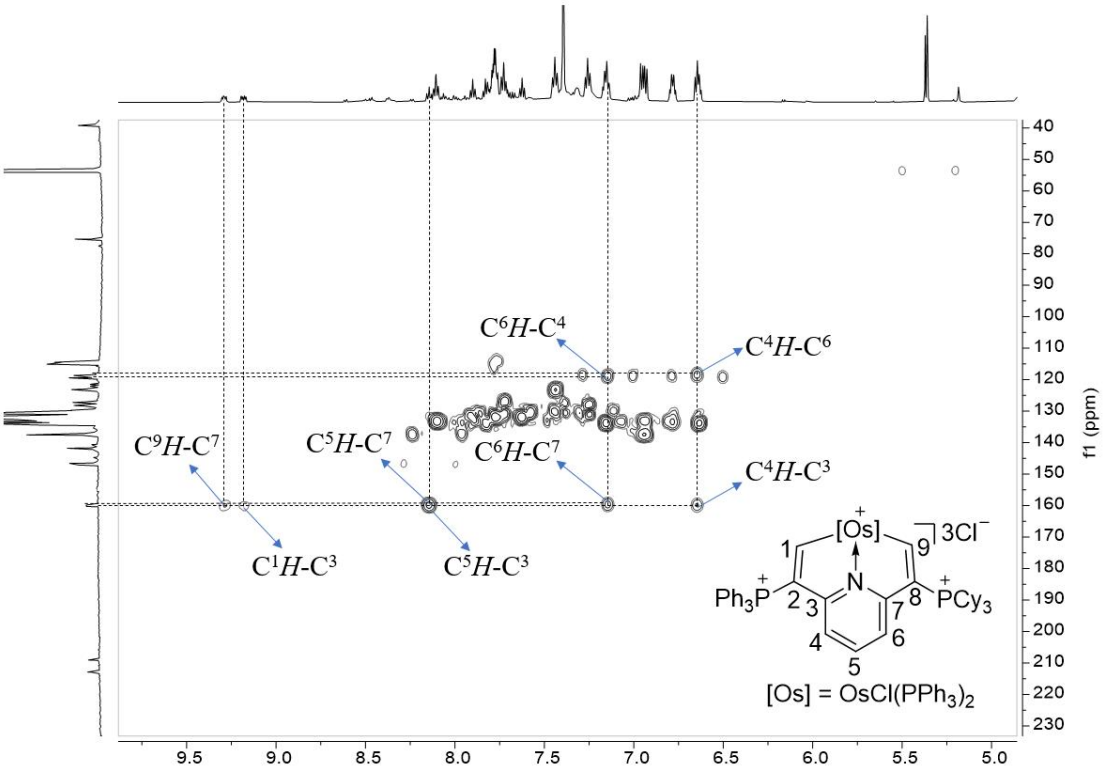


Figure S148. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **8d**.

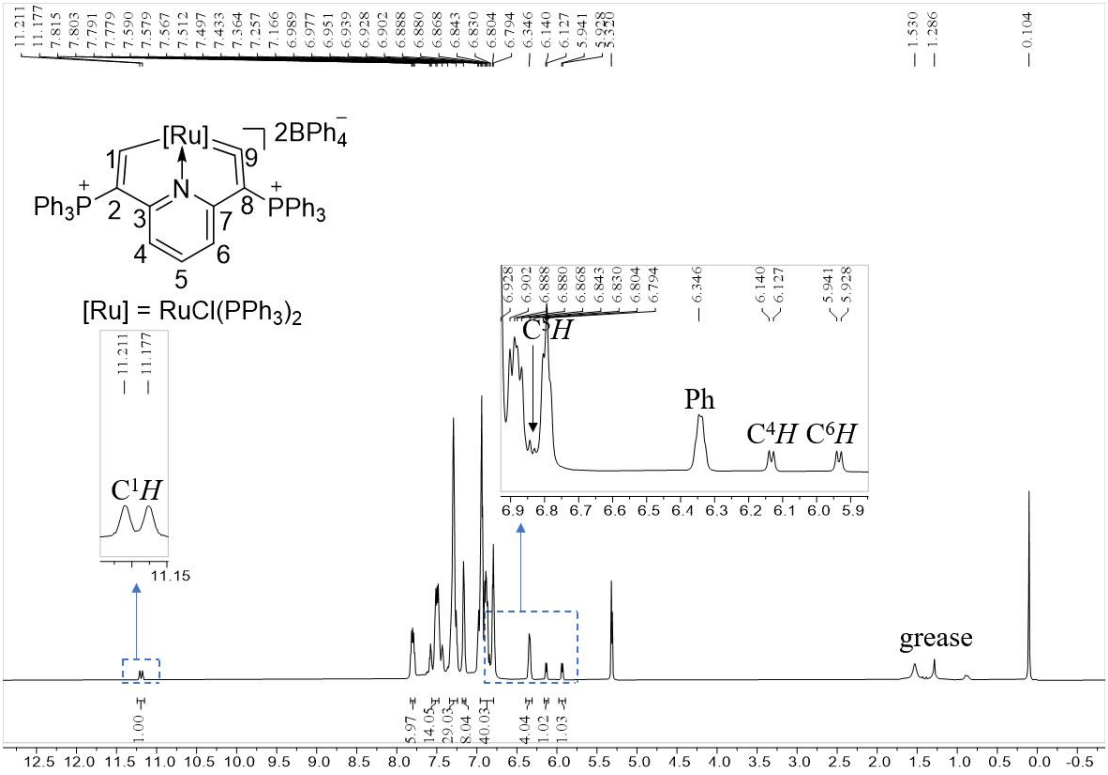


Figure S149. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **9**.

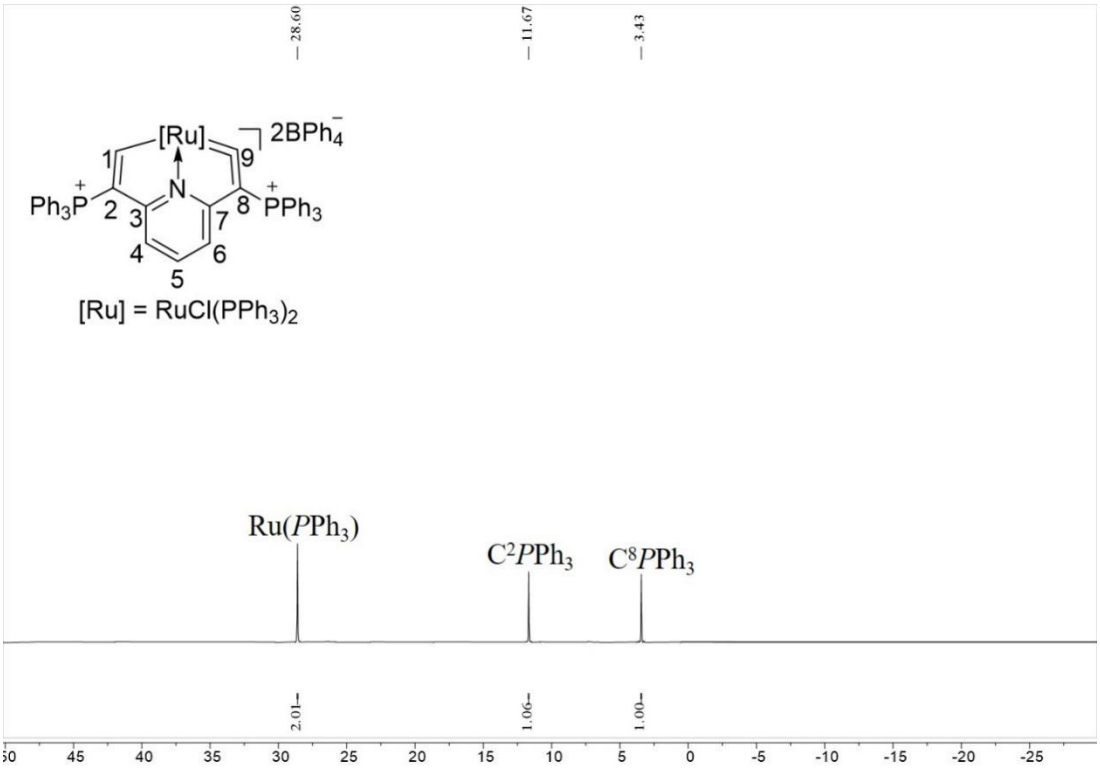


Figure S150. The $^{31}P\{^{1}H\}$ NMR (242.9 MHz, CD_2Cl_2) spectrum for complex **9**.

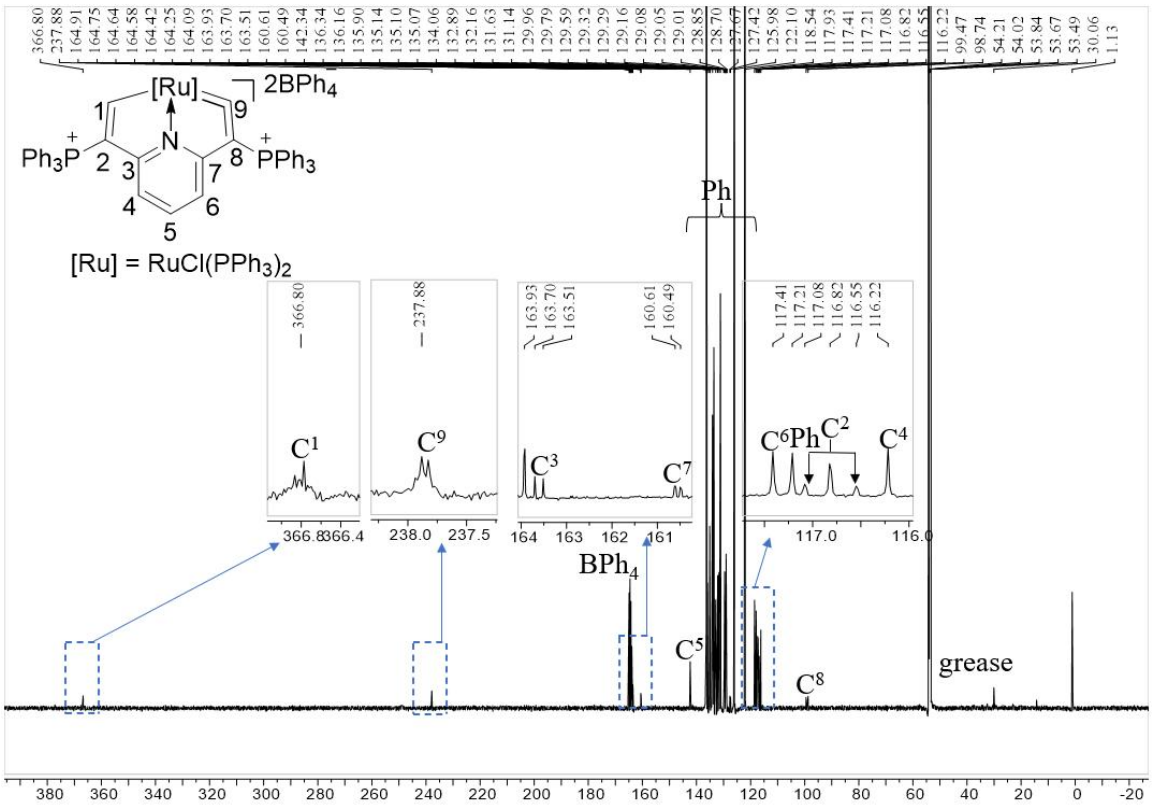


Figure S151. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **9**.

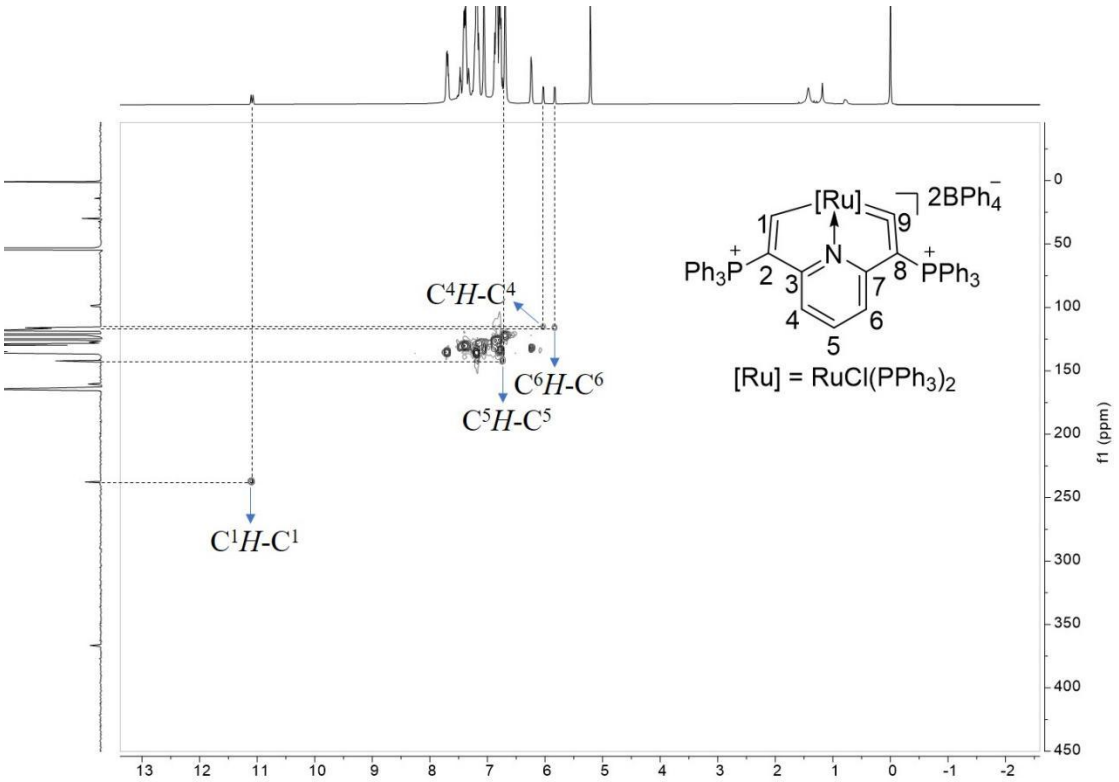


Figure S152. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **9**.

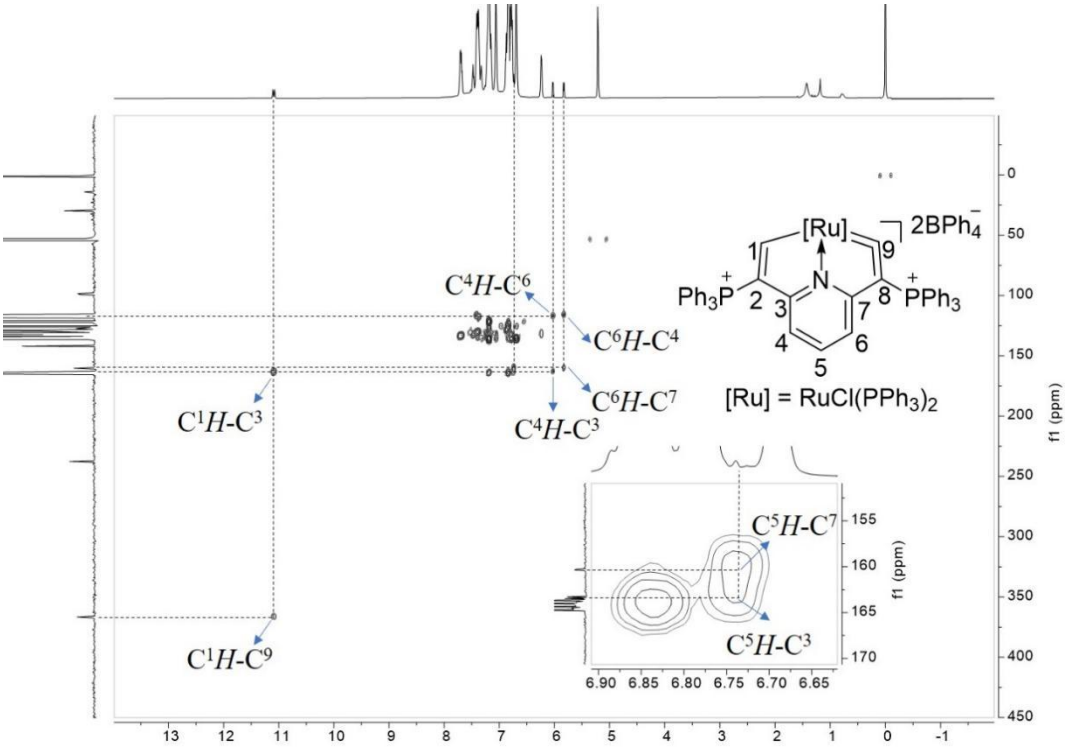


Figure S153. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **9**.

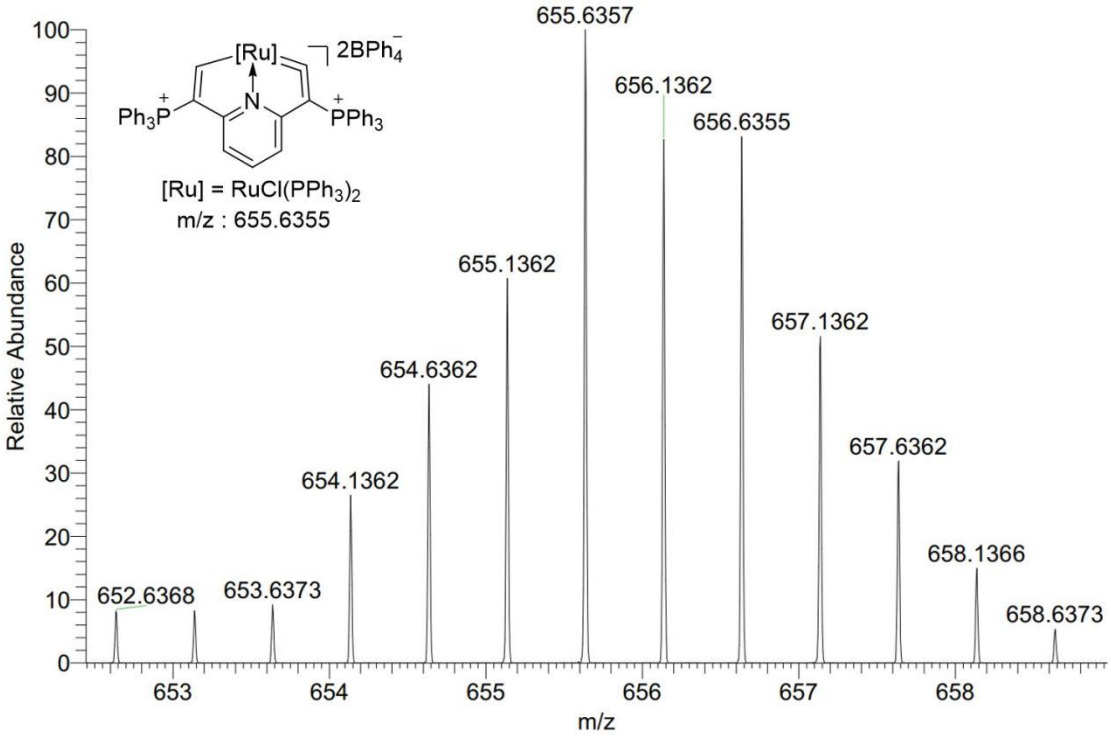


Figure S154. Positive-ion ESI-MS spectrum of [**9**]$^{+}$ measured in methanol

5. Thermal Stability Experiments

A solid sample of **1** could be heated at 120 °C for at least three hours without noticeable decomposition, partly decomposed at 130 °C and completely decomposed at 140 °C. A solid sample of **5a** could be heated at 130 °C for at least three hours without noticeable decomposition, partly decomposed at 140 °C and completely decomposed at 160 °C. A solid sample of **5b** could be heated at 140 °C for at least three hours without noticeable decomposition, partly decomposed at 150 °C and completely decomposed at 170 °C. A solid sample of **5c** could be heated at 150 °C for at least three hours without noticeable decomposition, partly decomposed at 160 °C and completely decomposed at180 °C. A solid sample of **7a** could be heated at 140 °C for at least three hours without noticeable decomposition, partly decomposed at 150 °C and completely decomposed at170 °C. A solid sample of **9** could be heated at 130 °C for at least three hours without noticeable decomposition, partly decomposed at 140 °C and completely decomposed at 150 °C.

Table S2. Thermal decomposition data of complex **1**, **5a**, **5b**, **5c**, **7a**, **9** in solid state.

Temperature (°C)	80	100	120	130	140	150	160	170	180
complex **1**	●	●	●	▲	■	—	—	—	—
complex **5a**	●	●	●	●	▲	▲	■	—	—
complex **5b**	●	●	●	●	●	▲	▲	■	—
complex **5c**	●	●	●	●	●	●	▲	▲	■
complex **7a**	●	●	●	●	●	▲	▲	■	—
complex **9**	●	●	●	●	▲	■	—	—	—

All reactions were performed for 3 h in air. ● = Stable; ▲ = Partly decomposed; ■ = Completely decomposed.

6. Theoretical Calculations

Computational details.

Geometry optimizations were carried out using the Gaussian 16 package[5] with the B3LYP functional[6, 7] augmented with the D3 version of Grimme's empirical dispersion correction.[8-10] the basis set SDD were used to describe the Os atoms[11], whereas the standard 6-31G* basis set was used for the C, N, S, P, Cl and H atoms. Frequency calculations at the same level of theory were performed to identify the number of imaginary frequencies (zero for local minimum and one for transition states) and provide the thermal corrections of Gibbs free energy. Transition states were submitted to intrinsic reaction coordinate calculations to determine two corresponding minima. The single-point energy calculations were performed at the TPSS-D3(BJ)/def2-TZVP level of theory for solution-phase.[12] The gas-phase geometry was used for all the solution phase calculations. The SMD method was used with the dichloromethane solvent[13]. The corrections of Gibbs free energy calculations were added to the single-point energies to obtain the Gibbs free energy in solution. All the energies reported in the paper correspond to the reference state of 1 mol/L, 298K. Natural bond orbital (NBO) calculations were carried out using NBO 7.0 program[14] at the B3LYP-D3/def2-TZVP level of theory.

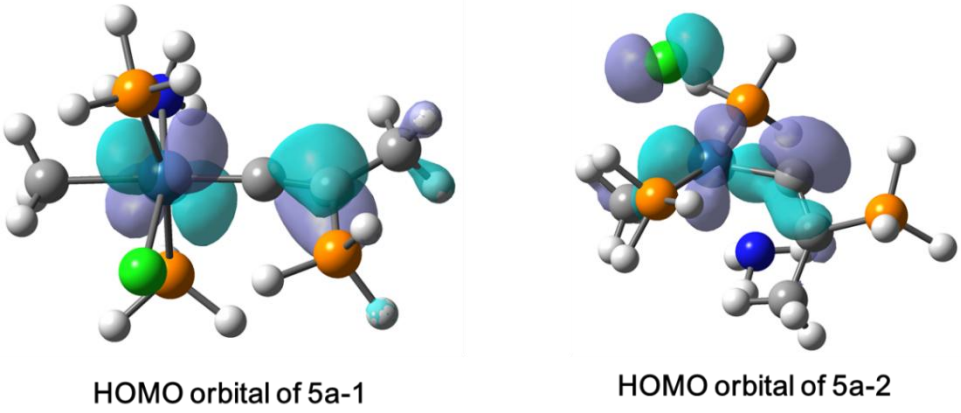


Figure S155. HOMO orbitals of linear (**5a-1**) and bent (**5a-2**) metal vinylidenes.

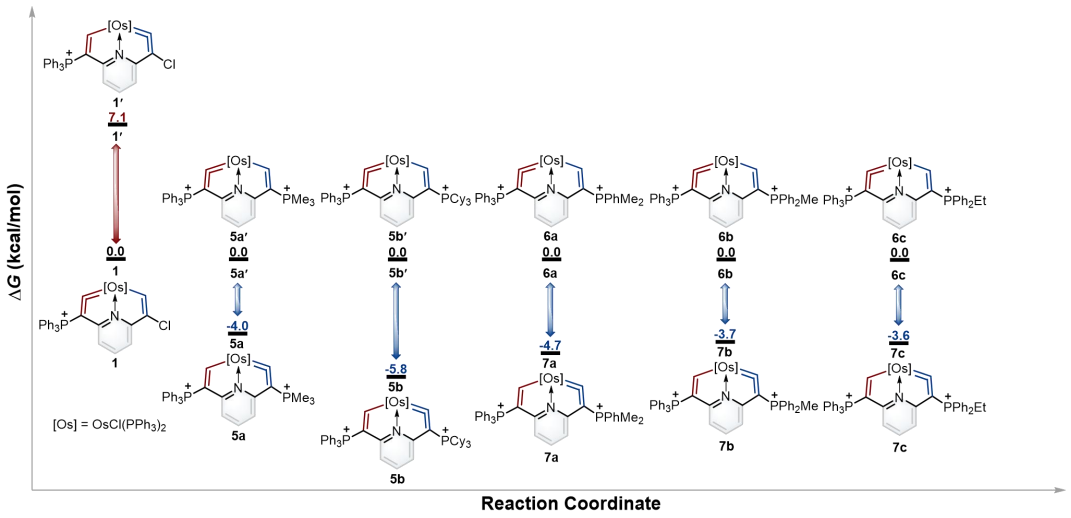
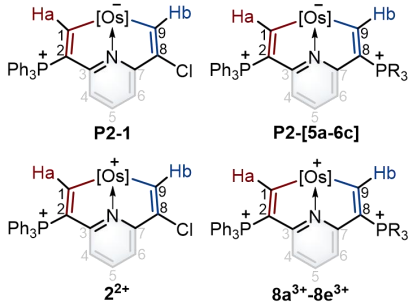


Figure S156. The relative energies between complexes **1'** and **1**, **5a'** and **5a**, **5b'** and **5b**, **6a** and **7a**, **6b** and **7b**, **6c** and **7c** at 298 K. Energies are given in kcal/mol



P2-5a: PR_3 = PMe_3
P2-5b: PR_3 = PCy_3
P2-6a: PR_3 = $PPhMe_2$
P2-6b: PR_3 = PPh_2Me
P2-6c: PR_3 = PPh_2Et

$8e^{3+}$: PR_3 = PMe_3
$8d^{3+}$: PR_3 = PCy_3
$8a^{3+}$: PR_3 = $PPhMe_2$
$8b^{3+}$: PR_3 = PPh_2Me
$8c^{3+}$: PR_3 = PPh_2Et

NBO Charges	Ha	Hb	NBO Charges	Ha	Hb
P2-1	**0.170**	0.186	**2^{2+}**	**0.246**	0.247
P2-5a	0.181	**0.155**	**$8e^{3+}$**	0.279	**0.246**
P2-5b	0.178	**0.160**	**$8d^{3+}$**	0.277	**0.259**
P2-6a	0.181	**0.165**	**$8a^{3+}$**	0.257	**0.243**
P2-6b	0.180	**0.165**	**$8b^{3+}$**	0.258	**0.248**
P2-6c	0.181	**0.154**	**$8c^{3+}$**	0.258	**0.226**

Figure S157. The calculated NBO charges of intermediates **P2-1**, **P2-5a-6c**, **2^{2+}**, and **$8a^{3+}$-$8e^{3+}$**.

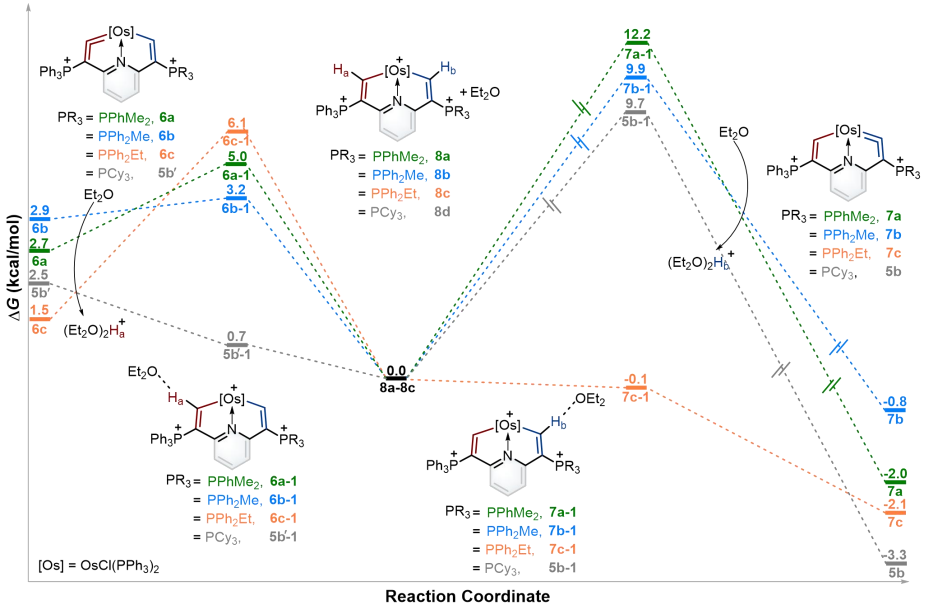
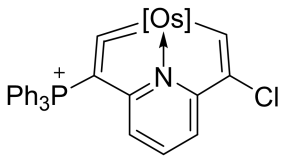


Figure S158. DFT-calculated the Gibbs energies for the formation of 7 and 5b at 298 K. Energies are given in kcal/mol.

7. Cartesian Coordinates



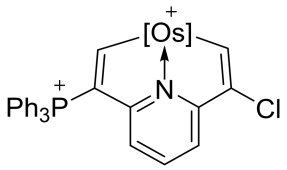
1

[Os] = $OsCl(PPh_3)_2$

E = -4521.992235 a.u.

Os	1.17270800	0.25081000	-0.49993200
Cl	3.76987100	1.23006100	3.29264300
Cl	1.99116900	0.41327300	-2.75685500
P	0.54816800	2.58462600	-0.54607700
P	1.99940800	-2.01308200	-0.35969100
P	-3.21376100	-0.79344400	0.12634900
N	0.44299500	0.09356200	1.49925400
C	-0.59355200	-0.28452000	-0.63266800
C	-1.49397500	-0.51477300	0.37721100
C	-0.84684400	-0.30797500	1.67846400
C	-1.35444000	-0.46043300	2.97031500
H	-2.36893400	-0.80503600	3.12129800
C	-0.53081900	-0.15944700	4.05539000
H	-0.91455100	-0.26546900	5.06556700
C	0.77740600	0.27102400	3.85519500
H	1.43329600	0.51022500	4.68169700
C	1.25039700	0.38298200	2.54719100
C	2.56688500	0.79277900	2.08744900
C	2.77352300	0.81193900	0.75995400
H	3.74580600	1.11971900	0.37995200
C	1.78284500	3.78933900	-1.16058500
C	1.44550000	5.15114500	-1.21977600
H	0.44985600	5.48016400	-0.94354700
C	2.38580800	6.09210300	-1.62992700
H	2.11368000	7.14247400	-1.67190700
C	3.67434200	5.68512300	-1.98601400
H	4.40687600	6.41978600	-2.30666900
C	4.01456800	4.33437700	-1.93333900
H	5.01089600	4.01027900	-2.21859600
C	3.07381100	3.38809100	-1.52356900
H	3.33589500	2.33995500	-1.51522600
C	0.19268000	3.17032100	1.14959700
C	1.20156300	3.76422000	1.91908600
H	2.16664600	3.98138700	1.47482200
C	0.97012200	4.07254300	3.26013000
H	1.76087500	4.52776900	3.84832500
C	-0.26702800	3.79351000	3.84259000
H	-0.44337700	4.03658800	4.88629400
C	-1.27622400	3.20074700	3.08033700
H	-2.24252100	2.97560300	3.52207200
C	-1.04456800	2.88486800	1.74431700
H	-1.82708600	2.41334500	1.16452300
C	-0.99204900	2.94297100	-1.47868300
C	-1.82371700	4.02289100	-1.14281100
H	-1.58496900	4.64948700	-0.2903600
C	-2.98059500	4.27767700	-1.87969100
H	-3.61417300	5.11928600	-1.61384600
C	-3.32251100	3.45209200	-2.95375100
H	-4.22796100	3.64486400	-3.52174900
C	-2.49479200	2.38196900	-3.29730900
H	-2.75556200	1.73486800	-4.12771700
C	-1.33273200	2.12840600	-2.56821400
H	-0.69070800	1.29850800	-2.83883700
C	3.66789300	-2.35399200	-1.02811600
C	4.55443800	-1.31673900	-1.33945300
H	4.23112100	-0.28869100	-1.26183000
C	5.84635500	-1.60711900	-1.77999800
H	6.52477000	-0.79545100	-2.02483300
C	6.25926000	-2.93201600	-1.91658500
H	7.26366200	-3.15614700	-2.26311300
C	5.37651100	-3.97178900	-1.61313800
H	5.69183800	-5.00507700	-1.72251100
C	4.08728000	-3.68592300	-1.17154700
H	3.40671800	-4.49907600	-0.94066000
C	2.12527800	-2.55781100	1.38357700
C	0.98591000	-2.94129000	2.10665300
H	0.02447300	-3.00618600	1.61333400
C	1.07365600	-3.22610200	3.46677900
H	0.18200400	-3.52278500	4.01100900
C	2.29806400	-3.11339700	4.12830100
H	2.36560300	-3.32848700	5.19052800
C	3.43349000	-2.71920200	3.42035900
H	4.38768100	-2.62023200	3.92833100
C	3.35027800	-2.44627500	2.05483800
H	4.23811800	-2.13865100	1.51371100
C	0.94120700	-3.25618700	-1.19608300
C	0.45482900	-2.93512900	-2.47359700
H	0.68580300	-1.96615100	-2.90609900
C	-0.30850800	-3.86104500	-3.18360600
H	-0.66814200	-3.61140300	-4.17769000
C	-0.60899000	-5.10585500	-2.62519200
H	-1.21132900	-5.82037900	-3.17806400
C	-0.11743200	-5.43371900	-1.36163800
H	-0.32801500	-6.40832900	-0.93050500
C	0.66437300	-4.51852800	-0.65265000
H	1.05666100	-4.79071500	0.32081600
C	-3.67439700	-2.43707900	0.72589700
C	-4.99778300	-2.77041600	1.05223100
H	-5.77869200	-2.01717900	1.02426300
C	-5.31005900	-4.08085200	1.40968400
H	-6.33152800	-4.33856800	1.67128000
C	-4.31408600	-5.06141800	1.42255200
H	-4.56430000	-6.08091300	1.69957500
C	-3.00376600	-4.73665100	1.06608300
H	-2.23168800	-5.49916600	1.05131000
C	-2.68118900	-3.42727800	0.71660400
H	-1.67083900	-3.17800600	0.41143400
C	-4.15184300	0.49342800	0.98555700
C	-4.14969700	1.77777800	0.41421400
H	-3.69341200	1.94963500	-0.55460300
C	-4.72402200	2.84291800	1.10200600
H	-4.71407000	3.83101600	0.65397300
C	-5.29438600	2.63954100	2.36158200
H	-5.73938800	3.47286600	2.89658700
C	-5.29122900	1.36633900	2.93413400
H	-5.73249700	1.20671100	3.91293400
C	-4.71886000	0.29240900	2.25153700
H	-4.71678300	-0.69279200	2.70467000
C	-3.60207500	-0.71574600	-1.63669200
C	-4.81953900	-0.17179900	-2.07005800
H	-5.51014800	0.26929100	-1.36009500
C	-5.13945400	-0.18580300	-3.42681200

H	-6.08017800	0.24068700	-3.76054200
C	-4.25367600	-0.74412900	-4.35032800
H	-4.50484900	-0.75124400	-5.40666000
C	-3.04900200	-1.30125400	-3.91509300
H	-2.36109000	-1.74296800	-4.62901000
C	-2.72334800	-1.29928500	-2.56084200
H	-1.79363900	-1.74540100	-2.23294200



2

[Os] = $OsCl(PPh_3)_2$

E= -4522.439699 a.u.

Os	-1.28885000	0.03013400	-0.41500400
Cl	-3.79539200	-0.14480200	3.49980300
Cl	-2.13083800	0.01651000	-2.57255600
P	-1.33550500	-2.42260400	-0.46889900
P	-1.37016300	2.46453500	-0.31634400
P	3.36708400	0.05768300	0.04350400
N	-0.37169200	-0.14136600	1.55374500
C	0.68451100	0.19480200	-0.61656900
C	1.60251200	0.06146500	0.37081700
C	0.98065900	-0.17166700	1.67066700
C	1.58179900	-0.38686500	2.91178400
H	2.65983100	-0.45419200	2.98934200
C	0.77498500	-0.51800100	4.04198400
H	1.22803900	-0.68366500	5.01388300
C	-0.60763600	-0.42499400	3.92403000
H	-1.26336700	-0.49840700	4.78218100
C	-1.15606900	-0.24369000	2.65623900
C	-2.55127000	-0.11071600	2.29284900
C	-2.75864000	0.07767000	0.98344700
H	-3.72995000	0.30449600	0.54261200
C	-2.85316100	-3.07491400	-1.24200700
C	-2.78908400	-4.08571200	-2.21060900
H	-1.83281700	-4.49371400	-2.51625300
C	-3.96111000	-4.57036100	-2.79274500
H	-3.90183700	-5.35149300	-3.54405400
C	-5.20081500	-4.05622100	-2.41340000
H	-6.10988100	-4.43611900	-2.86868300
C	-5.27085000	-3.04851100	-1.44825200
H	-6.23316800	-2.64470900	-1.14926400
C	-4.10382000	-2.55364700	-0.87173900
H	-4.17073900	-1.76708800	-0.12846400
C	-1.23583300	-3.14556200	1.20651900
C	-2.39900600	-3.45714100	1.92315100
H	-3.37231600	-3.36017700	1.45684900
C	-2.31151300	-3.91290100	3.23964100
H	-3.21958300	-4.15431100	3.78284600
C	-1.06620800	-4.06984800	3.84834400
H	-1.00153300	-4.43536900	4.86850300
C	0.09691300	-3.76452100	3.13691800
H	1.07140800	-3.88854400	3.59985000
C	0.01388700	-3.29688100	1.82876700
H	0.92389700	-3.05736600	1.29315900
C	0.04685800	-3.17764000	-1.39900500
C	0.51064700	-4.46440800	-1.07699000
H	0.07412100	-5.00836700	-0.24689100
C	1.53203000	-5.05005500	-1.82546800
H	1.87803700	-6.04801300	-1.57355900
C	2.09434000	-4.36431800	-2.90513200
H	2.88588700	-4.82525200	-3.48797600
C	1.61812100	-3.09747000	-3.24724100
H	2.03294600	-2.56797100	-4.09812800
C	0.59855600	-2.50722200	-2.50048700
H	0.21211500	-1.53949800	-2.79778100
C	-2.94478400	3.26502400	-0.76858400
C	-4.07063400	2.54084600	-1.18035400
H	-4.02430900	1.46526200	-1.29315200
C	-5.25618300	3.20861900	-1.49241200
H	-6.12258000	2.64120100	-1.81743800
C	-5.32328200	4.59812900	-1.39675700
H	-6.24572900	5.11545900	-1.64092700
C	-4.20003100	5.32676900	-0.99391000
H	-4.24792200	6.40890300	-0.92462800
C	-3.01494000	4.66642000	-0.68364200
H	-2.14560900	5.23845200	-0.37361500
C	-1.07350400	2.96404900	1.41271700
C	0.21945000	2.93882900	1.95768500
H	1.07199000	2.74755600	1.31718800
C	0.41269300	3.16320000	3.31871500
H	1.41749900	3.16110000	3.73089600
C	-0.68137600	3.39605200	4.15558000
H	-0.52895500	3.57040400	5.21610900
C	-1.97002700	3.41522200	3.62148500
H	-2.82508200	3.59919400	4.26404800
C	-2.16752300	3.20331700	2.25652500
H	-3.17291800	3.22414300	1.85078000
C	-0.12518800	3.30603100	-1.36443100
C	-0.08689200	2.95799900	-2.72533100
H	-0.74798100	2.18807800	-3.10838300
C	0.77237200	3.62468400	-3.59634900
H	0.77149000	3.36568900	-4.65084800
C	1.61791900	4.62974500	-3.11850700
H	2.28394900	5.15236000	-3.79844400
C	1.58576100	4.97734300	-1.76725800
H	2.22582100	5.77035100	-1.39284000
C	0.70848700	4.33036400	-0.89352600
H	0.66704200	4.64131800	0.14337700
C	4.21024200	1.47483000	0.77230100
C	5.41524600	1.90329800	0.18896200
H	5.80254800	1.41119400	-0.69724600
C	6.10945700	2.97501400	0.74682100
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C	5.60550400	3.62570300	1.87570900
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C	4.40715600	3.20155100	2.45457300
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C	3.70910500	2.12572200	1.91012000
H	2.78539000	1.79862000	2.36903300
C	4.01769000	-1.48098700	0.71457200
C	3.37782800	-2.68255700	0.36232100
H	2.53408000	-2.67895600	-0.32019400
C	3.84145500	-3.88503000	0.88799500
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C	4.93222200	-3.89251000	1.76394400
H	5.28913600	-4.83189300	2.17436200
C	5.56805900	-2.69824800	2.10944700
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C	5.11578900	-1.48633800	1.58543600
H	5.60899700	-0.55767700	1.85321100

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H	4.48378500	-1.84009000	-1.90211000
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H	4.86741800	-1.66210900	-4.33825700
C	4.03807000	0.32290500	-4.48654600
H	4.20837200	0.39911000	-5.55590200
C	3.46236900	1.39393600	-3.79563200
H	3.18403900	2.29932800	-4.32232000
C	3.25548100	1.31209900	-2.42143600
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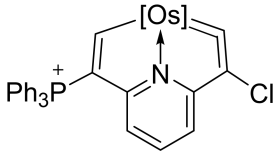

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N	0.27297200	0.04847300	-1.67111900
C	2.63404700	0.11513200	-1.15170600
C	2.42894500	0.14657300	-2.48765800
C	1.01965000	0.10296900	-2.81414100
C	0.39958700	0.09845900	-4.06918200
H	1.00953600	0.13914800	-4.96341900
C	-0.98753500	0.03298800	-4.12295600
H	-1.49144000	0.01758100	-5.08462300
C	-1.74308500	-0.01552800	-2.94770200
H	-2.82292300	-0.08186800	-2.99038900
C	-1.08302600	0.00553300	-1.71596700
C	-1.63864400	-0.03549400	-0.36281300
C	-0.69862600	-0.05324400	0.63660400
H	-1.02856100	-0.14204000	1.66932500
C	0.78832500	3.18142400	1.94660600
C	1.11777300	4.51355200	2.23938500
H	1.74910800	5.07763100	1.56117000
C	0.64319700	5.11830400	3.40221900
H	0.90774200	6.14902600	3.61825500
C	-0.16031500	4.39930100	4.28954600
H	-0.52224200	4.86940200	5.19913200
C	-0.48028600	3.07023900	4.01096700
H	-1.07626000	2.49301000	4.71229800
C	-0.00713300	2.46313700	2.84759300
H	-0.22354700	1.42193500	2.66304500
C	0.27502500	3.29195200	-0.87445700
C	-0.84467200	4.04325800	-0.49844100
H	-1.10604900	4.14271800	0.54888600
C	-1.60959600	4.69617000	-1.46691000
H	-2.45993700	5.29604400	-1.15860500
C	-1.28435100	4.57885600	-2.81796000
H	-1.87764300	5.09154500	-3.57002100
C	-0.17769800	3.81546700	-3.20129600
H	0.08892300	3.72509700	-4.24990900
C	0.60533700	3.18788100	-2.23602300
H	1.49234800	2.64177500	-2.53417600
C	2.99216000	3.17390400	0.07094900
C	3.15588900	4.39013100	-0.60731200
H	2.29553600	4.91037400	-1.01385000
C	4.43029500	4.93345000	-0.77539800
H	4.54786300	5.87191400	-1.30906300
C	5.54645800	4.27227500	-0.26269400
H	6.53785700	4.69463800	-0.39685300
C	5.38599400	3.06609000	0.42266800
H	6.25158100	2.54891900	0.82582200
C	4.11730400	2.51455500	0.58847300
H	3.99577800	1.57999900	1.12319000
C	0.89894400	-2.99233100	1.96222400
C	-0.45593500	-2.87931900	2.31191500
H	-1.17053600	-2.47474300	1.60248700
C	-0.89692400	-3.29516900	3.56561200
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C	1.35880400	-3.92775900	4.14997100
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C	-0.64611500	-4.89312800	-2.91052600
H	-1.10918100	-5.49279900	-3.68882000
C	-0.87900200	-5.18736700	-1.56649400
H	-1.51546600	-6.02420200	-1.29229500
C	-0.28460400	-4.41827500	-0.56243400
H	-0.46465900	-4.66296100	0.47791800
C	3.18404100	-3.01672600	0.17802800
C	4.29051000	-2.19633400	0.43572900
H	4.14175300	-1.15861300	0.70339100
C	5.58072300	-2.71991600	0.34943100
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C	-3.99690600	-3.62366900	-1.98347400
H	-2.35931900	-2.65767200	-0.97877100
C	-6.07320100	-2.38211200	-2.09657600
H	-6.06230700	-0.43895100	-1.17476700
C	-5.32888700	-3.52623800	-2.39144800
H	-3.41139800	-4.50328300	-2.22256800
H	-7.10620000	-2.30293800	-2.42031900
H	-5.78559100	-4.34026300	-2.94616900
C	-4.27606900	1.42448300	-0.39220000
C	-5.46437400	1.70462100	0.30564600
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H	-5.78536600	1.06215500	1.11918500
C	-4.63168500	3.37298600	-1.77406700
H	-2.92138400	2.08559400	-1.94813800

C	-5.81814600	3.64337800	-1.09186300
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C	-3.61707600	-0.42515400	1.74164100
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C	-4.28610500	-1.88125800	3.55041100
H	-4.37343700	-2.42974300	1.46710000
C	-3.45078800	0.34132700	4.02932400
H	-2.91367300	1.54118200	2.32796800
C	-3.94971800	-0.88778200	4.47096500
H	-4.68400900	-2.83131000	3.89338400
H	-3.19563000	1.11616000	4.74510900
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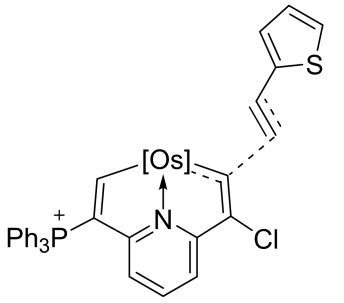

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P	1.25966000	-2.25414000	0.33620800
P	-3.57391700	-0.46697200	-0.68937100
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H	-0.86754900	-0.41149100	-1.73960800
C	-1.98312800	-0.15659100	0.05437900
C	-1.76408500	0.12678400	1.47070700
C	-2.69502600	0.27013500	2.49947400
H	-3.75456900	0.29072800	2.27574500
C	-2.23707700	0.38545000	3.81665400
H	-2.95228400	0.48901400	4.62706900
C	-0.87911800	0.35604400	4.08922600
H	-0.49167800	0.41326100	5.09798100
C	0.02263300	0.27478200	3.01965300
C	1.45915500	0.24077800	3.03987100
C	2.06057200	0.12612000	1.84494000
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C	4.75556600	-0.19207800	-1.46158200
C	5.20227000	-1.45818000	-1.83398400
H	4.98067900	-2.33667300	-1.24740000
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H	6.36197600	-2.37849000	-3.47089700
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C	2.81640200	3.35104600	-1.52096100
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H	1.55041800	5.25145600	1.01206100
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H	-0.79288900	4.12861000	5.37572600
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H	0.71249700	-3.59852300	-4.37115900
C	-0.73391200	-4.62038700	-3.13544100
H	-1.18294200	-5.16490700	-3.96126000

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H	-5.79159400	-5.50075900	0.79028300
C	-5.50090900	-4.07474000	-0.79845900
H	-6.01193000	-4.67626500	-1.54362900
C	-4.96340400	-2.84012900	-1.16071200
H	-5.05216300	-2.49443100	-2.18405700
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C	-4.01917600	0.44060700	-3.28954300
H	-4.61992100	1.22469300	-2.84334200
C	-3.86339400	0.38263900	-4.67504600
H	-4.35741200	1.11870700	-5.30166000
C	-3.07207500	-0.61198600	-5.25054400
H	-2.94629400	-0.64761000	-6.32831500
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H	-1.83002700	-2.34347100	-4.88448700
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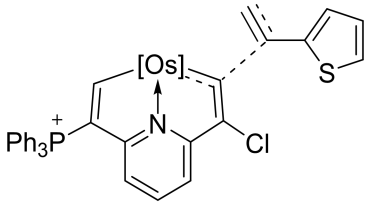
H	-2.13580100	-2.28928000	-2.44792200
C	-4.68663000	0.87412400	-0.22366600
C	-4.19011400	2.18723800	-0.28257900
H	-3.17202800	2.37429800	-0.60602100
C	-5.01753300	3.24923300	0.07184400
H	-4.63353200	4.26262100	0.01772400
C	-6.32842500	3.00550500	0.49254600
H	-6.96892800	3.83551600	0.77488700
C	-6.81941100	1.69933800	0.55106800
H	-7.83788000	1.51377100	0.87732000
C	-6.00195200	0.62768000	0.19031900
H	-6.37890700	-0.38891000	0.23756700



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P	-0.37579600	2.68202800	-0.33531800
P	3.68665000	-0.65195900	-0.08486400
N	0.11336900	0.05140700	1.60779400
C	1.07671700	-0.01984700	-0.73580700
H	1.45118800	-0.05203000	-1.75607100
C	1.99562000	-0.22412500	0.26778200
C	1.44621800	-0.22421000	1.62314600
C	2.09323900	-0.48419900	2.83316800
H	3.14822900	-0.72744700	2.84828800
C	1.35778700	-0.44660800	4.01892300
H	1.84932000	-0.65464500	4.96427600
C	-0.00079600	-0.15885500	3.99424800
H	-0.59553100	-0.13666500	4.89766200
C	-0.61235600	0.09214300	2.76065700
C	-1.99000300	0.46223400	2.50165500
C	-2.28308800	0.62510900	1.17593000
C	-4.11953100	1.19958700	0.91759600
C	-4.10497900	2.35283500	1.37741500
C	-2.93390200	-2.82060800	-0.87190500
C	-3.45961200	-2.39155800	-2.09791300
H	-3.07446600	-1.49469400	-2.56463000
C	-4.46989100	-3.12323700	-2.72168600
H	-4.86298800	-2.77957300	-3.67417800
C	-4.97235200	-4.28263700	-2.13254700
H	-5.75516200	-4.85262400	-2.62465200
C	-4.46213900	-4.70692700	-0.90514100
H	-4.84574100	-5.60811100	-0.43513900
C	-3.44310600	-3.98851100	-0.28147200
H	-3.03917600	-4.35225500	0.65558500
C	-0.22264700	-3.02905200	-1.32738100
C	0.01099900	-4.39158400	-1.08520000
H	-0.43494000	-4.87283900	-0.22152600
C	0.81296400	-5.13461900	-1.95057200
H	0.98459100	-6.18926000	-1.75374900
C	1.38181500	-4.53015100	-3.07541200
H	2.00686800	-5.11091300	-3.74749700
C	1.11575800	-3.18771300	-3.34654600
H	1.52779200	-2.71619300	-4.23329100
C	0.30999400	-2.44296000	-2.48266300
H	0.06347300	-1.41552300	-2.72195700
C	-1.15507700	-2.74099900	1.41828600
C	-2.21537700	-2.66007300	2.33396100
H	-3.17484000	-2.27608500	2.01023400
C	-2.04348900	-3.07360600	3.65399100
H	-2.87488300	-3.00513400	4.34876300
C	-0.80651500	-3.55875300	4.08148900
H	-0.67362900	-3.88051700	5.11017200
C	0.25994700	-3.61952600	3.18344200
H	1.23184300	-3.98135100	3.50651700
C	0.08862100	-3.20762200	1.86350100
H	0.92866200	-3.24795100	1.18377100
C	0.76610500	3.23389500	0.99237900
C	0.35530600	3.07914300	2.32706700
H	-0.62034300	2.65976700	2.54181100
C	1.18045700	3.48055200	3.37458900
H	0.84752900	3.35044200	4.39974600
C	2.42268600	4.06128900	3.10358900
H	3.05668600	4.39548900	3.92003300
C	2.83711200	4.21994400	1.78147300
H	3.79963100	4.67080700	1.56020200
C	2.02171300	3.79460800	0.73041600
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H	-4.74607600	4.41941100	-1.79458500
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H	-4.87445400	6.21571300	-0.07672000
C	-2.97602800	5.70724800	0.80860400
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H	0.64518100	1.44385500	-2.86978200
C	1.38933600	3.06017400	-4.06905200
H	1.67553700	2.40662900	-4.88751400
C	1.56413300	4.43867600	-4.17625100
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C	1.15097700	5.27176700	-3.13268000
H	1.27037100	6.34812300	-3.21247300
C	0.56613600	4.72427800	-1.99411800
H	0.22682300	5.38093800	-1.19928300
C	4.90966600	0.45643100	0.65349200
C	4.55525300	1.40538500	1.61913700
H	3.52384600	1.52696500	1.92302400
C	5.54490000	2.20814700	2.18867700
H	5.26732700	2.93913800	2.94034700
C	6.87504400	2.07574800	1.79196200
H	7.63995300	2.70294400	2.23964100
C	7.22640700	1.14329500	0.81051900
H	8.25919800	1.05004000	0.48984800
C	6.24828900	0.33510500	0.23913800
H	6.51948700	-0.38355900	-0.52873600
C	3.95223500	-0.56715800	-1.87045800
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H	4.26857600	-2.68360300	-2.17629900
C	4.42788900	-1.57629200	-4.01348700
H	4.63886200	-2.45919400	-4.60875000
C	4.36685000	-0.32029700	-4.61756700
H	4.53070800	-0.22470400	-5.68660500
C	4.10181800	0.81716600	-3.84882600
H	4.05268300	1.79600200	-4.31318800
C	3.89641900	0.69916900	-2.47780400
H	3.68592400	1.58391600	-1.88502200
C	4.02222200	-2.32877300	0.51081200
C	3.18602800	-3.36392700	0.06230100
H	2.38987200	-3.15973800	-0.64505400
C	3.37349700	-4.65923200	0.53829200
H	2.72425800	-5.45279400	0.18470400
C	4.38150100	-4.92502000	1.46889500
H	4.52056700	-5.93457000	1.84346300
C	5.20984400	-3.89526300	1.91851000
H	5.99209300	-4.10087800	2.64249500
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S	-5.55875000	0.31335800	-1.27091200
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C	-6.44080200	-1.16441400	-1.10055600
H	-6.67460600	-2.69908200	0.40748300
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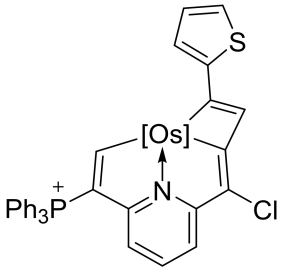

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S	5.82365100	0.67699300	-0.89464800
P	0.86141100	2.43289900	-0.10843100
P	1.17118000	-2.42421400	0.13587000
P	-3.73231900	-0.13132000	-0.47383500
N	-0.32921400	0.02840200	1.65881900
C	-0.97869000	-0.16030600	-0.75431200
H	-1.17235300	-0.25392700	-1.81589700
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C	-1.68503300	0.01451400	1.50273200
C	-2.53657900	0.10665000	2.60108700
H	-3.60900000	0.13623500	2.45547800
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C	-0.61983800	0.13714500	4.05270600
H	-0.15690300	0.18026600	5.02985500
C	0.20630100	0.09432600	2.91837500
C	1.62675300	0.15498500	2.89429100
C	2.17996800	0.21181600	1.66117500
C	3.46699900	0.32252800	1.10274700
H	4.42109500	0.42896300	1.62129300
C	3.21035100	0.09760200	-0.22575900
C	4.23962000	-0.05186700	-1.21471700
C	4.30296200	-0.80731300	-2.37172800
H	3.45756700	-1.36516700	-2.74092300
C	5.58294400	-0.80871700	-2.98511500
H	5.81198200	-1.35055800	-3.89562800
C	6.50048600	-0.04503800	-2.30904100
H	7.53112100	0.14811200	-2.57602500
C	2.33148300	3.36680500	-0.68441600
C	3.03347300	2.88319600	-1.79658100
H	2.75182200	1.94065800	-2.24734300
C	4.09585900	3.61437900	-2.32648100
H	4.64170100	3.21749200	-3.17687700
C	4.46153500	4.83510000	-1.75967200
H	5.29393900	5.39987000	-2.16904300
C	3.74923900	5.33321500	-0.66681200
H	4.02067600	6.28866000	-0.22739700
C	2.68356000	4.60909400	-0.13461100
H	2.13340600	5.01385700	0.70713300
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H	-0.55812700	5.01680900	0.10976300
C	-1.83845700	5.18006800	-1.60376900
H	-2.18971800	6.17119400	-1.33061800
C	-2.29376900	4.57215100	-2.77705800
H	-3.00673500	5.08622300	-3.41517400
C	-1.80577500	3.31625800	-3.13554500
H	-2.12851200	2.84567700	-4.05816000
C	-0.89044700	2.65293500	-2.31513000
H	-0.49114400	1.69398100	-2.61901900
C	0.52015900	3.05057500	1.58324100
C	1.57040600	3.24103700	2.49291500
H	2.59676800	3.10220400	2.17230200

C	1.30494000	3.59446800	3.81534200
H	2.12983500	3.73521300	4.50633600
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H	-2.09343700	3.64152100	3.68810900
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C	1.52445200	-3.17697100	2.88025700
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C	1.03450400	-3.45154300	4.15910300
H	1.73383200	-3.61636300	4.97285600
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C	-0.73749700	-3.03003400	2.05820500
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H	6.05412400	-2.93644400	0.93740800
C	3.93613600	-2.78214500	0.63006600
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C	-0.30541100	-3.07826800	-2.19145000
H	-0.02672900	-2.09666200	-2.55223800
C	-1.02712400	-3.94588900	-3.01559700
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C	-0.94695700	-5.64944100	-1.30974600
H	-1.18681400	-6.65029700	-0.96322900
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H	0.11947500	-5.14099200	0.48092000
C	-4.65791400	-1.60313300	0.03149100
C	-4.21906400	-2.40751100	1.09144900
H	-3.32328900	-2.14492700	1.63739700
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C	-6.55083900	-3.07493600	-0.30205600
H	-7.45353900	-3.33654200	-0.84507500
C	-5.82732700	-1.94251500	-0.66939900
H	-6.16056900	-1.33411300	-1.50443100
C	-3.77017100	-0.11920900	-2.27785200
C	-4.23618600	0.99305100	-2.98836200
H	-4.56777100	1.88082400	-2.46328400
C	-4.26827400	0.95518800	-4.38294400
H	-4.63579100	1.81506000	-4.93428600
C	-3.82963800	-0.18014900	-5.06423800
H	-3.85306000	-0.20390400	-6.14935000
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H	-3.03384000	-2.17764700	-4.88283400
C	-3.34359400	-1.27036700	-2.96174100
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C	-6.39016500	2.44261700	1.29436200
H	-7.35155200	2.39193100	1.79579600
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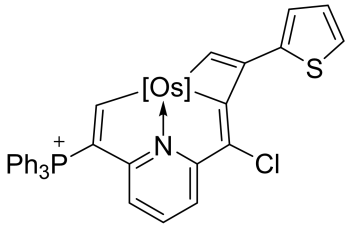

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P	-0.92491800	2.51819600	-0.42789500
P	3.86066000	-0.09343500	0.13936800
N	0.05479900	0.06426100	1.44237000
C	1.25680100	0.09632500	-0.77664700
H	1.69630600	0.11296400	-1.76742100
C	2.09240700	0.03959400	0.30859800
C	1.41247000	-0.00351700	1.59493700
C	1.98126400	-0.09056500	2.86323400
H	3.05449100	-0.18695300	2.97085400
C	1.15523500	-0.05090500	3.98938600
H	1.58976500	-0.10650600	4.98247200
C	-0.21494400	0.05715800	3.83414600
H	-0.88542300	0.09061500	4.68231000
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C	-2.43365900	0.03086800	0.88526900
C	-3.53660100	-0.08554900	-0.03159800
C	-2.82233500	0.03364300	-1.18440100
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H	-2.13548700	-1.84858900	-3.00611500
C	-3.67213500	-3.32917900	-3.27446700
H	-3.95947800	-2.95251700	-4.25179800
C	-4.32431600	-4.43659100	-2.72770400
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H	2.79059100	-3.02932900	-3.75506700
C	1.24916200	-2.73045700	-2.29026900
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C	-2.12679000	-2.96380000	1.96753800
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C	-2.15195600	-3.26878800	3.32797500
H	-3.10334100	-3.30164000	3.84886600
C	-0.96246400	-3.50884800	4.01708100
H	-0.98527400	-3.74295000	5.07725200
C	0.25560300	-3.43515400	3.34019700
H	1.18968400	-3.60181200	3.86878900
C	0.28256100	-3.13574100	1.97995600
H	1.23678400	-3.06848600	1.47374400
C	-0.72927800	3.10420800	1.30689200
C	-1.79105400	3.40613900	2.16515800
H	-2.80943200	3.41120800	1.80300800
C	-1.55110500	3.71742800	3.50553300
H	-2.38918100	3.94621000	4.15651100
C	-0.25013000	3.73349700	4.00436600
H	-0.06754100	3.97328100	5.04754900
C	0.81792600	3.44938400	3.15006400
H	1.83629700	3.46762100	3.52889600
C	0.57935500	3.13703000	1.81567500
H	1.41021800	2.92903100	1.15141500
C	-2.47383700	3.22200900	-1.10523300
C	-2.44352100	3.91801700	-2.32333400
H	-1.49936100	4.10820400	-2.81942600
C	-3.62743900	4.36502500	-2.91059900
H	-3.58582800	4.90168200	-3.85370900
C	-4.85520600	4.12453400	-2.29371300
H	-5.77484700	4.47275400	-2.75436300
C	-4.89663200	3.42813500	-1.08489200
H	-5.84402400	3.21777800	-0.59832700
C	-3.71759000	2.97336200	-0.50048000
H	-3.78183900	2.40427000	0.41515400
C	0.37179600	3.52266500	-1.26406900
C	1.11431800	3.02599100	-2.34090400
H	0.93614200	2.02042500	-2.69711600
C	2.04035100	3.84536100	-2.99237000
H	2.58985900	3.45532400	-3.84430900
C	2.24094700	5.15943700	-2.57231000
H	2.96140000	5.79309000	-3.08130400
C	1.49556700	5.66407300	-1.50363300
H	1.63399800	6.69056500	-1.17742500
C	0.56255100	4.85541400	-0.85940500
H	-0.01904700	5.26039300	-0.03822800
C	4.76236900	1.32091600	0.81989700
C	4.14082400	2.22675100	1.68897700
H	3.11099700	2.07708000	1.98291500
C	4.85451900	3.32005400	2.17807100
H	4.36632800	4.02644900	2.84233100
C	6.18697800	3.50865700	1.80864400
H	6.73987300	4.36181200	2.18944400
C	6.81040000	2.60537800	0.94313800
H	7.84468100	2.75578200	0.65022100
C	6.10159100	1.51592400	0.44227600
H	6.58058400	0.82914300	-0.24896700
C	4.30056200	-0.16337900	-1.60989600
C	4.81265400	-1.32973400	-2.18984300
H	4.94659800	-2.22603200	-1.59621100
C	5.14883100	-1.33524200	-3.54423400
H	5.55201700	-2.23785700	-3.99272300
C	4.96719100	-0.18835900	-4.31692800
H	5.22684100	-0.19805000	-5.37099400
C	4.45896000	0.97720000	-3.73535300
H	4.32555700	1.87153000	-4.33535000
C	4.13216400	0.99828400	-2.38303900
H	3.74465900	1.90753300	-1.93505200
C	4.41255100	-1.60573500	0.96309500
C	3.73462200	-2.79823200	0.65966700
H	2.92775100	-2.80167400	-0.06532800
C	4.10342400	-3.98132200	1.29470600
H	3.57827200	-4.89913300	1.05234500
C	5.13668500	-3.97795800	2.23614500
H	5.41759600	-4.90050800	2.73494600
C	5.80955200	-2.79228000	2.53727900
H	6.61184000	-2.79115200	3.26844900
C	5.45287200	-1.60263200	1.90101900
H	5.97326900	-0.68091000	2.13874200
H	-3.19056300	0.09294500	-2.20220800
C	-4.97248500	-0.28865200	0.11698800
C	-5.75551500	-1.03422800	-0.73823400
S	-5.96742700	0.51142700	1.31704500
C	-7.14572800	-0.96419600	-0.43737100
H	-5.33102700	-1.62224400	-1.54435100
C	-7.41437200	-0.16201900	0.63914900
H	-7.91163300	-1.49611700	-0.99043400
H	-8.37224100	0.05145600	1.09391800

Et_2O:
E = -233.802087 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

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E = -468.054149

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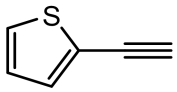
O	0.97909800	-0.28974300	-0.25595700
C	1.56552100	-0.54680500	1.06150300
H	2.13199900	0.33837700	1.36494800
H	0.70826500	-0.65509200	1.73088800
C	2.41383400	-1.80232800	1.03982900
H	3.26801700	-1.70570200	0.36311000
H	2.80644600	-1.98821200	2.04488800
H	1.82057000	-2.66898100	0.73429900
C	1.81985800	0.41537500	-1.22955700
H	2.82375900	-0.00348400	-1.13694400

H	1.41718700	0.12263300	-2.20154500
C	1.79427800	1.91893700	-1.03011700
H	2.43171700	2.39089600	-1.78481100
H	0.78181400	2.31686000	-1.14806800
H	2.17696700	2.20866000	-0.04645600
O	-1.34857600	0.30999800	-0.38448200
C	-2.04277400	-0.76917400	-1.10902700
H	-3.06044200	-0.40847100	-1.27399000
H	-1.52777900	-0.81096100	-2.07072400
C	-1.99710400	-2.09619500	-0.37672600
H	-2.53014000	-2.06221300	0.57778600
H	-2.48129100	-2.85759800	-0.99674400
H	-0.96432800	-2.41476000	-0.20233600
C	-1.99746000	0.80460300	0.83729300
H	-1.98630100	0.00777700	1.58668300
H	-3.03187400	1.01625100	0.55696300
C	-1.27464600	2.05009800	1.30478800
H	-1.78227300	2.44177200	2.19167900
H	-0.23674200	1.84102900	1.58260500
H	-1.28738100	2.82393700	0.53254800



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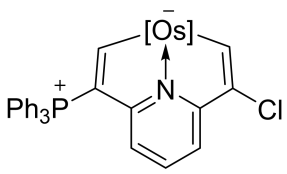
C	-0.29006200	1.37394600	0.00001000
C	0.49050200	0.23661100	-0.00009500
S	-0.51645100	-1.20295100	0.00021300
H	-2.92748800	-0.72941600	-0.00027600
H	-2.45194200	1.86136500	-0.00005400
H	0.13709200	2.36960800	0.00000900
C	1.89706700	0.13663200	-0.00018600
C	3.10347300	0.03536700	-0.00012200
H	4.16648100	-0.04331500	0.00037100



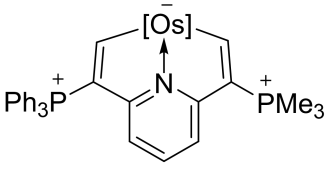
P2-1

[Os] = $OsCl(PPh_3)_2$

E = -4521.819890 a.u.

Os	-1.22411500	0.04829700	-0.39384500
Cl	-3.82945800	-0.12916400	3.50521800
Cl	-1.97927200	0.06666500	-2.81952800
P	-1.34823600	-2.30954800	-0.51801300
P	-1.39932300	2.39416500	-0.35358400
P	3.33752400	0.01280400	0.08632000
N	-0.41831800	-0.05287600	1.46401400
C	0.74029200	0.13942600	-0.84220700
C	1.59349400	0.06950200	0.27420500
C	0.94352000	-0.08143700	1.58065600
C	1.51983700	-0.23935300	2.84671500
H	2.59641500	-0.31038000	2.95519200
C	0.69060600	-0.31516800	3.96723500
H	1.13086700	-0.43264300	4.95332500
C	-0.69229600	-0.25202200	3.83082200
H	-1.35062800	-0.31228300	4.68727800
C	-1.24149100	-0.13238700	2.55007400
C	-2.64219500	-0.08420200	2.16101100
C	-2.98598100	-0.00541800	0.85256300
H	-4.06034600	0.03760000	0.65089500
C	-2.89075800	-3.06435600	-1.17168500
C	-2.99378400	-4.45208600	-1.34450900
H	-2.14174200	-5.09101900	-1.13634600
C	-4.18775400	-5.02115900	-1.78215400
H	-4.25759900	-6.09776700	-1.91202100
C	-5.29103000	-4.20763500	-2.05311000
H	-6.22227300	-4.65120000	-2.39515800
C	-5.19197800	-2.82629400	-1.88839700
H	-6.04316700	-2.18779000	-2.10760800
C	-3.99633000	-2.25379600	-1.45135200
H	-3.89986700	-1.18260900	-1.34188900
C	-1.21045800	-3.07754100	1.14513400
C	-2.36459200	-3.34339000	1.89317300
H	-3.34158600	-3.20917800	1.44241100
C	-2.26546800	-3.75979200	3.22085300
H	-3.17039800	-3.94844000	3.79082900
C	-1.01385500	-3.91703500	3.81715900
H	-0.93950300	-4.23740500	4.85277200
C	0.14113900	-3.64692000	3.08124500
H	1.12179300	-3.74651800	3.53830000
C	0.04185600	-3.22107100	1.75937500
H	0.94371400	-2.98599600	1.20949200
C	-0.01697100	-3.15507300	-1.48210100
C	0.48214000	-4.42429200	-1.15283200
H	0.08597300	-4.95544600	-0.29382000
C	1.51125800	-4.99818000	-1.90260800
H	1.88783300	-5.98268700	-1.63649300
C	2.05499200	-4.30958700	-2.98898000
H	2.86171400	-4.75328600	-3.56653400
C	1.54853500	-3.05476200	-3.33510400
H	1.95826000	-2.51473600	-4.18362500
C	0.51701700	-2.48113300	-2.59078800
H	0.10755300	-1.51429900	-2.86440600
C	-3.00458200	3.16375400	-0.80201900
C	-4.04585700	2.36919000	-1.29278700
H	-3.87333400	1.31034400	-1.43527000
C	-5.27324500	2.94994900	-1.61848700
H	-6.07565100	2.32715300	-2.00398800
C	-5.46719500	4.32140100	-1.45562800
H	-6.42404300	4.77070800	-1.70774400
C	-4.42708100	5.12006000	-0.97138300
H	-4.57279200	6.18954400	-0.84567500
C	-3.20035900	4.54429200	-0.64953900
H	-2.39508900	5.16768700	-0.27233100
C	-1.12479600	2.99458800	1.35793500
C	0.17682500	3.11388900	1.86638100
H	1.02129800	3.01191400	1.19406800
C	0.38946000	3.35319700	3.22219900
H	1.40285300	3.44623700	3.60438700
C	-0.69558500	3.45889500	4.09451400
H	-0.52938600	3.63223200	5.15403100
C	-1.99333300	3.33316300	3.59924200
H	-2.84407200	3.39661000	4.27100400
C	-2.20794700	3.10201600	2.24040300
H	-3.21941400	2.98448600	1.86874600
C	-0.19722200	3.35373800	-1.37402300
C	0.11871200	2.84697500	-2.64412300
H	-0.33562200	1.91652300	-2.97156700

C	0.99232300	3.54227700	-3.47980500
H	1.21380900	3.14463200	-4.46636600
C	1.58104700	4.73516100	-3.05343900
H	2.26718200	5.27196300	-3.70376500
C	1.27284600	5.24289800	-1.79001800
H	1.71976500	6.17393400	-1.45142600
C	0.37823900	4.56359700	-0.96052200
H	0.14007500	4.97323200	0.01526700
C	4.26857100	1.34352000	0.90797900
C	5.60006700	1.58787000	0.53501500
H	6.07045700	0.97912200	-0.23145100
C	6.31216800	2.62461200	1.13445400
H	7.34064200	2.81301500	0.84119300
C	5.69884100	3.42716100	2.10026200
H	6.25324700	4.23967700	2.56069700
C	4.37366700	3.19031000	2.46712200
H	3.89229000	3.81790900	3.21117000
C	3.65658800	2.15074400	1.87455800
H	2.63040700	1.96440100	2.16230800
C	3.98962200	-1.56716000	0.70458400
C	3.33826800	-2.73642700	0.27952700
H	2.50564900	-2.67676300	-0.41403800
C	3.75422200	-3.97559600	0.76016600
H	3.24302200	-4.87153000	0.42451100
C	4.80834900	-4.05388600	1.67397500
H	5.12335700	-5.02025500	2.05684900
C	5.45375600	-2.89192400	2.10052000
H	6.26968900	-2.95196800	2.81469700
C	5.04930900	-1.64715000	1.61612300
H	5.54665800	-0.74452400	1.95464700
C	3.76274600	0.17419000	-1.66632000
C	4.23397700	-0.91053800	-2.41361800
H	4.36330300	-1.88122800	-1.95002700
C	4.52462000	-0.74299100	-3.76826100
H	4.88695700	-1.58719700	-4.34718400
C	4.34707400	0.50069500	-4.37436800
H	4.57202800	0.62705200	-5.42937200
C	3.87724700	1.58438400	-3.62716600
H	3.72580200	2.55128500	-4.09456800
C	3.58471100	1.42723500	-2.27581800
H	3.20221700	2.26828900	-1.70644100
H	1.23679500	0.25872200	-1.81052400



P2-5a

[Os] = $OsCl(PPh_3)_2$

E = -4522.606889 a.u.

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P	1.23236200	-2.34056700	-0.67044500
P	-3.52306200	-0.11319200	0.45307700
N	0.38589800	0.11160900	1.34662200
C	-1.04645700	-0.15177500	-0.80296500
C	-1.75244400	-0.09368900	0.39636800
C	-0.96114600	0.06793700	1.61610600
C	-1.39965700	0.14582100	2.94333400
H	-2.45720900	0.11119700	3.17383200
C	-0.46169700	0.27433400	3.96694000
H	-0.79418300	0.34466900	4.99796500
C	0.89879300	0.31827200	3.67152300
H	1.61774100	0.42730400	4.47466300
C	1.31854400	0.22808900	2.33877100
C	2.67749400	0.21581300	1.79489500
C	2.80993400	0.13482400	0.41022400
H	3.84741300	0.09985400	0.05441400
C	2.32938900	3.13153500	-1.79426900
C	2.27344700	4.48124600	-2.17034200
H	1.38771300	5.07010100	-1.95462800
C	3.35115100	5.07309600	-2.82680600
H	3.29824700	6.11843100	-3.11682100
C	4.49203100	4.32101700	-3.11682700
H	5.32873900	4.78138500	-3.63436000
C	4.54806600	2.97474500	-2.75395100
H	5.42339800	2.38036600	-3.00048000
C	3.47045100	2.37916900	-2.09770200
H	3.48445400	1.32672900	-1.84960100
C	1.08006900	3.23053100	0.78272000
C	2.26852400	3.83591100	1.20953600
H	3.11752600	3.88683900	0.53603200
C	2.35810900	4.39393900	2.48718800
H	3.27719400	4.88576100	2.79565200
C	1.26863200	4.34175700	3.35830600
H	1.33957300	4.78160300	4.34914200
C	0.08093200	3.73649800	2.94059600
H	-0.77663200	3.68866000	3.60536200
C	-0.01088000	3.18816400	1.66417800
H	-0.93825900	2.72495400	1.35274200
C	-0.55633300	3.11242500	-1.58085300
C	-1.09834400	4.33204900	-1.14881800
H	-0.62381600	4.88359400	-0.34415400
C	-2.26093800	4.83552100	-1.73736700
H	-2.67163600	5.78191500	-1.39614200
C	-2.88878600	4.12803500	-2.76408900
H	-3.79433900	4.51925600	-3.21936100
C	-2.33997800	2.92432000	-3.21294400
H	-2.81726500	2.37314800	-4.01698900
C	-1.18011300	2.41724600	-2.62813700
H	-0.74179600	1.49009100	-2.98335700
C	2.57794600	-3.00602300	-1.71788600
C	3.67651500	-2.20072400	-2.04113800
H	3.66766900	-1.15865600	-1.75197700
C	4.74060700	-2.72802600	-2.77224300
H	5.58198100	-2.09265100	-3.03383300
C	4.71201600	-4.05880300	-3.19259800
H	5.53718100	-4.46525100	-3.77023300
C	3.61388200	-4.86399700	-2.88203000
H	3.58317100	-5.89739900	-3.21476400
C	2.55004000	-4.34036300	-2.14826600
H	1.69757800	-4.96879100	-1.90953600
C	1.58471500	-3.12338200	0.96502300
C	0.70628500	-2.90263700	2.03735000
H	-0.17117300	-2.28766700	1.89137800
C	0.94884700	-3.45598100	3.29326400
H	0.25106500	-3.26801600	4.10438300
C	2.08475500	-4.24035300	3.50392700
H	2.27410100	-4.67996900	4.47905600
C	2.97505700	-4.45636800	2.45015700

H	3.85834100	-5.07116600	2.60084000		0.05021300	2.60257900
C	2.72954600	-3.90116400	1.19130700			
H	3.42357100	-4.08844800	0.38021700			
C	-0.24266100	-3.25035000	-1.29209400			
C	-0.63359400	-2.98177600	-2.61588300			
H	-0.06772400	-2.26565500	-3.20495900			
C	-1.74079800	-3.62682200	-3.16126900			
H	-2.02067200	-3.42674200	-4.19159200			
C	-2.49013600	-4.52157400	-2.38975900			
H	-3.35446500	-5.02224800	-2.81734700			
C	-2.11984300	-4.77156900	-1.06855900			
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C	-5.56784000	-1.79931600	1.34695300	P	-0.18357300	-2.63987700	-0.88274000
H	-6.25526900	-1.07173100	0.92514200	P	-4.11694400	0.29727900	1.34853200
C	-6.06032900	-2.96456100	1.92952800	N	-0.13328700	0.04515600	0.96297900
H	-7.13158100	-3.13384600	1.97578700	C	-2.20906600	-0.23348100	-0.58751100
C	-5.17586900	-3.92000900	2.43999200	C	-2.47574400	-0.01493200	0.76265300
H	-5.56384500	-4.82990700	2.88778600	C	-1.32157700	0.15190800	1.64782600
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H	-3.10942800	-4.46085200	2.74428000	H	-2.23112500	0.48612400	3.57966600
C	-3.29896800	-2.54593800	1.78548100	C	-0.07849400	0.55840200	3.66895700
H	-2.23126400	-2.39276100	1.70021300	H	-0.05040600	0.76428400	4.73459500
C	-4.08841800	1.38902500	1.29447700	C	1.11275000	0.45004400	2.95590000
C	-3.54078600	2.60266600	0.84552000	H	2.05275000	0.57239200	3.47356200
H	-2.84767100	2.61662800	0.01065200	C	1.08618000	0.17762800	1.58017500
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H	-3.45475000	4.72606700	1.12517200	C	1.83117900	-0.18654000	-0.69478700
C	-4.75964200	3.78050100	2.56789000	H	2.64588000	-0.24449000	-1.41979100
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C	-4.96842100	1.37605000	2.38323400	C	1.58257200	2.68061600	-5.33478900
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C	-4.20288500	-0.15344200	-1.21874000	C	2.94350700	2.63659700	-5.03481900
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C	-5.30485700	0.88035000	-3.10213800	H	4.41639400	2.42302900	-3.46971900
H	-5.78225700	1.74563100	-3.55149100	C	2.40895400	2.29774300	-2.70398000
C	-5.17952700	-0.30681400	-3.82441800	H	2.72988400	2.15727100	-1.67717400
H	-5.56011400	-0.36594600	-4.83964500	C	0.30835100	3.29349500	-0.39969400
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H	-4.46725300	-2.34596400	-3.80164200	H	1.49153300	4.52528300	-1.72244900
C	-4.08544500	-1.35276700	-1.93994600	C	1.26355600	5.44902100	0.20245300
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H	4.93071400	-1.22099100	4.66222500	C	-0.24781400	3.21463500	0.88456400
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C	4.23718200	1.69779900	3.88933100	C	-1.77496000	2.71873500	-2.22791400
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H	4.39034600	2.55079800	3.22411200	H	-1.45704500	4.71949400	-1.46997100
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H	5.61392500	-0.85411300	1.31970800	C	-4.32275300	3.65523700	-2.95114100
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			H	C	-3.94859400	2.34168600	-3.24063900
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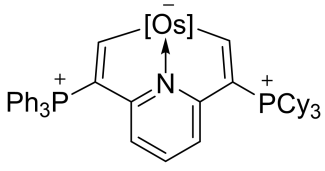

P2-5c

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H	3.33285200	-3.20507100	-4.33612700
C	2.26626500	-5.04527700	-3.98857700
H	2.84933700	-5.61328800	-4.70783500
C	1.22811700	-5.66295700	-3.28739300
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C	0.47198700	-4.93003500	-2.37397400
H	-0.33730100	-5.41183500	-1.83402100
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C	0.37333700	-3.46870800	3.11666100
H	-0.09352400	-3.15674500	4.04673100
C	1.42031900	-4.39341100	3.12527600
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H	2.84795200	-5.46842500	1.92065900
C	1.57025900	-4.22937400	0.71247400
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C	-1.86072900	-3.39968600	-0.99060000
C	-2.58786800	-3.14652200	-2.16711300
H	-2.14453900	-2.53131400	-2.94507000
C	-3.86636300	-3.67492500	-2.32660900
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C	-5.53322800	-2.84224600	4.39862300
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C	4.06482300	4.28170700	2.63813900
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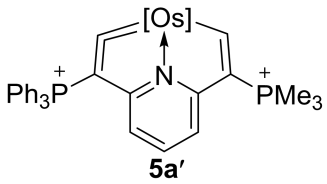

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C	1.66281100	0.00435200	0.58188500
C	0.82875600	-0.16354600	1.76971300
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H	0.46366700	-0.56797300	5.11645400
C	-1.14727000	-0.40226400	3.70068400
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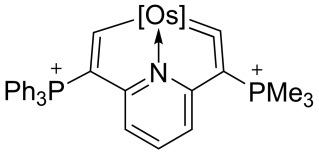
C	3.33711000	2.36615700	2.18551300
H	2.48549000	1.89791900	2.66488100
C	4.10376300	-1.22752700	1.51416200
C	3.67867000	-2.53201800	1.20666500
H	3.00656500	-2.70980300	0.37260300
C	4.14167600	-3.60012400	1.96891500
H	3.82128100	-4.60910900	1.72882000
C	5.01995300	-3.37168000	3.03432000
H	5.37857500	-4.20711700	3.62753100
C	5.44453300	-2.07578600	3.33377600
H	6.13237400	-1.90385200	4.15543700
C	4.99019500	-0.99644000	2.57305400
H	5.31965800	0.01225700	2.80133900
C	3.98416200	-0.04693100	-1.18136900
C	5.05950100	-0.89145000	-1.49083300
H	5.51686400	-1.50458700	-0.72220800
C	5.54062100	-0.93966600	-2.79917400
H	6.37699700	-1.58775000	-3.04071400
C	4.94664800	-0.15836600	-3.79249100

H	5.32404000	-0.19839900	-4.80973100
C	3.87129700	0.67905900	-3.48065000
H	3.41013200	1.29033000	-4.24890700
C	3.39186900	0.74864600	-2.17533700
H	2.57300800	1.41614400	-1.93926900
P	-4.30131900	-0.12709900	2.66436200
C	-4.59861900	-1.66992900	3.58178500
H	-5.49072200	-1.57282900	4.20781200
H	-4.73444700	-2.48453300	2.86638600
H	-3.73632200	-1.91293300	4.20678000
C	-4.28449600	1.26103000	3.83909000
H	-4.10770200	2.18752300	3.28570300



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[Os] = $OsCl(PPh_3)_2$

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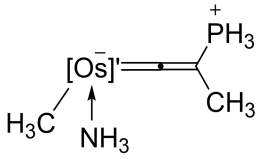
Os	-1.03468100	-0.01168700	-0.57999000
Cl	-1.43167600	0.03299800	-2.92904800
P	-1.18847100	2.40668400	-0.65027400
P	-1.01108300	-2.42964600	-0.75589400
P	3.55788300	0.09016100	0.42617100
P	-4.13118600	-0.08873800	2.74254400
N	-0.34086300	-0.08432900	1.43088300
C	1.01109600	0.09427100	-0.67100200
H	1.48767700	0.18941100	-1.64404400
C	1.76804100	0.05861000	0.46193200
C	0.99456000	-0.06613000	1.69594800
C	1.44605500	-0.13608300	3.01661800
H	2.50682400	-0.13757200	3.23227900
C	0.50995300	-0.20590100	4.05042600
H	0.84856500	-0.25906700	5.08036200
C	-0.85179000	-0.20736600	3.76691500
H	-1.58046100	-0.25933700	4.56721400
C	-1.26656000	-0.14978000	2.43199700
C	-2.60804300	-0.13753600	1.86565800
C	-2.56205200	-0.08941300	0.49525500
C	-2.55579300	3.02922200	-1.68175400
C	-2.47950500	4.30625900	-2.25756100
H	-1.58051700	4.90323200	-2.14518400
C	-3.56075500	4.81332500	-2.97767400
H	-3.49408100	5.80028500	-3.42467200
C	-4.72235200	4.05282800	-3.12557000
H	-5.56017100	4.44698100	-3.69235400
C	-4.80245300	2.78233200	-2.55132400
H	-5.69971600	2.18412600	-2.67936600
C	-3.72401600	2.26844700	-1.83322400
H	-3.77445500	1.27351500	-1.40620100
C	-1.48776200	3.18726500	0.98565600
C	-2.60495700	4.00934400	1.19837900
H	-3.29120900	4.21341100	0.38498600
C	-2.82996600	4.58561900	2.45103200
H	-3.68896900	5.23455900	2.59454700
C	-1.94860500	4.34690800	3.50740300
H	-2.12217500	4.80374200	4.47700600
C	-0.83667200	3.52657300	3.30548800
H	-0.14259600	3.33325400	4.11815600
C	-0.61085500	2.95246300	2.05577300
H	0.25415000	2.31995900	1.91237500
C	0.31167400	3.20752200	-1.33387700
C	0.57417100	3.03222000	-2.70425400
H	-0.10909100	2.45302000	-3.31626900
C	1.69923000	3.61924900	-3.27996500
H	1.87623400	3.50327900	-4.34508500
C	2.58840900	4.36051200	-2.49505800
H	3.46253900	4.81973300	-2.94690900
C	2.34499800	4.51332000	-1.12964300
H	3.03207400	5.08246400	-0.51117000
C	1.20434800	3.95019000	-0.55184300
H	1.00742100	4.11352700	0.50084100
C	0.52951300	-3.15651600	-1.42597900
C	1.13640500	-2.53665500	-2.52987400
H	0.68982100	-1.64767300	-2.96211300
C	2.29093700	-3.07936800	-3.09021400
H	2.75200100	-2.59128800	-3.94223200
C	2.85101000	-4.24365900	-2.55897200
H	3.74996600	-4.66566200	-2.99816800
C	2.24018600	-4.87665200	-1.47534800
H	2.65724100	-5.79580900	-1.07459300
C	1.08057800	-4.33984900	-0.91131900
H	0.60810600	-4.84455600	-0.07608800
C	-1.22979700	-3.23549200	0.87552800
C	-2.43069300	-3.87683800	1.20668700
H	-3.22431300	-3.95069200	0.47105300
C	-2.59840700	-4.44563600	2.47169400
H	-3.52202300	-4.96696600	2.70778500
C	-1.57517000	-4.37256900	3.41873900
H	-1.70481200	-4.82452800	4.39754100
C	-0.37416800	-3.73772300	3.09215500
H	0.43360200	-3.68622200	3.81606200
C	-0.20201500	-3.17551500	1.82954000
H	0.74147100	-2.70228800	1.58499400
C	-2.35174900	-3.11476200	-1.78440200
C	-3.57453700	-2.43538900	-1.89000600
H	-3.69148800	-1.46616200	-1.41893200
C	-4.62302300	-2.99677000	-2.61664100
H	-5.56443600	-2.46272700	-2.70612400
C	-4.45740500	-4.23099600	-3.24900000
H	-5.27225000	-4.66131600	-3.82293400
C	-3.23965900	-4.90634500	-3.15174100
H	-3.10510800	-5.86258400	-3.64757100
C	-2.18826200	-4.35288000	-2.42176500
H	-1.24376300	-4.88213600	-2.35455300
C	4.13647500	-1.33602900	1.36484500
C	5.12863100	-1.22842300	2.34758400
H	5.58805400	-0.26893000	2.56172900
C	5.51718000	-2.36634000	3.05642500
H	6.28479800	-2.28838500	3.81962200
C	4.92255900	-3.60021100	2.78399400
H	5.23031200	-4.48136100	3.33830000
C	3.93565600	-3.70583200	1.79858300
H	3.47659200	-4.66489000	1.58057900
C	3.53665000	-2.57694300	1.08884800
H	2.77404400	-2.66174500	0.32127600
C	4.12897100	-0.02078100	-1.27689800
C	3.88889000	1.07391200	-2.12531900
H	3.38740200	1.96116300	-1.75468500
C	4.31070900	1.01936700	-3.44996900
H	4.11945800	1.86113500	-4.10712100

C	4.98900300	-0.10838600	-3.92411500
H	5.32883000	-0.14123500	-4.95463000
C	5.24070000	-1.18642300	-3.07421100
H	5.77634100	-2.05638900	-3.44061100
C	4.80564700	-1.15240900	-1.74901000
H	4.99364800	-1.99574100	-1.09484100
C	4.21214600	1.62795400	1.10741700
C	3.39649600	2.49893800	1.84219600
H	2.36074300	2.24859800	2.02998700
C	3.91930700	3.69735800	2.32485200
H	3.28489800	4.37255200	2.89073600
C	5.25253300	4.02954300	2.07551100
H	5.65743400	4.96423800	2.45063500
C	6.06748100	3.16437500	1.33956500
H	7.10140500	3.42682500	1.14018900
C	5.55137000	1.96667000	0.84981300
H	6.17943700	1.30845100	0.25703000
C	-4.25122500	1.40494500	3.77288200

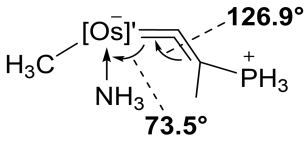


5a-1

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

E = -1793.19369948 a.u.

P	-0.75365800	-2.35305000	0.04984700
P	-0.75326100	2.35304200	0.05495200
P	3.35237300	-0.00115800	0.83928400
C	2.56333500	0.00067100	-0.73725700
C	1.21672500	0.00059400	-0.61811500
H	4.20372700	1.09629100	1.08084300
H	4.20387200	-1.09906500	1.07823000
H	-1.47765100	-2.80433600	1.16967100
H	-1.38906000	-3.11507400	-0.96133600
H	0.42044000	-3.12571000	0.18908100
H	-1.47413500	2.80193000	1.17773700
H	0.42094300	3.12593000	0.19220300
H	-1.39190700	3.11667300	-0.95295900
H	2.35794300	-0.00239100	1.84256100
C	-2.72965400	-0.00079700	0.51523500
H	-2.77026500	-0.00903300	1.60882000
H	-3.29676800	0.88319700	0.18315500
H	-3.29919100	-0.87814900	0.16967300
H	-1.29682000	0.82125800	-2.70202600
H	-1.29628100	-0.81437000	-2.70415800
H	-2.54472000	0.00213400	-2.01018900
C	3.37054800	0.00223600	-2.02579400
H	2.69051200	0.00329100	-2.88224900
H	4.00878600	0.89027000	-2.10621600
H	4.00877200	-0.88560700	-2.10838700
Os	-0.59515300	0.00024900	-0.16468100
Cl	-0.01998400	-0.00254900	2.25065000
N	-1.53062200	0.00263300	-2.13934000
H	-3.42992700	1.42527500	4.49411600
H	-5.20461200	1.42690600	4.30947200
H	-4.15977800	2.28592300	3.13177000
C	-4.36344500	-1.53719800	3.81826100
H	-4.29990500	-2.44371600	3.21144800
H	-5.33442600	-1.48619900	4.32021500
H	-3.57172700	-1.57719800	4.57094200
C	-5.46515000	-0.05878300	1.51423000
H	-5.35202800	0.82141500	0.87590800
H	-5.40867600	-0.95634900	0.89282900
H	-6.43362300	-0.02340400	2.02133900
H	-5.23969700	1.31634200	4.36979100
H	-3.47565800	1.14100600	4.56280000
C	-5.70540200	0.12467200	1.54238000
H	-5.58227300	1.05930600	0.98864900
H	-5.78399200	-0.70816900	0.83879200
H	-6.62488100	0.17679900	2.13301500
H	6.07472100	4.80906800	2.03297300



5a-2

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

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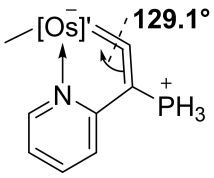
P	-1.72089100	-2.11307800	0.03192200
P	3.75869400	-0.78714000	-0.93474800
C	2.43914900	-0.14570000	0.07756500
C	1.24288900	-0.58230400	-0.43997400
H	4.66898800	-1.69912300	-0.35395900
H	4.64090300	0.18206200	-1.45983500
H	-0.83513500	3.02304500	-0.90358400
H	0.26234300	3.09456000	0.95480500
H	1.28377400	2.58467800	-0.86725000
H	-3.11136800	-2.05482500	0.25327900
H	-1.68873100	-2.79345300	-1.19894900
H	-1.39709800	-3.18011000	0.90682200
H	3.23596000	-1.46866100	-2.03831400
C	-1.85560700	0.86102300	1.59332800
H	-2.69606200	1.32422100	1.06305900
H	-2.26773800	0.08065300	2.24697600
H	-1.39352500	1.62106100	2.23403600
H	1.07768200	-1.51463900	1.77831400
H	0.98301500	-0.02520600	2.46114700
H	-0.26162400	-1.05456400	2.62192100
C	2.88966100	0.76934200	1.20907700
H	3.70990900	1.42231700	0.88585200
H	2.07949600	1.43186300	1.52621800
H	3.25335100	0.22250500	2.08926800
Os	-0.55543600	0.00432400	0.08440800
Cl	-1.92798300	0.46048800	-1.81289100
N	0.44959900	-0.73395600	1.96130800

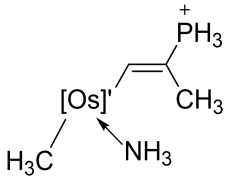


5a-3

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

E= -1944.49807271 a.u.

Os	0.84686500	-0.03193400	0.00001200
Cl	3.05527000	0.85679200	-0.00015100
P	1.06588900	-0.09326000	2.37310000
P	1.06578200	-0.09351900	-2.37308000
P	-2.64062500	2.83620700	-0.00008000
N	-1.24779800	-0.93702600	0.00011700
C	-0.35257900	1.38163400	-0.00000200
C	-1.73513000	1.35268100	0.00003100
C	-2.25826000	-0.00902600	0.00001900
C	-3.60473300	-0.39205200	-0.00005700
H	-4.38728000	0.36209800	-0.00015000
C	-3.93530400	-1.74153200	-0.00001500
H	-4.97536200	-2.05266500	-0.00007200
C	-2.90604400	-2.68405500	0.00008800
H	-3.11082200	-3.74874300	0.00011600
C	-1.58883000	-2.24180200	0.00015100
C	1.43615700	-2.13392100	0.00004000
H	2.53113800	-2.05782300	-0.00003100
H	1.14238100	-2.70215000	0.88904900
H	1.14227000	-2.70222700	-0.88888500
H	-1.73222200	3.89977700	0.00096100
H	-3.49835800	3.06797700	-1.09630600
H	-3.49985400	3.06691300	1.09518200
H	1.91941900	-1.08795300	2.89130000
H	1.60216700	1.05076900	2.99374700
H	-0.07300800	-0.31043600	3.18079900
H	-0.07297500	-0.31177900	-3.18068700
H	1.60113600	1.05077800	-2.99402900
H	1.92007900	-1.08766200	-2.89105900
H	-0.77282500	-2.94913400	0.00022800



5a-4

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

E = -1793.92170241 a.u.

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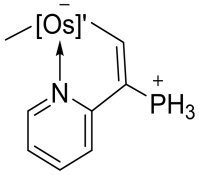
Cl	-0.78279200	-0.97515600	2.14246300
P	-1.32271800	-2.01240100	-0.87727300
P	-0.25001400	2.07701900	0.95183500
P	3.98725500	-0.83339100	0.17422300
C	2.58130500	0.07693700	-0.30352700
C	1.33415800	-0.53214700	-0.11124600
H	4.73759900	-0.47096800	1.32993200
H	5.06591300	-0.91920600	-0.74808100
H	-2.50995300	-2.54508600	-0.32156600
H	-1.63296900	-2.28910300	-2.24472000
H	-0.49159100	-3.14859200	-0.67693500
H	-1.20090400	2.48032700	1.92037000
H	0.91539000	2.31605200	1.72833400
H	-0.20974400	3.31428200	0.23283800
H	3.64766100	-2.16577300	0.44425600
C	-2.80585800	0.55968000	0.01318300
H	-3.03742600	1.47075900	0.58773000
H	-3.28654200	0.70474700	-0.97811400
H	-3.36173700	-0.24800600	0.50872100
H	-0.42660900	1.97133000	-2.12221600
H	-0.20540900	0.50453600	-2.82047400
H	-1.72121200	1.00379600	-2.39224900
C	2.83482700	1.49456400	-0.77921000
H	3.60059500	1.55050300	-1.56674600
H	1.90210800	1.88535600	-1.19634200
H	3.14512900	2.17779300	0.02424200
H	1.46124300	-1.57545900	0.22721600
N	-0.73863500	0.99980000	-2.10714700



5a-5

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

E = -1945.25244826 a.u.

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Cl	2.87626000	1.30529900	-0.02854000
P	1.18269500	-0.10172300	2.29630700
P	1.16098700	-0.31342900	-2.28396900
P	-2.91925500	2.63852400	-0.07192000
N	-1.13721400	-0.93570000	0.02918700
C	-0.38543000	1.57396600	-0.03778900
C	-1.78873100	1.32973000	-0.03009800
C	-2.20461200	-0.06278900	0.00905800
C	-3.52270700	-0.54590000	0.02383700
H	-4.35804200	0.15132200	0.00775000
C	-3.76844000	-1.91203700	0.05892200
H	-4.78730100	-2.28780800	0.07042400
C	-2.67897700	-2.78923700	0.07913200
H	-2.81727700	-3.86501200	0.10657400
C	-1.39498800	-2.26348200	0.06336000
C	1.94626900	-1.98803200	0.02558300
H	3.02116200	-1.76361200	0.06545500
H	1.71578700	-2.61711200	0.90207000
H	1.79032800	-2.64815700	-0.84554000
H	-2.19675900	3.83743900	-0.10861500
H	-3.82920700	2.76222800	-1.15665400
H	-3.83008400	2.82932300	1.00213300
H	2.33774000	-0.80621200	2.70304700
H	1.41314900	1.10205900	3.00363500
H	0.26617500	-0.68716800	3.21581800
H	0.52924100	-1.36231900	-3.00684700
H	0.92415800	0.71770200	-3.23055900
H	2.49868300	-0.59835300	-2.62832000
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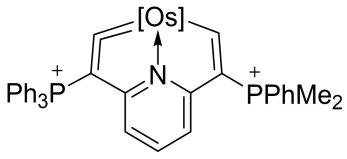

6a

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E =-4714.70543606 a.u.

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P	0.09153300	2.79051000	0.46047500
P	-3.38354700	-0.81150300	-1.18861000
N	0.59547900	-0.16826400	-1.09360900
C	-1.27404000	0.01333900	0.39859500
C	-1.69240100	-0.43200800	-0.82597700
C	-0.55005100	-0.56957200	-1.72646500
C	-0.49436300	-1.02669600	-3.04810000
H	-1.39322000	-1.37374500	-3.54268800
C	0.73704700	-1.05022000	-3.70068000
H	0.79830500	-1.41451100	-4.72140200
C	1.89028500	-0.61330600	-3.05066500
H	2.85086100	-0.65029100	-3.54932500
C	1.79283300	-0.16400700	-1.73031900
C	2.84398400	0.35288100	-0.85551100
C	2.43695700	0.64752400	0.41642300
H	3.15946900	1.05600200	1.12217000
C	1.86281100	-1.94213700	3.21872000
C	1.44457300	-2.62630100	4.36560300
H	0.47025700	-3.10037300	4.39358000
C	2.27940500	-2.69243100	5.48273900
H	1.94482200	-3.21908800	6.37096900
C	3.53460500	-2.08617300	5.45980500
H	4.18054200	-2.13869400	6.33060500
C	3.95949100	-1.40743600	4.31403900
H	4.93642600	-0.93353600	4.29382900
C	3.12490100	-1.32869100	3.20297100
H	3.45388600	-0.79410900	2.31794100
C	1.55354500	-2.99039100	0.53262200
C	2.77487300	-3.63321300	0.77179100
H	3.32198400	-3.43995000	1.68721400
C	3.27728100	-4.55360600	-0.15273800
H	4.21337400	-5.06268000	0.05714300
C	2.57485300	-4.83040500	-1.32609500
H	2.96312800	-5.55290100	-2.03785400
C	1.35602800	-4.19092700	-1.57104400
H	0.79147000	-4.40935600	-2.47260600
C	0.84697300	-3.28623300	-0.64452300
H	-0.12025500	-2.83555300	-0.82181900
C	-0.76192700	-2.67457700	2.20062100
C	-0.94213200	-4.04965000	1.98601900
H	-0.15734900	-4.63860500	1.52482900
C	-2.13489600	-4.66763100	2.36617600
H	-2.26862900	-5.73130200	2.19298700
C	-3.14370200	-3.92288300	2.97960400
H	-4.07003400	-4.40435500	3.27796800
C	-2.95472900	-2.56082700	3.22092000
H	-3.73205400	-1.98013500	3.70371800
C	-1.77476400	-1.93291300	2.82823500
H	-1.63558400	-0.87407400	3.01288000
C	0.92155200	4.00754800	1.53782600
C	2.09873000	3.69051900	2.22788900
H	2.47066000	2.67533800	2.22705900
C	2.76394200	4.66694700	2.96894200
H	3.66475300	4.40692900	3.51662800
C	2.25842700	5.96631100	3.02989200
H	2.77245400	6.72322000	3.61415300
C	1.08239500	6.28877800	2.34875400
H	0.68141500	7.29629400	2.39870600
C	0.41540100	5.31608100	1.60619700
H	-0.49736000	5.57442500	1.07934300
C	0.60347000	3.30691700	-1.22829300
C	0.10685000	2.61926400	-2.34617000
H	-0.58830100	1.80458900	-2.20592800
C	0.48055900	2.98658300	-3.63738200
H	0.08249100	2.44047600	-4.48788300
C	1.35786000	4.05539300	-3.83398400
H	1.64174100	4.35249000	-4.83900300
C	1.85782600	4.74799500	-2.72971800
H	2.52876200	5.58990400	-2.87356900
C	1.48992400	4.37516200	-1.43422300
H	1.87913300	4.92949700	-0.58843400
C	-1.68425900	3.22344600	0.60527700
C	-2.22354700	3.30271000	1.90116500
H	-1.58721200	3.13540700	2.76416300
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C	-2.51720000	3.42165600	-0.50187500
H	-2.11853300	3.38308100	-1.50780200
C	-4.11655000	0.42893200	-2.28261800
C	-5.48309000	0.72513500	-2.16768100
H	-6.09695500	0.20293700	-1.44130700
C	-6.04806200	1.71097200	-2.97612300
H	-7.10510800	1.93972800	-2.88569200
C	-5.25485500	2.40779500	-3.89042700
H	-5.69688600	3.17944300	-4.51295500
C	-3.89310300	2.11407000	-4.00540100
H	-3.27576200	2.65745100	-4.71394400
C	-3.32283400	1.12614700	-3.20624500
H	-2.26636900	0.90494800	-3.29839000
C	-3.42900400	-2.44262300	-1.95405700
C	-2.81339200	-3.50058600	-1.26216600
H	-2.37668700	-3.33759800	-0.28125800
C	-2.78126700	-4.76750200	-1.83720100
H	-2.31051600	-5.58715700	-1.30341800
C	-3.35706700	-4.98098400	-3.09464900
H	-3.32970600	-5.97041300	-3.54051000
C	-3.97391400	-3.93011300	-3.77616800
H	-4.42658500	-4.10158800	-4.74751400
C	-4.01420300	-2.65516000	-3.20824100
H	-4.49269000	-1.83551300	-3.73489700
C	-4.34284200	-0.82464000	0.33277600
C	-5.23862800	-1.87141200	0.59069300
H	-5.29743200	-2.72316700	-0.07795100
C	-6.05996500	-1.81039300	1.71657200
H	-6.75931400	-2.61606400	1.91581000
C	-5.98283500	-0.71646200	2.58068200
H	-6.62690200	-0.67070400	3.45360300
C	-5.08145300	0.32120200	2.32453300

H	-5.01925500	1.17281000	2.99352000
C	-4.26452400	0.27822000	1.19818200
H	-3.58322600	1.09458100	0.99641900
P	4.45509500	0.79112600	-1.47583800
C	4.27876100	2.08721700	-2.73935100
H	5.25370400	2.38479600	-3.13411600
H	3.65124100	1.72279400	-3.55544400
H	3.78402500	2.95064100	-2.28744900
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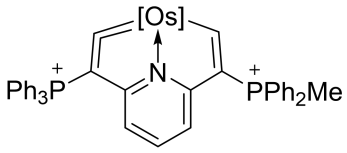
H	5.56949600	0.75186000	0.67178400
H	6.43519700	1.74879300	-0.51674100
H	4.97143300	2.39188000	0.27490700
C	5.31948200	-0.61983000	-2.18317300
C	4.89636100	-1.92147400	-1.87279100
C	6.43509600	-0.41509500	-3.01333900
C	5.59141000	-3.00964300	-2.39751400
H	4.03364500	-2.08649600	-1.23599900
C	7.12325300	-1.51066800	-3.52797800
H	6.77132900	0.58780600	-3.25983000
C	6.70018600	-2.80692800	-3.22102200
H	5.26113400	-4.01479700	-2.16204300
H	7.98527600	-1.35426300	-4.16823200
H	7.23709900	-3.65891200	-3.62616000



6b

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P	-0.16689900	2.46693700	1.32853100
P	-3.51250200	-0.34032400	-1.58318400
N	0.45492400	0.08183700	-0.97937000
C	-1.54797200	-0.10248900	0.33611300
C	-1.85425100	-0.14027400	-0.99742500
C	-0.63488200	-0.04858200	-1.79919900
C	-0.46317700	-0.10081100	-3.18618800
H	-1.31813400	-0.23850200	-3.83672800
C	0.82708100	-0.00714300	-3.70696700
H	0.97815700	-0.05285300	-4.78096000
C	1.92469000	0.14072600	-2.86141100
H	2.92514600	0.22011100	-3.26564400
C	1.71404500	0.18584400	-1.47922000
C	2.69115700	0.31682300	-0.39888700
C	2.15716900	0.25848500	0.85869600
H	2.81217700	0.31614700	1.72700400
C	1.41036700	-2.83795700	2.68213900
C	0.87889100	-3.43985700	3.82642300
H	-0.17883800	-3.67223900	3.87760100
C	1.70954000	-3.73277600	4.90987800
H	1.28972700	-4.19641800	5.79701300
C	3.06993900	-3.43280400	4.85453000
H	3.71275300	-3.66396900	5.69817900
C	3.60726600	-2.83981800	3.70779900
H	4.66968100	-2.61961600	3.65581100
C	2.78135300	-2.53692100	2.62870500
H	3.20543100	-2.09282800	1.73238800
C	1.04898600	-3.27514200	-0.15051000
C	2.00476700	-4.28842500	0.00986000
H	2.42297800	-4.49477100	0.98749100
C	2.40314800	-5.05936000	-1.08472100
H	3.12676300	-5.85597200	-0.93938100
C	1.86873100	-4.82004300	-2.35165100
H	2.18123800	-5.42303900	-3.19903900
C	0.91158400	-3.81549400	-2.51802000
H	0.46945100	-3.63007200	-3.49239400
C	0.49774500	-3.06162800	-1.42291400
H	-0.28576300	-2.33170200	-1.55476200
C	-1.26741000	-3.18628900	1.52053300
C	-1.53967300	-4.42994300	0.92972100
H	-0.78803600	-4.92644600	0.32682500
C	-2.78219600	-5.03794400	1.11631100
H	-2.98553800	-5.99804700	0.65147200
C	-3.75103200	-4.42164100	1.90900400
H	-4.71509700	-4.89803800	2.05888600
C	-3.47525900	-3.19508500	2.51575500
H	-4.22307900	-2.71391000	3.13558500
C	-2.24727400	-2.56918900	2.31454300
H	-2.04605200	-1.60983800	2.77582800
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C	1.81517700	2.78773700	3.30330700
H	2.20490300	1.83525800	2.97239000
C	2.46722300	3.48412100	4.32002900
H	3.37206500	3.07507600	4.75935300
C	1.94417800	4.68984000	4.79002300
H	2.44741500	5.22692900	5.58801000
C	0.76600100	5.19899100	4.23976800
H	0.35241600	6.13373100	4.60529600
C	0.11293000	4.50668200	3.22115700
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C	-0.08098600	3.14532300	-1.39285100
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H	-0.10543000	3.65621800	-3.48070400
C	1.12455600	5.01256200	-2.33718400
H	1.38637000	5.62774700	-3.19283500
C	1.62213600	5.32267100	-1.07068600
H	2.27867000	6.17730500	-0.93692300
C	1.26704700	4.54879900	0.03746600
H	1.64753400	4.81248100	1.01716700
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H	-1.96124500	2.09775300	3.54456500
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H	-2.26881100	3.73191600	-0.43372300
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C	-5.50616800	1.52676000	-2.11824900
H	-6.17397400	0.84551900	-1.60188400
C	-5.98982800	2.74119400	-2.60454100
H	-7.03832100	2.99136700	-2.47814000
C	-5.12693700	3.63524000	-3.24184400

H	-5.50557100	4.58307300	-3.61148100
C	-3.77688500	3.31191300	-3.40612900
H	-3.10551600	4.00743600	-3.89992700
C	-3.28792400	2.09792100	-2.93048700
H	-2.24058200	1.85309400	-3.06085200
C	-3.50551900	-1.64860500	-2.82305500
C	-2.93407400	-2.88291000	-2.46622200
H	-2.56116800	-3.04634400	-1.45905900
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H	-2.42192400	-4.85672900	-3.13854200
C	-3.35297000	-3.69504000	-4.70466800
H	-3.29371900	-4.49216900	-5.43924700
C	-3.92593600	-2.47090300	-5.05444300
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C	-4.00592000	-1.44167600	-4.11454500
H	-4.44904600	-0.48792600	-4.38300200
C	-4.58086500	-0.79604900	-0.20945700
C	-5.45262600	-1.88743200	-0.32170100
H	-5.43358400	-2.51929500	-1.20272000
C	-6.35438300	-2.15432400	0.70870500
H	-7.03511300	-2.99510400	0.62205400
C	-6.38458200	-1.33882100	1.84093400
H	-7.09397500	-1.54509300	2.63669700
C	-5.50641100	-0.25684000	1.95357600
H	-5.52611900	0.37842100	2.83254900
C	-4.60543300	0.02405100	0.93076100
H	-3.94176300	0.87470800	1.01636000
P	4.44348600	0.54584900	-0.64661600
C	5.12077000	1.32887000	0.85315400
H	6.16135400	1.60822300	0.67146800
H	4.54584800	2.23115800	1.07727200
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C	4.75020500	1.65516500	-2.03498100
C	5.68411100	1.32451400	-3.02798700
C	4.04261900	2.86692100	-2.09655100
C	5.91688300	2.21369700	-4.07698100
H	6.22103600	0.38320900	-2.98569100
C	4.28976000	3.74790700	-3.14548300
H	3.30042800	3.11830100	-1.34456500
C	5.22418700	3.42407900	-4.13327200
H	6.63941500	1.96091900	-4.84625400
H	3.74849400	4.68569600	-3.19224700
H	5.41078200	4.11607600	-4.94860400
C	5.30525700	-1.01065300	-0.91935400
C	6.69339300	-1.08346900	-0.70780400
C	4.60285200	-2.12664000	-1.39964900
C	7.37386700	-2.26740000	-0.98025700
H	7.24535700	-0.22420400	-0.33967200
C	5.29819000	-3.30275800	-1.67836800
H	3.52918300	-2.08455500	-1.55204100
C	6.67631200	-3.37463200	-1.47026300
H	8.44449600	-2.32519200	-0.81280800
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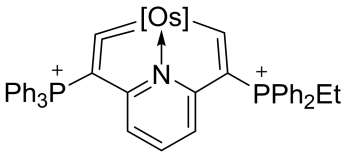

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P	0.27077400	-2.31344200	-1.32565100
P	-3.66755300	-0.30076700	1.43525500
N	0.32803900	0.02433600	0.91822200
C	-1.64551700	-0.12177900	-0.43963900
C	-1.98104800	-0.23528700	0.88367800
C	-0.77524600	-0.14903400	1.70923000
C	-0.63155500	-0.16873500	3.09843100
H	-1.49490200	-0.30668900	3.73193300
C	0.63502400	-0.00092500	3.65154200
H	0.75525100	-0.00040200	4.73033000
C	1.74859300	0.16347400	2.83014300
H	2.73209400	0.31034500	3.25516800
C	1.57305000	0.15355400	1.44573100
C	2.58355400	0.26080700	0.39095000
C	2.07738400	0.25747000	-0.87618300
H	2.74120700	0.30211700	-1.73573900
C	0.77888000	3.25444900	-2.64466000
C	0.09738200	3.90314000	-3.67911000
H	-0.98083000	4.00844100	-3.63912600
C	0.80418400	4.40722200	-4.77272600
H	0.26751200	4.90493800	-5.57428100
C	2.19015300	4.27259800	-4.83703300
H	2.73648200	4.66636600	-5.68836000
C	2.87674700	3.63165900	-3.80131100
H	3.95755800	3.53316700	-3.84491000
C	2.17450800	3.11888800	-2.71460600
H	2.71051600	2.62690800	-1.90837500
C	0.50066900	3.43766700	0.23155900
C	1.36629800	4.53514100	0.11771600
H	1.74628400	4.83114200	-0.85260800
C	1.72137600	5.27357300	1.24971400
H	2.37933800	6.13083200	1.14239000
C	1.22087800	4.92524300	2.50501800
H	1.48835000	5.50877600	3.38107100
C	0.35961700	3.83180300	2.62673400
H	-0.04339300	3.55423300	3.59599100
C	-0.00041500	3.09999200	1.49856300
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C	-2.22265600	4.35569300	-0.84467900
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C	-3.54592000	4.78573300	-0.94396400
H	-3.83267600	5.74636000	-0.52670700
C	-4.49681800	3.98570700	-1.58138000
H	-5.52725400	4.32056200	-1.65272400
C	-4.11829700	2.76282300	-2.13810200
H	-4.84983800	2.14153500	-2.64321500
C	-2.79821300	2.32533700	-2.03936300
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C	2.55616500	-2.18075500	-2.95230300
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C	3.76085100	-2.64822900	-3.48124600
H	4.27259500	-2.06832700	-4.24387000
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C	-0.06125600	-3.82430700	3.03373600
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C	-2.80764500	-3.28391900	-3.88831300
H	-3.47426300	-2.76038800	-4.56736200
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H	-3.55565400	-5.23837300	-4.40392800
C	-1.96091600	-5.34611300	-2.95660300
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H	-3.31443500	-0.95318600	4.30837100
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C	-3.48677500	2.39531600	1.91340500
H	-2.85084500	2.39995800	1.03612700
C	-3.78760400	3.59153300	2.55781000
H	-3.35841000	4.51727700	2.18932500
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C	5.05344200	-2.94329400	3.30422900
H	4.78771100	-0.81712800	3.46355700
C	5.03369200	-3.85547300	1.06251200
H	4.71544500	-2.46555400	-0.53485600
C	5.14845000	-4.03817600	2.44240800
H	5.14961900	-3.08225900	4.37641900
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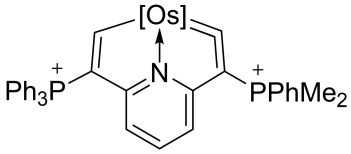

7a

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P	3.91223800	-0.05606100	0.41327500
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N	0.01882600	-0.06423100	1.42874700
C	1.36737300	0.10428500	-0.68199000
H	1.84944700	0.19654000	-1.65293700
C	2.12581800	0.02151700	0.44845600
C	1.35561800	-0.09294000	1.68480400
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H	2.87436800	-0.23437000	3.21010100
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H	-1.20689600	-0.25907800	4.56916500
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H	-2.89363900	6.01802000	-3.33967900
C	-4.15397300	4.27459000	-3.17995500
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C	-0.50302400	3.49664000	3.39880300
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C	-0.24255700	2.96467800	2.13692000
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C	1.07035800	3.08842000	-2.57780100
H	0.40180400	2.51292700	-3.20983000
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H	2.43110700	3.54028800	-4.17545800
C	3.08914100	4.39754100	-2.30533300
H	3.98261700	4.84648900	-2.72883900
C	2.80011900	4.56025200	-0.95020200
H	3.47047500	5.12833200	-0.31274000
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H	6.43723500	-2.78804800	3.70130600
C	4.99792500	-3.94736500	2.59063900
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H	3.49093800	-4.84357000	1.32594300
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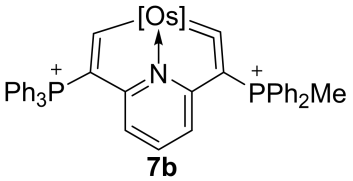

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H	3.69442100	4.54822500	5.30322800
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H	2.82249800	4.09431800	0.71674400
C	-1.18934000	3.24725500	1.28842300
C	-1.87462500	3.16900500	2.51363700
H	-1.43177800	2.63670900	3.34812000
C	-3.11544500	3.78710500	2.66196500
H	-3.62278600	3.74271400	3.62117200
C	-3.69811500	4.46826000	1.58860300
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C	-1.77746500	3.93149700	0.21665600
H	-1.25969400	4.02093300	-0.72980300
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H	-6.00828600	1.93034400	-1.84348800
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H	-6.35521300	4.13533600	-2.90429100
C	-4.29436000	4.35395000	-3.50287800
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C	-2.82538100	2.52157700	-2.93170000
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H	-3.15659100	-2.56206900	-1.25237300
C	-3.75094000	-3.47251000	-3.10895500
H	-3.46758600	-4.47150300	-2.79227600
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H	-5.74473700	-1.68362400	-0.77494300
C	-6.65690500	-0.89630400	1.00843500
H	-7.37482700	-1.70662700	1.08386600
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C	5.07015200	1.16330900	-1.20260400
C	5.10323600	1.49180100	-2.56735900
C	5.61658500	2.04645900	-0.25892300
C	5.70671800	2.67638600	-2.98227500
H	4.68866400	0.81318400	-3.30555200
C	6.22433800	3.22720700	-0.68293100
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C	6.27893000	3.53733500	-2.04290000

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H	6.76686600	4.44991000	-2.37121400
C	4.87288700	-1.67966100	-1.82844100
C	6.15249600	-1.61465600	-2.40615800
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H	6.80075400	-0.76593100	-2.21419800
C	4.48125800	-3.79820700	-2.91949800
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C	5.75006300	-3.73198000	-3.49834800
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H	6.08962700	-4.52970600	-4.15166900
C	4.98649300	-0.80322900	0.98259900
H	4.61733300	-0.08700400	1.72018600
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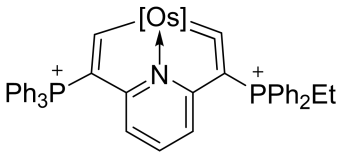

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P	-0.31665000	-2.31974900	-1.33521700
N	-0.18055500	0.08653800	1.01089800
C	-1.92480200	0.21821300	-0.64096700
C	-2.45746300	0.25831100	0.61875400
C	-1.40040000	0.18178600	1.62325900
C	-1.48609500	0.21569900	3.01693000
H	-2.44982900	0.31321300	3.50024300
C	-0.30967100	0.14596000	3.76209000
H	-0.35544100	0.17072200	4.84636000
C	0.92672100	0.05062100	3.12565500
H	1.84047100	-0.00546000	3.70318200
C	0.97151500	0.02595200	1.72756800
C	2.13066200	-0.06448400	0.83992500
C	1.82132300	-0.06540900	-0.49172700
H	2.61492900	-0.17090600	-1.22951800
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C	0.71544200	4.24221400	-3.37749900
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C	2.85255200	4.18249400	-4.51035700
H	3.53071300	4.58092400	-5.25856300
C	3.23698700	3.09060400	-3.72769200
H	4.21190400	2.63393600	-3.87149900
C	2.36217800	2.57109700	-2.77776500
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H	2.60308800	5.94905600	1.20660700
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C	-0.15042700	3.23901400	1.42364000
H	-0.94390100	2.50857700	1.48431400
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H	-5.23206900	4.49999900	-2.46418300
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H	-4.24496400	2.63956100	-3.79024300
C	-2.40335200	2.61710400	-2.68344800
H	-1.97978200	1.79785900	-3.25477400
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H	2.60642700	-2.46694800	-1.30270100
C	3.19959100	-3.42730400	-3.12644100
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C	2.77621100	-4.02361600	-4.31716400
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C	1.41429500	-4.12673800	-4.59596000
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C	0.75689000	-5.11231700	1.52609700
H	1.44515300	-5.94769900	1.61652400
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H	2.55457800	-4.45364100	3.53905600
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H	2.55377200	2.24944700	2.48585200
C	5.57353800	3.64074100	3.20582300
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C	-4.86857200	-4.02811400	2.67403500
H	-4.83560100	-4.70337600	0.62321000
H	-4.86864900	-3.06182100	4.60287200
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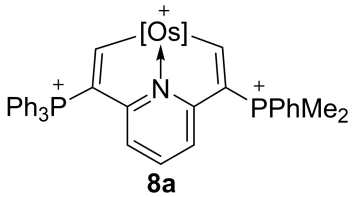

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H	0.66402600	-1.58411600	-4.69740500
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C	-4.39155300	-0.89935200	0.35863400
C	-5.03212700	-2.06409700	0.80234200
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C	-5.82764100	-2.01288600	1.94777800
H	-6.34127700	-2.90779900	2.28369200
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H	-5.44723400	1.27798900	2.74810800
C	-4.54685700	0.31243500	1.05687200
H	-4.09996300	1.22739400	0.68533800
H	-2.01765000	0.20603500	1.24383100
P	4.44656200	0.67680600	-1.56479300
C	5.44794400	1.28058600	-0.17342800
H	6.45426000	1.49639000	-0.54508400
H	5.02058400	2.19605100	0.24627400
H	5.52278600	0.50852300	0.59712000
C	4.30803600	2.02179200	-2.77678100
H	5.29704900	2.32926000	-3.12737900
H	3.70438600	1.69764700	-3.62748000
H	3.80979900	2.87142600	-2.30258900
C	5.19641500	-0.77010700	-2.30941000
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C	4.86711300	-2.04786100	-1.82433900
C	6.77842200	-1.74451700	-3.85837100
H	6.41309100	0.36333800	-3.71319800
C	5.50261700	-3.16386300	-2.36237300
H	4.12311400	-2.17354600	-1.04349500
C	6.45523000	-3.01456900	-3.37392800
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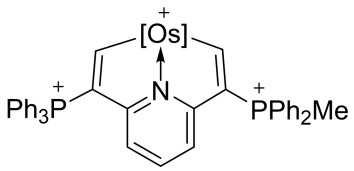

8b

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P	-0.19366600	2.52311200	1.30589100
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C	-1.63027600	-0.11646800	0.35443800
C	-1.89128100	-0.22514500	-0.96603000
C	-0.66681600	-0.18091200	-1.76232600
C	-0.51244700	-0.29372700	-3.14440500
H	-1.37583700	-0.45706200	-3.77653200
C	0.76835000	-0.21985400	-3.69015500
H	0.90581400	-0.31077800	-4.76261700
C	1.86904700	-0.02909000	-2.86083100
H	2.86683600	0.05088500	-3.27103700
C	1.66735700	0.07757600	-1.48431800
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C	1.41458000	-2.89495400	2.72947300
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H	-0.03881100	-4.29420000	3.50486400
C	1.74037700	-4.24928500	4.71118900
H	1.36721600	-4.99143300	5.40950400
C	3.00688000	-3.69438500	4.89094700
H	3.62116800	-4.00168100	5.73113500
C	3.48428400	-2.73943600	3.98779400
H	4.47109800	-2.30770600	4.12719300
C	2.69024800	-2.33674700	2.91786200
H	3.06839700	-1.59909200	2.21724200
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H	3.05123700	-3.54224300	0.68982400
C	2.98885200	-4.02912200	-1.40091200
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C	0.90930900	-3.58654300	-2.54481100
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H	-2.88318500	-6.02086800	0.55823100
C	-3.67151500	-4.51377300	1.88378700
H	-4.61786300	-5.02434000	2.03161000
C	-3.41477000	-3.31024800	2.54426300
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C	-2.20011200	-2.65476600	2.35858200
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H	2.16179900	1.96519800	3.03135700
C	2.32974300	3.63413700	4.36202600
H	3.22765400	3.25330200	4.83854100
C	1.76664300	4.83752900	4.79128600
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C	1.62700100	5.28460400	-1.15214000
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H	5.08519000	-0.89820300	-3.17057400
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C	6.13274400	1.64005200	-2.46439500
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H	6.85308200	0.87824400	-2.18441800
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H	2.91640500	2.65464800	-1.84334300
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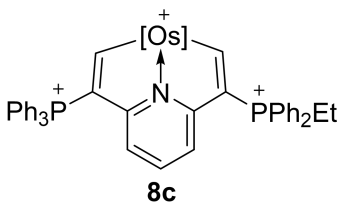

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C	-2.11329000	-0.09352600	-0.82027000
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C	2.60951900	3.11774200	4.48555600
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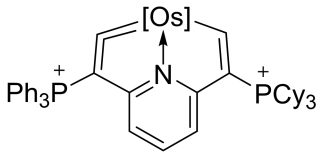

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P	4.15519200	-0.32741600	1.24012500
P	-3.99700800	-0.07076100	1.00367200
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C	2.43762800	-0.21364500	0.82193900
C	1.29243400	-0.42489100	1.70552700
C	1.29057500	-0.77173400	3.05820900
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H	0.02854700	-1.13158700	4.76011300
C	-1.12003200	-0.64608900	3.01590300
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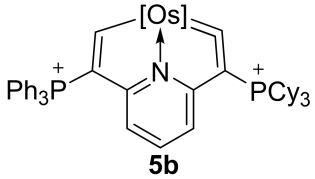

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H	0.31418300	-1.00554700	4.83207300
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H	-0.85761300	6.74109900	-3.22962700
C	-2.22502200	5.13223500	-3.67307600
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H	-3.40145600	3.34468100	-3.93593100
C	-1.77283600	3.02876900	-2.56741600
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C	0.23080600	2.70838600	2.10199500
H	0.93879900	1.89587300	2.04731500
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C	3.78660900	-2.83943000	-2.91978700
H	4.49302100	-2.32004600	-3.55853000
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H	5.08677700	-4.52585400	-2.57359300
C	3.20109500	-4.74494500	-1.55530700
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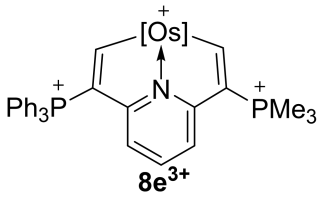
C	-6.13720400	1.70901200	0.79221500
H	-4.38336700	2.12149100	1.99391800
C	-4.41183600	3.94834500	-0.06446200
H	-4.05808400	2.05596200	-1.04623900
H	-2.81693300	2.49933900	0.11405100
C	-6.64121400	3.15991900	0.81518800
H	-6.36592400	1.27381600	-0.18674700

H	-6.67220600	1.11534900	1.53626100
C	-5.93188000	4.01121600	-0.24303400
H	-3.90499000	4.50432300	-0.86089200
H	-4.13601200	4.42541400	0.88566200
H	-7.72470500	3.16655900	0.65432800
H	-6.46790200	3.58792600	1.81263600
H	-6.27828100	5.04891400	-0.19024100
H	-6.19755100	3.64108500	-1.24342500



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P	-1.23236200	2.34056700	-0.67044500
P	3.52306200	0.11319200	0.45307700
N	-0.38589800	-0.11160900	1.34662200
C	1.04645700	0.15177500	-0.80296500
C	1.75244400	0.09368900	0.39636800
C	0.96114600	-0.06793700	1.61610600
C	1.39965700	-0.14582100	2.94333400
H	2.45720900	-0.11119700	3.17383200
C	0.46169700	-0.27433400	3.96694000
H	0.79418300	-0.34466900	4.99796500
C	-0.89879300	-0.31827200	3.67152300
H	-1.61774100	-0.42730400	4.47466300
C	-1.31854400	-0.22808900	2.33877100
C	-2.67749400	-0.21581300	1.79489500
C	-2.80993400	-0.13482400	0.41022400
H	-3.84741300	-0.09985400	0.05441400
C	-2.32938900	-3.13153500	-1.79426900
C	-2.27344600	-4.48124600	-2.17034200
H	-1.38771200	-5.07010100	-1.95462800
C	-3.35115000	-5.07309600	-2.82680600
H	-3.29824600	-6.11843100	-3.11682100
C	-4.49203000	-4.32101800	-3.11682700
H	-5.32873800	-4.78138600	-3.63436000
C	-4.54806600	-2.97474600	-2.75395100
H	-5.42339800	-2.38036700	-3.00048000
C	-3.47045100	-2.37916900	-2.09770200
H	-3.48445400	-1.32672900	-1.84960100
C	-1.08006900	-3.23053100	0.78272000
C	-2.26852400	-3.83591100	1.20953600
H	-3.11752600	-3.88683900	0.53603200
C	-2.35810800	-4.39393900	2.48718800
H	-3.27719300	-4.88576100	2.79565200
C	-1.26863100	-4.34175700	3.35830600
H	-1.33957200	-4.78160300	4.34914200
C	-0.08093200	-3.73649800	2.94059600
H	0.77663200	-3.68866000	3.60536200
C	0.01088000	-3.18816400	1.66417800
H	0.93825900	-2.72495400	1.35274200
C	0.55633300	-3.11242500	-1.58085300
C	1.09834500	-4.33204900	-1.14881800
H	0.62381700	-4.88359400	-0.34415400
C	2.26093900	-4.83552100	-1.73736700
H	2.67163700	-5.78191500	-1.39614200
C	2.88878700	-4.12803500	-2.76408900
H	3.79434000	-4.51925600	-3.21936100
C	2.33997800	-2.92432000	-3.21294400
H	2.81726500	-2.37314800	-4.01698900
C	1.18011300	-2.41724600	-2.62813700
H	0.74179600	-1.49009100	-2.98335700
C	-2.57794600	3.00602300	-1.71788600
C	-3.67651500	2.20072400	-2.04113800
H	-3.66766900	1.15865600	-1.75197700
C	-4.74060700	2.72802500	-2.77224300
H	-5.58198100	2.09265000	-3.03383300
C	-4.71201600	4.05880200	-3.19259800
H	-5.53718100	4.46525000	-3.77023300
C	-3.61388300	4.86399700	-2.88203000
H	-3.58317200	5.89739900	-3.21476400
C	-2.55004000	4.34036300	-2.14826600
H	-1.69757900	4.96879100	-1.90953600
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H	0.17117300	2.28766700	1.89137800
C	-0.94884700	3.45598100	3.29326400
H	-0.25106500	3.26801600	4.10438300
C	-2.08475500	4.24035300	3.50392700
H	-2.27410200	4.67996900	4.47905600
C	-2.97505700	4.45636800	2.45015700
H	-3.85834200	5.07116600	2.60084000
C	-2.72954600	3.90116400	1.19130700
H	-3.42357100	4.08844800	0.38021700
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H	0.06772400	2.26565500	-3.20495900
C	1.74079800	3.62682200	-3.16126900
H	2.02067200	3.42674200	-4.19159200
C	2.49013600	4.52157400	-2.38975900
H	3.35446400	5.02224800	-2.81734700
C	2.11984200	4.77156900	-1.06855900
H	2.69723500	5.46190400	-0.46026400
C	0.99154500	4.14932700	-0.52520900
H	0.69371000	4.38031100	0.49151400
C	4.18170600	1.58042900	1.28743500
C	5.56784000	1.79931700	1.34695300
H	6.25526900	1.07173200	0.92514200
C	6.06032900	2.96456200	1.92952800
H	7.13158100	3.13384700	1.97578700
C	5.17586900	3.92001000	2.43999200
H	5.56384400	4.82990800	2.88778600
C	3.79818700	3.71320400	2.36265500
H	3.10942800	4.46085200	2.74428000
C	3.29896800	2.54593800	1.78548100
H	2.23126400	2.39276100	1.70021300
C	4.08841800	-1.38902500	1.29447700
C	3.54078600	-2.60266600	0.84552000
H	2.84767100	-2.61662800	0.01065200
C	3.88210500	-3.79396100	1.48026500
H	3.45475100	-4.72606700	1.12517200
C	4.75964200	-3.78050000	2.56789000
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H	5.97912000	-2.56361800	3.86456700
C	4.96842100	-1.37604900	2.38323400
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C	4.81430900	-0.96394600	-1.79883900
H	4.90458700	-1.89186800	-1.24712500
C	5.30485700	-0.88034900	-3.10213800
H	5.78225700	-1.74563000	-3.55149100
C	5.17952700	0.30681500	-3.82441800
H	5.56011400	0.36594700	-4.83964500
C	4.56884200	1.42162800	-3.24282900
H	4.46725300	2.34596400	-3.80164200
C	4.08544500	1.35276700	-1.93994600
H	3.61457100	2.22184400	-1.49330200
H	1.64173700	0.29519900	-1.70864300
P	-4.07753400	-0.19203200	2.86977400
C	-4.06094900	1.24021900	3.99850700
H	-4.06602600	2.15374200	3.39772100
H	-4.93071400	1.22099000	4.66222500
H	-3.14581600	1.24090400	4.59376600
C	-4.23718200	-1.69780000	3.88933100
H	-5.07819900	-1.60830400	4.58362300
H	-4.39034600	-2.55079900	3.22411200
H	-3.31591700	-1.87723500	4.44751900
C	-5.61523100	-0.06540600	1.90981400
H	-5.61392500	0.85411200	1.31970800
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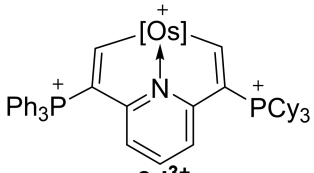

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P	-0.28622600	2.69960900	0.77266400
P	-4.12043400	-0.35528000	-1.35823600
N	-0.08194900	-0.13841600	-1.05092300
C	-2.02514400	0.07624600	0.40390700
C	-2.39441100	-0.16170200	-0.87329200
C	-1.24016800	-0.30431900	-1.75282400
C	-1.21434200	-0.59884100	-3.11669300
H	-2.13809600	-0.75856700	-3.65767200
C	0.01865300	-0.70452500	-3.75757800
H	0.06183700	-0.92934600	-4.81827400
C	1.19435800	-0.52518100	-3.03657300
H	2.15143900	-0.59786300	-3.53100700
C	1.12776700	-0.24686100	-1.66848000
C	2.21546000	-0.04151500	-0.71645600
C	1.73030200	0.19610600	0.52255200
H	2.33570000	0.35545600	1.41646500
C	1.05936200	-2.36777500	3.03388300
C	0.62618000	-2.64214600	4.33474800
H	-0.42807300	-2.78991100	4.54072200
C	1.55605500	-2.72728600	5.37436100
H	1.21484700	-2.94302300	6.38170100
C	2.91486400	-2.54200100	5.12172000
H	3.63268300	-2.61225800	5.93262100
C	3.35378900	-2.27995400	3.81894800
H	4.41449900	-2.15964800	3.61663800
C	2.43131600	-2.18852800	2.78077900
H	2.77752700	-2.01677200	1.76549000
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H	1.67842600	-4.49021900	1.72370300
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H	2.09843700	-6.29618700	0.10252500
C	0.89628100	-5.41275300	-1.45359500
H	1.07358300	-6.21848900	-2.15916500
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H	-0.39623600	-4.30184800	-2.78161900
C	-0.16813700	-3.31859200	-0.88640900
H	-0.85522500	-2.53055400	-1.15185300
C	-1.75188900	-2.76652800	2.17897800
C	-2.20257300	-4.02466800	1.74756300
H	-1.58119000	-4.64296100	1.11104800
C	-3.45161300	-4.49918800	2.15230500
H	-3.78538000	-5.47758700	1.82077700
C	-4.25628600	-3.73205600	2.99439300
H	-5.22088600	-4.11012700	3.31773500
C	-3.81100900	-2.48283200	3.43233000
H	-4.42894200	-1.88383200	4.09282000
C	-2.57079900	-1.99758300	3.02469000
H	-2.23196300	-1.03496500	3.38858700
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H	3.19758400	3.68203500	4.18061600
C	1.89958300	5.36925900	3.84488700
H	2.41101400	6.00656200	4.55919300
C	0.79265200	5.85357200	3.14383900
H	0.44565800	6.86900700	3.30590000
C	0.12387300	5.03216800	2.23860600
H	-0.73712500	5.41609600	1.70203500
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C	-0.17615800	2.84132300	-2.03801700
H	-0.97828100	2.11751900	-2.02739000
C	0.27476600	3.34440100	-3.25586200
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C	1.28653400	4.30784900	-3.28194800
H	1.62188000	4.71934900	-4.22854300
C	1.85705800	4.74471800	-2.08596000
H	2.64299800	5.49343600	-2.09932400
C	1.40589800	4.24324100	-0.86325200
H	1.84143300	4.61044500	0.05852100
C	-2.03268000	3.25298500	0.88031900
C	-2.63857800	3.22877600	2.15001300
H	-2.07516600	2.89918400	3.01696000
C	-3.94952300	3.67463600	2.30790600
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C	-4.67935800	4.12229000	1.20138900
H	-5.69798400	4.47565200	1.32791300
C	-4.08977700	4.12302500	-0.06322800
H	-4.64783300	4.46677900	-0.92812400
C	-2.76729100	3.70125200	-0.22429400
H	-2.31370200	3.75538600	-1.20541100
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C	-6.48659500	2.55874100	-2.92955900
H	-7.53322400	2.84021500	-2.87646300

C	-5.59620300	3.30783200	-3.70277700
H	-5.95286300	4.17351200	-4.25191400
C	-4.24820200	2.94336800	-3.77460900
H	-3.55794900	3.52586300	-4.37656500
C	-3.78782700	1.83180600	-3.07357000
H	-2.74272300	1.55520700	-3.13800000
C	-4.21865700	-1.86410200	-2.33047900
C	-3.63360700	-3.03383900	-1.81179000
H	-3.16070100	-3.02888500	-0.83387200
C	-3.68354600	-4.21003900	-2.55431100
H	-3.23846700	-5.11670500	-2.15677900
C	-4.30987500	-4.22290100	-3.80599700
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H	-5.38435200	-3.07775800	-5.28393500
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C	-5.12190400	-0.48805900	0.12870900
C	-5.84672300	-1.65388800	0.41036700
H	-5.79094600	-2.51287000	-0.24835900
C	-6.66019200	-1.69561900	1.54325500
H	-7.23819200	-2.58926100	1.75447000
C	-6.73977400	-0.59179200	2.39377600
H	-7.38118900	-0.62875700	3.26885500
C	-6.01023000	0.56853500	2.11329200
H	-6.08167800	1.43271700	2.76549700
C	-5.20994100	0.63143600	0.97655500
H	-4.68970900	1.55102600	0.73459800
H	-2.72264300	0.18976900	1.23641300
P	3.99163700	-0.30636600	-1.02295100
C	4.48414600	0.49909100	-2.60765300
C	3.81430600	1.86638800	-2.85050800
C	6.01475900	0.59118500	-2.79535700
H	4.11877700	-0.19442300	-3.37364700
C	4.13833300	2.34018200	-4.27591200
H	4.18875600	2.59684700	-2.12650000
H	2.73151000	1.81126900	-2.70702300
C	6.32389000	1.05148500	-4.22814700
H	6.42070500	1.32509400	-2.09170100
H	6.50327300	-0.36670900	-2.58381500
C	5.64955500	2.39453900	-4.53352600
H	3.68810100	3.32437900	-4.43725300
H	3.66460000	1.65656000	-4.99546400
H	7.40826300	1.12885200	-4.35616700
H	5.97665800	0.28727500	-4.93734100
H	5.84333900	2.68532300	-5.57078800
H	6.09599500	3.17441100	-3.90124500
C	4.84211200	0.42092100	0.45717300
C	6.37009800	0.19482000	0.57214200
C	4.54788400	1.93317500	0.61467400
H	4.37732500	-0.11744400	1.29654500
C	6.84893600	0.66103100	1.95703800
H	6.88474400	0.77603600	-0.19713800
H	6.64247900	-0.84776000	0.42212400
C	5.02698800	2.41266800	1.99302200
H	5.09433900	2.47749500	-0.16380200
H	3.48868800	2.16725700	0.47511800
C	6.51978300	2.13701500	2.20157200
H	7.92728300	0.49022700	2.03634900
H	6.37498800	0.03956700	2.73094800
H	4.80963100	3.48046600	2.09626800
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H	6.82090400	2.43084500	3.21216700
H	7.10229100	2.75821300	1.50802900
C	4.13925800	-2.17617200	-1.14170500
C	4.30715600	-2.67482800	-2.59374000
C	5.20690800	-2.81088200	-0.22766200
H	3.15569600	-2.50793900	-0.78198100
C	4.24337300	-4.20943300	-2.64794400
H	5.27085000	-2.33193800	-2.98989700
H	3.52443500	-2.26688200	-3.24120500
C	5.10149600	-4.34196000	-0.27425000
H	6.20481500	-2.51804600	-0.57212600
H	5.09797000	-2.45994400	0.80457000
C	5.25884600	-4.86428400	-1.70601800
H	4.41111700	-4.53402800	-3.68043000
H	3.22946400	-4.52513500	-2.37442200
H	5.86747300	-4.77215500	0.37936100
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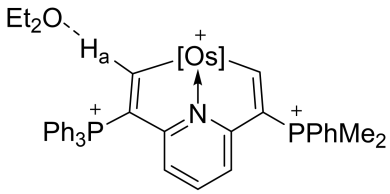

6a-1

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P	0.89942800	2.24342000	-0.90283400
P	-3.76435200	-0.58759200	-0.96205200
N	0.21901400	-1.02006700	-1.44073700
C	-1.29092800	0.13411100	0.09831000
C	-1.96773300	-0.49485200	-0.88708100
C	-1.07980900	-1.18727400	-1.81149100
C	-1.40979500	-1.93298400	-2.94457600
H	-2.44583300	-2.05716100	-3.23131500
C	-0.38711700	-2.51545800	-3.69088900
H	-0.62502100	-3.10300400	-4.57158100
C	0.93919900	-2.33868000	-3.30628000
H	1.73993600	-2.78489600	-3.88260600
C	1.22146500	-1.57666300	-2.17219200
C	2.51212100	-1.23375300	-1.59581500
C	2.38582400	-0.47018800	-0.48519600
H	3.23654500	-0.09257800	0.08452200
C	1.96337800	-1.82214300	3.01272700
C	1.64093000	-1.92123500	4.37205300
H	0.61418300	-2.07803000	4.68175300
C	2.64434400	-1.81594700	5.33776400
H	2.38572200	-1.89423000	6.38884400
C	3.97046700	-1.61428100	4.95689600
H	4.74623900	-1.53200700	5.71137000
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C	3.30224800	-1.61961500	2.63453600
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C	0.94556300	-3.42750900	0.78372700
C	2.09083500	-4.21635000	0.96067400
H	2.83494800	-3.94091700	1.69906100

C	2.25734500	-5.38701500	0.21489900
H	3.13292100	-6.00808300	0.38066800
C	1.28844800	-5.77857700	-0.71086600
H	1.41590500	-6.69598100	-1.27721100
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H	-0.63693900	-5.31346800	-1.57387300
C	-0.03354400	-3.83876100	-0.13531900
H	-0.94687800	-3.26876700	-0.24957800
C	-0.90646900	-2.18239800	2.62577400
C	-1.37459700	-3.48638600	2.85411600
H	-0.82447500	-4.33991100	2.47430000
C	-2.55018400	-3.68874600	3.57902000
H	-2.90351100	-4.69939000	3.75897600
C	-3.25829600	-2.59798200	4.08859100
H	-4.16737600	-2.76093200	4.65916000
C	-2.78235200	-1.30079300	3.88324800
H	-3.31802300	-0.45129900	4.29277600
C	-1.61253600	-1.09115000	3.15548000
H	-1.23357800	-0.08343000	3.03293400
C	2.06684400	3.43491100	-0.16751600
C	3.24163600	2.99569800	0.46197800
H	3.44501600	1.93802100	0.57576600
C	4.15457800	3.91778500	0.96852500
H	5.05156800	3.56793500	1.47030300
C	3.90406100	5.28749000	0.85199100
H	4.61043100	6.00566400	1.25604800
C	2.74146900	5.73116600	0.21970500
H	2.54353900	6.79405100	0.12596800
C	1.82454100	4.81169900	-0.28968900
H	0.92196400	5.16725100	-0.77371600
C	1.50077800	2.00862200	-2.61700900
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H	-0.19171600	0.82021700	-3.24396000
C	1.19504300	1.10406000	-4.85275000
H	0.59511300	0.53779700	-5.55878900
C	2.39667500	1.68835900	-5.26202400
H	2.73363000	1.58130300	-6.28849600
C	3.15186500	2.42876600	-4.34948100
H	4.07399600	2.90667800	-4.66671700
C	2.70849000	2.58960200	-3.03393200
H	3.28709300	3.19311800	-2.34386000
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H	-0.85034200	3.21579900	1.15687300
C	-2.41637600	4.30928700	0.20858200
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H	-0.77866600	3.32348500	-3.17016800
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C	-5.74835200	0.34380800	-2.64413500
H	-6.44359400	-0.11972300	-1.95009800
C	-6.23263300	1.03492800	-3.75137500
H	-7.30215700	1.09329700	-3.92461300
C	-5.34301200	1.66126800	-4.63071300
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C	-3.60695600	-3.15315100	0.01967800
H	-2.99724300	-2.71794300	0.80513500
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H	-3.43646700	-5.14333500	0.80398500
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H	-5.36948300	-2.29494100	-2.78644300
C	-4.47910400	0.20855400	0.48386900
C	-5.11809400	-0.52898600	1.49086000
H	-5.15939300	-1.61059900	1.44443500
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H	-3.98314900	2.18741800	-0.25689400
H	-1.77035800	0.71590300	0.88743100
O	-1.43546600	3.35586300	3.26609600
C	-0.54368500	4.12965700	4.07486300
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C	0.34978700	4.95300200	3.16409000
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H	-2.92725100	3.68912200	5.64708100
H	-1.60040600	1.80563500	4.63045700
P	4.12520600	-1.70379200	-2.22001700
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H	5.35966300	-1.35284400	-4.25754700
H	3.62434400	-1.60170500	-4.58872400
H	4.18018300	-0.03813700	-3.96839600
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H	3.58976400	-3.95314000	-2.90088500
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C	5.50870900	0.46399200	-1.21315300
C	6.93426600	-1.04693200	0.66761900
H	5.92500000	-2.76338700	-0.13739700
C	6.39282000	1.09195200	-0.33956000
H	4.95474200	1.05633900	-1.93574400
C	7.10547700	0.33782100	0.59852700
H	7.50135000	-1.63187400	1.38456100
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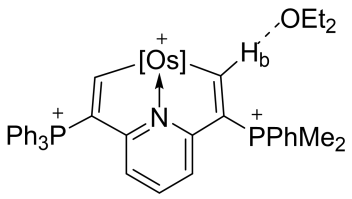

7a-1

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N	-0.02020400	-0.69282000	-1.09076200
C	-1.52822100	0.43619200	0.46431100
C	-2.21017200	-0.19247100	-0.51578300
C	-1.32310600	-0.87895600	-1.44597000
C	-1.65847000	-1.64123400	-2.56538100
H	-2.69668400	-1.80410200	-2.82236700
C	-0.63692800	-2.19137100	-3.33767300
H	-0.87816100	-2.78040800	-4.21651100
C	0.69030400	-1.98310700	-2.98285500
H	1.48948700	-2.40101200	-3.57747000
C	0.97942100	-1.23355400	-1.83832800
C	2.27615700	-0.88889700	-1.27267300
C	2.16310600	-0.10187200	-0.17309100
H	3.01465200	0.33713400	0.36758300
C	1.56001800	-1.51125100	3.47069800
C	1.17571900	-1.95042300	4.74538300
H	0.15956600	-2.28005800	4.92815300
C	2.10235200	-1.96530700	5.78883800
H	1.79561600	-2.30238800	6.77372400
C	3.41531000	-1.55110300	5.56696600
H	4.13430700	-1.56334800	6.37981700
C	3.80403900	-1.11704600	4.29657500
H	4.82519100	-0.79253000	4.12769400
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H	3.19224200	-0.73944800	2.27461300
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C	1.74644900	-3.97584100	1.63225700
H	2.42108300	-3.66323800	2.42107100
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H	1.09622400	-6.67669800	-0.33906800
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H	-0.73097300	-5.16898500	-1.10746300
C	-0.18062000	-3.57560800	0.22271000
H	-1.01703700	-2.95866300	-0.07907900
C	-1.26190600	-1.79666300	2.87570600
C	-1.85272100	-3.06599900	2.96409200
H	-1.36706500	-3.92972400	2.52565000
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H	2.95343600	2.63233300	1.26325900
C	3.42052300	4.69652900	1.57416400
H	4.22903900	4.47189900	2.26109100
C	3.11447900	6.02116500	1.26254100
H	3.69087500	6.83055900	1.69937200
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H	1.82764600	7.33286300	0.12987000
C	1.29874100	5.26901200	-0.14265200
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C	5.85156000	0.99467200	1.88970200
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H	7.19294100	3.14085600	0.73355500
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C	4.15279100	-3.11673400	-4.13111300
C	3.22986700	-5.31194400	-2.65721500
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C	4.08491600	-4.37741700	-4.72424500
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H	2.87578800	-6.16436500	-2.08826500
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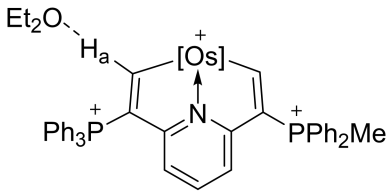

6b-1

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C	-1.52620900	-0.12603400	0.00632600
C	-1.84743300	-1.15295000	-0.81071100
C	-0.67383200	-1.73742600	-1.44673400
C	-0.60394400	-2.80692100	-2.34066700
H	-1.50727600	-3.31619000	-2.65069800
C	0.64443800	-3.21371200	-2.81176000
H	0.71810100	-4.05280200	-3.49586300
C	1.79452200	-2.54385300	-2.40293000
H	2.77348300	-2.85956200	-2.74253700
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H	2.83244800	1.05684000	0.38517900
C	1.67349600	-0.11754500	3.52961700
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H	0.17396200	0.03756000	5.07702400
C	2.03018400	0.94629800	5.67460400
H	1.65295400	1.23842200	6.64938900
C	3.34320900	1.24714800	5.31380400
H	3.98885400	1.77710300	6.00678700
C	3.82958600	0.85724200	4.06170300
H	4.85371800	1.07902300	3.77823400
C	2.99976400	0.18192400	3.17171300
H	3.39599500	-0.13373400	2.21113700
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C	2.41177100	-3.04047600	2.71959100
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C	2.21972600	-5.19524400	1.62662100
H	2.55802700	-6.21946700	1.50214800
C	1.12991900	-4.72313000	0.88919400
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C	0.67990800	-3.41880800	1.07184900
H	-0.19964300	-3.08652300	0.53911800
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C	-1.18386100	-2.58214700	3.73763500
H	-0.41675100	-3.34421400	3.66322300
C	-2.37338300	-2.86660200	4.41054000
H	-2.51839600	-3.84711900	4.85345500
C	-3.36379200	-1.89018700	4.53013800
H	-4.28395300	-2.11269900	5.06144100
C	-3.15940000	-0.62162100	3.98268700
H	-3.91955800	0.14515700	4.08490600
C	-1.97756200	-0.33247400	3.30366900
H	-1.82014600	0.66468100	2.91035100
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C	1.93147300	3.99681200	-0.19881900
H	2.39848800	3.11795900	0.22772700
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H	3.35373100	5.33053900	0.70565700
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H	2.29910400	7.37773900	-0.23148900
C	0.74045300	6.29265400	-1.24948600
H	0.27462000	7.18342100	-1.65845200
C	0.18971700	5.04027300	-1.52050300
H	-0.69946200	4.96832400	-2.13665700
C	0.91144500	1.80989200	-2.99888700
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H	3.12706100	3.07244000	-5.26347600
C	1.85293100	2.67769300	-3.57570500
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C	-2.21221900	2.38529900	-3.08531600
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H	-3.23197400	-0.32771600	-5.66340600
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C	-6.35947600	0.48793400	1.79588900
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H	4.00032300	-0.92192500	-3.84515900
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C	5.24346800	0.69077700	-0.52248400
C	6.05604000	0.33088900	0.56357300
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H	4.38102800	2.33166300	-1.65850100
C	6.40411500	2.67511400	1.05285700
H	7.28140700	1.05549600	2.17570500
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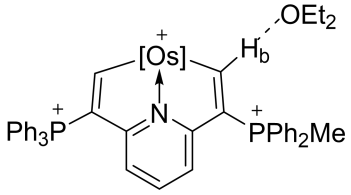

7b-1

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C	2.48661000	-0.08465400	0.60786100
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C	-0.58878100	-0.37112600	3.47231700
H	-1.42873600	-0.44583100	4.14616100
C	-0.79899200	-0.16828900	2.10497200
C	-2.05137000	-0.00531400	1.37621600
C	-1.85164200	0.06869900	0.03955200
H	-2.65685800	0.16752100	-0.69408600
C	-1.36728100	-2.95032500	-2.35585900
C	-1.04660600	-3.66619200	-3.51618700
H	-0.01151600	-3.85572000	-3.77585600
C	-2.06602600	-4.14680600	-4.34053000
H	-1.81224700	-4.69716600	-5.24075800
C	-3.40306900	-3.93650200	-4.00253100
H	-4.19150900	-4.32617300	-4.63857800
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H	-2.08532200	-4.39677600	-0.31298900
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H	1.49881500	-2.57644600	1.21254300
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H	-1.47774900	6.28757400	-3.72835500
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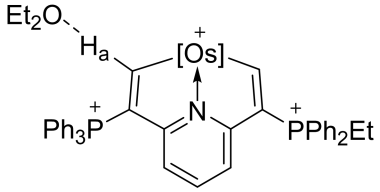

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H	1.87815200	4.31961800	-5.42270400
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H	4.23843700	4.08960500	-4.68743600
C	3.72319000	3.17500700	-2.80306700
H	4.75173200	3.07960900	-2.47079900
C	2.69155400	2.72602300	-1.98212500
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H	0.36951100	5.52857800	3.47501500
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H	-1.49793300	3.90276600	3.15262100
C	-0.78205500	3.23886200	1.24229900
H	-1.61958700	2.57386200	1.09461600
C	-1.55457200	2.89933300	-2.00595500
C	-2.16171000	4.09382100	-1.58837600
H	-1.70329900	4.70070100	-0.81633600
C	-3.35458100	4.51728700	-2.17795900
H	-3.81186700	5.44718100	-1.85408500
C	-3.94313500	3.76291500	-3.19338500
H	-4.86458800	4.10056000	-3.65688000
C	-3.33350600	2.58310000	-3.62601600
H	-3.77969200	1.99924700	-4.42398600
C	-2.14869300	2.14963200	-3.03585400
H	-1.67209700	1.24653100	-3.40073600
C	1.15993300	-3.45878700	-1.82450800
C	2.45247200	-2.96242900	-2.04355200
H	2.75403400	-1.99718900	-1.65922200
C	3.38029800	-3.71197300	-2.76240200
H	4.37037400	-3.30291300	-2.92011300
C	3.02446700	-4.96068700	-3.27560800
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C	1.74024400	-5.46360800	-3.05788100
H	1.46047900	-6.43564200	-3.45130500
C	0.81013600	-4.72127400	-2.33122400
H	-0.18015600	-5.12721500	-2.15920700
C	0.36136300	-3.18150900	0.92895800
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H	-1.33233700	-2.21978200	1.84950200
C	-0.17009700	-3.28432000	3.29909900
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C	1.76602900	-4.45209700	2.44907000
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H	2.11226900	-4.30034800	0.33245400
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C	-2.01157100	-3.06730000	-2.59591600
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H	-7.09253700	2.30222400	-2.70103500
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H	-2.44299400	-0.15985800	-1.53554700
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H	4.16608000	0.67013100	-4.39979300
H	5.01246300	-0.88033700	-4.56694400
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H	2.72229600	-2.07106800	3.74019500
C	3.80962100	-0.43717900	6.51741900
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H	3.84223000	-0.55112100	7.59631700
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H	3.15177400	2.80394700	2.21913500
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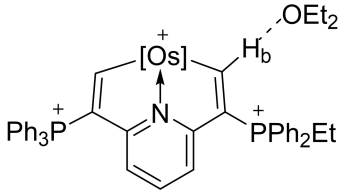

7c-1

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P	3.57907200	-1.70644900	1.13442300
N	-0.40741200	-1.07980000	1.01714500
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C	1.90469000	-1.09625400	0.88192200
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C	0.63514500	-2.72733600	2.41294100
H	1.53605000	-3.20263300	2.77885600
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H	-0.70633200	-3.96272600	3.55685700
C	-1.76828000	-2.52251700	2.36245700
H	-2.75167500	-2.85310400	2.67318500
C	-1.63540700	-1.47460600	1.44874400
C	-2.67339100	-0.66243800	0.83141800
C	-2.15789000	0.24608000	-0.02843800
H	-2.76443500	0.96715900	-0.57993100
C	-1.43753000	-0.32447800	-3.64749700
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H	0.12136200	-0.30109800	-5.14339900
C	-1.70220400	0.56655700	-5.88329400
H	-1.28467500	0.77830100	-6.86240700
C	-3.02576900	0.90174100	-5.59988000
H	-3.63974000	1.37807400	-6.35753400
C	-3.56278900	0.61651000	-4.34046900
H	-4.59504500	0.86729400	-4.11664900
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C	-1.12749600	-2.67460700	-1.94010700
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H	-2.73851700	-2.57559500	-3.37834600
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H	1.46948100	2.15633300	3.84572700
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C	5.86195100	-1.45372000	4.48421800
H	6.87919000	-1.70175100	4.76882800
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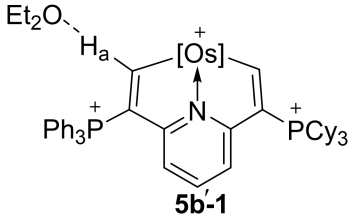

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H	1.10420300	3.03086700	4.16852000
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H	0.21000400	2.36352800	-7.04034300
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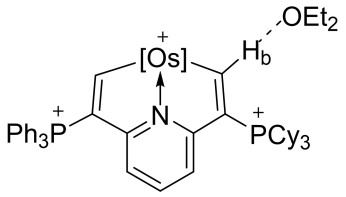

5b-1

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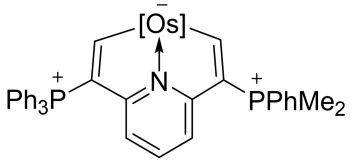

P2-6a

[Os] = $OsCl(PPh_3)_2$

E = -4715.46277896

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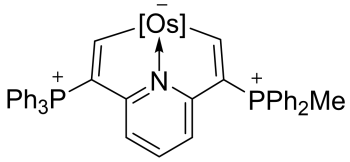
Cl	-0.96689700	-0.06565600	-3.13622800
P	-0.39892800	-2.45681200	-0.89101300
P	-1.03161300	2.22011300	-0.75165700
P	3.83665700	0.33334000	0.55243500
N	-0.07603600	-0.17498700	1.30335400
C	1.41136700	0.20915600	-0.79166200
C	2.07589600	0.18274300	0.43260800
C	1.25442000	-0.05013000	1.62180500
C	1.64871300	-0.11947700	2.96336300
H	2.69237100	-0.01723600	3.23391400
C	0.68583800	-0.33713400	3.94811400
H	0.98640400	-0.41537100	4.98836000
C	-0.65757900	-0.46518900	3.60233500
H	-1.39398700	-0.66195900	4.37226300
C	-1.03694000	-0.36113700	2.25902300
C	-2.37273200	-0.41646900	1.66491100
C	-2.45285000	-0.36812600	0.27492200
H	-3.47364600	-0.41707500	-0.11584400
C	-1.69426900	-3.32731800	-1.85196500
C	-1.54584100	-4.68292100	-2.17933200
H	-0.63242300	-5.20875500	-1.92063100
C	-2.56675500	-5.36182300	-2.84169400
H	-2.44229800	-6.41100400	-3.09356700
C	-3.74350200	-4.69185700	-3.18579200
H	-4.53638500	-5.22059500	-3.70712000
C	-3.89158500	-3.34071800	-2.87116100
H	-4.79554800	-2.81006800	-3.15645600
C	-2.87048500	-2.65761700	-2.20947600
H	-2.95822500	-1.60130700	-1.99679400
C	-0.48190400	-3.29824700	0.74288600
C	-1.66049400	-3.90966100	1.18777800
H	-2.51175800	-3.98407300	0.51908700
C	-1.73763500	-4.43910700	2.47806900
H	-2.64897100	-4.93484800	2.80239100
C	-0.64556500	-4.35283700	3.34307000
H	-0.70661100	-4.77110300	4.34386500
C	0.53156600	-3.73973300	2.90765200
H	1.39021500	-3.66349800	3.56837700
C	0.61045900	-3.21789300	1.61957400
H	1.52748200	-2.74347500	1.29556600
C	1.18214000	-3.08050500	-1.59969500
C	1.79676000	-4.26560300	-1.16850200
H	1.34069100	-4.86069900	-0.38443700
C	3.00891800	-4.67629800	-1.72808200
H	3.47550200	-5.59676100	-1.38766700
C	3.61576400	-3.90912100	-2.72434300
H	4.56074200	-4.22721500	-3.15583200
C	2.99593800	-2.74063900	-3.17355300
H	3.45673100	-2.14391700	-3.95446700
C	1.78509100	-2.32728900	-2.61860800
H	1.29181100	-1.42889500	-2.97550800
C	-2.40679300	2.78146900	-1.82406500
C	-3.45094000	1.90317700	-2.13592500
H	-3.37978900	0.86891800	-1.83063900
C	-4.54998400	2.35197000	-2.86823200
H	-5.34902300	1.65876400	-3.11494900
C	-4.61036000	3.67709900	-3.30312200
H	-5.46189200	4.02295500	-3.88214500
C	-3.56439400	4.55475400	-3.00745400
H	-3.60127400	5.58384700	-3.35267200
C	-2.46633800	4.10925700	-2.27229200
H	-1.65583900	4.79438100	-2.04364100
C	-1.47239700	2.99496400	0.86847900
C	-0.62573400	2.80410200	1.97163300
H	0.27451300	2.21673400	1.85733600
C	-0.92888000	3.35146000	3.21687000
H	-0.25458000	3.18557200	4.05223600
C	-2.09670100	4.09828600	3.38732800
H	-2.33568500	4.52919200	4.35532500
C	-2.95439300	4.28789400	2.30194600
H	-3.86219800	4.87300000	2.42071000
C	-2.64470500	3.74274200	1.05257300
H	-3.31065400	3.91641800	0.21511300
C	0.38498800	3.23540700	-1.34551700
C	0.81696700	3.00723500	-2.66398200
H	0.31036500	2.26179900	-3.27024000
C	1.89144500	3.72715100	-3.18079500
H	2.20338800	3.55645100	-4.20719900
C	2.56734700	4.65913200	-2.38603800
H	3.40564200	5.21880300	-2.79178100
C	2.15831300	4.86892300	-1.06913600
H	2.67950000	5.58682300	-0.44219600
C	1.06248900	4.16959100	-0.55421800
H	0.73354500	4.36752400	0.45985800
C	4.35220900	1.83359400	1.42862700
C	5.71469600	2.15386800	1.54510400
H	6.47028500	1.48394000	1.14489500
C	6.09615500	3.34538100	2.15721000
H	7.14925800	3.59281900	2.24748800
C	5.12399000	4.22659400	2.64089300
H	5.42551700	5.15730200	3.11189300
C	3.76953700	3.91893200	2.50780500
H	3.01267100	4.60837200	2.86960300
C	3.38137400	2.72483100	1.90089900
H	2.33196500	2.49325900	1.77445000
C	4.49100700	-1.13300900	1.39283500
C	4.07665200	-2.37982900	0.89456000
H	3.43198700	-2.43653000	0.02341800
C	4.48760500	-3.55037300	1.52675700
H	4.16290900	-4.50812600	1.13331400
C	5.30187500	-3.48420800	2.66066900
H	5.61617900	-4.39745400	3.15685900
C	5.71017400	-2.24558700	3.15888700
H	6.33992700	-2.19408700	4.04173500

C	5.30819000	-1.06737700	2.52770600
H	5.61764700	-0.10692100	2.92557100
C	4.56704600	0.45204500	-1.09473900
C	5.29622600	-0.59914900	-1.66239900
H	5.45310600	-1.52048900	-1.11472400
C	5.81931700	-0.45856100	-2.94807800
H	6.38723300	-1.27280300	-3.38744600
C	5.61122300	0.71990100	-3.66531600
H	6.01763900	0.82347500	-4.66688900
C	4.88427600	1.76926400	-3.09593300
H	4.71775500	2.68652600	-3.65058000
C	4.36596400	1.64344700	-1.81085900
H	3.80339900	2.46201800	-1.37476000
H	2.02806300	0.41015300	-1.67177300
P	-3.83548700	-0.41383200	2.66180100
C	-3.82373400	0.91668700	3.91276400
H	-4.76815200	0.90861200	4.46446400
H	-2.99095600	0.79177100	4.60659600
H	-3.70099100	1.87651100	3.40552900
C	-4.09559200	-1.97576100	3.56732800
H	-4.98017700	-1.92151500	4.20822500
H	-4.19596800	-2.79465100	2.85204800
H	-3.21045900	-2.17988300	4.17516700
C	-5.26299700	-0.10176100	1.60431200
C	-6.25935900	-1.06457900	1.40322100
C	-5.33649400	1.13535400	0.94143000
C	-7.32285400	-0.79124000	0.54159100
H	-6.21110100	-2.02610700	1.90298900
C	-6.39714100	1.39853200	0.08036300
H	-4.55286200	1.87459200	1.07284100
C	-7.39042100	0.43538100	-0.11990200
H	-8.09348300	-1.53937900	0.38489800
H	-6.43539000	2.34519200	-0.44823900
H	-8.21587800	0.64107000	-0.79456500



P2-6b

[Os] = $OsCl(PPh_3)_2$

E = -4907.31989416

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P	0.35823500	2.60347000	0.44887600
P	-3.92151600	-0.28941400	-1.00774500
N	0.09176200	-0.30568200	-1.08459900
C	-1.75826600	0.27583200	0.64117500
C	-2.20164700	-0.11756400	-0.61915200
C	-1.17217500	-0.46157600	-1.60130300
C	-1.32456700	-0.88015800	-2.92863600
H	-2.31268800	-1.00636000	-3.35345200
C	-0.19065300	-1.15318400	-3.69511600
H	-0.30247700	-1.50501600	-4.71608300
C	1.08214200	-0.98225200	-3.15518200
H	1.96143700	-1.22776000	-3.73957500
C	1.21246300	-0.52544200	-1.83741000
C	2.42805900	-0.21976200	-1.08575700
C	2.27203900	0.13230200	0.25441400
H	3.21352100	0.36815300	0.76049700
C	1.43945900	-2.29124300	3.09633200
C	1.23479000	-3.39473900	3.93604300
H	0.35677700	-4.01952100	3.80866100
C	2.15460600	-3.69315700	4.94093900
H	1.98557800	-4.54769900	5.58971500
C	3.28482500	-2.89215700	5.11538700
H	3.99813300	-3.12274300	5.90147700
C	3.48842600	-1.78766800	4.28644700
H	4.35537300	-1.14939400	4.43171900
C	2.56767600	-1.48369400	3.28471600
H	2.69654400	-0.60785900	2.66409100
C	0.75869500	-3.24226600	0.47853300
C	1.88215900	-4.06332900	0.63625400
H	2.51928500	-3.94631400	1.50550700
C	2.17280200	-5.05214200	-0.30797600
H	3.03736400	-5.69342500	-0.16044700
C	1.35628100	-5.22135000	-1.42698500
H	1.57988600	-5.99535000	-2.15595400
C	0.24270500	-4.39479200	-1.60040100
H	-0.40224700	-4.51207600	-2.46643900
C	-0.05354300	-3.41891000	-0.65300600
H	-0.93300300	-2.80349000	-0.78662400
C	-1.32503700	-2.57695100	2.31766900
C	-1.76714200	-3.88829800	2.09073000
H	-1.14315700	-4.58563200	1.54237600
C	-3.01682100	-4.30353700	2.55901900
H	-3.34956700	-5.32163700	2.37591700
C	-3.83020800	-3.41573000	3.26387400
H	-4.80281900	-3.73800300	3.62529300
C	-3.38288100	-2.11599600	3.51471200
H	-4.00758700	-1.42193200	4.06812900
C	-2.13882000	-1.69625400	3.04757900
H	-1.78288900	-0.69130000	3.25058300
C	1.44876200	3.60837900	1.52539800
C	2.54940100	3.01516600	2.15424600
H	2.68664700	1.94577200	2.08288100
C	3.43228700	3.79263400	2.90361500
H	4.27526000	3.31899200	3.39837000
C	3.21878800	5.16540500	3.03897500
H	3.90122200	5.76790700	3.63165900
C	2.11433700	5.76122800	2.42525000
H	1.93691200	6.82696300	2.53623200
C	1.23173800	4.98643800	1.67329200
H	0.37397200	5.45312800	1.19907400
C	0.91132500	3.11678400	-1.24095000
C	0.29799600	2.54031700	-2.36446900
H	-0.46577900	1.78864200	-2.22737300
C	0.65437300	2.92175800	-3.65695200
H	0.15973400	2.45872700	-4.50623200
C	1.64525500	3.88580200	-3.85374600
H	1.92401000	4.18888700	-4.85875200
C	2.27916400	4.45325100	-2.74678200
H	3.05144100	5.20440900	-2.88726500
C	1.91630700	4.07287100	-1.45137900
H	2.40318700	4.54001000	-0.60310400
C	-1.26924100	3.45125100	0.62452100
C	-1.85600600	3.44225000	1.90237400
H	-1.34029700	2.95181600	2.72267800
C	-3.09230300	4.05013500	2.10797100
H	-3.52614700	4.05297000	3.10390000
C	-3.77283700	4.64960600	1.04284600
H	-4.73700500	5.12319800	1.20626800

C	-3.20645600	4.63723300	-0.23169700
H	-3.72914700	5.09371800	-1.06744200
C	-1.95360100	4.05179300	-0.43808600
H	-1.51134200	4.07925200	-1.42746600
C	-4.48107000	0.90590300	-2.24950500
C	-5.84201900	0.99375500	-2.58476600
H	-6.56270600	0.32310000	-2.12568800
C	-6.27078000	1.96030600	-3.49145700
H	-7.32278000	2.02859300	-3.75040300
C	-5.35007700	2.84948000	-4.05466000
H	-5.68960400	3.60565100	-4.75603200
C	-4.00052300	2.77546900	-3.70770200
H	-3.28580100	3.47398900	-4.13241400
C	-3.56430700	1.80653300	-2.80461200
H	-2.52285600	1.76079800	-2.51524900
C	-4.21059600	-1.97939600	-1.59381400
C	-3.66374600	-3.01223500	-0.81437400
H	-3.13627400	-2.78437200	0.10588500
C	-3.79309800	-4.33535300	-1.22782600
H	-3.36620100	-5.12684200	-0.62008200
C	-4.45824500	-4.63294700	-2.42039500
H	-4.55284800	-5.66448100	-2.74608600
C	-4.99955500	-3.60625900	-3.19674600
H	-5.51342100	-3.83802600	-4.12458700
C	-4.87898100	-2.27743200	-2.78723100
H	-5.28840900	-1.48146200	-3.40005900
C	-4.93321600	0.01230800	0.45594000
C	-5.61384300	-1.02071400	1.10989300
H	-5.54888100	-2.03949300	0.74683800
C	-6.37373000	-0.73340500	2.24413400
H	-6.90419700	-1.53382400	2.75048900
C	-6.44523000	0.57295500	2.72833600
H	-7.03470200	0.79089800	3.61387700
C	-5.76255800	1.60309000	2.07450600
H	-5.81217400	2.61991500	2.44953400
C	-5.01269500	1.33026200	0.93483300
H	-4.48982500	2.13445800	0.42849200
H	-2.53423600	0.55178400	1.35978300
P	3.98446300	-0.02808900	-1.90917200
C	3.84733500	1.13160500	-3.31178800
H	3.53740100	2.10897100	-2.93777800
H	4.80814000	1.22180500	-3.82486800
H	3.08824900	0.77715500	-4.01072800
C	5.17700300	0.68882100	-0.75863600
C	6.22081700	-0.08083300	-0.23045000
C	5.00223300	2.02037100	-0.34616100
C	7.08891300	0.48309900	0.70532200
H	6.35091800	-1.11145100	-0.54284700
C	5.87124700	2.57404000	0.58931100
H	4.17546400	2.61132900	-0.72724600
C	6.91477100	1.80611400	1.11422000
H	7.89775700	-0.11307600	1.11605700
H	5.72042900	3.59600200	0.92071400
H	7.59041000	2.23969000	1.84537500
C	4.64896500	-1.57605800	-2.56538000
C	5.79386400	-1.57195300	-3.37961500
C	4.01311700	-2.78395600	-2.24923200
C	6.29673500	-2.77207700	-3.87442200
H	6.29902600	-0.63983700	-3.61602700
C	4.52044800	-3.98075300	-2.75608300
H	3.13298100	-2.78898900	-1.61531800
C	5.65676100	-3.97625600	-3.56517000
H	7.18375800	-2.76986500	-4.50024600
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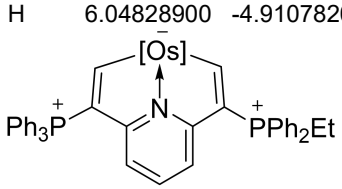
H	6.04828900	-4.91078200	-3.95573000



P2-6c

[Os] = $OsCl(PPh_3)_2$

Os	0.09340600	-0.15178200	-1.09720600
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P	-0.06352600	-2.51353700	-1.18318000
P	-3.86245500	0.40614400	1.21997200
N	0.12870600	0.01127500	0.92168200
C	-1.90912700	0.00975800	-0.70456900
C	-2.20672900	0.14827100	0.64677800
C	-1.07058200	0.16755600	1.57338700
C	-1.08742000	0.29458500	2.96501500
H	-2.02492800	0.40369700	3.49609800
C	0.12219700	0.29907900	3.65714600
H	0.12660400	0.42104100	4.73608400
C	1.32918700	0.16458100	2.97840500
H	2.25421200	0.19371200	3.52929800
C	1.32713800	-0.00320000	1.58723900
C	2.43809400	-0.25356900	0.65909600
C	2.11801000	-0.37529700	-0.69126900
H	2.96315500	-0.65622400	-1.33660600
C	1.60182500	2.79050300	-2.55072900
C	1.82798900	4.16330300	-2.73007400
H	1.23574600	4.88810700	-2.18063500
C	2.81613000	4.60606600	-3.60704100
H	2.98483700	5.67099800	-3.73780700
C	3.58188400	3.68057400	-4.32244600
H	4.34484600	4.02637900	-5.01427700
C	3.35132900	2.31377300	-4.15885700
H	3.92926100	1.59101200	-4.72773600
C	2.36438200	1.86794400	-3.27683200
H	2.15260000	0.81232800	-3.16799800
C	0.96563900	2.95867800	0.23849400
C	2.31858500	3.25516200	0.43857800
H	3.01565500	3.17860900	-0.38454000
C	2.78034900	3.66592500	1.69074800
H	3.83501700	3.89405000	1.82141500
C	1.89184000	3.79936700	2.75784600
H	2.24945100	4.12328400	3.73116200
C	0.53607400	3.52419400	2.56329000
H	-0.17002400	3.62479600	3.38227600
C	0.08115300	3.10112700	1.31819100
H	-0.96780600	2.87442000	1.18692700
C	-1.15142600	3.18422900	-1.69321500
C	-1.35308200	4.47724000	-1.18681200
H	-0.59763900	4.94035900	-0.56096500
C	-2.53788000	5.16500600	-1.45680100
H	-2.68216200	6.16656800	-1.06058300
C	-3.53223200	4.56838000	-2.23509500
H	-4.45625400	5.10203400	-2.43947300
C	-3.32763200	3.29033100	-2.75967800
H	-4.09200400	2.82260500	-3.37246300
C	-2.14379600	2.60100000	-2.49541700

H	-1.97463200	1.61465600	-2.91459100
C	0.78372100	-3.36724900	-2.56468000
C	1.84513300	-2.74024700	-3.22819400
H	2.08190000	-1.71279000	-2.98873100
C	2.54943600	-3.41871200	-4.22251000
H	3.36200900	-2.91972400	-4.74286400
C	2.19397600	-4.72346900	-4.56822300
H	2.73766200	-5.24743400	-5.34902300
C	1.12793400	-5.34993000	-3.91875000
H	0.84118600	-6.36148200	-4.19112200
C	0.42463600	-4.67513700	-2.92145800
H	-0.40321500	-5.16564300	-2.41881800
C	0.64663200	-3.37069000	0.29419000
C	0.22016200	-2.99649000	1.57856500
H	-0.54728800	-2.24342600	1.68972500
C	0.78409500	-3.56366500	2.71942000
H	0.44266700	-3.24365500	3.69949600
C	1.78902800	-4.52637400	2.59814000
H	2.22485700	-4.97870400	3.48483600
C	2.21853400	-4.91356300	1.32729800
H	2.99083600	-5.67045900	1.21990700
C	1.65437000	-4.33934400	0.18457600
H	2.00185700	-4.64952700	-0.79376600
C	-1.77508200	-3.17720200	-1.30474900
C	-2.49327700	-2.85412100	-2.46945000
H	-2.02776700	-2.23156600	-3.22855800
C	-3.79081800	-3.32920000	-2.64262300
H	-4.32790700	-3.09326000	-3.55680000
C	-4.40101100	-4.10046000	-1.64746000
H	-5.41396800	-4.46870900	-1.78482500
C	-3.70216900	-4.39678800	-0.47729500
H	-4.16980500	-4.98982200	0.30350100
C	-2.38778500	-3.94894800	-0.31197700
H	-1.84074600	-4.21811300	0.58502700
C	-4.44980900	-0.93959500	2.28235200
C	-5.76537600	-0.93289000	2.77388100
H	-6.42617400	-0.09870200	2.55624000
C	-6.22922500	-2.00935400	3.52606900
H	-7.24606700	-2.00419200	3.90611000
C	-5.39075700	-3.09968200	3.77865200
H	-5.75804800	-3.93959000	4.36061000
C	-4.08979900	-3.11613900	3.27466100
H	-3.44184300	-3.96790500	3.45819600
C	-3.61770100	-2.03907600	2.52489700
H	-2.61711500	-2.05773300	2.11286500
C	-3.94406200	1.97996100	2.11657600
C	-3.45966800	3.11635800	1.44674300
H	-3.09859400	3.04118300	0.42594100
C	-3.42886800	4.34611200	2.09922000
H	-3.05220400	5.21659600	1.57217600
C	-3.86863200	4.44764700	3.42177100
H	-3.83767800	5.40578000	3.93170300
C	-4.34509600	3.31826700	4.09000800
H	-4.68338600	3.39592000	5.11870700
C	-4.38571600	2.08324200	3.44120100
H	-4.74649100	1.20650500	3.96813700
C	-5.00402400	0.45851000	-0.17942700
C	-5.60204500	1.64748300	-0.61340400
H	-5.40537000	2.58272300	-0.10405000
C	-6.45669800	1.62661500	-1.71576200
H	-6.92138300	2.54881800	-2.05069300
C	-6.71181900	0.42840500	-2.38340500
H	-7.37619500	0.41728700	-3.24219800
C	-6.11770700	-0.75851000	-1.94589400
H	-6.31197800	-1.69252100	-2.46207200
C	-5.26844100	-0.75013400	-0.84374200
H	-4.80986400	-1.67475400	-0.51042800
H	-2.75953100	-0.01312100	-1.39111900
P	4.12987900	-0.56033100	1.10786900
C	4.42690100	-0.58697400	2.89091500
C	4.76650300	0.59246300	3.57125800
C	4.18290800	-1.76531200	3.61201900
C	4.86827900	0.58719300	4.96107800
H	4.92984900	1.51101500	3.01815700
C	4.28756900	-1.76245400	5.00169000
H	3.88208400	-2.67316800	3.10031400
C	4.63033400	-0.58888600	5.67656500
H	5.13020000	1.50096600	5.48539400
H	4.09801500	-2.67560400	5.55740500
H	4.71027600	-0.58981800	6.75936700
C	5.27282600	0.65426500	0.38319100
C	6.57474600	0.79002400	0.89480500
C	4.88984900	1.40291600	-0.73742900
C	7.46827300	1.67879200	0.29887600
H	6.88719500	0.21647800	1.76113700
C	5.78840300	2.28780700	-1.33167900
H	3.89344500	1.30564400	-1.14633600
C	7.07585800	2.42978000	-0.81189700
H	8.47017400	1.78456500	0.70349100
H	5.46990200	2.86106700	-2.19667000
H	7.77468800	3.12252400	-1.27106400
C	4.60866700	-2.20669300	0.44924300
H	3.89561700	-2.92400300	0.86687300
H	4.39853000	-2.16454600	-0.62430900
C	6.05900000	-2.61639200	0.71402400
H	6.23895700	-3.61277800	0.29879300
H	6.76306100	-1.92460000	0.24327600
H	6.27956200	-2.65400700	1.78539000

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