Supplementary Information

Synthesis and Characterization of Metallapentalenoxazetes from the [2+2] Cycloaddition of Metallapentalynes with Nitrosoarenes

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Contents

1. General Information

Unless otherwise stated, all manipulations were carried out under an inert atmosphere (N_2) using standard Schlenk techniques or a glovebox. Nitrogen was purified by passing through columns of supported P_2O_5. Solvents were distilled from sodium/benzophenone (hexane and diethyl ether) or calcium hydride (dichloromethane) under N_2 prior to use. The metallopentalyne **1**[1] and **A**[2] were synthesized according to previously published procedures. All other reagents were used as received from commercial sources without further purification. Column chromatography was performed on silica gel (200-300 mesh) in air. NMR spectroscopic experimentals was recorded using a Bruker Advance II 400 spectrometer (^{1}H, 400.1 MHz; ^{13}C, 100.6 MHz; ^{31}P, 162.0 MHz), a Bruker Advance III 500 spectrometer (^{1}H, 500.2 MHz; ^{13}C, 125.8 MHz; ^{31}P, 202.5 MHz) or a Bruker Ascend III 600 spectrometer (^{1}H, 600.1 MHz; ^{13}C, 150.9 MHz; ^{31}P, 242.9 MHz) at room temperature. The ^{1}H and ^{13}C{^{1}H} NMR chemical shifts (δ) are relative to tetramethylsilane, and the ^{31}P{^{1}H} NMR chemical shifts are relative to 85% H_3PO_4. The absolute values of the coupling constants are given in hertz (Hz). Two-dimensional and one-dimensional NMR are abbreviated as heteronuclear single quantum coherence (HSQC), heteronuclear multiple bond correlation (HMBC), and distortionless enhancement by polarization transfer (DEPT). The multiplicities are abbreviated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad). Elemental analyses were performed on a Vario EL III elemental analyzer. High-resolution mass spectrometry (HRMS) was conducted using a Bruker En Apex-Ultra 7.0 T FT-MS instrument. Absorption spectra were recorded on a SHIMADZU UV2550 ultraviolet–visible spectrophotometer. CV was performed with a CHI660E electrochemical workstation in anhydrous acetonitrile containing nBu$_4$NPF$_6$ (0.1 M) as supporting electrolyte. All potentials were recorded versus Ag/AgCl (saturated) as a reference electrode. The scan rate was 0.1 Vs^{-1}.

2. Theoretical Calculations

Computational Methods

All of the structures were optimized at the B3LYP/6-31+G(d) level of DFT with a double-ζ valence (LanL2DZ) basis set to describe P, Cl, and Os atoms[3],[4],[5]. In all calculations, the effective core potentials (ECPs) of Hay and Wadt with polarization functions were added for P (ζ(d) = 0.34), S (ζ(d) = 0.421), Cl (ζ(d) = 0.514), and Os (ζ(f) = 0.886)[6]. In TD-DFT calculations, a PCM model with a solvent of acetonitrile was used[7]. The frequency calculations were performed to confirm the characteristics of the calculated structures as minima. All the optimizations were performed with the Gaussian 09 software package[8].

Results

Table S1. Orbital distributions in HOMO/LUMO and energy levels of **2-4**, and **6**.

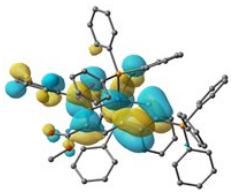
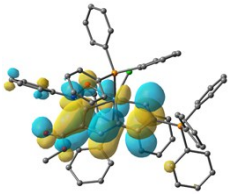
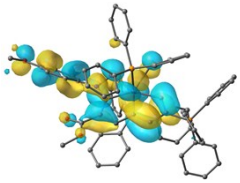
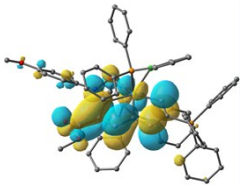
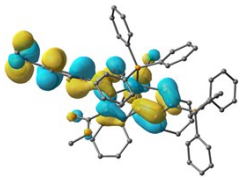
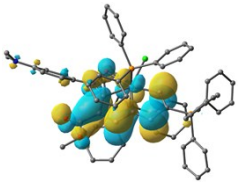
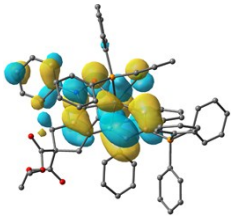
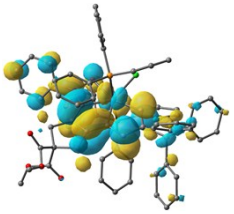
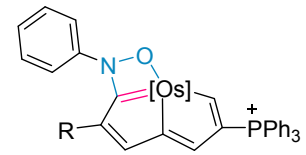
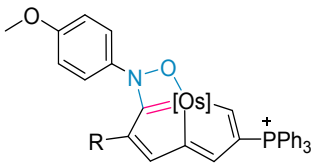
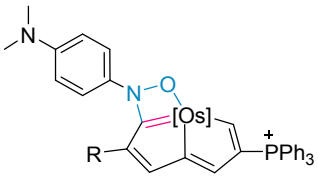
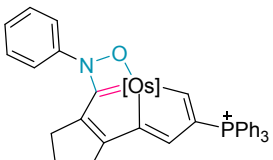
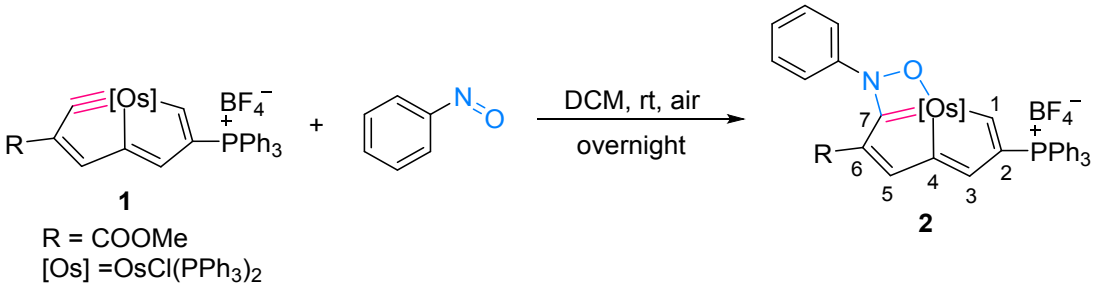
Compound (ΔE)	**HOMO** (Energy level)	**LUMO** (Energy level)
2		
(2.94 eV)	(-7.15 eV)	(-4.21 eV)
3		
(2.86 eV)	(-7.01 eV)	(-4.15 eV)
4		
(2.5 eV)	(-6.52 eV)	(-4.02 eV)
6		
(3.18 eV)	(-6.93 eV)	(-3.75 eV)

Table S2. TD-DFT calculations of the first excited states for **2**, **3**, **4** and **6**.

Compound	λ_{max} Calc.(Exp.) [nm]	f	Excitation	percentage (%)
 R = COOMe [Os] =$OsCl(PPh_3)_2$ **2**	511.0 (507.1)	0.1180	HOMO→LUMO	90.9%
 R = COOMe [Os] =$OsCl(PPh_3)_2$ **3**	525.0 (509.6)	0.1407	HOMO→LUMO	93.3%
 R = COOMe [Os] =$OsCl(PPh_3)_2$ **4**	531.7 (513.3)	0.1884	HOMO→LUMO	97.6%
 R = COOMe [Os] = $OsCl(PPh_3)_2$ **6**	455.8 (468.4)	0.1134	HOMO→LUMO HOMO→LUMO+4	63.3% 23.8%

3. Synthesis of Metal Complexes.

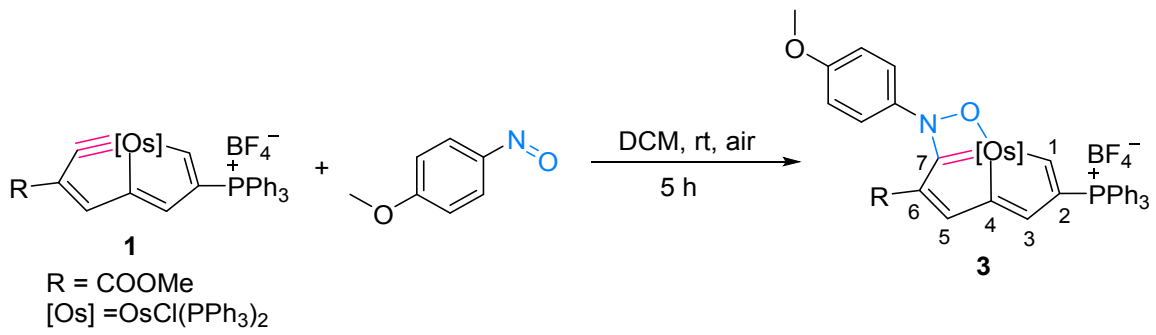
Preparation of complex 2:



A mixture of **1** (249 mg, 0.2 mmol) and nitrosobenzene (107 mg, 1.0 mmol) in dichloromethane (10 mL) was stirred overnight at room temperature under air atmosphere to give a red solution. The solution was evaporated under vacuum to a volume of ca. 2 mL, then diethyl ether (20 mL) was added to the solution to give a red precipitate. The precipitate was collected by filtration, washed with diethyl ether (2 × 5 mL) and dried under vacuum to give **2** (246 mg, 91%) as a red solid.

^{1}H NMR plus HSQC (500.1 MHz, CD_2Cl_2): δ = 12.65 (d, J(PH) = 16.0 Hz, 1H, H1), 7.70 (d, J(PH) = 2.6 Hz, 1H, H3), 7.49 (s, 1H, H5), 3.09 (s, 3H, COOCH_3), 7.76–6.52 ppm (m, other aromatic protons). ^{31}P NMR (202.4 MHz, CD_2Cl_2): δ = 10.84 (s, CPPh$_3$), –14.87 ppm (s, OsPPh$_3$). ^{13}C NMR plus DEPT-135 and HSQC (125.7 MHz, CD_2Cl_2): δ = 210.93 (m, C1), 178.04 (d, J(PC) = 23.3 Hz, C4), 173.30 (t, J(PC) = 5.5 Hz, C7), 163.44 (s, C5), 159.88 (s, COOCH$_3$, confirmed by HMBC), 146.24 (d, J(PC) = 20.5 Hz, C3), 144.69 (s, C6), 118.92 (d, J(PC) = 89.1 Hz, C2), 50.06 (s, COOCH$_3$), 134.02–122.16 ppm (m, other aromatic carbon atoms). HRMS (ESI): (m/z) calcd for [M]$^+$ requires 1266.2767, found 1266.2775. Anal. Calcd (%) for $C_{69}H_{56}BClF_4NO_3OsP_3$: C 61.27, H 4.17, N 1.04; Found: C 61.53, H 4.09, N 1.10.

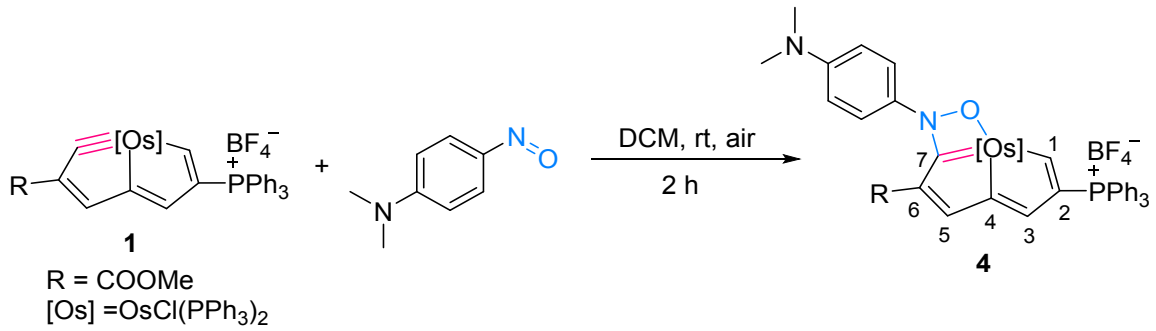
Preparation of complex 3:



A mixture of **1** (249 mg, 0.2 mmol) and 4-methoxy-nitrosobenzene (55 mg, 0.4 mmol) in dichloromethane (10 mL) was stirred at room temperature under air atmosphere for 5 h to give a red solution. The solution was evaporated under vacuum to a volume of ca. 2 mL, and then diethyl ether (20 mL) was added to the solution to afford a red solid. The solid was purified by column chromatography (neutral alumina, eluent: dichloromethane/acetone = 5:1) to yield complex **3** (227 mg, 82%) as a red solid.

^{1}H NMR plus HSQC (500.1 MHz, CD_2Cl_2): δ (ppm) = 12.62 (d, J(PH) = 15.4 Hz, 1H, H1), 7.65 (d, J(PH) = 1.8 Hz, 1H, H3), 7.42 (s, 1H, H5), 3.78 (s, 3H, CH_3O), 3.21 (s, 3H, COOCH_3), 7.85–6.49 (m, other aromatic protons). ^{31}P NMR (202.4 MHz, CD_2Cl_2): δ (ppm) = 10.89 (s, CPPh$_3$), –14.82 (s, OsPPh$_3$). ^{13}C NMR plus DEPT-135 and HSQC (125.7 MHz, CD_2Cl_2): δ (ppm) = 210.98 (m, C1), 177.83 (d, J(PC) = 22.6 Hz, C4), 172.65 (t, J(PC) = 5.3 Hz, C7), 163.13 (s, C5), 159.88 (s, COOCH$_3$, confirmed by HMBC), 145.91 (d, J(PC) = 20.6 Hz, C3), 138.50 (s, C6), 118.96 (d, J(PC) = 89.3 Hz, C2), 54.79 (s, CH$_3$O), 50.14 (s, COOCH$_3$), 132.97–112.15 (m, other aromatic carbon atoms). HRMS (ESI): (*m/z*) calcd for $[M]^+$ requires 1296.2877, found 1296.2835. Anal. Calcd (%) for $C_{70}H_{58}BClF_4NO_4OsP_3$: C 60.81, H 4.23, N 1.01; Found: C 61.20, H 4.09, N 1.08.

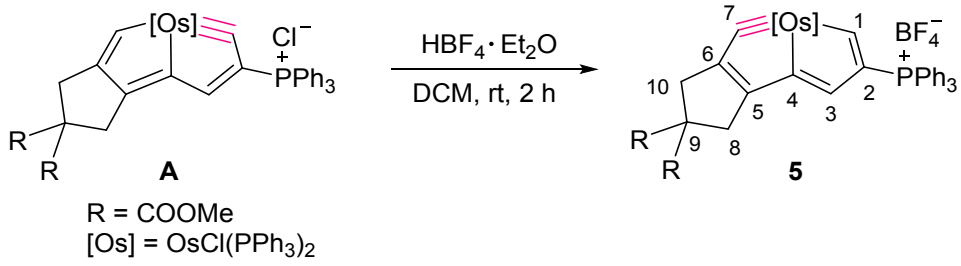
Preparation of complex 4:



A mixture of **1** (249 mg, 0.2 mmol) and N, N-dimethyl-4-nitroso-Benzenamine (60 mg, 0.4 mmol) in dichloromethane (10 mL) was stirred at room temperature under air atmosphere for 2 h to give a red solution. The solution was evaporated under vacuum to a volume of ca. 2 mL, and then diethyl ether (20 mL) was added to the solution to afford a red solid. The solid was purified by column chromatography (neutral alumina, eluent: dichloromethane/acetone = 4:1) to yield complex **4** (237 mg, 85%) as a deep red solid.

^{1}H NMR plus HSQC (600.1 MHz, CD_2Cl_2): δ (ppm) = 12.57 (d, J(PH) = 16.3 Hz, 1H, H1), 7.58 (d, J(PH) = 2.5 Hz, 1H, H3), 7.33 (s, 1H, H5), 3.13 (s, 3H, COOCH_3), 2.87 (s, 6H, (CH_3)$_2$N), 7.76–6.31 (m, other aromatic protons). ^{31}P NMR (242.9 MHz, CD_2Cl_2): δ (ppm) = 10.72 (s, CPPh$_3$), –15.11 (s, OsPPh$_3$). ^{13}C NMR plus DEPT-135 and HSQC (150.9 MHz, CD_2Cl_2): δ (ppm) = 211.21 (m, C1), 177.56 (d, J(PC) = 23.8 Hz, C4), 171.36 (t, J(PC) = 5.5 Hz, C7), 162.36 (s, C5), 159.90 (s, COOCH$_3$, confirmed by HMBC), 145.19 (d, J(PC) = 21.2 Hz, C3), 134.58 (s, C6), 118.97 (d, J(PC) = 88.7 Hz, C2), 50.12 (s, COOCH$_3$), 39.27 (s, (CH$_3$)$_2$N), 133.01–109.27 (m, other aromatic carbon atoms). HRMS (ESI): (m/z) calcd for $[M]^+$ requires 1309.3188, found 1309.3158. Anal. Calcd (%) for $C_{71}H_{61}BClF_4N_2O_3OsP_3$: C 61.10, H 4.41, N 2.01; Found: C 60.75, H 4.63, N 2.16.

Preparation of stating material 5:

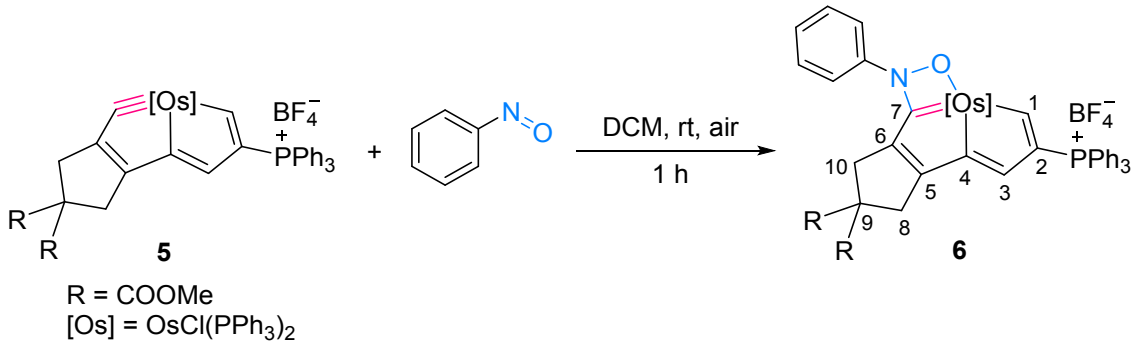


Complex **A** was synthesized according to the literature method previously reported by our group.[2] A solution of $HBF_4 \cdot Et_2O$ (340 μL, 2 mmol) was added to a solution of **A** (258 mg, 0.2 mmol) in dichloromethane (10 mL). The mixture was stirred at room temperature under dinitrogen atmosphere for 2 h to give a brown solution. The solution was evaporated under vacuum to a volume of ca. 2 mL, and then diethyl ether (20 mL) was added to the solution to afford a brown solid. The solid was collected by filtration, washed with diethyl ether (2 × 5 mL) and dried under vacuum to yield complex **5** (255 mg, 95%).

^{1}H NMR plus HSQC (600.1 MHz, CD_2Cl_2): δ (ppm) = 12.87 (d, J(PH) = 17.4 Hz, 1H, H1), 8.15 (s, 1H, H3), 3.56 (s, 6H, COOCH_3), 2.99 (s, 2H, H10), 2.18 (s, 2H, H8), 7.79–6.87 (m, other aromatic protons). ^{31}P NMR (242.9 MHz, CD_2Cl_2): δ (ppm) = 13.80 (s, CPPh$_3$), 6.69 (s, OsPPh$_3$). ^{13}C NMR plus DEPT-135 and HSQC (150.9 MHz, CD_2Cl_2): δ (ppm) = 317.26 (m, C7), 218.53 (m, C1), 182.46 (s, C5), 173.44 (d, J(PC) = 19.3 Hz, C4), 169.44 (s, COOCH$_3$,

confirmed by HMBC), 162.21 (s, C6), 138.37 (d, *J*(PC) = 21.9 Hz, C3), 131.74 (d, *J*(PC) = 72.1 Hz, C2), 63.99 (s, C9), 52.35 (s, COO*C*H$_3$), 37.65 (s, C8), 31.96 (s, C10), 134.29–126.93 (m, other aromatic carbon atoms). HRMS (ESI): (*m/z*) calcd for [M]$^+$ requires 1257.2763, found 1257.2790.

Preparation of complex 6:



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

A mixture of **5** (269 mg, 0.2 mmol) and nitrosobenzene (43 mg, 0.4 mmol) in dichloromethane (10 mL) was stirred at room temperature under air atmosphere for 2 h to give an orange solution. The solution was evaporated under vacuum to a volume of ca. 2 mL, and then diethyl ether (20 mL) was added to the solution to afford an orange solid. The solid was purified by flash column chromatography (silica gel, eluent: dichloromethane/acetone = 4:1) to yield **6** (255 mg, 88%) as an orange solid.

^{1}H NMR plus HSQC (600.1 MHz, CD_2Cl_2): δ (ppm) = 12.31 (d, *J*(PH) = 16.0 Hz, 1H, H1), 7.13 (s, 1H, H3), 3.73 (s, 6H, COOC*H*$_3$), 3.07 (s, 2H, H10), 2.53 (s, 2H, H8), 7.76–6.67 (m, other aromatic protons). ^{31}P NMR (242.9 MHz, CD_2Cl_2): δ (ppm) = 11.01 (s, C*P*Ph$_3$), –10.72 (s, Os*P*Ph$_3$). ^{13}C NMR plus DEPT-135 and HSQC (150.9 MHz, CD_2Cl_2): δ (ppm) = 205.10 (m, C1), 174.63 (s, C5), 171.81 (d, *J*(PC) = 23.4 Hz, C4), 170.31 (s, *C*OOCH$_3$, confirmed by HMBC), 165.41 (t, *J*(PC) = 5.5 Hz, C7), 139.32 (s, C6), 136.44 (d, *J*(PC) = 20.2 Hz, C3), 121.20 (d, *J*(PC) = 80.1 Hz, C2), 63.83 (s, C9), 52.69 (s, COO*C*H$_3$), 35.68 (s, C10), 34.75 (s, C8), 142.56–118.94 (m, other aromatic carbon atoms). HRMS (ESI): (*m/z*) calcd for [M]$^+$ requires 1364.3135, found 1364.3120. Anal. Calcd (%) for $C_{74}H_{62}BClF_4NO_5OsP_3$: C 61.27, H 4.31, N 0.97; Found: C 61.58, H 4.17, N 1.13.

4. X-ray Crystallographic Analysis

Single-crystal X-ray diffraction data were collected on a Rigaku R-AXIS SPIDER IP CCD Area Detector with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) or a Rigaku XtaLAB Synergy-S diffractometer coupled to a RigakuHypix detector with Cu Kα radiation (λ = 1.54184 Å). All data were corrected for absorption effects using the multi-scan technique. The structures were solved by Patterson methods, expanded by difference Fourier syntheses and refined by full-matrix least-squares refinement of F^2 using the 2014 version of the program SHELXL[9]. Non-H atoms were refined anisotropically unless otherwise stated. The 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 layered with hexane. Some of the solvent molecules (CH_2Cl_2) in **2** was disordered and refined with suitable restraints. CCDC 1890223 (**2**) and CCDC 1890305 (**6**) contain the supplementary crystallographic data for this paper. Further details on the crystal data, data collection, and refinements are provided in Supplementary Tables S5. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

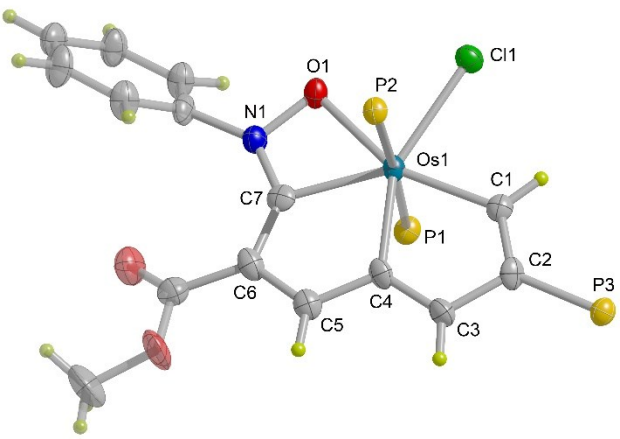


Figure S1. Molecular structure of **2**. Thermal ellipsoids are set at 50% probability level. The phenyl groups in the PPh_3 moieties are omitted for clarity. Selected bond distances and angles for complex **2** are summarized in Supplementary Table S3.

Table S3. Selected bond distances and angles for complex **2**.

Bond Distances(Å)					
Os1−C1	2.070(10)	Os1−C7	2.078(10)	Os1−O1	2.146(7)
Os1−Cl1	2.444(2)	Os1−C4	2.127(9)	C7−N1	1.296(13)
C1−C2	1.345(14)	C2−C3	1.454(14)	C3−C4	1.359(15)
C4−C5	1.425(15)	C5−C6	1.370(15)	C6−C7	1.404(14)
N1−O1	1.389(11)				
Bond Angles(º)					
Os(1)−C(1)−C(2)	123.7(8)		C(1)−C(2)−C(3)	111.6(9)	
C(2)−C(3)−C(4)	112.4(9)		Os(1)−C(4)−C(3)	120.4(7)	
C(4)−Os(1)−C(1)	72.0(4)		Os(1)−C(4)−C(5)	118.2(8)	
C(4)−C(5)−C(6)	116.3(9)		C(5)−C(6)−C(7)	108.8(9)	
Os(1)−C(7)−C(6)	125.2(8)		C(7)−Os(1)−C(4)	71.4(4)	
C(7)−Os(1)−O(1)	61.4(3)		Os(1)−O(1)−N(1)	92.9(5)	
O(1)−N(1)−C(7)	106.8(8)		Os(1)−C(7)−N(1)	98.9(7)	

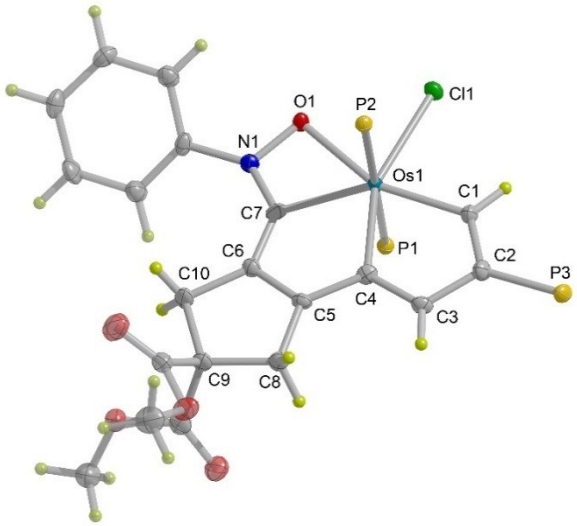


Figure S2. Molecular structure of **6**. Thermal ellipsoids are set at 50% probability level. The phenyl groups in the PPh_3 moieties are omitted for clarity. Selected bond distances and angles for complex **6** are summarized in Supplementary Table S4.

Table S4. Selected bond distances and angles for complex **6**.

Bond Distances(Å)					
Os1−C1	2.069(4)	Os1−C7	2.064(4)	Os1−O1	2.164(3)
Os1−Cl1	2.4556(8)	Os1−C4	2.152(4)	C7−N1	1.298(5)
C1−C2	1.368(6)	C2−C3	1.436(6)	C3−C4	1.357(6)
C4−C5	1.434(6)	C5−C6	1.351(6)	C6−C7	1.416(6)
N1−O1	1.367(4)	C5−C8	1.493(5)	C8−C9	1.560(6)
C9−C10	1.572(5)	C6−C10	1.504(5)		
Bond Angles(º)					
Os(1)−C(1)−C(2)	123.3(3)		C(1)−C(2)−C(3)	112.2(3)	
C(2)−C(3)−C(4)	112.4(3)		Os(1)−C(4)−C(3)	120.5(3)	
C(4)−Os(1)−C(1)	71.57(15)		Os(1)−C(4)−C(5)	117.6(3)	
C(4)−C(5)−C(6)	115.9(3)		C(5)−C(6)−C(7)	110.0(3)	
Os(1)−C(7)−C(6)	125.0(3)		C(7)−Os(1)−C(4)	71.41(15)	
C(7)−Os(1)−O(1)	60.23(13)		Os(1)−O(1)−N(1)	93.61(19)	
O(1)−N(1)−C(7)	105.6(3)		Os(1)−C(7)−N(1)	100.5(3)	

Table S5. Crystal data and structure refinement for **2** and **6**.

	2·0.25CH_2Cl_2	**6**·3CH_2Cl_2
Empirical formula	$C_{69.25}H_{56.5}BCl_{1.5}F_4NO_3OsP_3$	$C_{77}H_{68}BCl_7F_4NO_5OsP_3$
Formula weight	1373.75	1705.39
Temperature/K	173(2)	100.00(10)
Crystal system	orthorhombic	triclinic
Space group	$P2_12_12_1$	P-1
a/Å	13.604(3)	12.28710(10)
b/Å	13.735(3)	14.71150(10)
c/Å	34.365(7)	21.50510(10)
α/°	90	93.4950(10)
β/°	90	103.8640(10)
γ/°	90	101.6860(10)
Volume/Å^3	6421(2)	3671.23(5)
Z	4	2
ρ_{calc}g/cm^3	1.421	1.543
μ/mm^{-1}	2.181	6.756
F(000)	2762.0	1716.0
Crystal size/mm^3	0.25 × 0.2 × 0.13	0.3 × 0.2 × 0.1
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2θ range for data collection/°	5.99 to 49.998	7.09 to 129.998
Index ranges	-16 ≤ h ≤ 16, -16 ≤ k ≤ 16, -40 ≤ l ≤ 40	-14 ≤ h ≤ 14, -17 ≤ k ≤ 17, -25 ≤ l ≤ 25
Reflections collected	41679	41192
Independent reflections	11264 [R_{int} = 0.0506, R_{sigma} = 0.0582]	12474 [R_{int} = 0.0470, R_{sigma} = 0.0405]
Data/restraints/parameters	11264/9/775	12474/0/894
Goodness-of-fit on F^2	1.108	1.051
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0419, wR_2 = 0.1223	R_1 = 0.0384, wR_2 = 0.1015
Final R indexes [all data]	R_1 = 0.0448, wR_2 = 0.1246	R_1 = 0.0447, wR_2 = 0.1048
Largest diff. peak/hole / e Å^{-3}	2.15/-0.63	1.83/-1.70

5 Thermal Stability Tests

Table S6. Thermal stability tests for complexes **2-4** and **6** in the solid state under air condition.[a]

	100 ℃ (15 h)	120 ℃ (15 h)	140 ℃ (15 h)	160 ℃ (15 h)	180 ℃ (15 h)	200 ℃ (5 h)	200 ℃ (10 h)	200 ℃ (15 h)
2	○	○	○	○	Δ	▲	■	●
3	○	○	○	○	Δ	▲	■	●
4	○	○	○	○	Δ	▲	■	●
6	○	○	○	○	○	Δ	▲	■

[a] ○ = stable; Δ = Slightly decomposed (< 10%); ▲ = Partly decomposed (< 30%); ■ = Partly decomposed (< 60%); ● = Completely decomposed.

6. HRMS and NMR Spectra

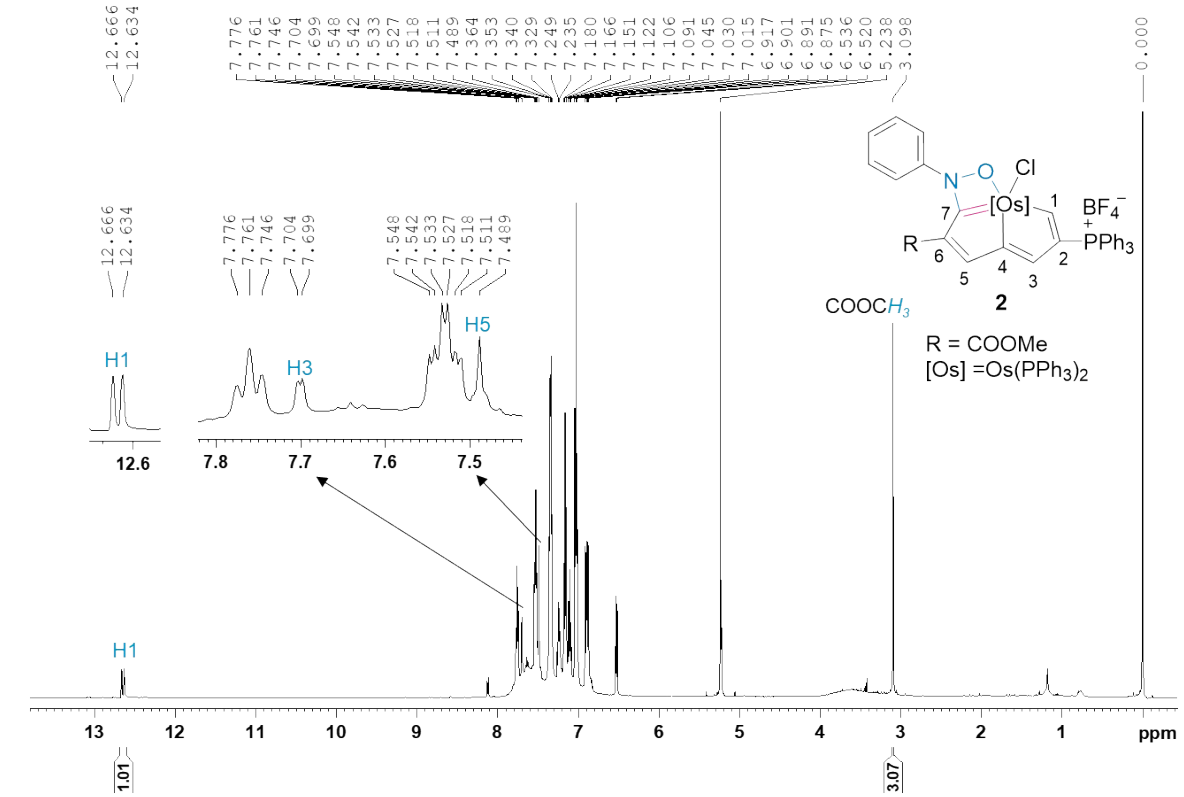


Figure S3. The ^{1}H NMR (500.1 MHz, CD_2Cl_2) spectrum for complex **2**.

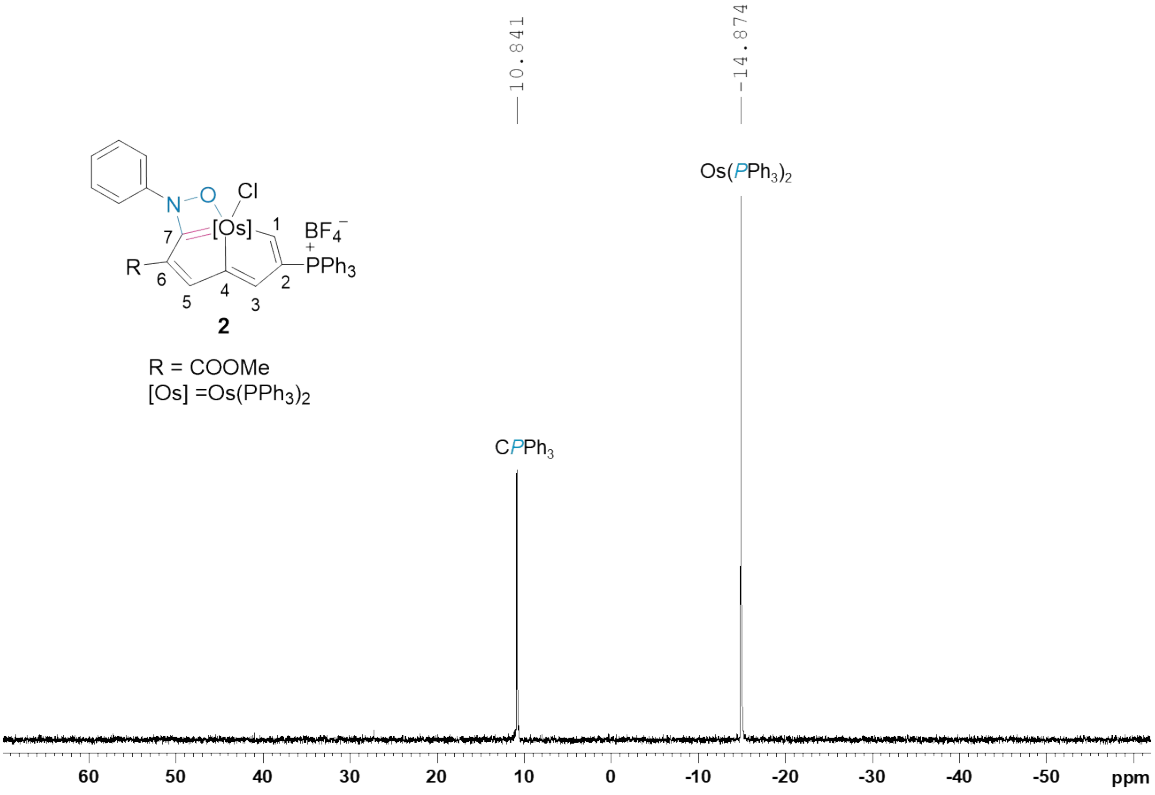


Figure S4. The $^{31}P\{^{1}H\}$ NMR spectrum (202.4 MHz, CD_2Cl_2) for complex **2**.

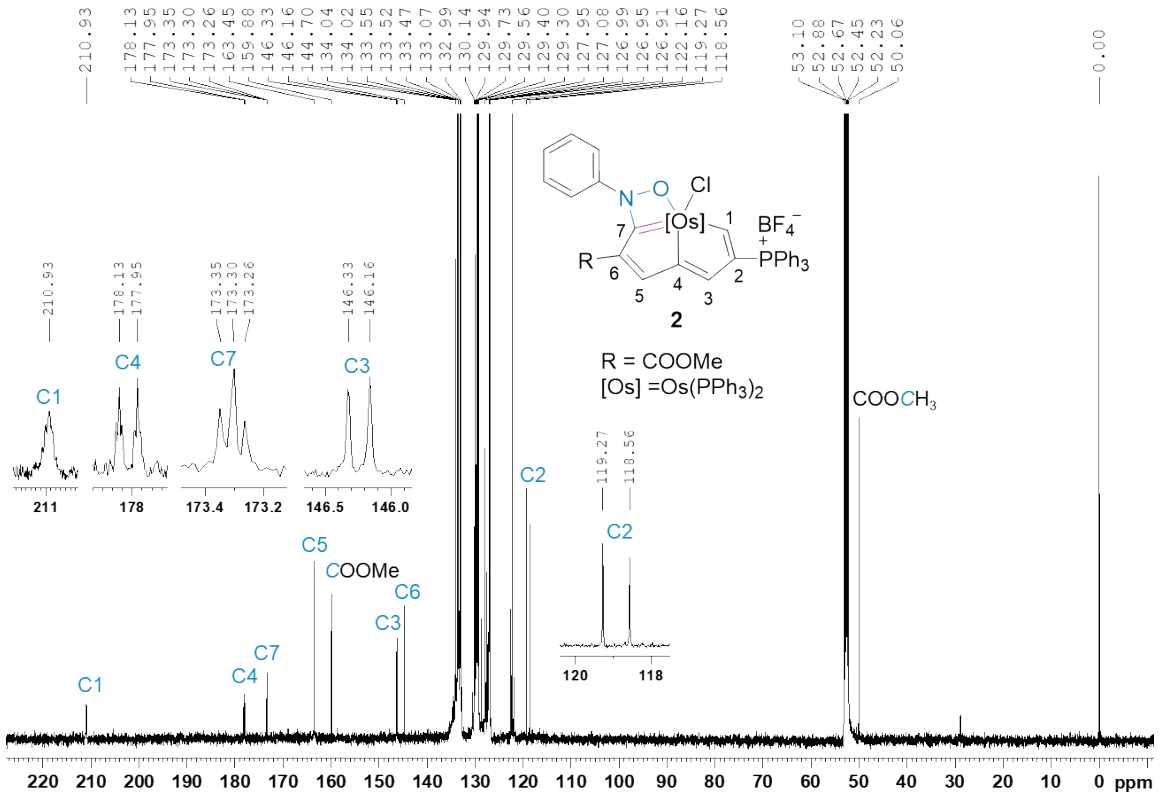


Figure S5. The $^{13}C\{^{1}H\}$ NMR (125.7 MHz, CD_2Cl_2) spectrum for complex **2**.

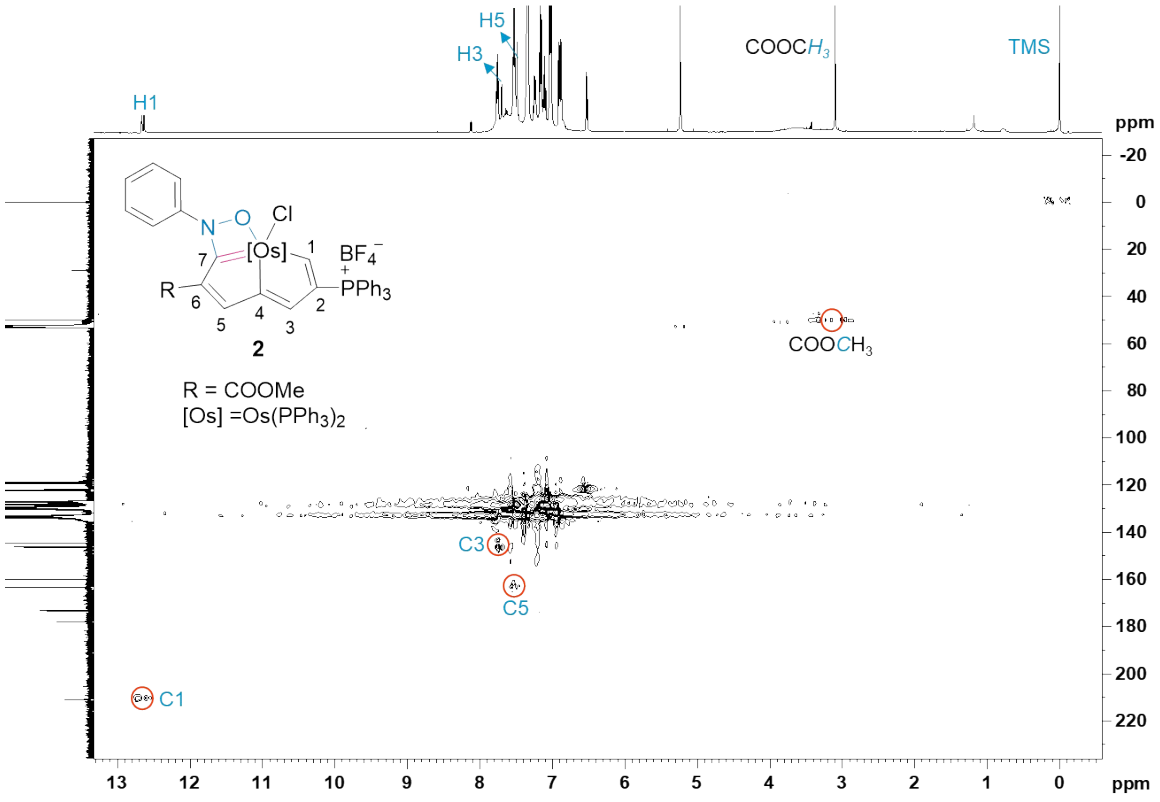


Figure S6. The ^{1}H-^{13}C HSQC (125.7 MHz, CD_2Cl_2) spectrum for complex **2**.

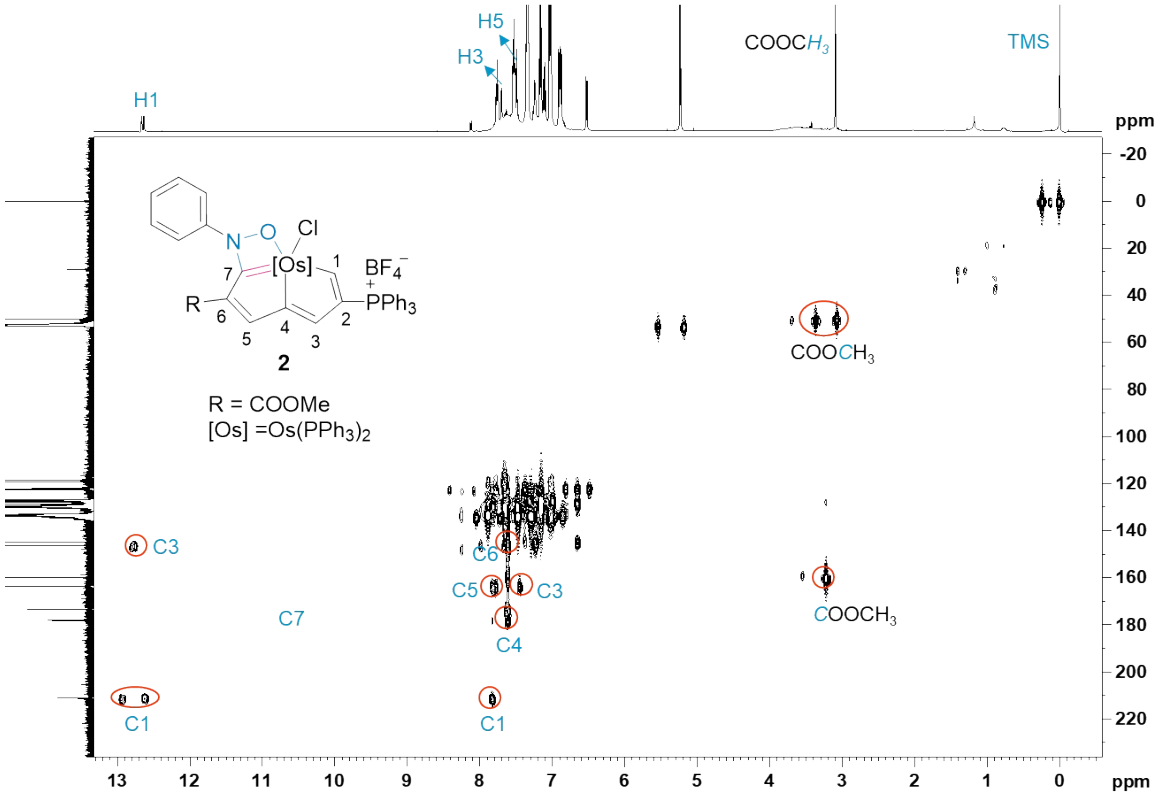


Figure S7. The ^{1}H-^{13}C HMBC (125.7 MHz, CD_2Cl_2) spectrum for complex **2**.

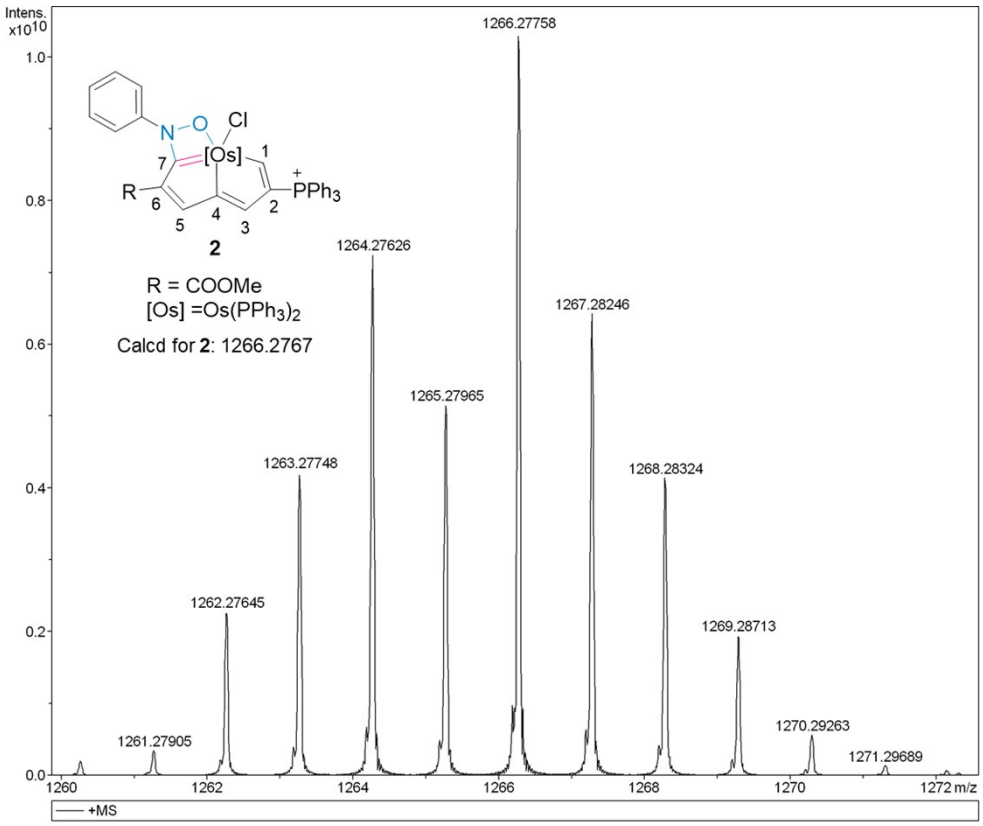


Figure S8. Positive-ion ESI-MS spectrum for complex **2** measured in methanol.

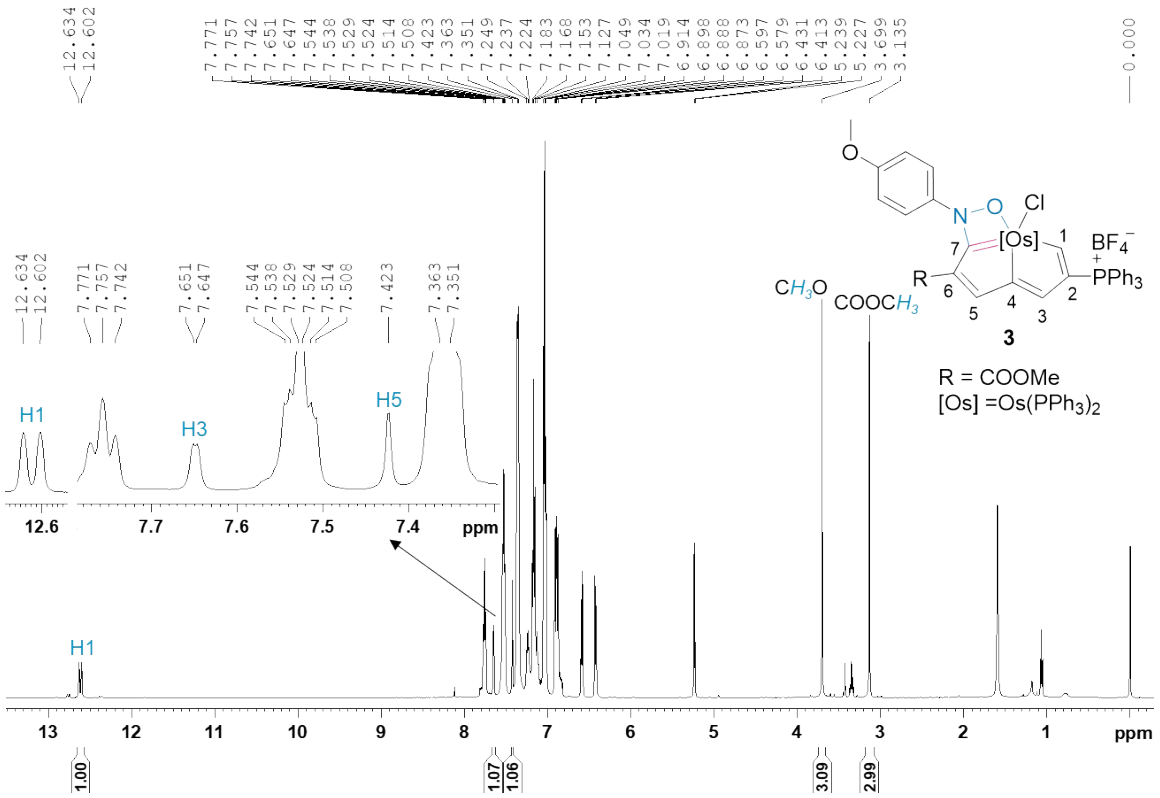


Figure S9. The ^{1}H NMR (500.1 MHz, CD_2Cl_2) spectrum for complex **3**.

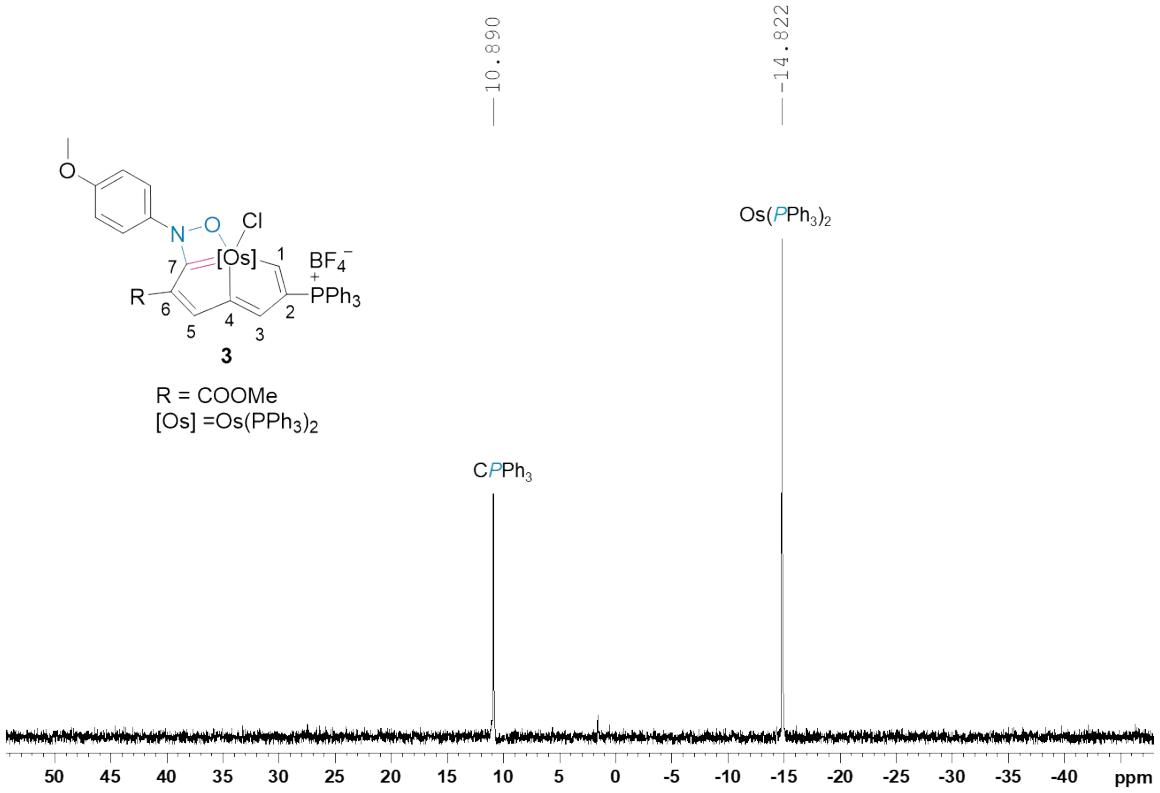


Figure S10. The $^{31}P\{^{1}H\}$ NMR spectrum (202.4 MHz, CD_2Cl_2) for complex **3**.

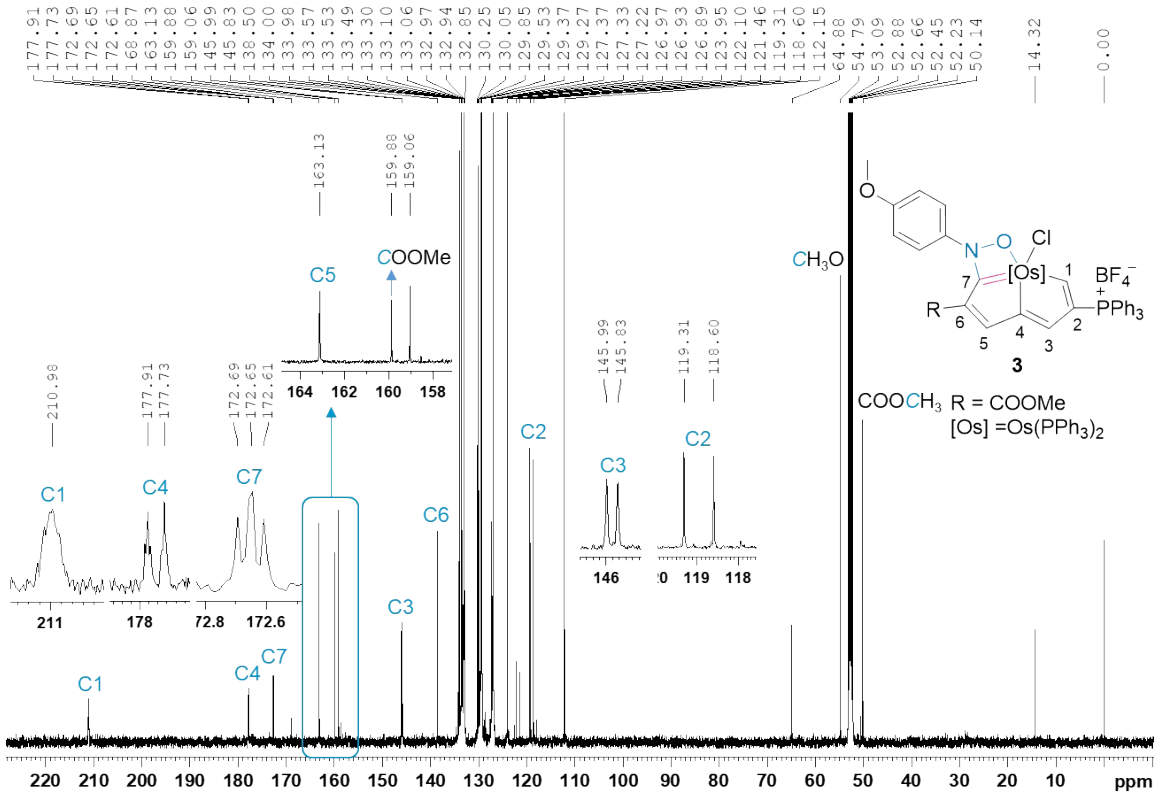


Figure S11. The $^{13}C\{^{1}H\}$ NMR (125.7 MHz, CD_2Cl_2) spectrum for complex **3**.

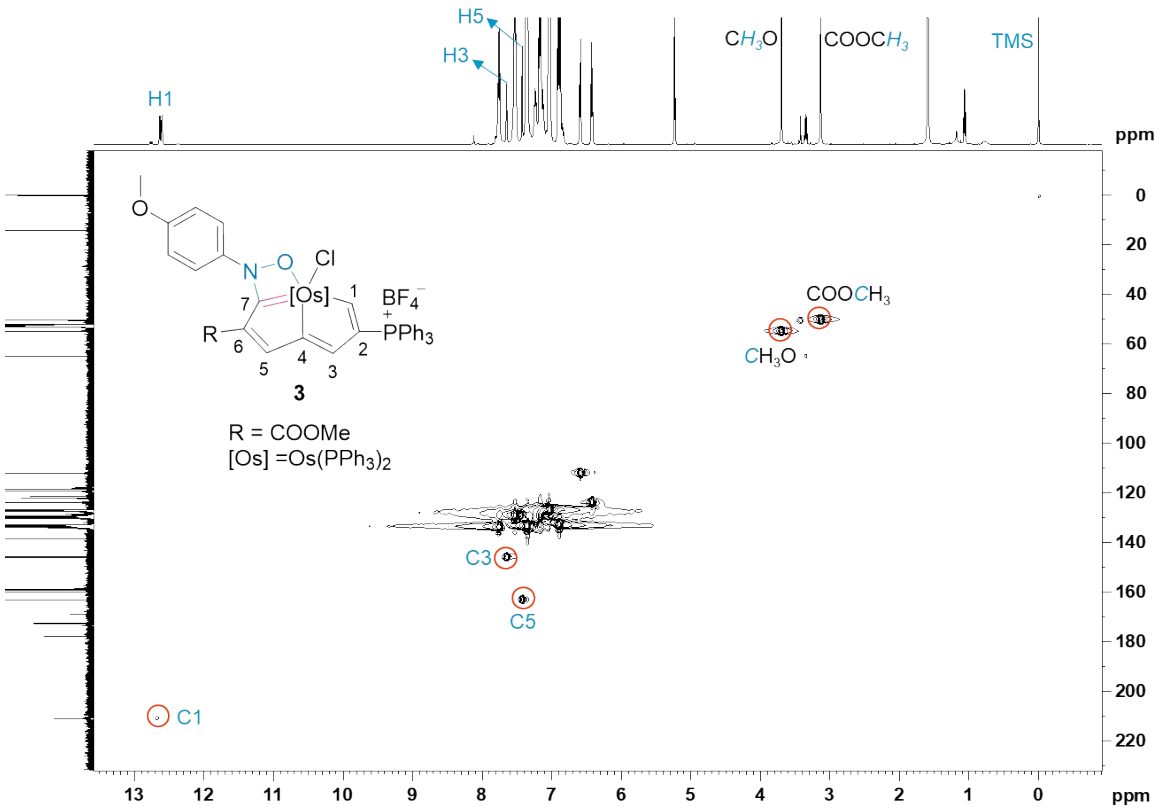


Figure S12. The ^{1}H-^{13}C HSQC (125.7 MHz, CD_2Cl_2) spectrum for complex **3**.

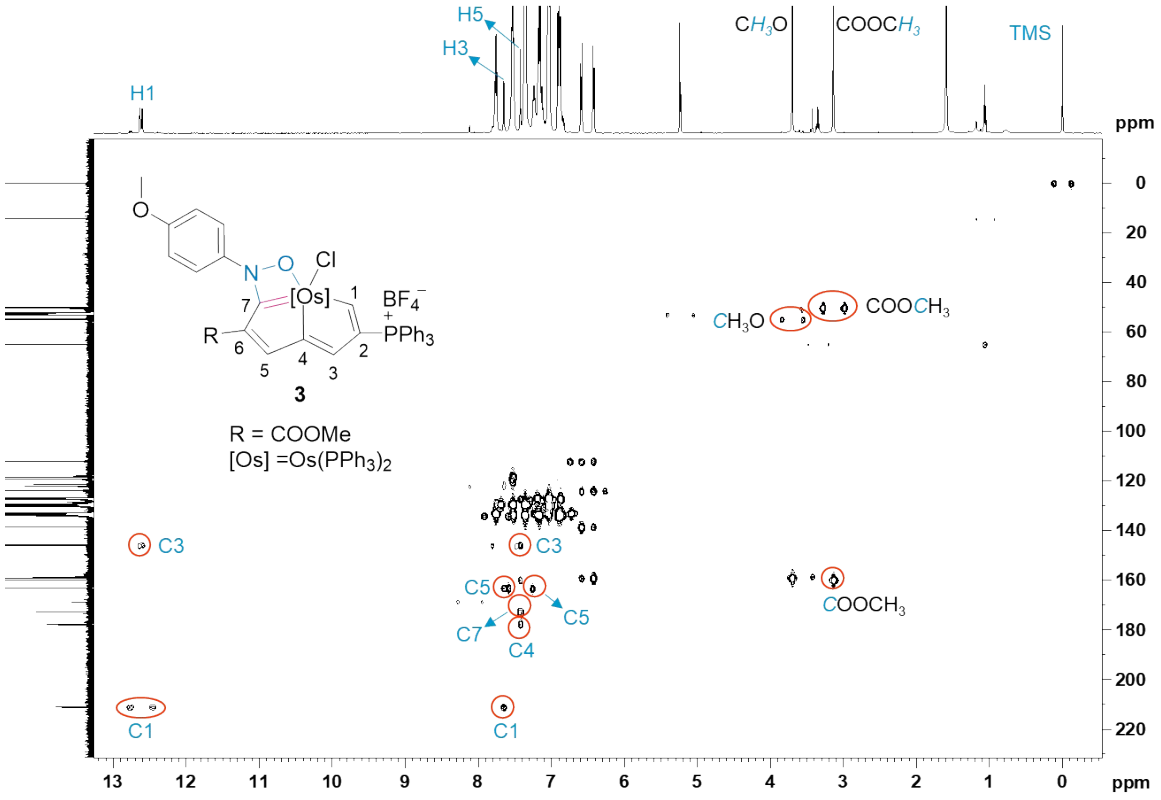


Figure S13. The ^{1}H-^{13}C HMBC (125.7 MHz, CD_2Cl_2) spectrum for complex **3**.

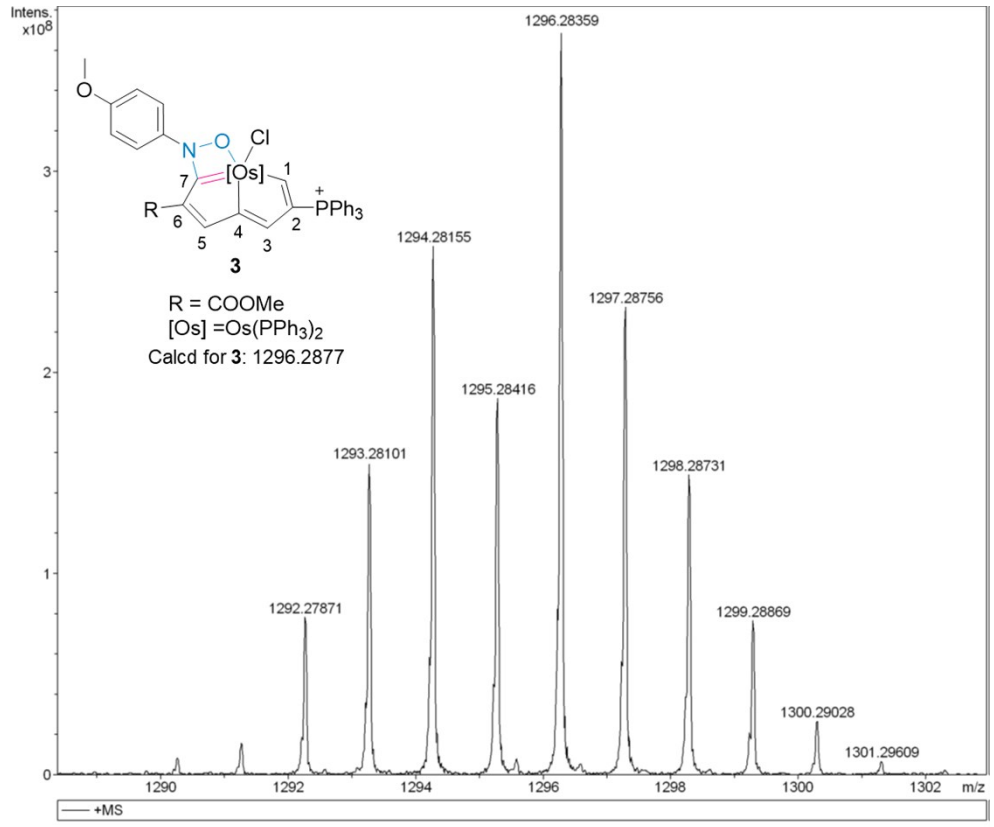


Figure S14. Positive-ion ESI-MS spectrum for complex **3** measured in methanol.

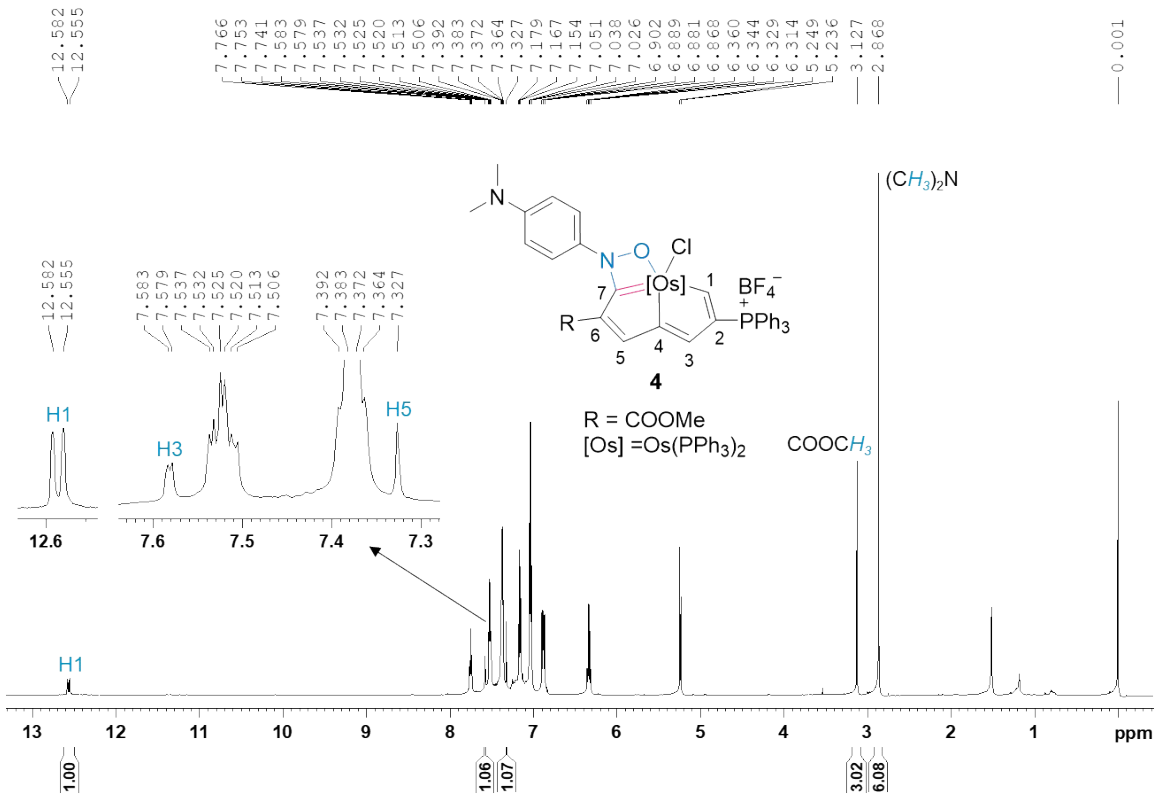


Figure S15. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **4**.

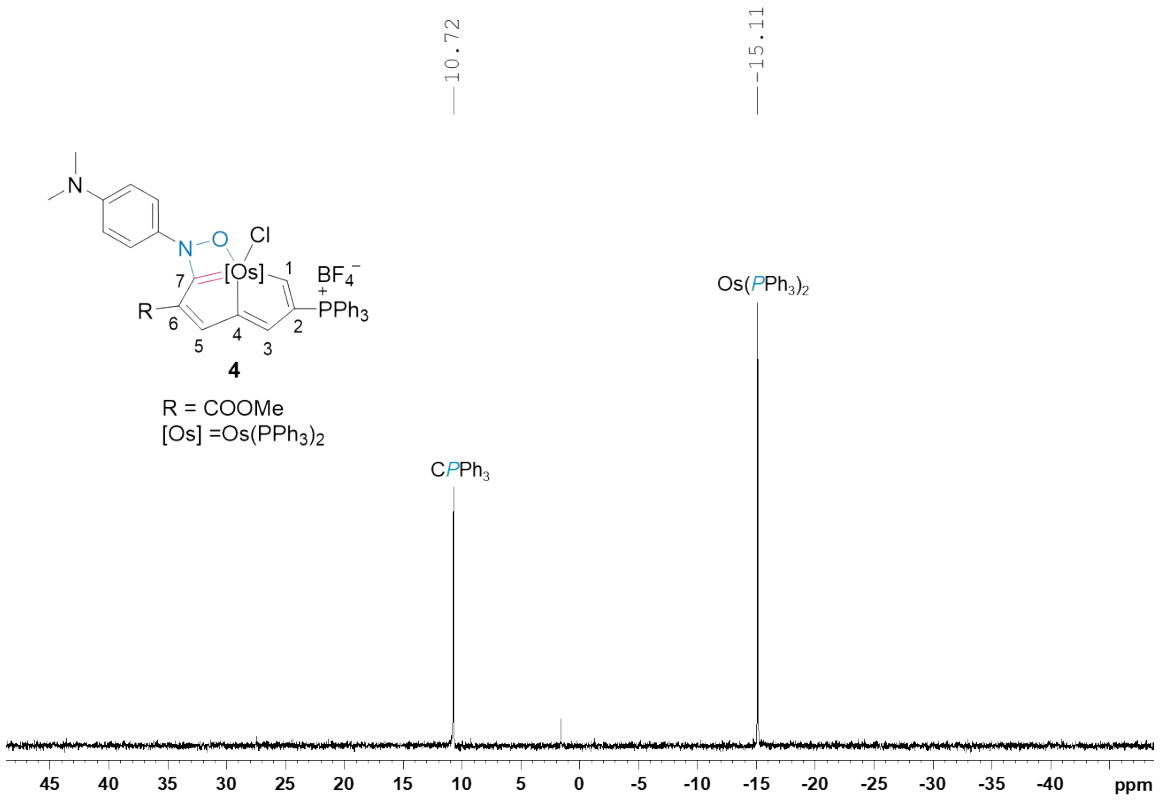


Figure S16. The $^{31}P\{^{1}H\}$ NMR spectrum (242.9 MHz, CD_2Cl_2) for complex **4**.

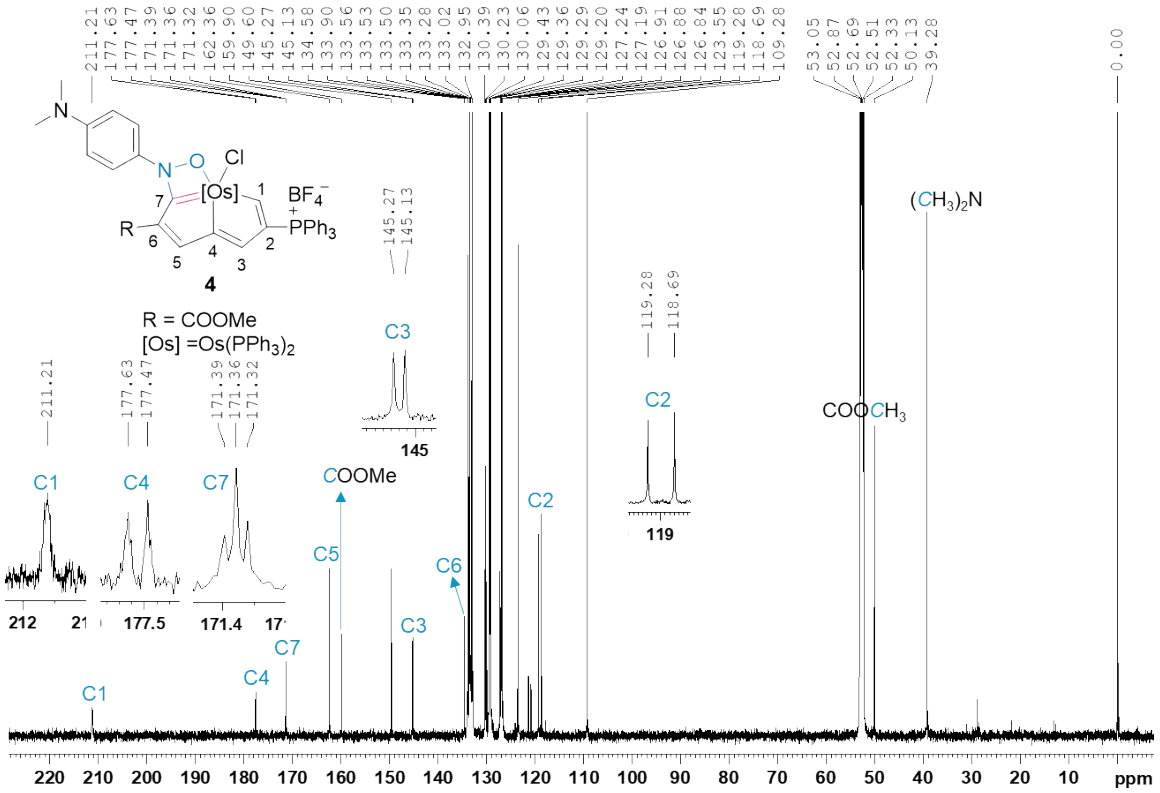


Figure S17. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **4**.

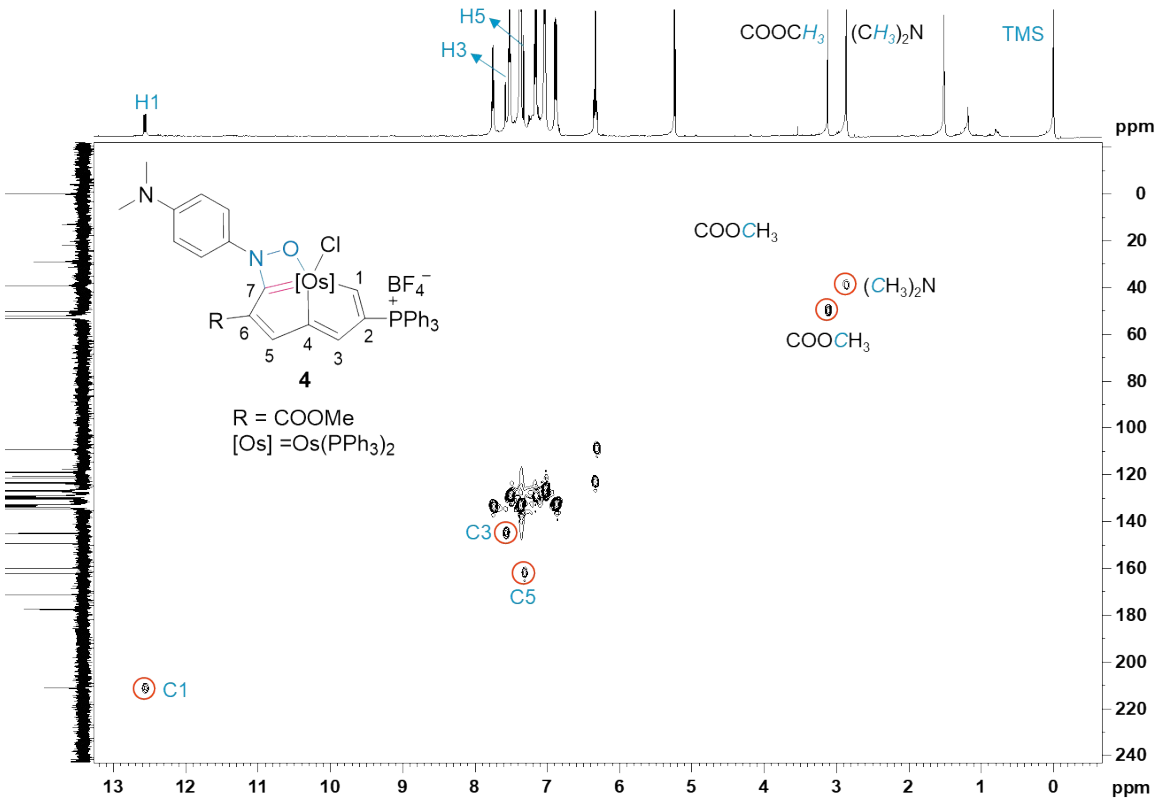


Figure S18. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **4**.

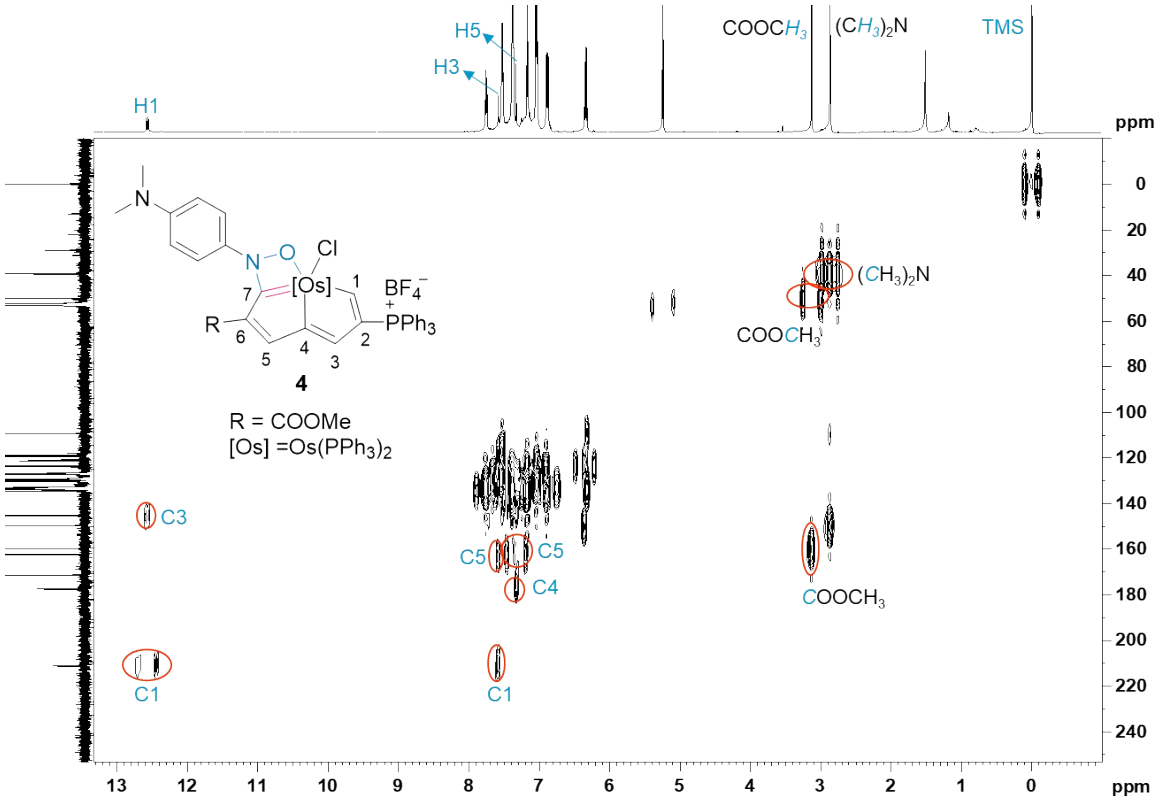


Figure S19. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **4**.

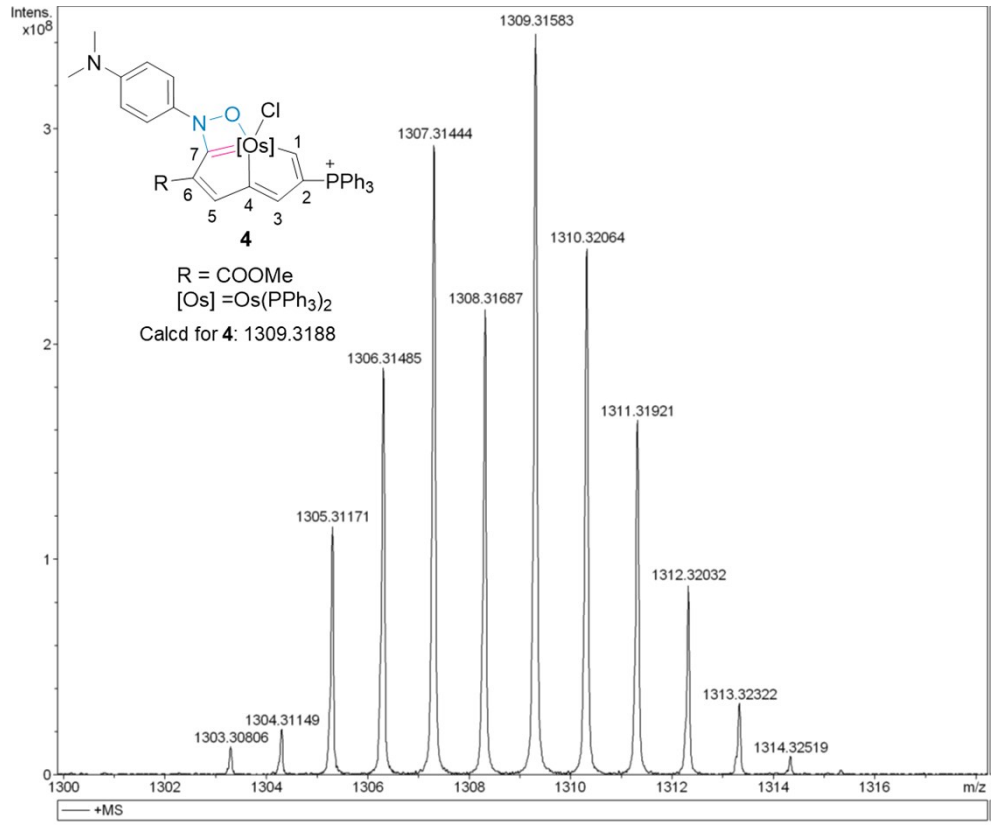


Figure S20. Positive-ion ESI-MS spectrum for complex **4** measured in methanol.

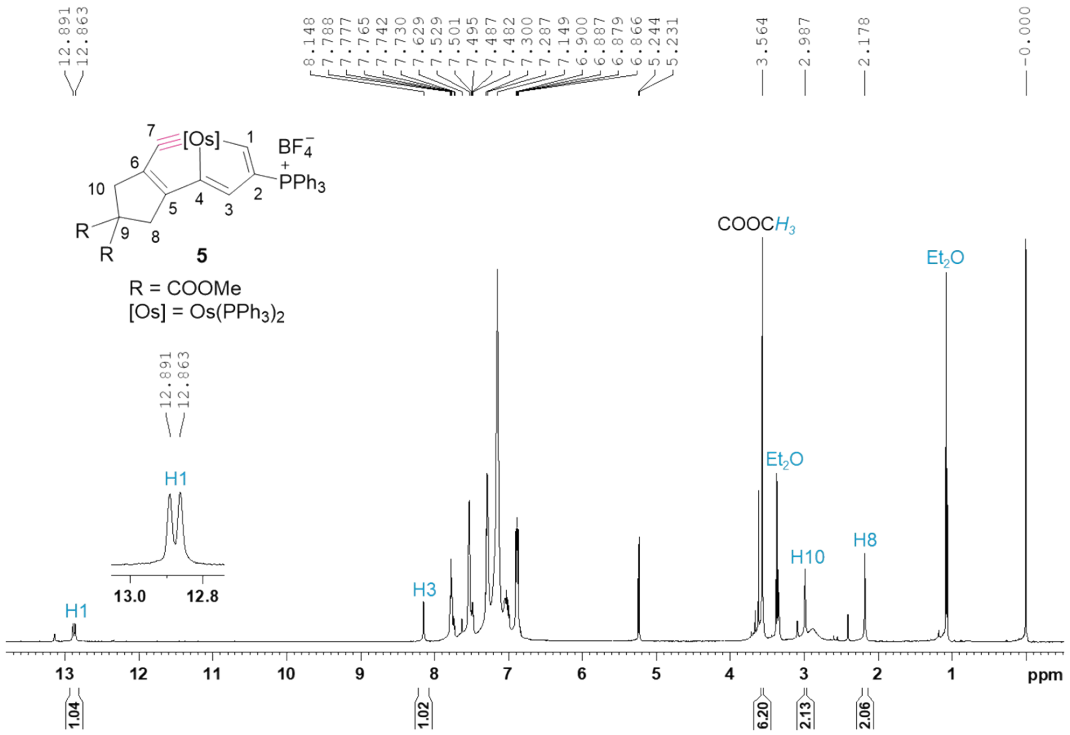


Figure S21. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **5**.

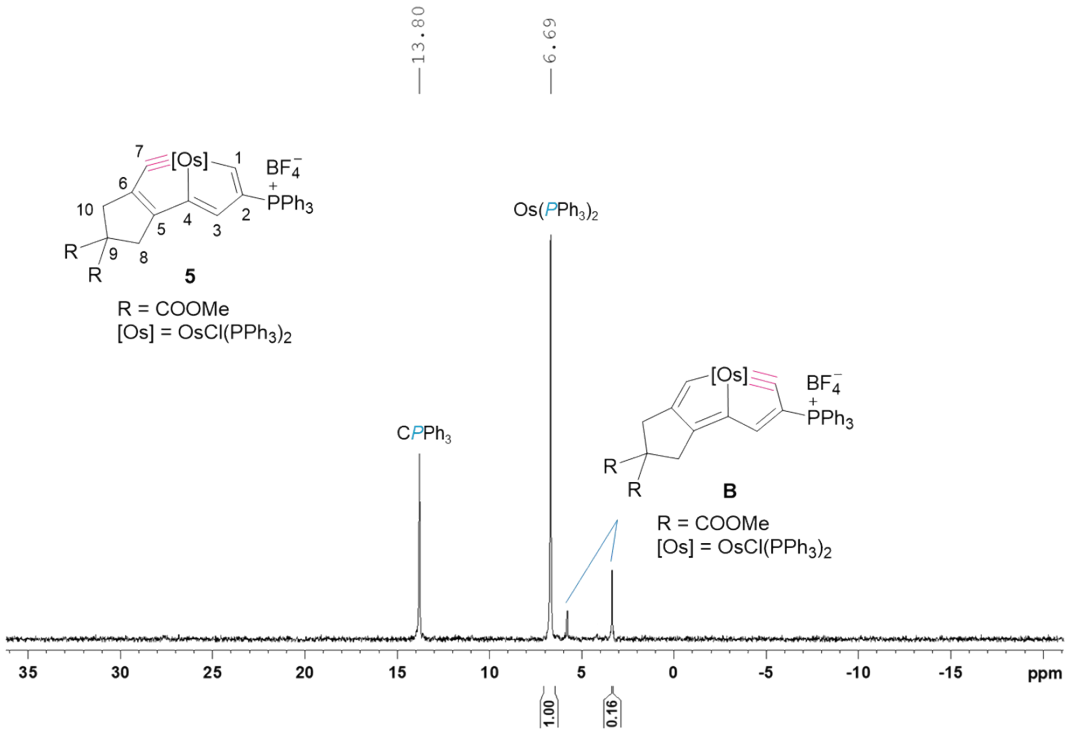


Figure S22. The ^{31}P $\{^{1}H\}$ NMR spectrum (242.9 MHz, CD_2Cl_2) for complex **5**. There is an equilibrium between complexes **5** and **B** due to the shift of the metal carbyne bonds, which chemistry has been reported in Nat. Commun. 2014, 5, 3265. Thus, the two isomers (**5** and **B**) always appear in a ratio of 1/0.16 in the solution.

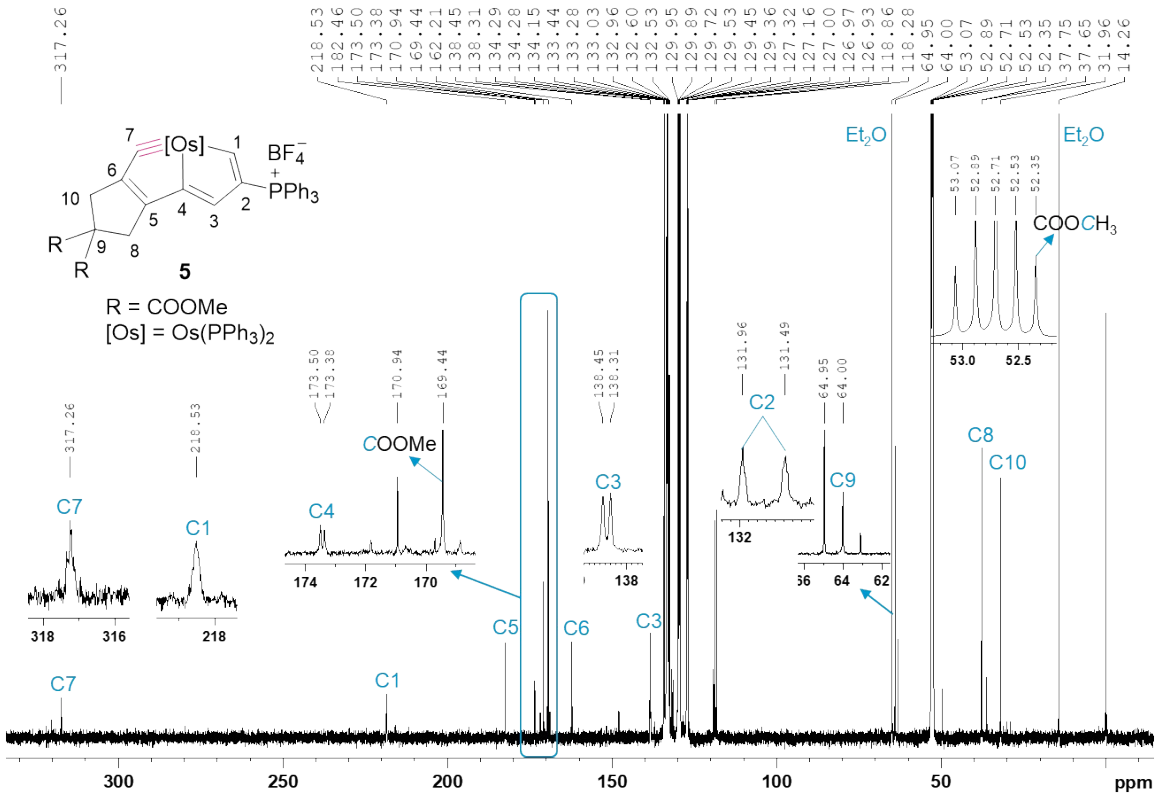


Figure S23. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **5**.

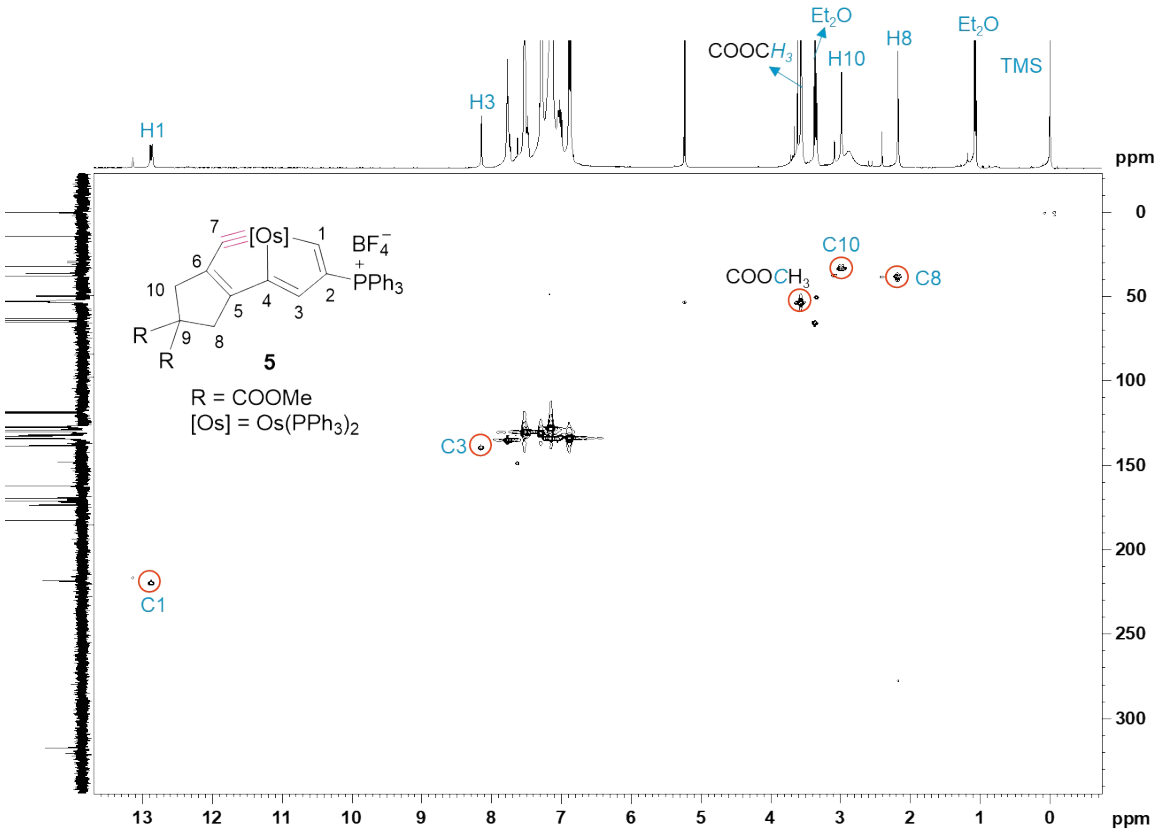


Figure S24. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **3**.

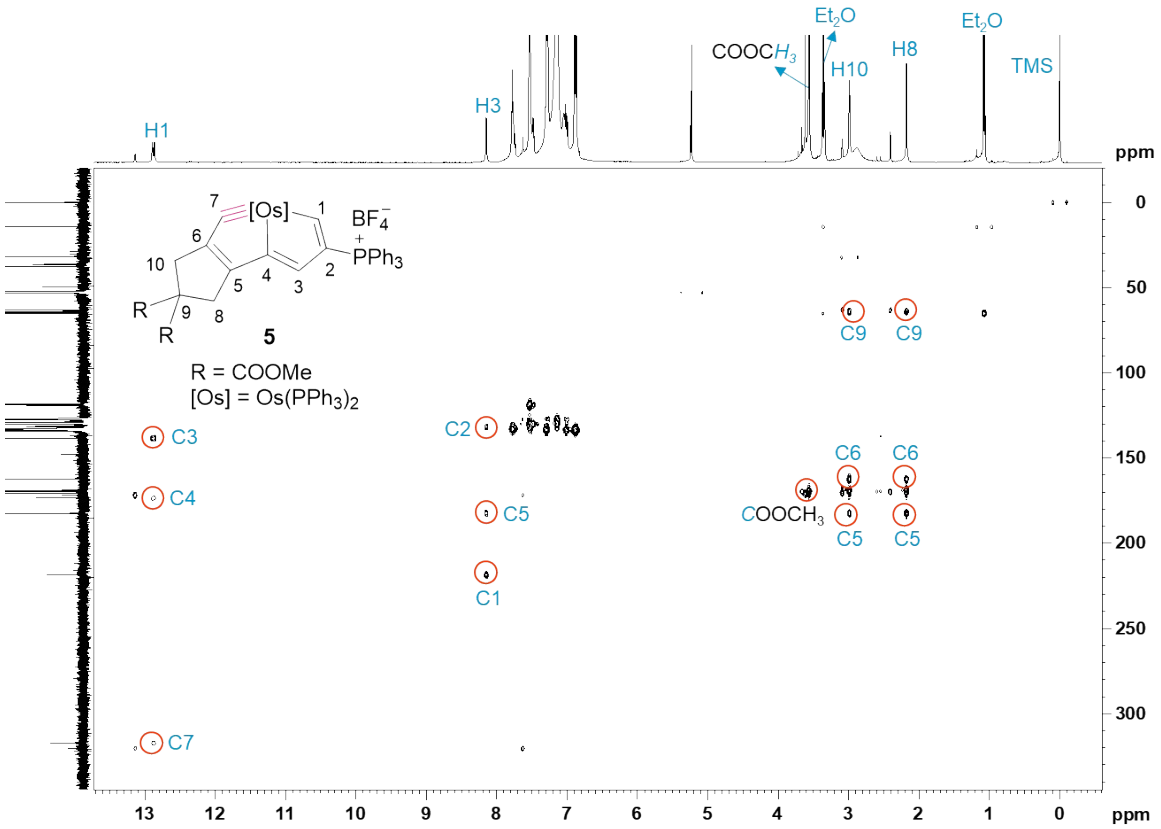


Figure S25. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **5**.

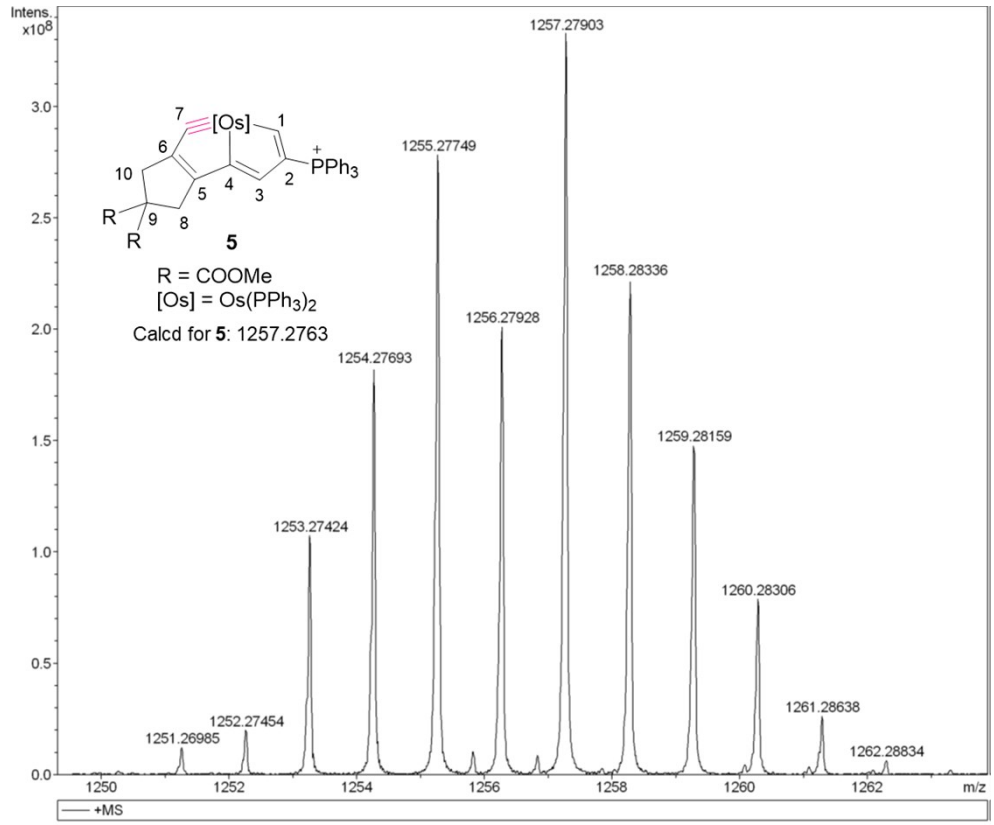


Figure S26. Positive-ion ESI-MS spectrum for complex **5** measured in methanol.

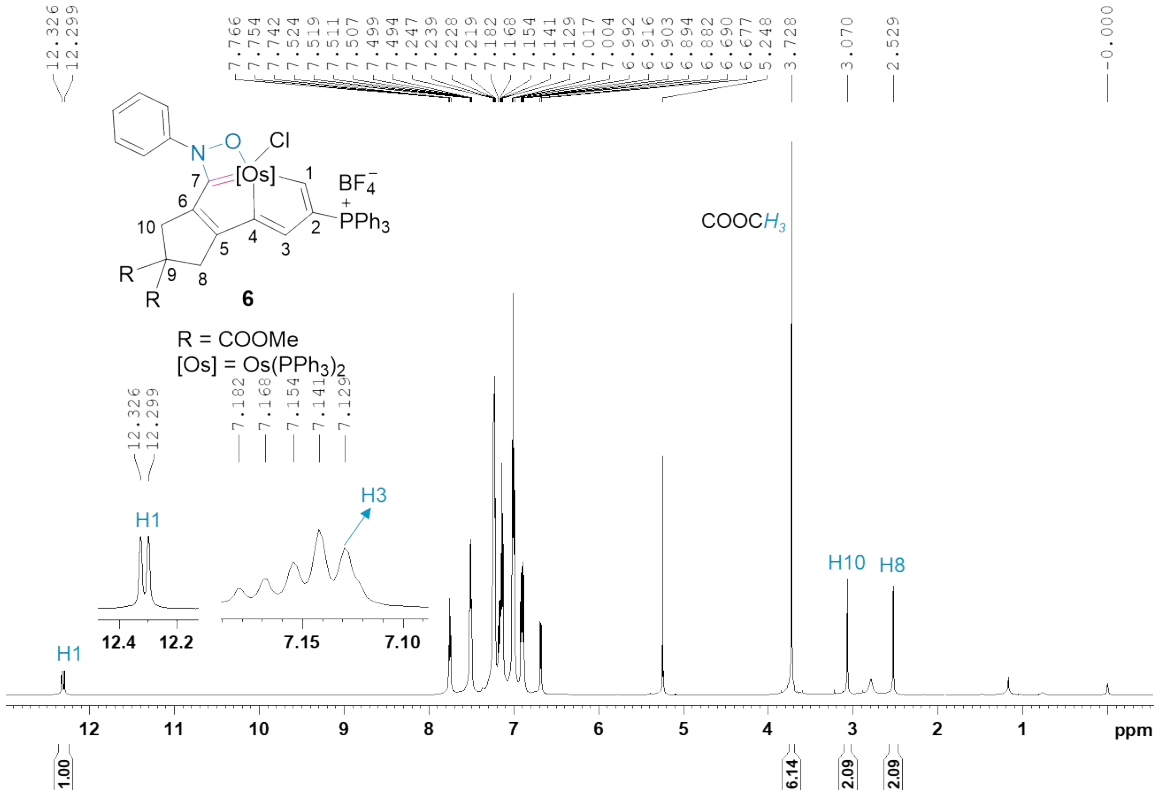


Figure S27. The ^{1}H NMR (600.1 MHz, CD_2Cl_2) spectrum for complex **6**.

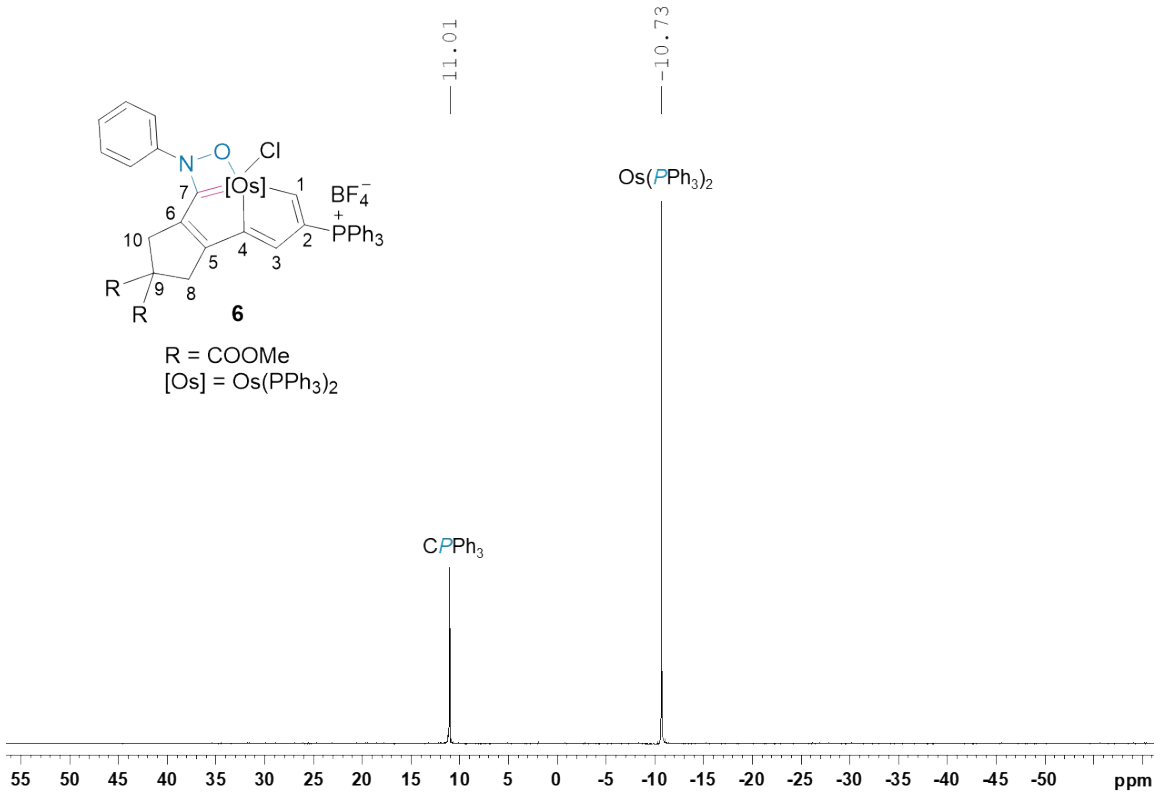


Figure S28. The $^{31}P\{^{1}H\}$ NMR spectrum (242.9 MHz, CD_2Cl_2) for complex **6**.

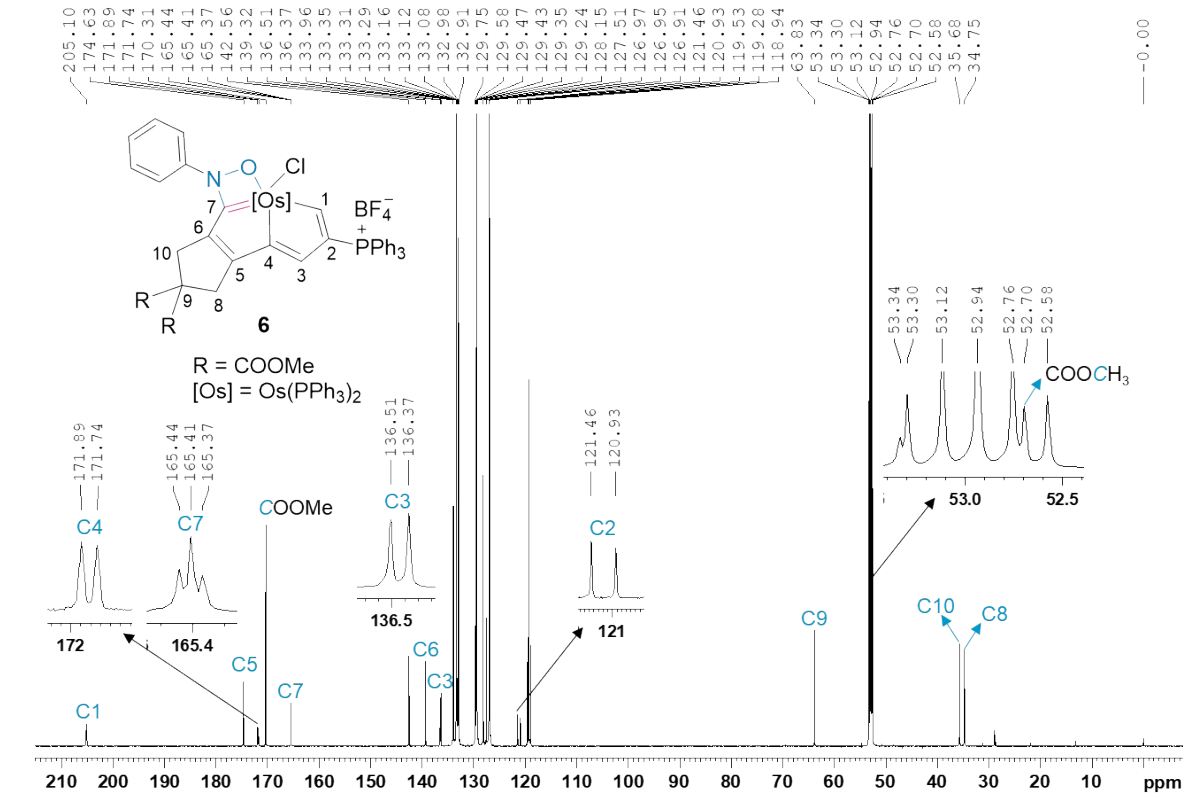


Figure S29. The $^{13}C\{^{1}H\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for complex **6**.

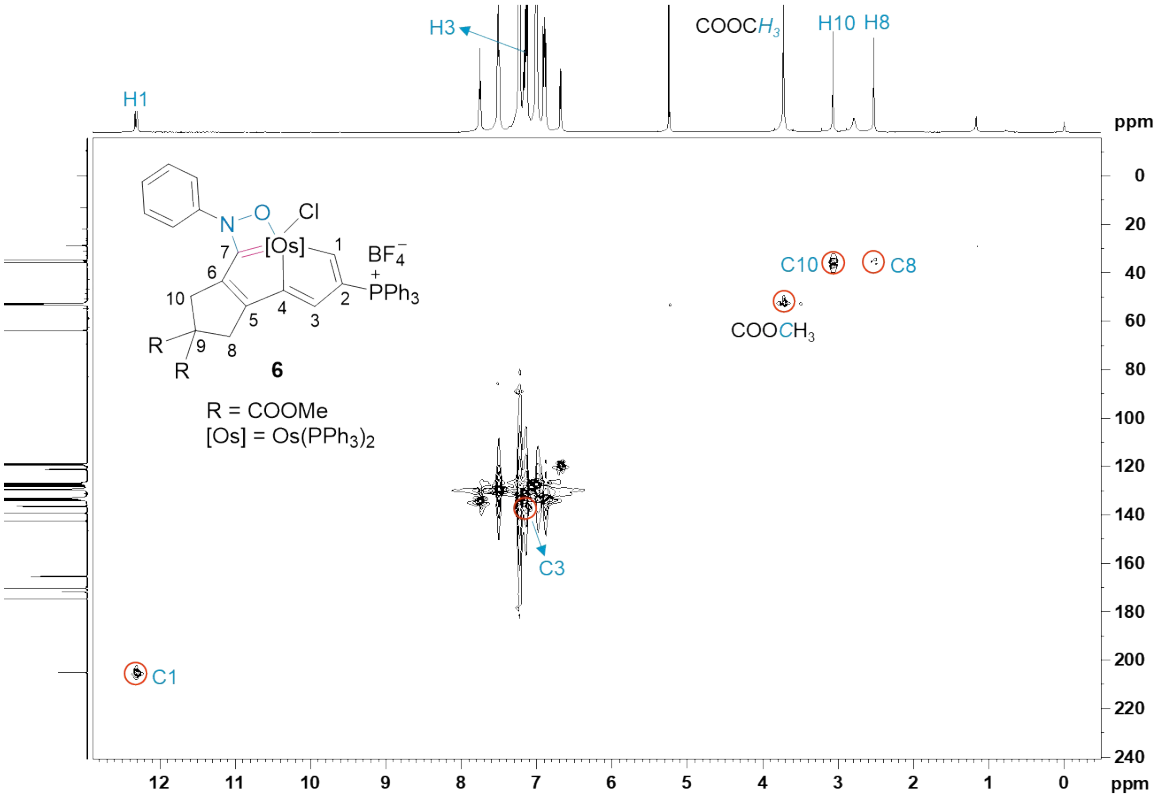


Figure S30. The ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2) spectrum for complex **6**.

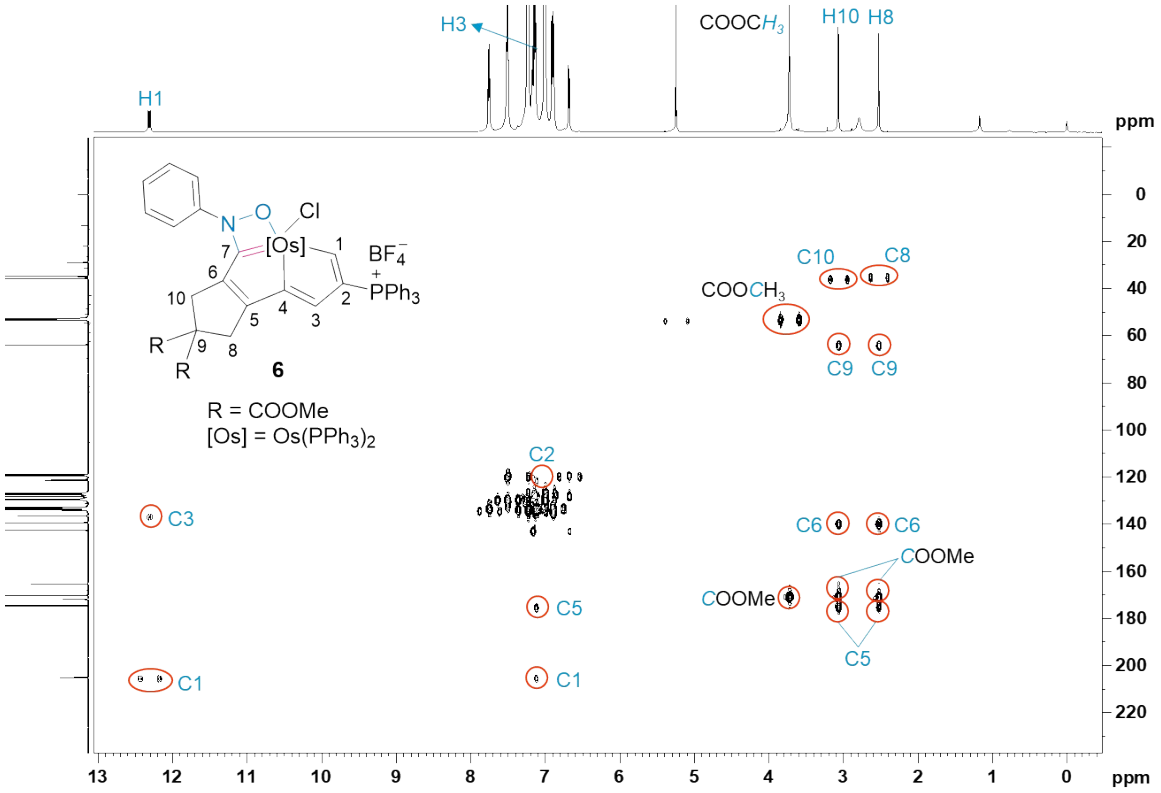


Figure S31. The ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2) spectrum for complex **6**.

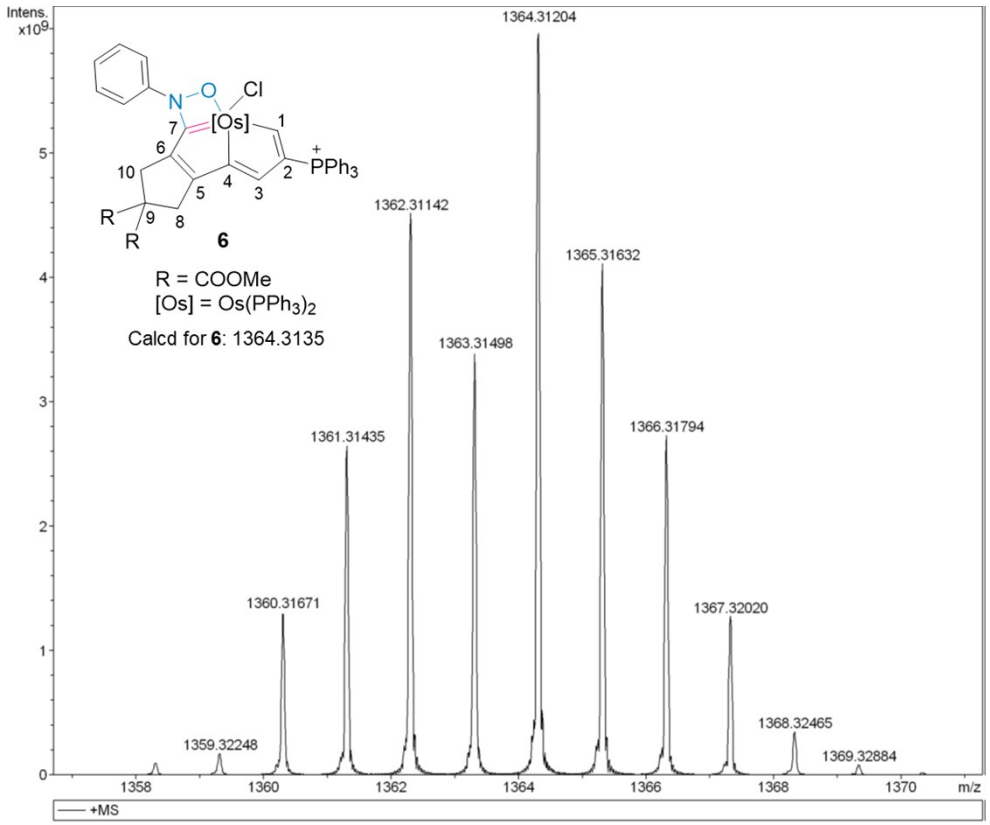
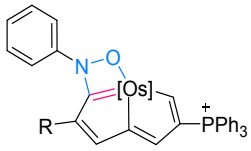


Figure S32. Positive-ion ESI-MS spectrum for complex **6** measured in methanol.

7. Cartesian coordinates together with the electronic energies for all the complexes calculated in this study

2



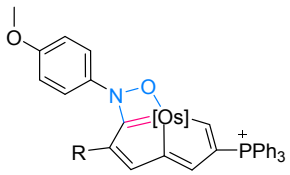
R = COOMe
[Os] =$OsCl(PPh_3)_2$

E = -3068.16864078

N	-3.319636	-0.162954	0.031842
C	4.587315	1.368610	1.696018
C	1.383724	0.061177	-0.602099
H	1.814375	0.063372	-1.597163
C	2.201067	0.100577	0.512132
C	1.450473	0.100479	1.733472
H	1.889689	0.151847	2.727306
C	0.090866	0.035195	1.516742
C	-0.819851	-0.040018	2.608226
H	-0.486573	-0.039010	3.641052
C	-2.149319	-0.164913	2.274061
C	-2.284236	-0.128915	0.851207
C	-3.205354	-0.417746	3.261045
C	-3.744932	-0.435988	5.621605
H	-3.237243	-0.134382	6.535488
H	-4.662475	0.136146	5.471775
H	-3.982878	-1.501721	5.634971
C	-2.666343	-3.998113	2.749650
H	-3.694991	-4.237708	2.995588
C	6.517484	-3.125361	0.992879
H	7.489853	-3.437465	0.627663
C	2.521828	-5.180042	-1.099552
H	2.909579	-6.074572	-0.622777
C	-2.875993	-5.479660	-2.391252
H	-3.026364	-6.544172	-2.243584
C	5.967714	-1.917510	0.551008
H	6.516227	-1.306547	-0.156940
C	-3.694142	3.182837	-3.571282
H	-4.445617	2.611913	-4.106890
C	-1.510205	3.722095	3.377808
H	-0.949153	3.701994	4.306557
C	-2.914471	2.544737	-2.597542
H	-3.060635	1.494409	-2.384865
C	4.484011	-0.431050	-2.206324
H	3.927199	-1.347218	-2.042523
C	1.484072	3.093979	-1.895861
H	1.192682	2.264665	-2.531906
C	0.691571	3.428398	-0.779030
C	-6.806821	0.860831	0.842602
H	-7.332227	1.570862	1.472118
C	3.933619	2.616648	1.738754
H	3.088943	2.818446	1.089535
C	-1.931551	3.267176	-1.898087
C	2.617394	3.849826	-2.211265
H	3.208724	3.587272	-3.081904
C	-3.490120	-4.823042	-3.465737
H	-4.120332	-5.377646	-4.153438
C	-4.741552	-0.115017	0.067933
C	5.753500	1.004682	-3.694047
H	6.166132	1.205340	-4.676983
C	-1.649650	3.219565	0.993990
C	-3.505830	4.537613	-3.857861
H	-4.109991	5.025527	-4.615990
C	-1.747341	4.635769	-2.191075
H	-0.993823	5.214102	-1.669715
C	1.058935	4.534802	0.009386
H	0.448519	4.832056	0.852906
C	-2.945333	3.769908	0.975649
H	-3.507549	3.804660	0.050522
C	-1.028686	-3.226394	1.115042
C	-1.856446	-3.381977	-1.680728
C	-5.448377	-0.964544	-0.795370
H	-4.905866	-1.654996	-1.429788
C	1.490655	-2.887108	-2.327533
H	1.077417	-2.015061	-2.823837
C	-0.941504	3.197259	2.213252
H	0.052281	2.767495	2.253208
C	-5.411522	0.811242	0.877303
H	-4.851207	1.482738	1.515534
C	0.914481	-3.347679	-1.126248
C	-2.466666	-2.730988	-2.766901
H	-2.309836	-1.674120	-2.920640
C	-3.514986	4.286228	2.146829
H	-4.512439	4.712387	2.112696

C	4.558383	-3.524070	2.365367
H	4.011546	-4.146814	3.065045
C	4.001251	-2.318840	1.928606
H	3.025113	-2.016094	2.289261
C	2.198900	5.286835	-0.309711
H	2.458655	6.148640	0.297381
C	4.376622	3.601590	2.626155
H	3.872984	4.561621	2.652713
C	-3.279616	-3.453866	-3.651622
H	-3.741540	-2.939432	-4.488021
C	5.677797	1.117752	2.549736
H	6.182068	0.158572	2.530072
C	-7.524932	0.008443	-0.004680
H	-8.608434	0.054902	-0.029529
C	-2.354313	-3.553308	1.459720
H	-3.147489	-3.460151	0.727797
C	4.703550	-1.507265	1.018221
C	5.969320	1.907582	-2.646850
H	6.552078	2.806927	-2.813971
C	3.089652	-4.716700	-2.290104
H	3.919157	-5.249906	-2.743110
C	-6.842767	-0.898870	-0.825295
H	-7.395618	-1.557009	-1.486928
C	5.437352	1.654451	-1.377649
H	5.604431	2.362249	-0.574902
C	-0.341645	-3.789647	3.386987
H	0.442382	-3.880374	4.132420
C	5.461590	3.349379	3.475477
H	5.799259	4.115298	4.165524
C	-2.060489	-4.767983	-1.508608
H	-1.582977	-5.295282	-0.690302
C	-0.028618	-3.336126	2.101316
H	0.994253	-3.068117	1.865073
C	1.435225	-4.508504	-0.524844
H	0.991276	-4.907199	0.378751
C	4.690126	0.483989	-1.153288
C	-2.530168	5.263473	-3.162917
H	-2.374820	6.315661	-3.378565
C	2.565140	-3.572841	-2.905052
H	2.976249	-3.224823	-3.848092
C	-1.661135	-4.124301	3.714224
H	-1.902367	-4.478025	4.711250
C	-2.799578	4.266981	3.348572
H	-3.239920	4.674318	4.252693
C	6.109472	2.108914	3.437152
H	6.947350	1.910942	4.096658
C	5.010672	-0.162331	-3.472316
H	4.845554	-0.864799	-4.281881
C	2.979838	4.947221	-1.419248
H	3.851915	5.540983	-1.674034
C	5.815201	-3.928469	1.899076
H	6.244142	-4.865171	2.238525
O	-2.710034	-0.159660	-1.272870
O	-2.784681	-0.144781	4.546604
O	-4.338613	-0.859295	3.018255
P	-0.904600	2.488612	-0.548087
P	-0.652021	-2.507517	-0.554940
P	4.007838	0.110083	0.499683
Cl	-0.366122	0.114686	-2.953021
Os	-0.680047	-0.016666	-0.482795

3



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E = -3182.65307035

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C	1.619230	0.076287	-0.595986
H	2.060105	0.082989	-1.586665
C	2.423788	0.132216	0.526640
C	1.660311	0.122329	1.740512
H	2.088405	0.184090	2.738635
C	0.304447	0.032825	1.510008
C	-0.616086	-0.054401	2.592677
H	-0.292753	-0.045384	3.628571
C	-1.940252	-0.200088	2.246772
C	-2.062737	-0.173743	0.821697
C	-3.000592	-0.454893	3.228493
C	-3.548609	-0.474013	5.587291
H	-3.042805	-0.177414	6.503913
H	-4.464561	0.100921	5.437866
H	-3.789490	-1.539161	5.595911
C	-2.388842	-4.041616	2.732893
H	-3.414745	-4.300818	2.970482

C	6.791781	-3.014509	1.061375	C	1.790092	-2.874675	-2.312931
H	7.772259	-3.311388	0.705243	H	1.364241	-2.013188	-2.816963
C	2.855647	-5.140365	-1.064120	C	-0.789103	3.178981	2.185321
H	3.256924	-6.024549	-0.579282	H	0.211471	2.766683	2.236586
C	-2.527996	-5.542146	-2.405101	C	-5.216915	0.703757	0.788887
H	-2.660978	-6.608620	-2.254896	H	-4.686525	1.404755	1.421105
C	6.224750	-1.818366	0.609539	C	1.213182	-3.339938	-1.113808
H	6.768393	-1.201255	-0.096838	C	-2.163815	-2.787858	-2.787056
C	-3.477487	3.097130	-3.631008	H	-2.024420	-1.728845	-2.943116
H	-4.209632	2.510114	-4.175928	C	-3.381187	4.220254	2.089544
C	-1.379021	3.696959	3.342444	H	-4.385655	4.628658	2.043935
H	-0.827167	3.689770	4.276871	C	4.828996	-3.440787	2.420195
C	-2.696957	2.475999	-2.646956	H	4.287398	-4.069714	3.118424
H	-2.823570	1.422968	-2.434915	C	4.254670	-2.247349	1.973448
C	4.740980	-0.365904	-2.167454	H	3.270708	-1.959607	2.324998
H	4.196350	-1.289957	-2.007093	C	2.340414	5.315952	-0.313138
C	1.678824	3.106294	-1.898706	H	2.579520	6.183942	0.293655
H	1.408547	2.269768	-2.534579	C	4.515408	3.680383	2.647914
C	0.869530	3.430585	-0.790943	H	3.994197	4.631205	2.665486
C	-6.612935	0.721671	0.748340	C	-2.956067	-3.528100	-3.676227
H	-7.150686	1.432709	1.362208	H	-3.419979	-3.024754	-4.518237
C	4.098623	2.683832	1.760785	C	5.861784	1.220247	2.594502
H	3.256593	2.867683	1.102892	H	6.383557	0.270311	2.583935
C	-1.738544	3.219288	-1.935471	C	-7.295091	-0.173557	-0.088642
C	2.802151	3.880295	-2.205566	C	-2.073788	-3.596485	1.443803
H	3.406542	3.624841	-3.069320	H	-2.861891	-3.522104	0.704301
C	-3.144190	-4.900108	-3.487193	C	4.950002	-1.427948	1.064715
H	-3.758856	-5.467934	-4.178156	C	6.194106	1.994631	-2.598819
C	-4.507985	-0.216219	0.010669	H	6.764334	2.902638	-2.762334
C	6.003086	1.085967	-3.645831	C	3.423892	-4.672577	-2.252706
H	6.422414	1.290758	-4.625085	H	4.267254	-5.191969	-2.696103
C	-1.484903	3.184779	0.958911	C	-6.577426	-1.080465	-0.888279
C	-3.314134	4.455488	-3.915978	H	-7.131228	-1.754332	-1.530303
H	-3.918500	4.930249	-4.682285	C	5.653450	1.736066	-1.334408
C	-1.579425	4.591327	-2.227016	H	5.801347	2.448124	-0.531663
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C	1.210365	4.545568	-0.002498	H	0.704279	-3.857310	4.143049
H	0.587170	4.834938	0.834497	C	5.596771	3.451538	3.508353
C	-2.790324	3.710962	0.925864	H	5.914131	4.226374	4.198096
H	-3.343264	3.732763	-0.005282	C	-1.733038	-4.813121	-1.517933
C	-0.751683	-3.245361	1.109515	H	-1.253288	-5.329068	-0.693723
C	-1.552012	-3.424287	-1.693074	C	0.241204	-3.331264	2.105334
C	-5.190263	-1.102705	-0.841554	H	1.260498	-3.043354	1.877312
H	-4.627279	-1.792257	-1.458664	C	1.751552	-4.487040	-0.501793

H	1.308430	-4.889181	0.400662
C	4.922396	0.554573	-1.114620
C	-2.362869	5.202038	-3.209104
H	-2.226798	6.257141	-3.423666
C	2.882256	-3.542436	-2.878145
H	3.294133	-3.191474	-3.819766
C	-1.390178	-4.143995	3.707090
H	-1.633545	-4.497960	4.703519
C	-2.677756	4.218044	3.298492
H	-3.134401	4.620317	4.196810
C	6.267224	2.222819	3.481477
H	7.102386	2.042787	4.149529
C	5.276261	-0.091956	-3.428722
H	5.130106	-0.798699	-4.238210
C	3.137945	4.986273	-1.413829
H	4.002251	5.594052	-1.661972
C	6.096275	-3.825547	1.965723
H	6.538547	-4.753196	2.312853
O	-2.462169	-0.215982	-1.306553
O	-2.585154	-0.180721	4.516496
O	-4.133588	-0.895978	2.983590
P	-0.711502	2.462143	-0.573246
P	-0.373087	-2.525158	-0.559606
P	4.229617	0.174226	0.532643
Cl	-0.107674	0.091179	-2.965361
Os	-0.444825	-0.036624	-0.496911
C	-9.496854	0.654063	0.592308
H	-9.334018	0.488081	1.663167
H	-9.300103	1.703165	0.343828
H	-10.522713	0.399950	0.330895
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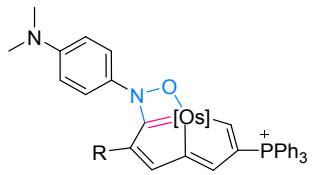
4



R = COOMe
[Os] =$OsCl(PPh_3)_2$

E = -3202.10081686

Os	-0.357802	-0.023281	-0.570898
Cl	-0.042517	0.089393	-3.004833
P	-0.383316	-2.427026	-0.562933
P	-0.339454	2.375797	-0.493221
P	4.261444	0.083815	0.492887
O	-2.583414	-0.089135	4.416843
O	-2.362287	-0.114945	-1.329936
O	-4.046752	-0.735561	2.840669
N	-2.943089	-0.072634	-0.067794
C	-0.823739	3.026743	1.193048
C	0.367520	-0.035724	1.423728
C	-2.171688	3.419826	1.354706
H	-2.754779	3.409989	0.629240
C	-1.961173	-0.060743	0.740205
C	-0.544023	-0.084995	2.514876
H	-0.267132	-0.119222	3.401627
C	-2.940858	-0.324539	3.098377
C	1.258545	3.186594	-0.934903
C	1.943104	4.119187	-0.177077
H	1.655138	4.281563	0.693396
C	-2.321236	2.733605	-2.470081
H	-2.407548	1.807559	-2.488830
C	-4.368339	-0.051428	0.004559
C	-1.435462	3.358438	-1.609966
C	1.703518	0.024635	-0.650805
H	2.114522	0.030854	-1.483918
N	-8.548891	0.317013	-0.074493
C	1.725534	-0.001301	1.691703
H	2.098069	-0.010220	2.543934
C	2.488709	0.048962	0.456076
C	1.188677	-3.281654	-0.936765
C	2.789074	-5.116865	-0.633151
H	3.072377	-5.873376	-0.170863
C	-1.482686	-3.309817	-1.769762
C	-1.265910	4.736041	-1.593204
H	-0.627511	5.124523	-1.038909
C	-5.113379	-0.956933	-0.726094
H	-4.695396	-1.624303	-1.222455
C	-1.853786	-0.081289	2.147198
C	4.376439	2.172114	2.273114
H	3.795456	1.653181	2.779117
C	-0.940542	-3.074825	1.060174
C	-4.993296	0.973726	0.739949
H	-4.498438	1.584053	1.235697
C	-2.610861	3.810788	2.581900
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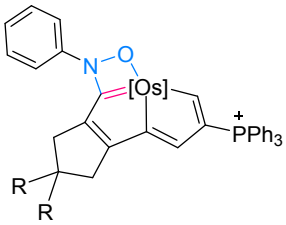
C	-1.777310	-4.693512	-1.549918
H	-1.421904	-5.104195	-0.795010

C	1.650276	-4.436902	-0.234892	H	-8.840471	1.881735	1.144835
H	1.174857	-4.738608	0.504758	H	-10.083743	1.565878	0.242144
C	0.035018	3.021677	2.229772	H	-8.830376	2.278233	-0.372675
H	0.912245	2.729210	2.109021	C	3.067945	-3.535940	-2.422736
C	-3.103929	3.578265	-3.334198	H	3.561769	-3.224301	-3.147749
H	-3.711243	3.184124	-3.916658	C	-3.067831	-4.774541	-3.508960
C	-2.984212	4.932416	-3.329007	H	-3.612785	-5.259980	-4.083915
H	-3.491052	5.458970	-3.904412	C	4.124863	-2.355982	1.709454
C	-2.055657	5.526495	-2.410701	H	3.404792	-2.498576	1.139073
H	-1.982263	6.451387	-2.363992	C	4.806888	3.458390	2.702317
C	-6.501596	-0.852578	-0.707624	H	4.501220	3.780611	3.518762
H	-6.997554	-1.503788	-1.151665	C	3.498727	4.569538	-1.911074
C	-0.399376	3.457359	3.496344	H	4.254863	5.007373	-2.229986
H	0.196184	3.484214	4.210961	C	5.874472	-0.931832	2.511928
C	4.894678	1.721936	1.015481	H	6.293762	-0.101460	2.535872
C	-7.170031	0.130879	-0.088710	C	-0.577412	-3.696799	3.341204
C	4.789434	-1.159904	1.667432	H	0.024588	-3.832086	4.038790
C	-6.396720	1.038057	0.696383	C	2.829246	3.652430	-2.708945
H	-6.837120	1.690767	1.193208	H	3.102554	3.508758	-3.586071
C	1.911959	-2.888806	-2.038987	C	5.749919	2.440117	0.238155
H	1.614137	-2.165365	-2.540051	H	6.029151	2.117641	-0.588274
C	-2.519965	-5.407989	-2.352293	C	-9.303211	-0.576837	-0.862056
H	-2.687989	-6.304238	-2.173687	H	-8.975546	-0.562751	-1.763624
C	3.486973	-4.663334	-1.712325	H	-10.225831	-0.308939	-0.850781
H	4.256704	-5.112034	-1.980199	H	-9.223931	-1.463744	-0.504621
C	3.034719	4.821645	-0.651450	C	-2.765839	-3.795885	2.432183
H	3.450304	5.460563	-0.117969	H	-3.663661	-4.011412	2.544055
C	-2.037867	-2.667077	-2.877102	C	4.509207	-3.367139	2.596092
H	-1.910682	-1.754258	-3.003663	H	4.026589	-4.158555	2.674034
C	-2.318786	-3.347046	1.197363	C	-1.846312	-3.938679	3.560637
H	-2.905763	-3.228031	0.487210	H	-2.150140	-4.190785	4.401579
C	-1.709128	3.844196	3.672399	C	5.637744	4.225675	1.970427
H	-2.002063	4.127636	4.507634	H	5.880405	5.083363	2.234181
C	-2.785429	-3.405470	-3.790786	C	5.666869	-3.126800	3.367018
H	-3.099464	-3.010991	-4.573601	H	5.987085	-3.796259	3.927140
C	-3.585534	-0.339307	5.399160	C	6.159220	3.569026	0.670559
H	-4.337886	0.235044	5.242237	H	6.805543	4.023230	0.177072
H	-3.227127	-0.162970	6.273076	C	6.314551	-1.962938	3.309494
H	-3.865419	-1.255831	5.345751	C	4.669683	0.409147	-2.250066
C	-0.087001	-3.253060	2.134123	H	4.084330	1.129579	-2.207293
H	0.821771	-3.074021	2.039958	C	5.274745	0.075082	-3.456122
C	1.740924	2.944371	-2.179809	H	5.094205	0.573047	-4.220139
H	1.336071	2.286286	-2.699655	C	6.149269	-1.002799	-3.518958
C	-9.124522	1.623185	0.264609	C	6.418820	-1.746658	-2.375730

H	7.004203	-2.467013	-2.418446
C	5.813177	-1.414020	-1.170611
C	4.938685	-0.336091	-1.107856
H	7.198028	-1.827432	3.897794
H	6.615270	-1.260333	-4.447124
H	6.019951	-1.987505	-0.291247

6



R = COOMe
[Os] = $OsCl(PPh_3)_2$

E = -3412.66443258

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P	0.343167	1.853024	-2.053384
P	-3.966282	0.473609	1.026891
O	2.064265	-0.953674	-2.148006
O	2.616579	3.599985	3.161349
N	2.977746	-0.526746	-1.129443
O	3.208756	1.261153	5.713422
O	4.744300	2.851893	3.543540
O	4.298173	-0.474699	4.688638
C	1.062670	-4.103922	-1.242524
C	2.189434	-0.117982	-0.151934
C	1.196863	-2.990335	1.435769
C	-1.730198	-0.192281	-0.579842
H	-2.405929	-0.474418	-1.380510
C	2.450090	0.317979	1.169179
C	-1.179221	0.573135	1.571318
H	-1.359222	0.987661	2.560128
C	1.271528	0.554558	1.825937
C	3.694248	1.630924	-4.471491
H	4.055748	0.957077	-5.241174
C	-5.020488	0.404916	-0.465105
C	1.521229	-3.873534	-2.550609
H	1.481139	-2.879631	-2.968485
C	2.478060	1.359924	-3.836570
H	1.916593	0.475378	-4.106517
C	0.600245	-2.626177	2.658945
H	-0.414652	-2.246662	2.671549
C	0.672998	3.548582	0.205711
H	1.322824	2.772049	0.584439
C	0.014782	3.378401	-1.028204
C	4.443557	2.758800	-4.115748
H	5.386934	2.964573	-4.611120
C	6.233402	-1.967430	-2.146144
H	6.616915	-2.879063	-2.591698
C	1.109893	-5.416040	-0.722546
H	0.746328	-5.621853	0.278136
C	1.989780	2.227391	-2.835823
C	4.860966	-1.832109	-1.927930
H	4.167705	-2.618839	-2.200372
C	0.073764	0.328426	1.069822
C	2.530557	-3.443299	1.447048
H	3.016016	-3.725630	0.520473
C	3.968223	3.620910	-3.122309
H	4.536745	4.503851	-2.847643
C	-0.856121	2.089987	-3.462745
C	-1.379776	-3.564125	0.082156
C	2.746848	3.361637	-2.487701
H	2.385409	4.052257	-1.736152
C	1.496332	0.990683	3.253114
H	1.153536	0.224014	3.957843
H	0.990986	1.927597	3.504658
C	3.659956	0.494581	2.052899
H	4.460379	1.098885	1.618934
H	4.106351	-0.466419	2.334465
C	7.113472	-0.937209	-1.787655
H	8.179136	-1.050195	-1.955404
C	5.240643	0.399770	-1.017035
H	4.839285	1.335038	-0.645626
C	2.025461	-4.935931	-3.315606
H	2.368522	-4.743866	-4.327159
C	3.058604	1.177606	3.340832
C	-2.219744	0.272074	0.624003
C	4.372616	-0.651702	-1.346783
C	0.518672	4.724388	0.948989
H	1.051117	4.823987	1.887697
C	-3.409031	3.190093	1.459715
H	-2.637181	3.074096	0.706728
C	-0.439416	2.529849	-4.731547

H	0.608302	2.706619	-4.934252	H	6.311390	4.141827	3.764076
C	-3.829704	-4.962238	0.194209	C	-2.231863	1.889352	-3.238192
H	-4.766115	-5.509398	0.232488	H	-2.579767	1.560766	-2.267107
C	-4.570848	-0.820481	2.179671	C	3.405654	2.667853	3.345114
C	-3.494865	-4.213078	-0.941381	C	3.667692	0.787825	7.032276
H	-4.164788	-4.191686	-1.796009	H	3.254903	1.502018	7.740990
C	3.616454	0.549392	4.615762	H	4.758672	0.781664	7.064884
C	-5.175067	-0.819010	-1.148310	H	3.290063	-0.219212	7.219852
H	-4.678086	-1.715359	-0.793176	C	1.306910	-2.744491	3.860970
C	-1.717483	-4.330817	1.212029	H	0.823864	-2.479527	4.796869
H	-1.030144	-4.417858	2.043807	C	-5.979736	-0.880389	-2.289148
C	-2.735175	2.536692	-5.520418	H	-6.092928	-1.821572	-2.815880
H	-3.456704	2.703182	-6.313717	C	-6.493040	1.481081	-2.068890
C	1.617709	-6.467286	-1.488469	H	-7.009841	2.368350	-2.418313
H	1.647268	-7.469236	-1.072624	C	3.240884	-3.541462	2.649122
C	2.078093	-6.229457	-2.790303	H	4.269135	-3.886964	2.637345
H	2.466660	-7.047674	-3.388107	C	-0.966175	5.595930	-0.753545
C	-1.373458	2.745937	-5.752630	H	-1.594168	6.392373	-1.140592
H	-1.030338	3.079671	-6.726456	C	-3.607665	4.438349	2.058727
C	-2.938152	-5.016648	1.268887	H	-2.987797	5.274588	1.757014
H	-3.179334	-5.605378	2.148175	C	2.630787	-3.199429	3.860523
C	-4.202487	2.092867	1.850705	H	3.186487	-3.268498	4.788371
C	6.613911	0.244245	-1.227038	C	-5.929818	-1.192472	2.183272
H	7.289536	1.053975	-0.973008	H	-6.618463	-0.762607	1.464390
C	-0.302788	5.752006	0.469275	C	-5.514218	-2.697982	4.038792
H	-0.412722	6.671342	1.036449	H	-5.878664	-3.423512	4.758210
C	-5.683506	1.555945	-0.929718	C	-4.589052	4.599686	3.044020
H	-5.577059	2.499335	-0.407234	H	-4.736420	5.568924	3.508581
C	-0.807689	4.421497	-1.500094	C	-6.395586	-2.128688	3.112138
H	-1.313153	4.330974	-2.452403	H	-7.442371	-2.412686	3.109353
C	-6.640430	0.266296	-2.748923	C	-4.162257	-2.334073	4.034824
H	-7.270261	0.211192	-3.630426	H	-3.477378	-2.778910	4.748621
C	-3.161958	2.112821	-4.256062	C	-3.687941	-1.399627	3.109678
H	-4.216548	1.947901	-4.062282	H	-2.638729	-1.127640	3.107075
C	-2.284686	-3.513520	-0.998430	C	-5.187403	2.258406	2.843899
H	-2.025723	-2.952712	-1.890685	H	-5.794745	1.418557	3.161387
C	5.242417	4.239681	3.590522	C	-5.377137	3.510377	3.435746
H	4.756340	4.779178	4.405350	H	-6.134012	3.632483	4.202954
H	5.038764	4.741823	2.642865				

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