Supplementary Information

Ring Contraction of Metallacyclobutadiene to Metallacyclopropene Driven by π- and σ-Aromaticity Relay

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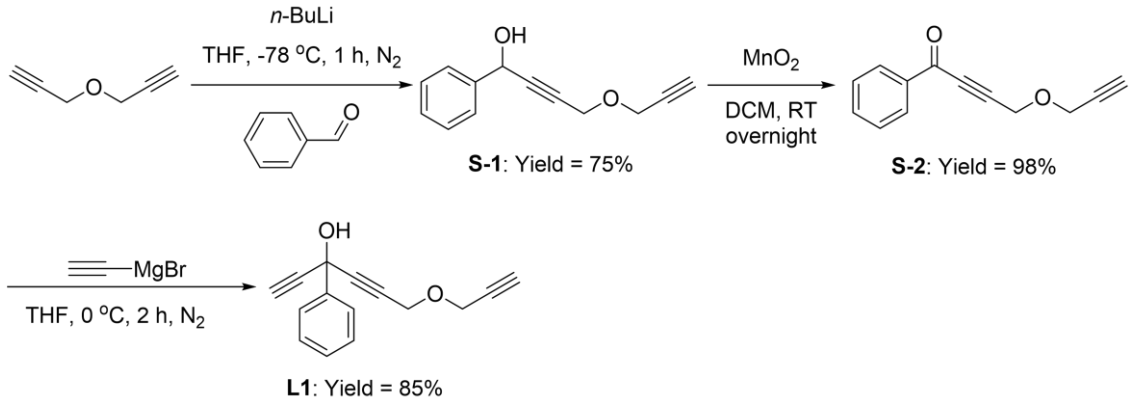
Supplementary Methods

1. 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 (tetrahydrofuran and diethyl ether) or calcium hydride (dichloromethane) under N_2 prior to use. Other reagents were used as received from commercial sources without further purification. Column chromatography was performed on alumina gel (200–300 mesh) or silica gel (200–300 mesh) in air. Nuclear magnetic resonance (NMR) spectroscopic experiments were performed on a Bruker AVIII-400 (^{1}H, 400.0 MHz; ^{13}C, 100.6 MHz; ^{31}P, 161.9 MHz), a Bruker AVIII-500 (^{1}H, 500.2 MHz; ^{13}C, 125.8 MHz; ^{31}P, 202.5 MHz) or a Bruker Ascend III 600 (^{1}H, 600.1 MHz; ^{13}C, 150.9 MHz; ^{31}P, 242.9 MHz) spectrometer 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. The absolute values of the coupling constants are given in Hertz (Hz). Assignments of signals in ^{1}H and ^{13}C NMR spectra were done by reference to heteronuclear single quantum coherence (HSQC), heteronuclear multiple bond correlation (HMBC), and distortionless enhancement by polarization transfer (DEPT) NMR spectra. Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t), multiplet (m), and broad (br). High-resolution mass spectroscopy (HRMS) experiments were conducted on an Agilent 1290-6545XT (**1** and **2a**) or Bruker En Apex Ultra 7.0T FTMS (**2b**, **2c**, **3a**–**3c**, **4A**, **5a**, **5b** and **6a**). The theoretical molecular ion peak was calculated by mmass_v5.5.0_msw[1-3] (**1** and **2a**) or Compass Isotope Pattern software supplied by Bruker Co (**2b**, **2c**, **3a**–**3c**, **4A**, **5a**, **5b** and **6a**). Elemental analyvses were performed on a Vario EL III elemental analyzer. Absorption spectra were recorded on an Agilent Cary5000 UV–Vis–NIR spectrophotometer (**1**, **2a**–**2c**) or JascoV-780 UV–Vis–NIR (**3a**–**3c**, **5a**, **5b** and **6a**) spectrophotometer.

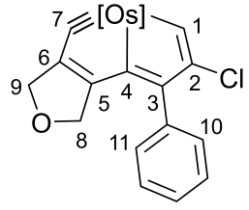
2. Synthesis and Characterization

General procedure for the synthesis of compounds S-1, S-2 and L1.



Compounds **S-1**, **S-2** and **L1** were synthesized according to the literature.[4] Compound **S-1**: ^{1}H-NMR (400.0 MHz, $CDCl_3$): δ = 7.54 (d, J_{H-H} = 7.08 Hz, 2H), 7.34-7.40 (m, 3H), 5.50 (s, 1H), 4.35 (d, J_{H-H} = 1.68 Hz, 2H), 4.26 (d, J_{H-H} = 2.36 Hz, 2H), 2.89 (br, 1H), 2.48 ppm (t, J_{H-H} = 2.35 Hz, 1H); ^{13}C-NMR (100.6 MHz, $CDCl_3$): δ = 140.4, 128.7, 128.4, 126.6, 86.92, 81.59, 78.84, 75.24, 64.47, 56.85, 56.60 ppm. Compound **S-2**: ^{1}H-NMR (400.0 MHz, $CDCl_3$): δ = 8.13 (d, J_{H-H} = 7.05 Hz, 2H), 7.62 (t, J_{H-H} = 6.32 Hz, 1H), 7.49 (t, J_{H-H} = 6.63 Hz, 2H), 4.56 (s, 2H), 4.35 (s, 2H), 2.53 ppm (s, 1H); ^{13}C-NMR (100.6 MHz, $CDCl_3$): δ = 177.3, 136.3, 134.4, 129.6, 128.7, 89.04, 84.45, 78.30, 75.86, 57.19, 56.53 ppm. Compound **L1**: ^{1}H-NMR (400.0 MHz, $CDCl_3$): δ = 7.81 (dd, J_{H-H} = 8.10 Hz, J_{H-H} = 1.53 Hz, 2H), 7.38-7.44 (m, 3H), 4.38 (s, 2H), 4.27 (d, J_{H-H} = 2.32 Hz, 2H), 3.22 (br, 1H), 2.80 (s, 1H), 2.48 ppm (t, J_{H-H} = 2.33 Hz,1H); ^{13}C-NMR (100.6 MHz, $CDCl_3$): δ = 141.0, 128.9, 128.6, 125.7, 86.69, 83.53, 80.53, 78.72, 75.33, 73.65, 64.81, 56.72 ppm. All spectra were consistent with those previously reported.

Preparation and characterization of complex 1.

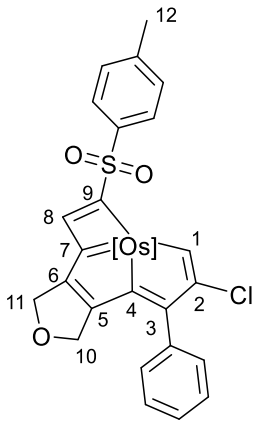


[Os] = $OsCl(PPh_3)_2$

1

Under a N_2 atmosphere, a mixture of **L1** (256 mg, 1.14 mmol), $OsCl_2(PPh_3)_3$ (1.00 g, 0.95 mmol) and *n*-Bu_4NCl (1.00 g, 3.60 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 15 min to give a brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (alumina gel, eluent: CH_2Cl_2) to give **1** (425 mg, 45%) as a yellow solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.42 (s, 1H, C^1*H*), 7.53-7.32 (m, 33H, other aromatic protons), 6.71 (d, $J_{H\text{-}H}$ = 7.60 Hz, 2H, C^{10}*H* and C^{11}*H*), 4.56 (s, 2H, C^9*H*), 2.75 ppm (s, 2H, C^8*H*); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = 2.62 ppm (s, Os*P*Ph$_3$); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 310.0 (t, $J_{P\text{-}C}$ = 15.59 Hz, C^7), 202.0 (t, $J_{P\text{-}C}$ = 9.56 Hz, C^1), 175.0 (s, C^4), 160.7 (s, C^6), 157.9 (s, C^5), 152.8 (s, C^3), 142.2 (t, $J_{P\text{-}C}$ = 5.03 Hz, C^2), 139.7-127.4 (m, other aromatic carbons), 71.15 (s, C^8), 64.89 ppm (s, C^9); HRMS (ESI): m/z calcd for $[C_{51}H_{40}Cl_2OOsP_2+Na^+]^+$: 1015.1425, found: 1015.1440.

Preparation and characterization of complex 2a.



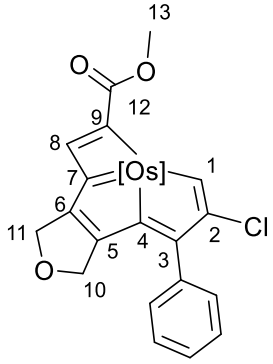
[Os] = $OsCl(PPh_3)_2$

2a

Under a N_2 atmosphere, a mixture of complex **1** (500 mg, 0.50 mmol) and *p*-toluenesulfonylacetylene (400 mg, 2.50 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 5 min to give a brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then mixed solvent (Et_2O/PE = 1:4, v/v, 50 mL) was added to the solution. The brown precipitate was collected by filtration, washed with mixed solvent (Et_2O/PE = 1:4, v/v, 2 × 50 mL) and dried under vacuum to give **2a** (527 mg, 90%) as a brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, $CDCl_3$): δ = 13.29 (t, $J_{P\text{-}H}$ = 1.60 Hz, 1H, C^1*H*), 7.68-7.07 (m, 37H, other aromatic protons), 6.01 (d, $J_{H\text{-}H}$ = 7.66 Hz, 2H, C^{12}*H* and C^{13}*H*), 5.41 (t, $J_{P\text{-}H}$ = 2.80 Hz, 1H, C^8*H*), 4.19 (s, 2H, C^{11}*H*), 2.35 (s, 3H, C^{14}*H*), 2.30 ppm (s, 2H, C^{10}*H*); ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = -12.07 ppm (s, Os*P*Ph$_3$); ^{13}C-NMR plus DEPT-

135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2): δ = 229.6 (s, C^{1}), 173.3 (t, $J_{P\text{-}C}$ = 5.28 Hz, C^{7}), 172.4 (s, C^{4}), 170.2 (s, C^{3}), 164.4 (t, $J_{P\text{-}C}$ = 8.30 Hz, C^{9}), 163.9 (s, C^{5}), 153.8 (t, $J_{P\text{-}C}$ = 5.28 Hz, C^{8}), 147.4 (s, C^{6}), 133.9 (s, C^{2}), 143.0-126.2 (m, other aromatic carbons), 72.43 (s, C^{10}), 64.72 (s, C^{11}), 21.24 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{48}Cl_2O_3OsP_2S\text{-}Cl^-]^+$: 1137.2094, found: 1137.2045; Elemental analysis calcd (%) for $C_{60}H_{48}Cl_2O_3OsP_2S$: C 61.48, H 4.13, found: C 61.58, H 4.39.

Preparation and characterization of complex 2b.

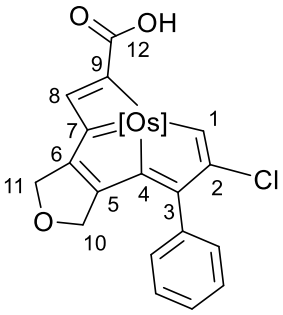


[Os] = $OsCl(PPh_3)_2$

2b

Under a N_2 atmosphere, a mixture of complex **1** (500 mg, 0.50 mmol) and methyl propiolate (200 μL, 2.50 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 5 min to give a brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then mixed solvent (Et_2O/PE = 1:4, v/v, 50 mL) was added to the solution. The brown precipitate was collected by filtration, washed with mixed solvent (Et_2O/PE = 1:4, v/v, 2 × 50 mL) and dried under vacuum to give **2b** (495 mg, 92%) as a brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.94 (s, 1H, $C^{1}H$), 7.71-7.27 (m, 33H, other aromatic protons), 6.54 (s, 1H, $C^{8}H$), 6.33 (d, $J_{H\text{-}H}$ = 7.20 Hz, 2H, $C^{12}H$ and $C^{13}H$), 4.01 (s, 2H, $C^{11}H$), 3.54 (s, 3H, $C^{15}H$), 2.22 ppm (s, 2H, $C^{10}H$); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -10.02 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 227.5 (t, $J_{P\text{-}C}$ = 6.20 Hz, C^{1}), 173.0 (s, C^{4}), 172.0 (t, $J_{P\text{-}C}$ = 5.66 Hz, C^{7}), 171.2 (s, C^{14}), 169.2 (s, C^{3}), 164.9 (d, $J_{P\text{-}C}$ = 7.04 Hz, C^{9}), 162.4 (s, C^{5}), 156.0 (t, $J_{P\text{-}C}$ = 5.24 Hz, C^{8}), 145.2 (s, C^{6}), 134.9 (s, C^{2}), 139.1-125.0 (m, other aromatic carbons), 72.32 (s, C^{10}), 64.15 (s, C^{11}), 50.33 ppm (s, C^{15}); HRMS (ESI): m/z calcd for $[C_{55}H_{44}Cl_2O_3OsP_2\text{-}Cl^-]^+$: 1041.2056, found: 1041.2099; Elemental analysis calcd (%) for $C_{55}H_{44}Cl_2O_3OsP_2$: C 61.39, H 4.12, found: C 61.26, H 4.21.

Preparation and characterization of complex 2c.

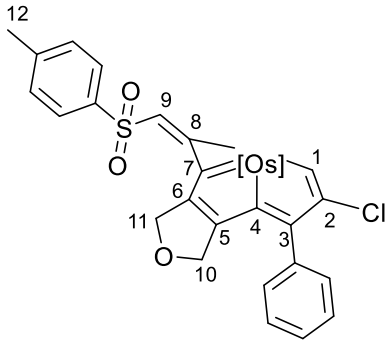


[Os] = $OsCl(PPh_3)_2$

2c

Under a N_2 atmosphere, a mixture of complex **1** (500 mg, 0.50 mmol) and propiolic acid (153 μL, 2.50 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 5 min to give a brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then mixed solvent (Et_2O/PE = 1:4, v/v, 50 mL) was added to the solution. The brown precipitate was collected by filtration, washed with mixed solvent (Et_2O/PE = 1:4, v/v, 2 × 50 mL) and dried under vacuum to give **2c** (504 mg, 95%) as a brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 13.05 (s, 1H, C^1*H*), 7.54-7.29 (m, 34H, COO*H*, other aromatic protons), 7.14 (s, 1H, C^8*H*), 6.51 (d, $J_{H\text{-}H}$ = 7.20 Hz, 2H, C^{12}*H* and C^{13}*H*), 4.16 (s, 2H, C^{11}*H*), 2.18 ppm (s, 2H, C^{10}*H*); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -9.22 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 225.9 (t, $J_{P\text{-}C}$ = 7.45 Hz, C^1), 175.1 (s, C^4), 174.1 (t, $J_{P\text{-}C}$ = 5.60 Hz, C^7), 170.7 (s, C^{14}), 169.4 (s, C^3), 166.0 (t, $J_{P\text{-}C}$ = 7.75 Hz, C^9), 163.1 (s, C^5), 159.9 (t, $J_{P\text{-}C}$ = 4.73 Hz, C^8), 145.8 (s, C^6), 128.8 (s, C^2), 138.5-125.9 (m, other aromatic carbons), 72.26 (s, C^{10}), 64.38 ppm (s, C^{11}); HRMS (ESI): m/z calcd for $[C_{54}H_{42}Cl_2O_3OsP_2\text{-}Cl^-]^+$: 1027.1900, found: 1027.1982; Elemental analysis calcd (%) for $C_{54}H_{42}Cl_2O_3OsP_2$: C 61.07, H 3.99, found: C 61.06, H 4.32.

Preparation and characterization of complex 3a.

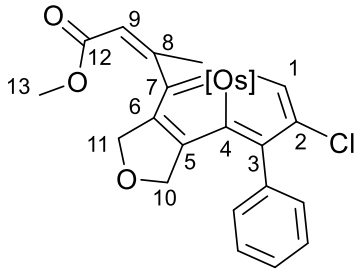


[Os] = $OsCl(PPh_3)_2$

3a

Under a N_2 atmosphere, trifluoroacetic acid (500 μL, 6.73 mmol) was added to a solution of complex **2a** (500 mg, 0.43 mmol) in CH_2Cl_2 (25 mL). The reaction mixture was stirred at rt for 3 h to give a mandarin red solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **3a** (200 mg, 40%) as a reddish-brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 12.81 (s, 1H, C^1*H*), 7.51-7.12 (m, 37H, other aromatic protons), 6.71 (d, $J_{H\text{-}H}$ = 6.00 Hz, 2H, C^{12}*H* and C^{13}*H*), 6.45 (s, 1H, C^9*H*), 4.64 (s, 2H, C^{11}*H*), 3.03 (s, 2H, C^{10}*H*), 2.39 ppm (s, 3H, C^{14}*H*); ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = -17.85 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (150.9 MHz, CD_2Cl_2): δ = 225.8 (q, $J_{P\text{-}C}$ = 25.66 Hz, $J_{P\text{-}C}$ = 11.00 Hz, C^1), 179.3 (s, C^4), 176.0 (t, $J_{P\text{-}C}$ = 3.60 Hz, C^7), 172.5 (s, C^6), 164.0 (s, C^5), 159.0 (s, C^3), 152.6 (t, $J_{P\text{-}C}$ = 4.53 Hz, C^8), 144.4 (s, C^2), 142.7-126.5 (m, other aromatic carbons), 113.6 (s, C^9), 71.11 (s, C^{10}), 68.14 (s, C^{11}), 21.25 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{48}Cl_2O_3OsP_2S+Na^+]^+$: 1195.1666, found: 1195.1680; Elemental analysis calcd (%) for $C_{60}H_{48}Cl_2O_3OsP_2S$: C 61.48, H 4.13, found: C 61.49, H 4.16.

Preparation and characterization of complex 3b.

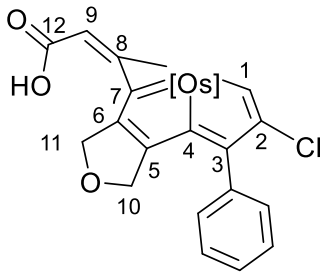


[Os] = $OsCl(PPh_3)_2$

3b

Under a N_2 atmosphere, trifluoroacetic acid (500 μL, 6.73 mmol) was added to a solution of complex **2b** (500 mg, 0.46 mmol) in CH_2Cl_2 (25 mL). The reaction mixture was stirred at rt for 3 h to give a reddish-brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **3b** (260 mg, 52%) as a reddish-brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.84 (s, 1H, C^1*H*), 7.49-7.30 (m, 33H, other aromatic protons), 6.66 (d, $J_{H\text{-}H}$ = 7.60 Hz, 2H, C^{12}*H* and C^{13}*H*), 6.15 (s, 1H, C^9*H*), 4.51 (s, 2H, C^{11}*H*), 3.56 (s, 3H, C^{15}*H*), 3.10 ppm (s, 2H, C^{10}*H*); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -16.16 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 224.7 (t, $J_{P\text{-}C}$ = 10.56 Hz, C^1), 178.8 (s, C^4), 178.2 (t, $J_{P\text{-}C}$ = 3.84 Hz, C^7), 171.6 (s, C^6), 166.9 (s, C^{14}), 162.8 (s, C^5), 158.7 (s, C^3), 152.2 (t, $J_{P\text{-}C}$ = 4.92 Hz, C^8), 149.0 (s, C^2), 134.2-126.5 (m, other aromatic carbons), 106.1 (s, C^9), 71.32 (s, C^{10}), 67.69 (s, C^{11}), 50.90 ppm (s, C^{15}); HRMS (ESI): m/z calcd for $[C_{55}H_{44}Cl_2O_3OsP_2\text{-}Cl^-]^+$: 1041.2056, found: 1041.2086; Elemental analysis calcd (%) for $C_{55}H_{44}Cl_2O_3OsP_2$: C 61.39, H 4.12, found: C 61.34, H 4.24.

Preparation and characterization of complex 3c.

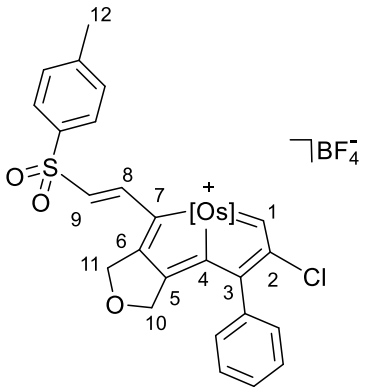


[Os] = $OsCl(PPh_3)_2$

3c

Under a N_2 atmosphere, trifluoroacetic acid (500 μL, 6.73 mmol) was added to a solution of complex **2c** (500 mg, 0.47 mmol) in CH_2Cl_2 (25 mL). The reaction mixture was stirred at rt for 3 h to give a reddish-brown solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **3c** (300 mg, 52%) as a reddish-brown solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.83 (s, 1H, C^1*H*), 7.47-7.22 (m, 34H, COO*H*, other aromatic protons), 6.59 (d, $J_{H\text{-}H}$ = 5.60 Hz, 2H, C^{12}*H* and C^{13}*H*), 6.12 (s, 1H, C^9*H*), 4.51(s, 2H, C^{11}*H*), 3.12 ppm (s, 2H, C^{10}*H*); ^{31}P-NMR (161.9 MHz, CF_3COOD:CD_2Cl_2 = 1:100, v/v)): δ = -15.71 ppm (s, Os*P*Ph$_3$); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CF_3COOD:CD_2Cl_2 = 1:100, v/v): δ = 227.3 (s, C^1), 176.5 (s, C^4), 175.2 (s, C^7), 173.0 (s, C^{14}), 161.4 (s, C^5), 159.8 (s, C^3), 156.4 (s, C^8), 154.8 (s, C^6), 139.3 (s, C^2), 133.7-126.2 (m, other aromatic carbons), 103.1 (s, C^9), 71.25 (s, C^{10}), 67.93 ppm (s, C^{11}); HRMS (ESI): m/z calcd for [$C_{54}H_{42}Cl_2O_3OsP_2$-Cl$^-$]$^+$: 1027.1900, found: 1027.1975; Elemental analysis calcd (%) for $C_{54}H_{42}Cl_2O_3OsP_2$: C 61.07, H 3.99, found: C 61.33, H 4.24.

Preparation and characterization of complex 4A.



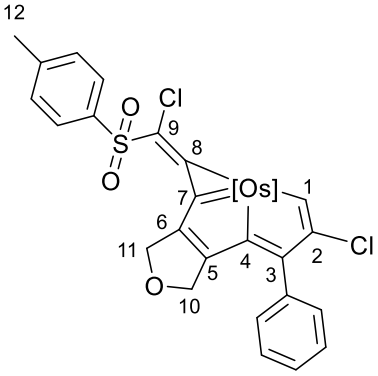
[Os] = OsCl(PPh$_3$)$_2$

4A

Under a N_2 atmosphere, a solution of HBF_4·Et_2O (50-55% w/w HBF_4, 100 μL, 0.60 mmol) was added to a solution of complex **2a** (50 mg, 42.5 μmol) in CH_2Cl_2 (0.5 mL). The reaction mixture was stirred at rt for 30 min to give an orange solution of **4A** (in approximately 80% yield based on ^{1}H- and ^{31}P-NMR), which was characterized by *in situ* ^{1}H-NMR, ^{31}P-NMR and ^{13}C-NMR. Complex **4A** is stable only under strong acidic conditions. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 11.74 (s, 1H, C^1*H*), 7.80-7.25 (m, 37H, other aromatic protons), 6.99 (d, 1H, $J_{H\text{-}H}$ = 14.40 Hz, C^8*H*), 6.47 (d,

2H, $J_{H\text{-}H}$ = 6.80 Hz, $C^{12}H$ and $C^{13}H$), 6.10 (d, 1H, $J_{H\text{-}H}$ = 14.40 Hz, $C^{9}H$), 4.57 (s, 2H, $C^{11}H$), 3.69 (s, 2H, $C^{10}H$), 2.47 ppm (s, 3H, $C^{14}H$); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = 17.45 ppm (s, Os*P*Ph$_3$); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 215.8 (t, $J_{P\text{-}C}$ = 8.75 Hz, C^7), 214.1 (t, $J_{P\text{-}C}$ = 8.97 Hz, C^1), 176.1 (s, C^4), 170.4 (s, C^6), 169.1 (s, C^5), 166.9 (s, C^3), 146.7 (t, $J_{P\text{-}C}$ = 3.98 Hz, C^2), 135.0-126.3 (m, other aromatic carbons), 123.6 (s, C^8), 120.7 (s, C^9), 70.68 (s, C^{10}), 67.27 (s, C^{11}), 21.42 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{49}Cl_2O_3OsP_2S]^+$: 1173.1846, found: 1173.1898.

Preparation and characterization of complex 5a.

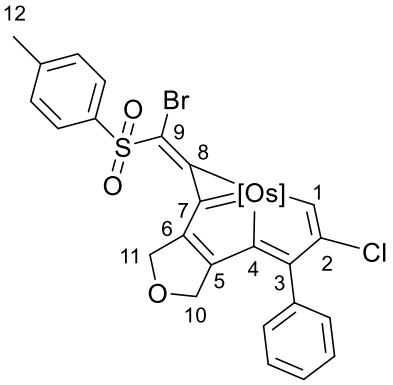


[Os] = OsCl(PPh$_3$)$_2$

5a

Under a N_2 atmosphere, a mixture of complex **3a** (500 mg, 0.43 mmol) and NCS (73 mg, 0.55 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 10 min to give a mandarin red solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **5a** (489 mg, 95%) as a mandarin red solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.69 (s, 1H, C^1H), 7.50-7.11 (m, 37H, other aromatic protons), 6.63 (d, $J_{H\text{-}H}$ = 6.80 Hz, 2H, $C^{12}H$ and $C^{13}H$), 4.66 (s, 2H, $C^{11}H$), 3.07 (s, 2H, $C^{10}H$), 2.42 ppm (s, 3H, $C^{14}H$); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -14.13 ppm (s, Os*P*Ph$_3$); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 225.7 (t, $J_{P\text{-}C}$ = 10.56 Hz, C^1), 180.6 (t, $J_{P\text{-}C}$ = 4.42 Hz, C^7), 179.8 (s, C^4), 170.3 (s, C^6), 163.4 (s, C^5), 160.2 (s, C^3), 151.8 (t, $J_{P\text{-}C}$ = 4.73 Hz, C^8), 135.5 (t, $J_{P\text{-}C}$ = 3.63 Hz, C^2), 136.2-126.5 (m, other aromatic carbons), 118.5 (s, C^9), 71.06 (s, C^{10}), 68.54 (s, C^{11}), 21.33 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{47}Cl_3O_3OsP_2S\text{-}Cl^-]^+$: 1171.1690, found: 1171.1709; Elemental analysis calcd (%) for $C_{60}H_{47}Cl_3O_3OsP_2S$: C 59.73, H 3.93, found: C 59.81, H 3.95.

Preparation and characterization of complex 5b.

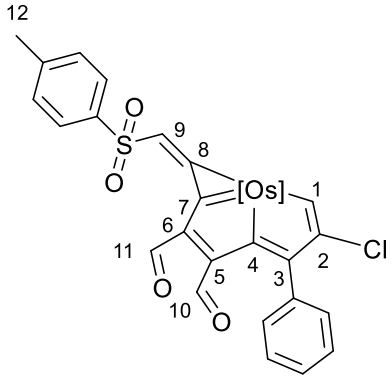


[Os] = $OsCl(PPh_3)_2$

5b

Under a N_2 atmosphere, a mixture of complex **3a** (500 mg, 0.43 mmol) and N-bromosuccinimide (NBS) (84 mg, 0.55 mmol) was stirred in CH_2Cl_2 (25 mL) at rt for 10 min to give a mandarin red solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **5b** (511 mg, 95%) as a mandarin red solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 12.76 (s, 1H, C^1*H*), 7.50-7.10 (m, 37H, other aromatic protons), 6.64 (d, $J_{H\text{-}H}$ = 6.00 Hz, 2H, C^{12}*H* and C^{13}*H*), 4.64 (s, 2H, C^{11}*H*), 3.13 (s, 2H, C^{10}*H*), 2.42 ppm (s, 3H, C^{14}*H*); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -14.11 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 225.3 (t, $J_{P\text{-}C}$ = 10.51 Hz, C^1), 181.4 (t, $J_{P\text{-}C}$ = 4.14 Hz, C^7), 179.6 (s, C^4), 169.9 (s, C^6), 163.6 (s, C^5), 160.3 (s, C^3), 152.0 (t, $J_{P\text{-}C}$ = 4.83 Hz, C^8), 138.0 (t, $J_{P\text{-}C}$ = 3.67 Hz, C^2), 139.3-126.6 (m, other aromatic carbons), 108.8 (s, C^9), 71.09 (s, C^{10}), 68.72 (s, C^{11}), 21.32 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{47}Cl_2BrO_3OsP_2S\text{-}Cl^-]^+$: 1215.1178, found: 1215.1254; Elemental analysis calcd (%) for $C_{60}H_{47}Cl_2BrO_3OsP_2S$: C 57.60, H 3.79, found: C 57.91, H 3.99.

Preparation and characterization of complex 6a.



[Os] = $OsCl(PPh_3)_2$

6a

Under a N_2 atmosphere, a mixture of complex **3a** (500 mg, 0.43 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (500 mg, 2.25 mmol) was stirred in dichloromethane (25 mL) at 40°C for 2 d to give a mandarin red solution. The solution was evaporated under vacuum to a volume of approximately 2 mL. Then the solution was purified by column chromatography (silica gel, eluent: CH_2Cl_2 and CH_2Cl_2/Me_2CO = 100:1, v/v) to give **6a** (357 mg, 70%) as a mandarin red solid. ^{1}H-NMR plus ^{1}H-^{13}C HSQC (400.0 MHz, CD_2Cl_2): δ = 13.39 (s, 1H, C^1*H*), 10.00 (s, 1H, C^{11}*H*), 9.04 (s, 1H, C^{10}*H*), 7.59-7.12 (m, 37H, other aromatic protons), 6.72 (s, 1H, C^9*H*), 6.46 (d, $J_{H\text{-}H}$ = 7.20 Hz, 2H, C^{12}*H* and C^{13}*H*), 2.43 ppm (s, 3H, C^{14}*H*); ^{31}P-NMR (161.9 MHz, CD_2Cl_2): δ = -19.15 ppm (s, Os*P*Ph_3); ^{13}C-NMR plus DEPT-135, ^{1}H-^{13}C HSQC and ^{1}H-^{13}C HMBC (100.6 MHz, CD_2Cl_2): δ = 240.6 (t, $J_{P\text{-}C}$ = 10.56 Hz, C^1), 192.7 (s, C^{10}), 188.9 (s, C^{11}), 187.8 (t, $J_{P\text{-}C}$ = 4.35 Hz, C^7), 183.5 (s, C^4), 167.6 (s, C^5), 167.0 (s, C^3), 156.7 (t, $J_{P\text{-}C}$ = 4.53 Hz, C^8), 152.9 (t, $J_{P\text{-}C}$ = 2.35 Hz, C^6), 143.1 (t, $J_{P\text{-}C}$ = 3.33 Hz, C^2), 140.3-126.9 (m, other aromatic carbons), 117.1 (s, C^9), 21.28 ppm (s, C^{14}); HRMS (ESI): m/z calcd for $[C_{60}H_{46}Cl_2O_4OsP_2S+Na^+]^+$: 1209.1459, found: 1209.1487; EA calcd (%) for $C_{60}H_{46}Cl_2O_4OsP_2S$: C 60.76, H 3.91, found: C 60.95, H 4.

3. Control Experiments

As shown in Fig. S1, reaction of complex **2a** (8.5 μmol, 10 mg) with 10 equiv. of CF_3COOH (85 μmol, 6.3 μL), product **3a** can be obtained exclusively within 25 min.

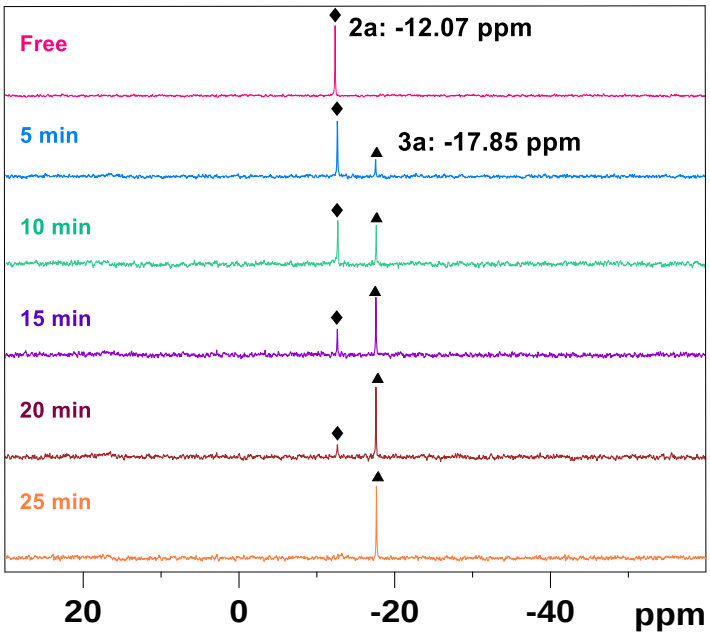


Fig. S1. The *in situ* ^{31}P-NMR (161.9 MHz) spectra for complex **2a** (8.5 μmol, 10 mg) with CF_3COOH (10 eq., 6.3 μL) in CH_2Cl_2 (0.5 mL) measured per 5 min. Complex **2a** (δ = -12.07 ppm) converted into **3a** (δ = -17.85 ppm) within 25 min.

However, when the reaction was carried in the presence of 20 equiv. of CF_3COOH (170 μmol**,** 12.6 μL), a new singlet at = 17.45 ppm in $^{31}P\{^1H\}$ NMR spectrum attributed to species **4a**, was observed. A series of parallel experiments showed that the content of **4a** increased gradually as the amount of acid increased (10 equiv. (85 μmol, 6.3 μL), 20 equiv. (170 μmol, 12.6 μL), 30 equiv. (255 μmol 19.0 μL) and 50 equiv. (425 μmol 31.6 μL) of CF_3COOH, respectively). After the acid exceeds 50 equiv., the relative ratio of **3a** and **4a** is almost unchanged (Fig. S2).

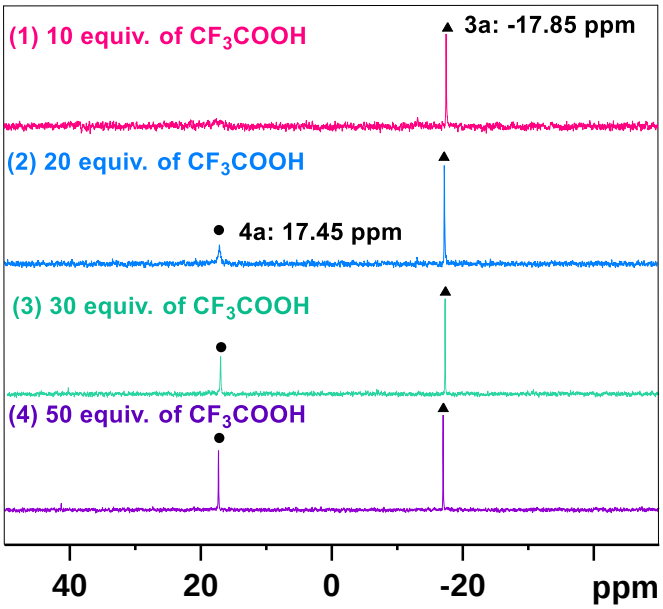


Fig. S2. Investigation of the formation of **4a** by $^{31}P\{^{1}H\}$ NMR spectroscopy. Parallel reactions of 10 equiv. (6.3 μL), 20 equiv. (12.6 μL), 30 equiv. (19.0 μL) and 50 equiv. (31.6 μL) of CF_3COOH with **2a**

Further, dilution experiments were conducted on the reaction system No. (3) containing 30 equiv. of CF_3COOH in (19.0 μL) in 0.5 mL CH_2Cl_2. The mixture of **3a** and **4a** was diluted to 5/7 (by addition of 0.2 mL CH_2Cl_2), 5/9 (total addition of 0.4 mL CH_2Cl_2) and 1/2 (total addition of 0.5 mL CH_2Cl_2) of its original concentration gradually, it can be observed that compound **4a** was gradually converted into **3a** with decreasing acid concentration. (Fig. S3)

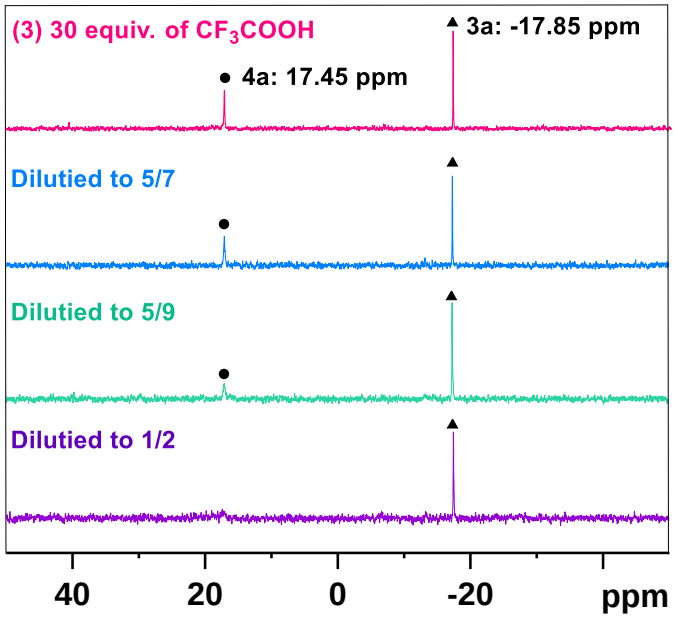


Fig. S3. The *in situ* ^{31}P-NMR (161.9 MHz) spectra of dilution experiments. The *in situ* reaction system (30 equiv. of CF_3COOH with **2a**) was diluted to 5/7, 5/9 and 1/2 of its original concentration. Compound **4a** converts to complex **3a** finally.

4. X-ray Crystallographic Analysis

Single-crystal X-ray diffraction data were collected on a Rigaku XtaLAB Synergy, Dualflex, HyPix diffractometer with $Mo_{K\alpha}$ radiation (λ = 0.71073 Å) for **2a** or $Cu_{K\alpha}$ radiation (λ = 1.54184 Å) for **3a**–**3c**, **4A** and **5b**, and by the SuperNova, Dual, Cu at home/near, Atlas diffractometer with $Mo_{K\alpha}$ radiation (λ = 0.71073 Å) for **6a**. The crystals were kept at 100 K during data collection. All single crystals suitable for X-ray diffraction were obtained by recrystallization from a solution of CH_2Cl_2 layered with diethyl ether (**2a**) or *n*-hexane (**3a**–**3c**, **4A**, **5b** and **6a**). With Olex2,[5] the structures were solved with the ShelXT[6] solution program using intrinsic phasing method and refined with the ShelXL[7] refinement package using least-squares minimization. Non-hydrogen atoms were refined anisotropically unless otherwise stated. The hydrogen atoms were introduced at their geometric positions and refined as riding atoms unless otherwise stated. The disordered solvents were removed from the dataset using the Solvent Mask routine of Olex 2 which was reported in the CIF. CCDC 2103042 (**2a**), 2103166 (**3a**), 2103167 (**3b**), 2103168 (**3c**), 2103171 (**4A**), 2103169 (**5b**) and 2103170 (**6a**) contain the supplementary crystallographic data for this paper. Further details on the crystal data, data collection, and refinements are provided in Tables S1-S10. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

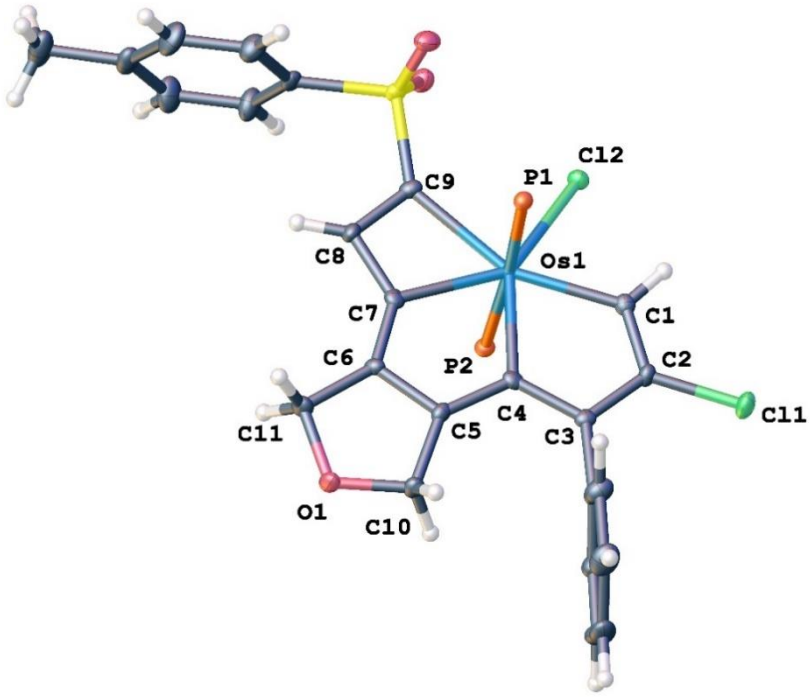


Fig. S4. X-ray crystal structure for complex **2a** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S1. Selected bond distances and angles for complex **2a**.

Bond Distances(Å)					
Os1–C1	2.046(3)	C1−C2	1.372(4)	C5−C6	1.396(4)
Os1–C4	2.127(3)	C2−C3	1.383(5)	C6−C7	1.381(5)
Os1–C7	2.064(3)	C3−C4	1.397(4)	C7–C8	1.425(4)
Os1–C9	2.218(3)	C4−C5	1.411(5)	C8–C9	1.338(5)
Bond Angels(°)					
Os1–C1–C2	122.1(3)		C5–C6–C7	111.7(3)	
C1–C2–C3	114.6(3)		C6–C7–Os1	123.0(2)	
C2–C3–C4	110.9(3)		C7–Os1–C4	72.87(13)	
C3–C4–Os1	120.1(2)		Os1–C7–C8	102.4(2)	
C4–Os1–C1	72.05(14)		C7–C8–C9	100.2(3)	
Os1–C4–C5	117.9(2)		C8–C9–Os1	98.2(2)	
C4–C5–C6	114.4(3)		C9–Os1–C7	59.21(13)	

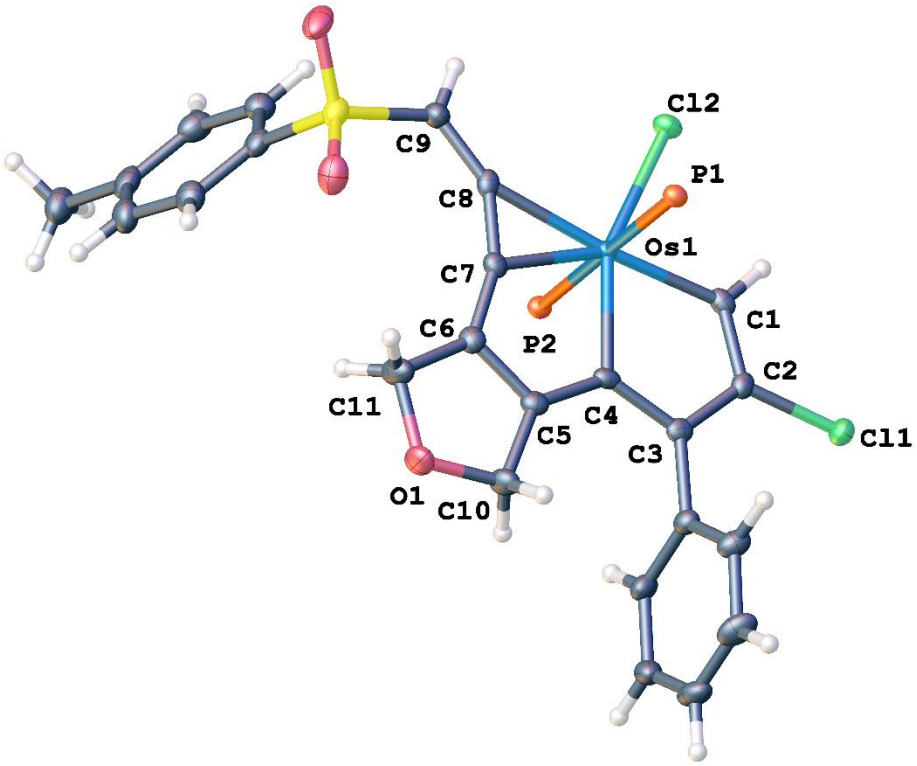


Fig. S5. X-ray crystal structure for complex **3a** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S2. Selected bond distances and angles for complex **3a**.

Bond Distances(Å)					
Os1–C1	2.027(2)	C1–C2	1.377(3)	C5–C6	1.384(3)
Os1–C4	2.116(2)	C2–C3	1.403(3)	C6–C7	1.370(3)
Os1–C7	2.008(2)	C3–C4	1.404(3)	C7–C8	1.363(3)
Os1–C8	2.169(2)	C4–C5	1.395(3)	C8–C9	1.325(3)

Bond Angels(°)			
Os1–C1–C2	119.46(16)	C6–C7–Os1	123.29(17)
C1–C2–C3	116.3(2)	C7–Os1–C4	73.57(9)
C2–C3–C4	111.24(19)	Os1–C7–C8	77.49(13)
C3–C4–Os1	117.94(16)	C7–C8–Os1	64.67(13)
C4–Os1–C1	75.01(9)	C8–Os1–C7	37.84(9)
Os1–C4–C5	116.88(16)	Os1–C8–C9	151.38(18)
C4–C5–C6	114.3(2)	C7–C8–C9	143.9(2)
C5–C6–C7	111.9(2)		

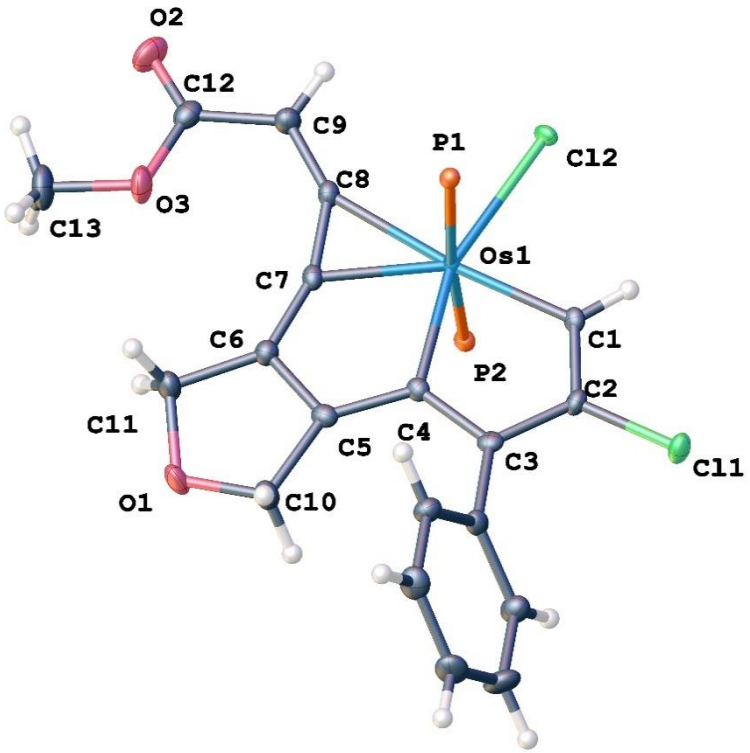


Fig. S6. X-ray crystal structure for complex **3b** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S3. Selected bond distances and angles for complex **3b**.

Bond Distances(Å)					
Os1–C1	2.026(2)	C1–C2	1.379(3)	C5–C6	1.384(3)
Os1–C4	2.110(2)	C2–C3	1.405(3)	C6–C7	1.368(3)
Os1–C7	2.017(2)	C3–C4	1.403(3)	C7–C8	1.352(3)
Os1–C8	2.154(2)	C4–C5	1.408(3)	C8–C9	1.338(3)
Bond Angels(°)					
Os1–C1–C2	119.24(15)		C6–C7–Os1	122.79(16)	
C1–C2–C3	116.34(19)		C7–Os1–C4	73.65(8)	
C2–C3–C4	111.03(19)		Os1–C7–C8	76.69(13)	
C3–C4–Os1	118.13(15)		C7–C8–Os1	65.66(12)	
C4–Os1–C1	75.13(8)		C8–Os1–C7	37.65(9)	
Os1–C4–C5	117.21(15)		Os1–C8–C9	150.71(17)	
C4–C5–C6	113.54(19)		C7–C8–C9	143.6(2)	
C5–C6–C7	112.7(2)				

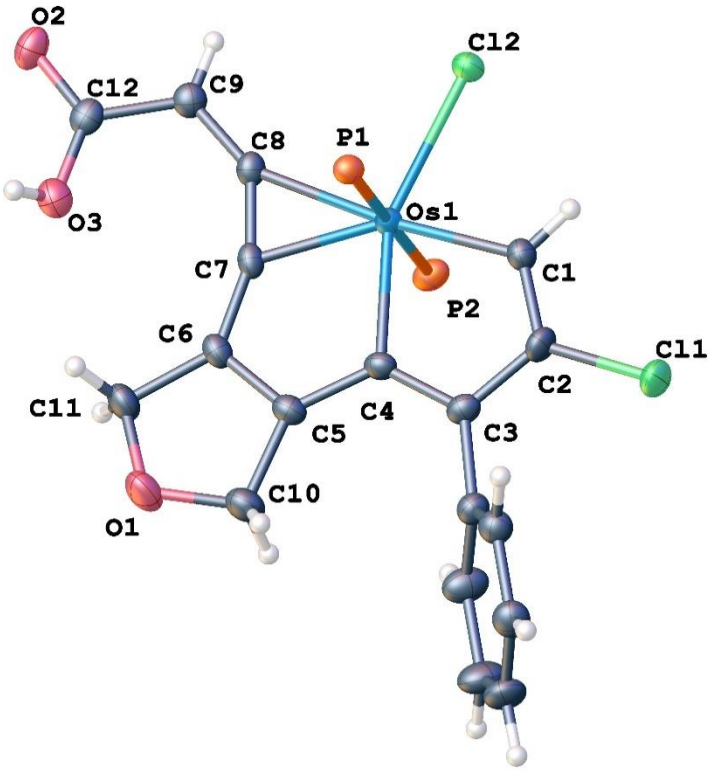


Fig. S7. X-ray crystal structure for complex **3c** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S4. Selected bond distances and angles for complex **3c**.

Bond Distances(Å)					
Os1–C1	2.018(3)	C1−C2	1.375(4)	C5−C6	1.378(4)
Os1–C4	2.119(3)	C2−C3	1.405(4)	C6−C7	1.378(4)
Os1–C7	2.010(3)	C3−C4	1.397(4)	C7–C8	1.349(4)
Os1–C8	2.153(3)	C4−C5	1.414(4)	C8–C9	1.346(4)

Bond Angels(°)			
Os1–C1–C2	119.9(2)	C6–C7–Os1	123.5(2)
C1–C2–C3	116.0(2)	C7–Os1–C4	73.66(11)
C2–C3–C4	111.3(2)	Os1–C7–C8	76.91(16),
C3–C4–Os1	117.91(19)	C7–C8–Os1	65.47(15)
C4–Os1–C1	74.89(11)	C8–Os1–C7	37.62(11)
Os1–C4–C5	116.57(19)	Os1–C8–C9	153.6(2)
C4–C5–C6	114.4(2)	C7–C8–C9	140.5(3)
C5–C6–C7	111.9(2)		

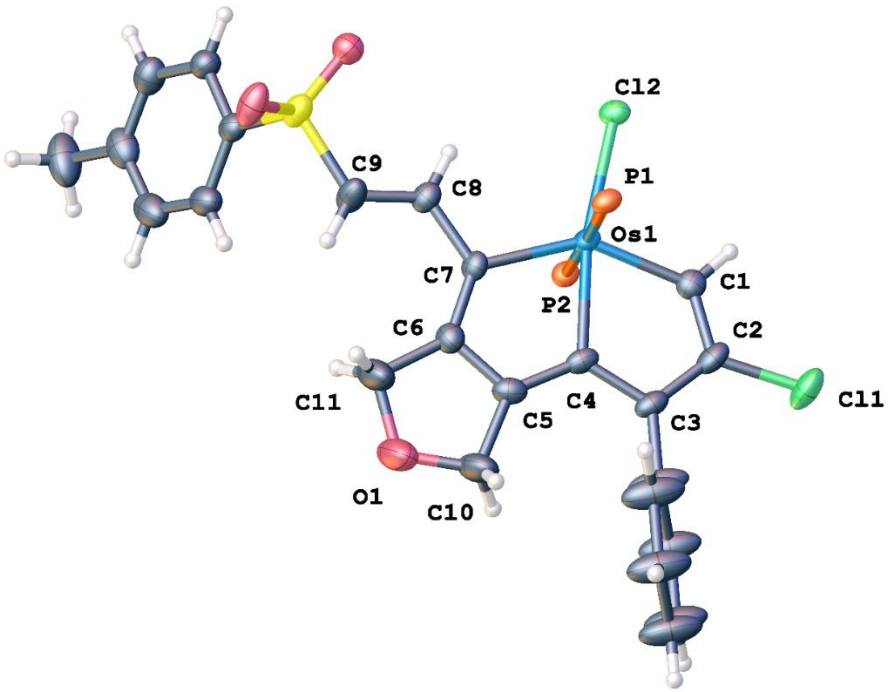


Fig. S8. X-ray crystal structure for the cation of complex **4A** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S5. Selected bond distances and angles for complex **4A**.

Bond Distances(Å)					
Os1–C1	1.962(6)	C2–C3	1.403(10)	C6–C7	1.377(9)
Os1–C4	2.163(6)	C3–C4	1.413(8)	C7–C8	1.464(8)
Os1–C7	2.021(5)	C4–C5	1.389(9)	C8–C9	1.323(9)
C1–C2	1.364(9)	C5–C6	1.377(9)		
Bond Angels(°)					
Os1–C1–C2	126.2(5)		C4–C5–C6	114.0(5)	
C1–C2–C3	113.7(6)		C5–C6–C7	113.0(6)	
C2–C3–C4	109.4(5)		C6–C7–Os1	123.4(4)	
C3–C4–Os1	118.8(5)		C7–Os1–C4	72.6(2)	
C4–Os1–C1	71.7(3)		Os1–C7–C8	110.1(4)	
Os1–C4–C5	117.0(4)		C7–C8–C9	123.0(6)	

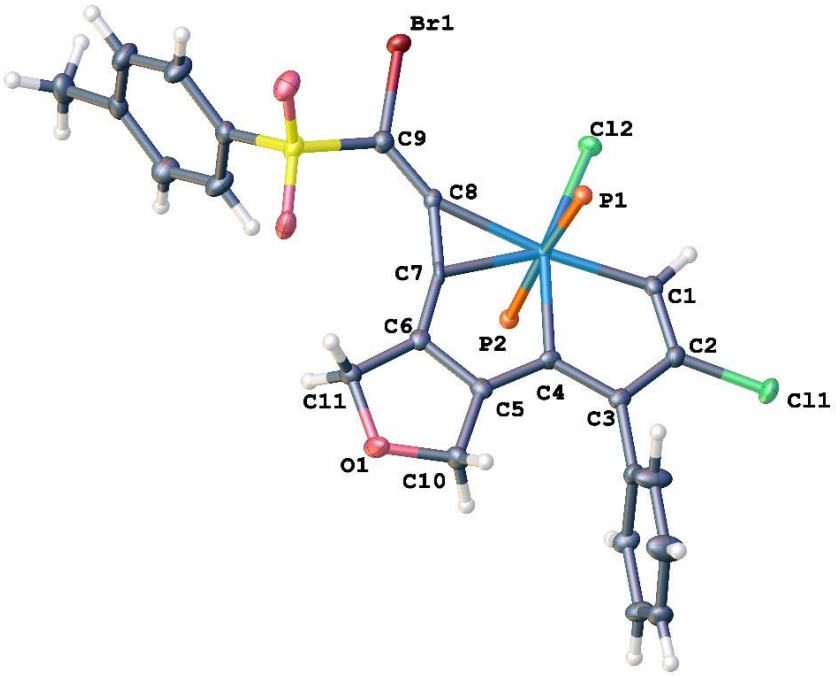


Fig. S9. X-ray crystal structure for complex **5b** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S6. Selected bond distances and angles for complex **5b**.

Bond Distances(Å)					
Os1–C1	2.020(3)	C2–C3	1.402(4)	C7–C8	1.363(4)
Os1–C4	2.108(3)	C3–C4	1.399(4)	C8–C9	1.334(4)
Os1–C7	2.007(3)	C4–C5	1.413(4)	C9–Br1	1.908(3)
Os1–C8	2.162(3)	C5–C6	1.378(4)		
C1–C2	1.377(4)	C6–C7	1.373(4)		
Bond Angels(°)					
Os1–C1–C2	119.1(2)		C6–C7–Os1	123.3(2)	
C1–C2–C3	116.6(3)		C7–Os1–C4	73.68(11)	
C2–C3–C4	110.9(3)		Os1–C7–C8	77.16(17)	
C3–C4–Os1	118.2(2)		C7–C8–Os1	64.89(15)	
C4–Os1–C1	75.18(11)		C8–Os1–C7	37.95(11)	
Os1–C4–C5	116.8(2)		Os1–C8–C9	154.9(2)	
C4–C5–C6	114.0(3)		C7–C8–C9	139.6(3)	
C5–C6–C7	112.1(3)		C8–C9–Br1	125.7(2)	

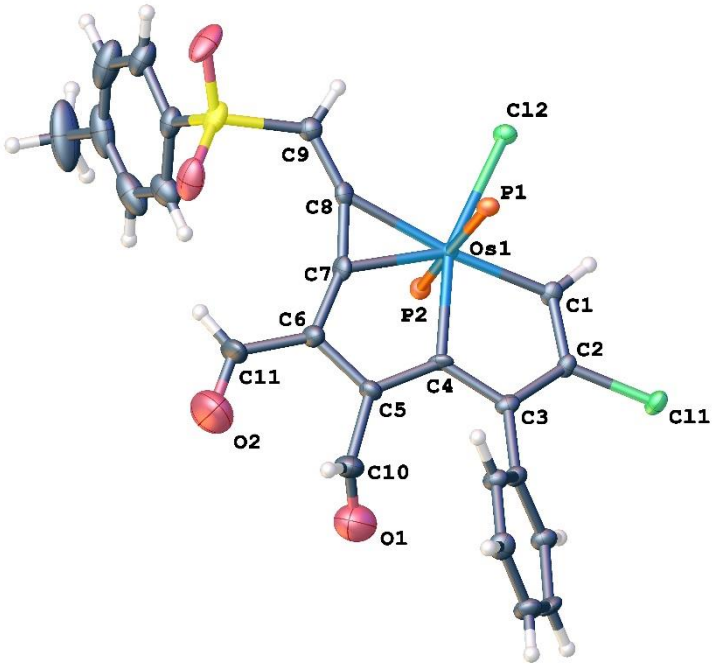


Fig. S10. X-ray crystal structure for complex **6a** drawn at the 50% probability level. The phenyl groups in PPh_3 are omitted for clarity.

Table S7. Selected bond distances and angles for complex **6a**.

Bond Distances(Å)					
Os1–C1	2.013(4)	C3–C4	1.414(5)	C5–C10	1.495(6)
Os1–C4	2.099(3)	C4–C5	1.399(5)	C6–C11	1.473(6)
Os1–C7	1.999(4)	C5–C6	1.414(5)	C10–O1	1.162(6)
Os1–C8	2.143(4)	C6–C7	1.386(5)	C11–O2	1.193(6)
C1–C2	1.380(5)	C7–C8	1.358(5)		
C2–C3	1.404(5)	C8–C9	1.322(5)		
Bond Angels(°)					
Os1–C1–C2	119.3(3)	C5–C6–C7	110.7(3)	C7–C8–C9	149.1(4)
C1–C2–C3	116.0(3)	C6–C7–Os1	124.2(3)	C4–C5–C10	129.3(4)
C2–C3–C4	111.1(3)	C7–Os1–C4	73.42(15)	C6–C5–C10	117.7(3)
C3–C4–Os1	117.3(3)	Os1–C7–C8	76.7(2)	C5–C6–C11	124.1(4)
C4–Os1–C1	75.75(15)	C7–C8–Os1	65.2(2)	C7–C6–C11	125.2(4)
Os1–C4–C5	118.5(3)	C8–Os1–C7	38.07(15)	C5–C10–O1	128.3(5)
C4–C5–C6	113.0(3)	Os1–C8–C9	145.6(3)	C6–C11–O2	122.4(5)

Table S8. Crystal data and structure refinement for **2a**, **3a** and **3b**.

Complex	**2a**	**3a**	**3b**+CH_2Cl_2
Empirical formula	$C_{60}H_{48}Cl_2O_3OsP_2S$	$C_{60}H_{48}Cl_2O_3OsP_2S$	$C_{56}H_{46}Cl_4O_3OsP_2$
Mol. weight	1172.08	1172.08	1160.87
Temperature [K]	100.0(3)	99.9(4)	100.00(10)
Crystal system	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$	Pbca	$P2_1/c$
a [Å]	12.4254(2)	12.6801(3)	16.80610(10)
b [Å]	16.8772(3)	20.3505(4)	12.64840(10)
c [Å]	25.9137(5)	37.4827(7)	22.36290(10)
α [°]	90	90	90
β [°]	95.196(2)	90	98.6850(10)
γ [°]	90	90	90
V [Å^3]	5411.93(17)	9672.3(3)	4699.18(5)
Z	4	8	4
ρ_{calcd} [g cm^{-3}]	1.439	1.610	1.641
μ [mm^{-1}]	2.596	7.407	8.231
F(000)	2352.0	4704.0	2320.0
Crystal size [mm^3]	0.12 × 0.08 × 0.07	0.05 × 0.05 × 0.02	0.2 × 0.1 × 0.05
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range [°]	3.974 to 62.252	4.716 to 129.998	7.998 to 129.998
Coll. refl.	53610	31933	55930
Indep. refl.	14757	8205	7986
data/restraints/params	14757/0/623	8205/0/623	7986/0/596
GOF on F^2	1.055	1.034	1.022
R_1/wR_2 [$I \geq 2\sigma(I)$]	0.0378/0.0967	0.0199/0.0474	0.0194/0.0464
R_1/wR_2 (all data)	0.0506/0.1017	0.0214/0.0480	0.0212/0.0476
Largest peak/hole [e Å^{-3}]	1.81/-1.78	0.75/-0.57	0.93/-0.51

Table S9. Crystal data and structure refinement for **3c** and **4A**.

Complex	**3c**	**4A**
Empirical formula	$C_{54}H_{42}Cl_2O_3OsP_2$	$C_{60}H_{49}BCl_2F_4O_3OsP_2S$
Mol. weight	1060.91	1259.90
Temperature [K]	99.9(4)	100.00(10)
Crystal system	trigonal	triclinic
Space group	R-3	P-1
a [Å]	46.4049(5)	12.1295(2)
b [Å]	46.4049(5)	14.0041(3)
c [Å]	11.2611(2)	18.3704(4)
α [°]	90	78.501(2)
β [°]	90	77.643(2)
γ [°]	120	84.961(2)
V [Å^3]	21001.0(6)	2983.65(11)
Z	18	2
ρ_{calcd} [g cm^{-3}]	1.511	1.402
μ [mm^{-1}]	7.203	6.139
F(000)	9540.0	1260.0
Crystal size [mm^3]	0.2 × 0.1 × 0.05	0.5 × 0.5 × 0.2
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2θ range [°]	6.598 to 152.206	6.448 to 129.992
Coll. refl.	81505	29576
Indep. refl.	9526	10124
data/restraints/params	9526/72/559	10124/93/710
GOF on F^2	1.048	1.031
R_1/wR_2 [$I \geq 2\sigma(I)$]	0.0273/0.0638	0.0532/0.1484
R_1/wR_2 (all data)	0.0298/0.0657	0.0570/0.1517
Largest peak/hole [e Å^{-3}]	0.64/-0.84	2.61/-0.86

Table S10. Crystal data and structure refinement for **5b** and **6a**.

Complex	**5b**	**6a**
Empirical formula	$C_{60}H_{47}BrCl_2O_3OsP_2S$	$C_{60}H_{46}Cl_2O_4OsP_2S$
Mol. weight	1250.98	1186.07
Temperature [K]	99.9(3)	100.00(10)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/c$
a [Å]	12.15060(10)	19.6126(3)
b [Å]	22.0023(2)	12.8418(2)
c [Å]	19.6911(2)	22.5429(4)
α [°]	90	90
β [°]	104.6050(10)	99.739(2)
γ [°]	90	90
V [Å^3]	5094.14(8)	5595.86(16)
Z	4	4
ρ_{calcd} [g cm^{-3}]	1.631	1.408
μ [mm^{-1}]	7.958	2.513
F(000)	2488.0	2376.0
Crystal size [mm^3]	0. 5 × 0.2 × 0.1	0.2 × 0.1 × 0.05
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)
2θ range [°]	6.136 to 149.494	6.752 to 57.404
Coll. refl.	33270	44221
Indep. refl.	9962	12679
data/restraints /params	9962/0/632	12679/1/632
GOF on F^2	1.032	1.041
R_1/wR_2 [$I \geq 2\sigma(I)$]	0.0290 / 0.0697	0.0387/0.0931
R_1/wR_2 (all data)	0.0319 / 0.0710	0.0477/0.0991
Largest peak/hole [e Å^{-3}]	0.83/-1.04	2.62/-1.48

5. Thermal Stability Tests

Temp. (°C)	90[a]	100	110	120	140	160	180	200	220
2a	● [b]	▲ [c]	▲	■ [d]	–	–	–	–	–
2b	●	●	▲	■	–	–	–	–	–
2c	●	▲	▲	▲	▲	■	–	–	–
3a	●	●	●	●	●	●	●	▲	■
3b	●	●	●	●	●	●	▲	▲	■
3c	●	●	●	●	●	▲	▲	■	–

[a] All reactions were carried out for 3 hours in air. [b] ● = Stable. [c] ▲= Partly decomposed. [d]■ = Completely decomposed.

Fig. S11. Thermal stability of **2a**–**2c** and **3a**–**3c** in the solid state.

6. Computational Methods

All structures were optimized at the B3LYP level of density functional theory.[8-10] Frequency calculations were performed to confirm the characteristics of all the calculated structures as minima. Compounds **2a**, **3a** and **4A** are simplified through the way that the PH_3 groups were used to replace the PPh_3 ligands and phenyl attached at C3 was omitted, which are named simplified model compounds **2a'**, **3a'** and **4A'**.All these structures evaluated were optimized by B3LYP-D3BJ/6–31G* ;[11-15] The nucleus-independent chemical shifts(NICS)[16-18] and anisotropy of the induced current density (AICD)[19-20] calculations were performed at the B3LYP/6-31G* level. The effective core potentials (ECPs) of Hay and Wadt with a double-ζ valence basis set LanL2DZ[21-22] for **2a'**, **3a'**, **4A'** were used to describe Os, P, Cl, and S atoms, and SDD[23] for the others were used to describe Os atom Polarization functions were added for Os (ζ(f) = 0.886), P (ζ(d) = 0.340), Cl (ζ(d) = 0.514), S (ζ(d) = 0.421).[24-25] The single-point energy calculations were performed on the mechanism using the B3LYP-D3BJ/Def 2-TZVP method with the SMD solvation method in DCM.[26-27] All the orbital isosurfaces and $NICS(1)_{ZZ}$ grids were visualized by Multiwfn.[28] The iso-chemical shielding surfaces (ICSS) analysis[29] were used to support the measurement of aromaticity, and we chose the ZZ component of ICSS ($ICSS_{zz}$),[30] which was also carried out by Multiwfn.[28] All the calculations were performed with the Gaussian 09 software package,[31] whereas the CMO-NICS calculations were carried out with the NBO 7.0 program[32] interfaced with the Gaussian 16 program.[33]

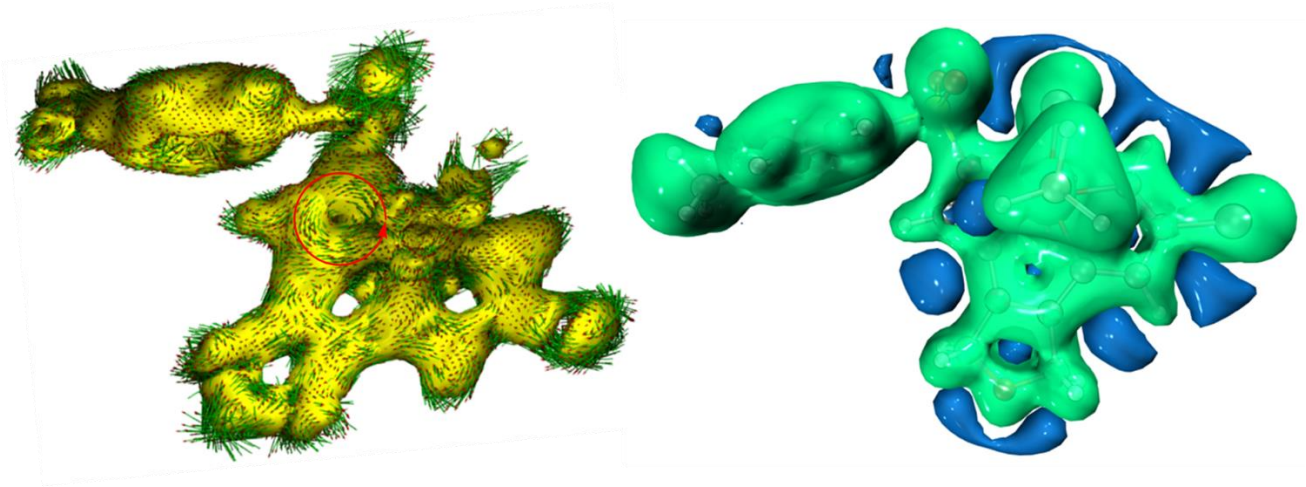


Fig. S12. The ACID plot of **2a'** (left) is displayed with an isosurface value of 0.030 a.u. The paratropic ring currents (red arrows) are shown correspondingly. The $ICSS_{zz}$ plot of **2a'** (right) with an isosurface value of 5.0 ppm displays shielding (green) and deshielding (blue) surfaces.

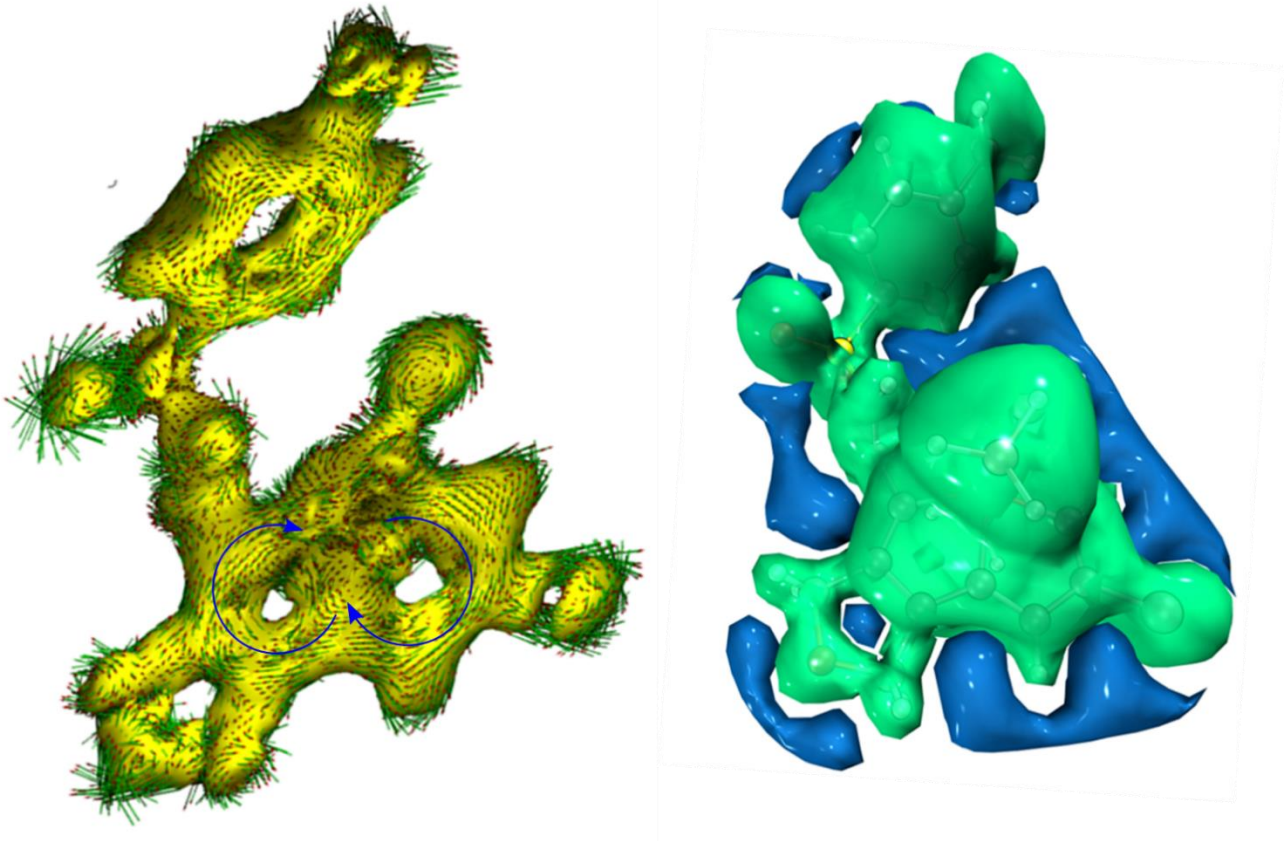


Fig. S13. The ACID plot of **4A'** (left) is displayed with an isosurface value of 0.030 a.u. The diatropic ring currents (blue arrows) are shown correspondingly. The $ICSS_{zz}$ plot of **4A'** (right) with an isosurface value of 5.0 ppm displays shielding (green) and deshielding (blue) surfaces.

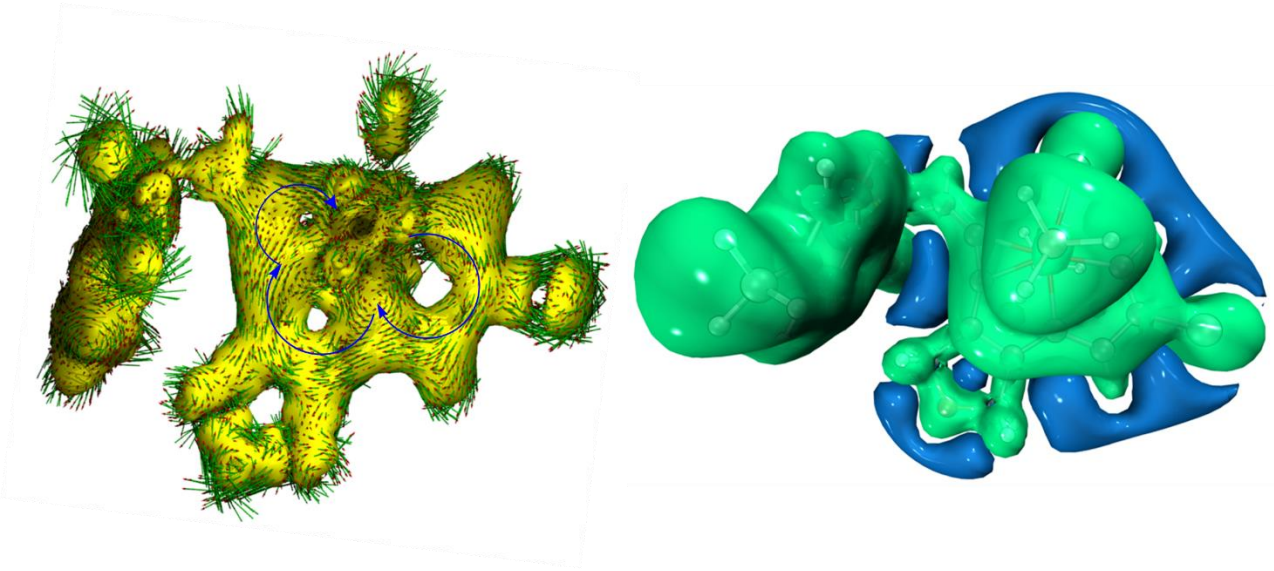
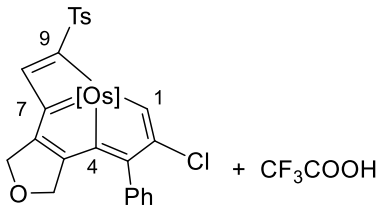


Fig. S14. The ACID plot of **3a'** (left) is displayed with an isosurface value of 0.030 a.u. The diatropic ring currents (blue arrows) are shown correspondingly. The $ICSS_{zz}$ plot of **3a'** (right) with an isosurface value of 5.0 ppm displays shielding (green) and deshielding (blue) surfaces.

Cartesian Coordinates

Part 1: the mechanism of ring contraction



2a

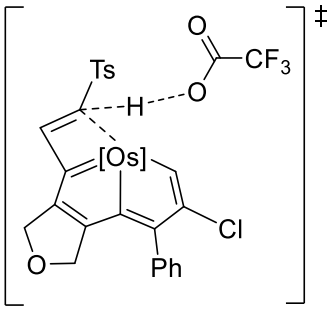
[Os] = $OsCl(PPh_3)_2$

E = -5161.54410582 a.u.

Os	-0.26979100	-0.04284500	0.10860400
Cl	1.81390400	0.51259300	-1.19776500
P	-0.75975700	2.22337900	0.89081000
P	-0.04280900	-2.36410400	-0.63810300
S	2.96731400	0.15443100	2.14069900
Cl	-2.97500100	1.10258100	-3.55413200
O	3.06108000	0.05917800	3.61207500
C	-2.39815800	-0.44449600	0.09584000
C	-0.78375400	-0.64950300	2.02837900
O	-4.19605900	-0.96009000	3.28132000
C	-2.07934800	-0.94135600	2.37787000
C	-0.36461600	2.45714000	2.67370600
C	-2.97205900	-0.85615200	1.30767800
C	-0.60339200	-2.53679800	-2.38715600
C	-2.52940900	2.72640100	0.66036300
O	3.40455700	1.43520400	1.52862600
C	-3.15717600	-0.09115800	-1.03510900
C	-2.34905000	0.53995600	-2.00756800
C	1.54057800	-3.31344100	-0.70850100
C	0.07630300	3.67110600	0.13183200
C	-2.85045700	3.64981100	-0.34647300
H	-2.06989500	4.06140700	-0.97357100
C	-1.06056500	-3.50681200	0.38688100
C	0.97355700	2.74701900	2.98137700
H	1.68840800	2.92159800	2.18777200
C	-4.59141700	-0.38434700	-1.20324700
C	2.71861300	-2.70761900	-1.16810000
H	2.75576700	-1.63370000	-1.29215400
C	-1.25670200	2.21179600	3.72521100
H	-2.29913200	2.00728800	3.53496300
C	0.46941900	-0.58802000	2.72659300
H	0.68658900	-0.71176600	3.78661300
C	-5.07169500	-1.69033200	-1.00890500
H	-4.38085400	-2.47647500	-0.72195900
C	-1.96035900	-2.45052900	-2.73501600
H	-2.71123700	-2.34902800	-1.96956200
C	-0.65773800	-3.66120200	1.72401200
H	0.23145200	-3.15061400	2.07735800
C	-4.16957900	4.05889500	-0.55044200
H	-4.38762800	4.77794100	-1.33480700
C	0.60513000	3.62282200	-1.16131200
H	0.66307000	2.68252400	-1.68824400
C	3.82398100	-3.48888000	-1.50436500
H	4.71553700	-3.00466800	-1.88618300
C	-5.19481500	3.55710000	0.24982500
H	-6.21990400	3.88338600	0.09884600
C	-3.57977100	2.19389600	1.42607500
H	-3.39252000	1.43013000	2.16482000
C	-2.17540500	-4.22177400	-0.06322700
H	-2.46646200	-4.18167800	-1.10440600
C	-6.42403200	-1.98203000	-1.17383800
H	-6.77820600	-2.99816300	-1.02583200
C	-0.81609800	2.24322800	5.04970000
H	-1.52625800	2.05777500	5.85107300
C	-4.89404300	2.61472700	1.23377800
H	-5.68195500	2.19501600	1.85249200

C	-5.49762100	0.62303100	-1.57163200
H	-5.13674400	1.63328000	-1.71410800
C	0.34173400	-2.61723000	-3.42043200
H	1.39754100	-2.67831900	-3.19124900
C	1.51625500	-4.70748000	-0.53484500
H	0.61636300	-5.20026900	-0.18739400
C	3.78751400	-4.87319500	-1.34445400
H	4.64790000	-5.47852700	-1.61630500
C	1.28076200	-0.21989900	1.70530900
C	-2.90721500	-5.02443800	0.81704300
H	-3.77378500	-5.56716800	0.44979400
C	-2.36490300	-2.46114800	-4.06738800
H	-3.42236400	-2.38439200	-4.30167500
C	0.52049800	2.51254100	5.34275700
H	0.86425200	2.52021700	6.37302200
C	-2.51755600	-5.14598200	2.14984100
H	-3.08591200	-5.77188400	2.83159400
C	0.04645300	4.90006200	0.81528000
H	-0.37446500	4.95398500	1.81342900
C	-4.35294200	-1.11835900	1.86211300
H	-5.11410100	-0.41390200	1.51904500
H	-4.69365700	-2.13728300	1.62567400
C	1.41306000	2.76987400	4.30244500
H	2.46073700	2.96041800	4.50868500
C	-1.37587700	-4.47569200	2.59625100
H	-1.04439900	-4.58533900	3.62501500
C	-7.31911900	-0.96963100	-1.52331200
H	-8.37475600	-1.19404000	-1.64615200
C	0.54804900	6.05081800	0.21564300
H	0.52532900	6.99266100	0.75651700
C	-2.83573900	-1.26204100	3.63485400
H	-2.73278600	-2.32192400	3.91964900
H	-2.55871300	-0.64014700	4.49182700
C	1.07560800	5.99362800	-1.07754000
H	1.47224300	6.89098100	-1.54392200
C	-0.06299300	-2.61592900	-4.75562100
H	0.68823600	-2.67431000	-5.53793400
C	2.63794500	-5.47807600	-0.83602000
H	2.60054700	-6.55506800	-0.69740000
C	-6.85176000	0.33266900	-1.71628800
H	-7.54416100	1.12550500	-1.98428100
C	4.01330900	-1.14093300	1.50196400
C	-1.41562300	-2.54133900	-5.08580300
H	-1.72695400	-2.53809300	-6.12630700
C	1.09994300	4.78211400	-1.76294400
H	1.52774500	4.72300200	-2.75665400
C	3.90009400	-2.41428000	2.06847000
H	3.10166100	-2.62912500	2.77107000
C	5.90586000	-3.08788500	0.87822000
C	5.03833800	-0.82590000	0.61631000
H	5.10200000	0.15788300	0.16646000
C	5.98364200	-1.80859300	0.31909900
H	6.79474100	-1.56953600	-0.36357800
C	4.84091200	-3.38165200	1.74480800
H	4.75746700	-4.37692200	2.17290500
C	6.91966600	-4.14937200	0.53668800
H	6.46246100	-4.94000800	-0.07167600
H	7.31783500	-4.62732100	1.43909600
H	7.76003000	-3.73488500	-0.02788900
C	-1.00990300	0.57185100	-1.71182600
H	-0.32212200	0.91926600	-2.47665400
C	4.40572800	3.51794800	-2.75987100
C	4.48605700	2.61104200	-1.51406900
O	5.17981500	1.61884800	-1.51229900

O	3.69750000	3.06057400	-0.56173400
H	3.58881400	2.37145700	0.15130000
F	4.28348700	4.81769700	-2.43884700
F	5.49301100	3.37174800	-3.52504100
F	3.32490300	3.16961900	-3.49521600



TS1

[Os] = $OsCl(PPh_3)_2$

E = -5161.51886988 a.u.

Os	-0.49051500	0.13578700	-0.32921800
Cl	0.84734600	0.55017300	-2.28877900
P	-0.96311300	2.42926300	0.43930500
P	-0.01306700	-2.19387500	-0.89791500
S	3.71873600	0.48248900	2.27760200
Cl	-4.45117300	0.49056000	-2.74946100
O	3.45796500	0.13926000	3.69850100
C	-2.36294500	-0.62611900	0.45269600
C	-0.16994000	-0.26402400	1.63472300
O	-2.75016500	-1.13470600	4.09440300
C	-1.17375100	-0.75116000	2.46232600
C	-0.10546700	2.81671800	2.01963100
C	-2.36912300	-0.98493400	1.81205400
C	-0.83750700	-2.59958400	-2.47949400
C	-2.77873000	2.65952200	0.68544500
O	4.42631400	1.73652600	1.95649500
C	-3.51411400	-0.55105700	-0.32906400
C	-3.24738200	0.17855800	-1.51537600
C	1.72222100	-2.71333800	-1.16886300
C	-0.53163700	3.90772200	-0.55310500
C	-3.50277700	3.38904100	-0.27009600
H	-2.98798700	3.84248800	-1.10857500
C	-0.54984800	-3.42876900	0.35216000
C	1.18199800	3.36699500	1.91544700
H	1.57668600	3.65955800	0.95169000
C	-4.80553100	-1.16887700	0.01686400
C	2.78381400	-1.80789900	-1.25028400
H	2.64792900	-0.75946100	-1.03923000
C	-0.57012900	2.42440000	3.28237500
H	-1.56015500	2.01498800	3.41097600
C	1.18770900	-0.12612500	2.08565300
H	1.39437200	-0.50157800	3.09505500
C	-4.84594700	-2.52442500	0.38320800
H	-3.92363000	-3.09458300	0.40819200
C	-2.23667500	-2.67743000	-2.56689500
H	-2.84644800	-2.57620400	-1.68018400
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C	0.15394700	3.83021000	-1.76669200
H	0.44516000	2.87090600	-2.16657800
C	4.04870300	-2.24886500	-1.63864900
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C	-3.48639000	2.05582200	1.73672800
H	-2.98094600	1.42329800	2.45035500
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H	-5.38436700	1.76571200	2.69586100
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H	-5.98296000	0.60644100	-0.30295600
C	-0.07619600	-2.68263400	-3.65404600
H	1.00255000	-2.59560900	-3.60785900
C	1.95493100	-4.07919700	-1.41483800
H	1.13919700	-4.79238700	-1.34101800
C	4.27007800	-3.59696400	-1.90777800
H	5.25607000	-3.93585100	-2.21261000
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H	-2.79857300	-5.89131600	1.04774000
C	-2.86001200	-2.86118300	-3.79904000
H	-3.94332400	-2.91618000	-3.84631700
C	1.53362700	3.06953700	4.28957400
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C	-1.27931300	-5.19674200	2.41065200
H	-1.56607800	-5.87480100	3.20897600
C	-0.85561800	5.16911200	-0.01913200
H	-1.37241500	5.23893300	0.93307900
C	-3.36453500	-1.46327400	2.83991600
H	-4.33672500	-0.96577500	2.78497800
H	-3.52979700	-2.54786900	2.75880800
C	1.99425900	3.48783400	3.04205500
H	3.00527800	3.86042100	2.92656200
C	-0.19458900	-4.33189900	2.57955500
H	0.37289000	-4.34179100	3.50576200
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C	-1.32382400	-1.06879300	3.92178100
H	-0.85403300	-2.02973900	4.18585800
H	-0.92900900	-0.29505600	4.58650500
C	0.17508400	6.24490400	-1.92122400
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C	-0.70501800	-2.85833000	-4.88644700
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C	-7.20924800	-1.05011900	0.31763600
H	-8.12882100	-0.47242500	0.29539600
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H	3.46048900	-2.37163200	2.57484700
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H	7.50794000	-1.47000400	-0.14407300
C	5.13539400	-3.23481100	1.52795100
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H	7.63443100	-4.64198300	1.16989800
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C	-1.94885200	0.55105300	-1.67995700
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C	3.62754500	2.01531600	-1.30066700
O	4.30310800	1.00298500	-1.38517200
O	2.66553400	2.28682700	-0.47841400
H	2.40961600	1.42367800	0.21017200
F	3.66156700	4.37700100	-1.76866400
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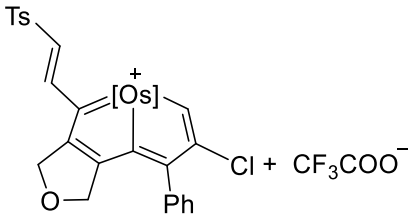

Int 4a

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P	1.04787800	-2.24265500	-1.11856800
S	-3.79045000	-0.90573000	-2.11346600
Cl	3.87875000	-1.38682800	2.99912700
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C	-0.12283800	0.70196000	-1.15481500
O	2.33539900	2.81581100	-2.85627600
C	0.79688000	1.60581900	-1.63808500
C	-2.43786200	1.51227400	1.94111700
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C	2.39130100	-3.25096200	-0.37441900
C	0.17328100	2.88571100	1.60690000
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C	2.76228300	-0.75396800	1.81318800
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H	2.05142200	2.20794800	2.44305900
C	1.69058700	-1.43997700	-2.63239600
C	-3.20542600	1.10778200	3.04638800
H	-2.73408100	0.63833200	3.90101600
C	4.53214300	0.60723600	0.58750400
C	-1.12267700	-4.08391500	-1.14767200
H	-1.50175400	-3.56624100	-0.27595800
C	-3.07429700	2.11262200	0.84611400
H	-2.52987400	2.44774300	-0.02856800
C	-1.50490100	0.47703900	-1.53150600
C	5.48795700	-0.36101500	0.23697400
H	5.19050400	-1.40267100	0.16472300
C	2.08073600	-3.91047000	0.82564600
H	1.09670800	-3.78865600	1.26860500
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H	3.23109900	4.33567400	2.03068100
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H	-0.58077500	-1.13916300	3.68438500
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H	-2.67761400	-5.56125100	-1.10498100
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C	-0.49110900	3.96250300	1.01215200
H	-1.53997200	3.92942500	0.75527300

C	2.95288700	-0.82880800	-2.67367700
H	3.62796100	-0.90156300	-1.83095200
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H	7.53338200	-0.74130600	-0.30192800
C	-4.44835300	2.35133700	0.87409400
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C	4.92695600	1.94470600	0.70615600
H	4.19509700	2.69116000	0.98752500
C	3.63761500	-3.47033000	-0.96973500
H	3.87921500	-3.01925100	-1.92381600
C	0.50798200	-4.32086400	-2.92128900
H	1.40598100	-3.98353400	-3.42733100
C	-1.31729700	-5.89506900	-2.74378200
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C	2.46243800	0.09898900	-4.85318900
H	2.75675400	0.70781900	-5.70203000
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H	-6.27756600	2.13523500	1.99471600
C	2.96920000	2.46977100	-1.62790300
H	3.95656000	2.05453500	-1.84311400
H	3.09837800	3.35476200	-0.98395900
C	-4.58249500	1.32360200	3.05530200
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H	0.40915300	3.55793900	-2.43655600
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H	0.45920700	2.77081600	6.54249800
C	4.57955800	-4.29197000	-0.34398200
H	0.39651600	0.48898700	7.53338000
C	-0.16582700	-5.44246700	-3.39402800
H	0.20945600	-5.96547700	-4.26875400
C	6.24894700	2.31439600	0.46083500
H	6.54234700	3.35572600	0.55669800
C	-4.37885200	-1.88617100	-0.74832000
C	4.27883100	-4.91332600	0.86673000
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C	-4.64800100	-1.26354800	0.47132800
H	-4.54225300	-0.19177700	0.57347800
C	-5.05857000	-2.04438200	1.54566200
H	-5.26181700	-1.56327900	2.49776300
C	-4.93273500	-4.02782800	0.17819000
H	-5.05973100	-5.10150600	0.06341000
C	-5.59335100	-4.27140200	2.60971300

H	-6.37873000	-3.78321400	3.19657800
H	-4.73676700	-4.42559100	3.27868500
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H	1.05641200	-1.82472600	2.51091400
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H	-2.11034800	1.38617700	-1.62316300
O	-1.82050200	3.26186000	-1.83276400
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O	-2.93069700	4.91670100	-0.74645900
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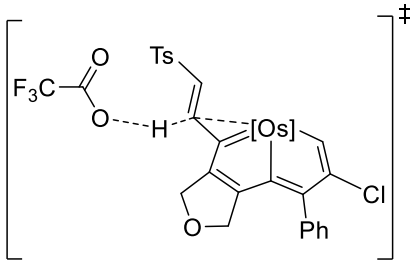

TS2

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S	-4.18425100	0.26281000	-1.30317100
Cl	4.48974800	-2.09969800	1.97317600
O	-4.48832500	-0.04798300	-2.71250200
C	2.25466000	0.27872100	-0.32304500
C	-0.10880500	0.82199400	-0.90494700
O	2.11982600	2.59405600	-3.22588500
C	0.80768500	1.58380500	-1.61694100
C	-1.34586300	1.61913400	2.82678000
C	2.12384100	1.24806000	-1.33028800
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C	1.03608800	2.80054100	1.57295700
O	-4.48514100	1.59934800	-0.76240400
C	3.46203200	-0.26518800	0.12931400
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C	-1.12662700	-2.94263000	-1.82673000
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H	3.08928000	2.18525500	1.85262000
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H	-0.84463200	1.41419800	4.92292100
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C	-1.97340500	-3.56021300	-0.88766300
H	-1.65878100	-3.66613900	0.14268500
C	-2.37548700	1.90500000	1.92064300
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H	4.04371900	4.21167400	0.80846400
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C	2.81073200	-2.03232500	-2.74253300
H	3.27085600	-2.71106000	-2.03450900
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H	-4.42369500	2.43039300	1.63847700
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H	0.08888500	2.35434700	-3.53281700
C	2.54220100	0.16587400	6.13962400
H	3.36695100	2.15596400	6.05758400
C	2.23051700	-6.03227100	-1.26139700
H	3.04712700	-0.09470600	7.06528300
C	-2.82409000	-3.27409700	-3.52520700
H	-3.14949000	-3.15767900	-4.55428000
C	6.57772500	1.68084800	-0.79818600
H	6.94625700	2.70112800	-0.74245500
C	-4.99141100	-0.97889100	-0.29454000
C	2.18648500	-6.42661600	0.07757500
H	2.63324300	-6.70242600	-2.01540500
C	1.69150000	-0.75349500	5.52153700
H	2.56318200	-7.40220600	0.37082500
C	-5.90527900	-1.84339600	-0.89002900
H	-6.11366300	-1.74762400	-1.94974100
C	-6.20346600	-2.96326000	1.24908700
C	-4.67081100	-1.08210900	1.06012800
H	-3.95165000	-0.40924200	1.51339600
C	-5.27166200	-2.08254000	1.81847600

H	-5.01130600	-2.18064300	2.86895800
C	-6.51393800	-2.82564100	-0.11033700
H	-7.23264600	-3.50269200	-0.56527200
C	-6.87186500	-4.02077800	2.09269600
H	-7.70126500	-3.59400600	2.67153300
H	-6.17089700	-4.46222400	2.80932700
H	-7.28293000	-4.82584000	1.47550700
C	1.90042900	-1.39415600	1.47181100
H	1.62714300	-2.00590000	2.32473300
H	-2.34863200	-1.17776600	-0.72717000
H	-1.89505000	2.05061100	-1.51172900
O	-2.07454200	3.07962000	-2.16799700
C	-2.36272900	4.10684400	-1.43964800
C	-2.30705100	5.41799300	-2.26350300
O	-2.57417400	4.18108800	-0.23876500
F	-2.77452600	5.28100700	-3.51250700
F	-1.00087700	5.80806000	-2.35667500
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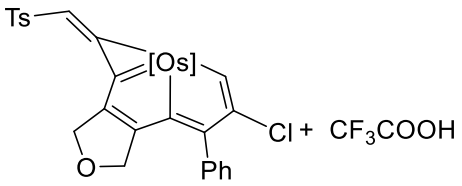

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P	0.30851600	-2.66782600	-0.35946900
S	-3.84196200	0.26201800	-0.50784800
Cl	5.20187100	-1.55921400	0.86982000
O	-3.32559800	0.04829200	-1.87617200
C	1.95953900	0.08078500	-0.82649100
C	-0.51197900	0.35279400	-0.58871600
O	0.46683200	1.59543800	-3.88700700
C	-0.03784400	0.93017200	-1.73953300
C	-0.51238700	2.11004600	2.83381800
C	1.34527100	0.77614400	-1.88655300
C	1.44148700	-4.03679700	0.09854300
C	1.42643200	2.98094100	0.81196500
O	-4.28810400	1.65766800	-0.18075800
C	3.31052800	-0.31720800	-0.75408600
C	3.57771400	-1.00238500	0.45591700
C	-1.30975400	-3.53234700	-0.17774000
C	2.31790700	1.66506600	3.19345300
C	2.71620300	2.98773100	0.25363100
H	3.41814200	2.20189600	0.51158900
C	0.46977900	-2.42042500	-2.16341600
C	-0.52303900	2.16464300	4.23453200
H	0.37379500	1.92991800	4.79514800
C	4.31647800	-0.13432500	-1.82414400
C	-1.99534200	-3.47586200	1.04297100
H	-1.62882600	-2.83358400	1.83510400
C	-1.69096100	2.40176200	2.13204000
H	-1.72059900	2.36005100	1.05339400
C	-1.36345200	-0.11898200	0.34486300
C	4.97544100	-1.24999100	-2.36867500
H	4.76981100	-2.23805700	-1.97105000
C	1.74217300	-4.20176200	1.45905700
H	1.33731100	-3.50621300	2.18722300
C	-0.63154700	-1.94043900	-2.88946000
H	-1.60048600	-1.83022900	-2.41425500
C	3.10931500	4.01185700	-0.60426700
H	4.12116400	4.02377500	-0.99990500
C	2.60769700	0.54511600	3.98560300

H	2.04183500	-0.36749200	3.84856400
C	-3.12899800	-4.26286400	1.24672000
H	-3.65135000	-4.20943700	2.19749300
C	2.21175900	5.02780400	-0.94628000
H	2.51646500	5.81953200	-1.62455700
C	0.54427000	4.01713100	0.48750900
H	-0.44384100	4.06710000	0.92296500
C	1.72342900	-2.47582400	-2.78682800
H	2.59031900	-2.80164400	-2.22626400
C	5.88631800	-1.09757400	-3.41063500
H	6.37824400	-1.97225400	-3.82664200
C	-2.85123400	2.76557600	2.81080700
H	-3.73874700	3.00245500	2.23447100
C	0.93181600	5.02720700	-0.39800500
H	0.22845400	5.81571300	-0.63902700
C	4.62403900	1.13603700	-2.32643500
H	4.13595200	2.00322400	-1.90162600
C	1.90878200	-4.97827300	-0.82785300
H	1.64939900	-4.88939500	-1.87674800
C	-1.77987000	-4.38315400	-1.18992300
H	-1.25594800	-4.44374900	-2.13747100
C	-3.58942400	-5.11189800	0.23999300
H	-4.46785600	-5.72932400	0.40602700
C	-2.64623300	-0.30117100	0.65833000
C	1.87246300	-2.08676000	-4.11686700
H	2.85617000	-2.12209700	-4.57574400
C	2.53581400	-5.26911200	1.87577500
H	3.80117500	-0.25610600	5.58192300
C	-2.85422000	2.81688400	4.20487100
H	2.76568500	-5.38478500	2.93104200
C	0.76938300	-1.62621400	-4.83754600
H	0.88576700	-1.30363300	-5.86763300
C	3.00068300	2.86726700	3.43369700
H	-3.75904800	3.09480000	4.73846900
C	1.71479700	1.39554900	-3.21309700
H	2.34703100	0.75912300	-3.83638000
H	2.22679700	2.35910800	-3.06559800
C	-1.69038400	2.51260300	4.91318800
H	2.77269700	3.74948000	2.84676400
C	-0.47989800	-1.55489300	-4.22066800
H	-1.68666400	2.54752800	5.99898800
C	6.17297000	0.17420400	-3.91366200
H	6.88586400	0.29263600	-4.72452000
C	3.97938600	2.93598800	4.42441900
H	-1.33732600	-1.17225800	-4.76542400
C	-0.61397100	1.61425000	-2.94181700
H	-0.91795000	2.64659600	-2.72444700
H	-1.47340700	1.08642000	-3.36216400
C	4.28012900	1.81087200	5.19348200
H	4.50535600	3.87115200	4.59430400
C	2.71020000	-6.03960700	-0.40573200
H	5.04596000	1.86479300	5.96213400
C	-2.91733600	-5.16402800	-0.98269900
H	-3.26859600	-5.82087900	-1.77362900
C	5.54502300	1.29067700	-3.36207700
H	5.76876200	2.28502300	-3.73808500
C	-5.24837900	-0.79506600	-0.23362500
C	3.03264000	-6.18248100	0.94423200
H	3.07749500	-6.75711300	-1.13414500
C	3.58563100	0.62023700	4.97740100
H	3.65895100	-7.00803700	1.27013800
C	-5.15501900	-2.13520800	-0.61348100
H	-4.24496300	-2.52115100	-1.05936600
C	-7.42724300	-2.48120600	0.18587100

C	-6.40097800	-0.28203000	0.35777200
H	-6.43848500	0.76335500	0.64230200
C	-7.48534900	-1.13322500	0.56276100
H	-8.39003600	-0.74517500	1.02296200
C	-6.24849500	-2.96703200	-0.39930100
H	-6.18278800	-4.01219000	-0.68663200
C	-8.61377000	-3.39119100	0.38379700
H	-9.19940200	-3.47617600	-0.54081100
H	-9.28300600	-3.01384400	1.16297500
H	-8.29929200	-4.40251500	0.66250100
C	2.51654400	-1.19112300	1.32157600
H	2.70832100	-1.73079200	2.24442000
H	-3.02708200	-0.72098200	1.58109500
H	-3.72907600	2.82624500	-1.21231200
O	-3.41319800	3.53054900	-1.85715200
C	-2.81150500	4.51019700	-1.21317200
C	-2.29019400	5.56357500	-2.21539000
O	-2.63239900	4.62360000	-0.02179900
F	-3.23501500	5.92142400	-3.09637100
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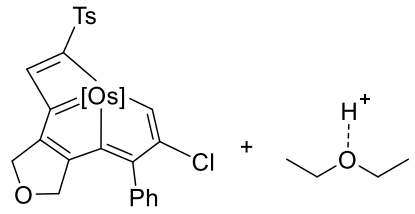

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P	0.33184500	-2.22621000	-1.02598100
S	3.61278000	0.62235900	0.10590300
Cl	-4.20008100	-0.01483100	-2.75142500
O	3.95317300	1.95758800	0.65318200
C	-2.01061400	-0.77828800	0.51163600
C	0.21404900	-0.42200300	1.64657900
O	-2.27746200	-1.29397400	4.15550400
C	-0.73830600	-0.92968100	2.48870900
C	0.00221100	2.96570000	1.93276100
C	-1.96747300	-1.14853200	1.86003200
C	-0.79198000	-2.87149300	-2.33394700
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O	3.88921200	0.38907300	-1.32377600
C	-3.19123300	-0.76309100	-0.25331900
C	-2.96722300	-0.15268200	-1.51128800
C	1.96833000	-2.67060300	-1.72897600
C	-1.04327700	3.68349500	-0.61403900
C	-3.74390300	2.76483200	0.40916800
H	-3.54208700	3.21877400	-0.55324200
C	0.25021300	-3.36332400	0.41907700
C	1.38204500	3.10136900	1.73306900
H	1.84241200	2.74706800	0.82331100
C	-4.47061500	-1.36716900	0.15665600
C	2.62963200	-1.78361700	-2.58372200
H	2.23382200	-0.79105800	-2.73973700
C	-0.56126300	3.46628200	3.11566000
H	-1.63009400	3.42084900	3.27968800
C	1.61683500	-0.15656500	1.76030300
H	2.25933100	-0.32101500	2.62494400
C	-4.51933700	-2.69586000	0.61185500
H	-3.60437300	-3.27448900	0.67348800
C	-2.15214500	-3.10711000	-2.08379000
H	-2.55386200	-2.95396000	-1.09705400

C	1.30914500	-3.29504600	1.34112200
H	2.16494200	-2.66307600	1.13830600
C	-5.05563200	2.74296500	0.88782000
H	-5.84924000	3.17790200	0.28721000
C	-1.41300300	3.51137500	-1.95574500
H	-1.58051000	2.51877600	-2.34591900
C	3.81365300	-2.16795500	-3.21665000
H	4.32703300	-1.45994400	-3.85934900
C	-5.34452000	2.17194300	2.12644300
H	-6.36469700	2.15655300	2.49767900
C	-3.00324000	1.63925400	2.41094900
H	-2.22154400	1.19975100	3.01605200
C	-0.81291900	-4.23340600	0.68155700
H	-1.60998100	-4.35786800	-0.03866400
C	-5.72948000	-3.27682900	0.98271300
H	-5.75082700	-4.30735200	1.32418000
C	0.25103200	4.05464700	4.08737400
H	-0.19996700	4.43620300	4.99865400
C	-4.31249900	1.61731300	2.88616500
H	-4.51801400	1.16738200	3.85290600
C	-5.66794200	-0.63716600	0.07204100
H	-5.64144200	0.38725800	-0.27458200
C	-0.31606000	-3.04593300	-3.64304900
H	0.72796400	-2.87557500	-3.87324000
C	2.49415300	-3.96084700	-1.53695200
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H	5.26816700	-3.73398500	-3.49388500
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C	-3.01189400	-3.51420700	-3.10000600
H	-4.06005200	-3.68349900	-2.87349200
C	1.62833100	4.16100600	3.88831900
H	2.25499100	4.61611200	4.64973500
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C	-0.85653800	4.98742100	-0.12825200
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C	-2.92006200	-1.64610300	2.92324300
H	-3.90489600	-1.17691300	2.89872300
H	-3.05046400	-2.73593000	2.85689300
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C	1.28699500	-4.05440900	2.50813300
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C	-6.90956700	-2.53413800	0.91572800
H	-7.85306400	-2.98384700	1.20976100
C	-1.02304700	6.08815700	-0.96947500
H	-0.88042300	7.08966500	-0.57408300
C	-0.85680300	-1.27818500	3.94741900
H	-0.41376500	-2.26177500	4.16812000
H	-0.42274100	-0.53694300	4.62477600
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H	-1.51126300	6.76294000	-2.95983900
C	-1.18052800	-3.44422000	-4.66369200
H	-0.79157200	-3.57342400	-5.66931400
C	3.67779600	-4.33803400	-2.16610900
H	4.07673700	-5.33554600	-2.00672600
C	-6.87326700	-1.21301400	0.46356200
H	-7.78838600	-0.63108800	0.40949100
C	4.50787600	-0.60742000	1.04014100
C	-2.52877700	-3.68161300	-4.39790900
H	-3.19747600	-3.99178000	-5.19504800

C	-1.57833600	4.61272400	-2.79628200
H	-1.86504700	4.45671400	-3.83190300
C	4.92888700	-0.31743700	2.33806300
H	4.79492200	0.68131200	2.73959800
C	5.70041800	-2.61619100	2.56703800
C	4.68499800	-1.87523600	0.48201700
H	4.37001000	-2.07215700	-0.53428800
C	5.27732800	-2.87041400	1.25286200
H	5.41494800	-3.85978500	0.82529300
C	5.52440900	-1.32768400	3.09177100
H	5.85900600	-1.11369100	4.10309700
C	6.36183800	-3.69858300	3.38209600
H	5.91005400	-4.67700500	3.18868200
H	6.29302800	-3.49303000	4.45443500
H	7.42704000	-3.77794900	3.13021200
C	-1.66569900	0.20320800	-1.74313500
H	-1.39211400	0.53075500	-2.74262300
H	2.15414400	2.59829500	-1.99199500
C	4.07045000	3.12739400	-2.65770000
H	4.13369600	2.04129000	-2.65020400
O	2.82523400	3.39163500	-1.88609100
C	2.14909700	4.70098300	-2.04719100
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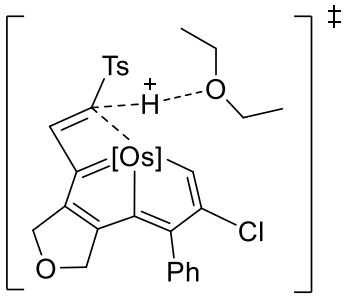
H	2.47752400	5.10511200	-3.00784800
H	3.89707100	3.50328500	-3.67006200
C	2.47331600	5.60216500	-0.87725700
H	1.92118600	6.53883200	-1.00146900
H	2.15952800	5.14248500	0.06244400
H	3.53961300	5.83231000	-0.82184200
C	5.25331200	3.75911000	-1.96300000
H	5.29959800	3.41042900	-0.92834800
H	6.16442400	3.44237000	-2.48214900
H	5.21939500	4.85201700	-1.98641600



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P	0.12756400	-2.02667400	1.38510700
S	-4.17834000	0.39449400	-0.25364500
Cl	4.73586800	0.53020800	1.95421500
O	-4.58882500	1.67607000	-0.87334000
C	1.97549400	-0.64927600	-0.66879300
C	-0.40756100	-0.31885200	-1.32627700
O	1.51041900	-1.34386300	-4.26407900
C	0.35436500	-0.85278200	-2.34202900
C	-0.28914400	2.83079500	-2.06436200
C	1.67175800	-1.07676100	-1.96818900
C	1.47396300	-2.31550700	2.58847600
C	2.47906100	2.56560000	-1.20417000
O	-4.68960500	0.07159300	1.09850400
C	3.27833800	-0.57633900	-0.16405300
C	3.29687300	0.20025400	1.02062700
C	-1.36294900	-2.53953400	2.32163900
C	0.54553600	3.93333600	0.43675400
C	3.41382800	3.35026600	-0.51851800
H	3.11836700	3.90532500	0.36395700
C	0.12106700	-3.33614200	0.09308700

C	-1.68059600	2.86896400	-1.88880400
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C	4.44745000	-1.24586100	-0.75447200
C	-2.53735200	-1.78997300	2.30625800
H	-2.55740500	-0.83988700	1.79582100
C	0.23551600	3.17156500	-3.31985100
H	1.30442100	3.21003500	-3.47975100
C	-1.83463300	-0.20692700	-1.30539700
H	-2.39495500	-0.65786000	-2.13028700
C	4.37122400	-2.60674700	-1.09938800
H	3.44439800	-3.14700200	-0.93828600
C	2.78307800	-2.65100500	2.21474800
H	3.03293500	-2.83204400	1.18082300
C	-1.00363700	-3.35076600	-0.74942600
H	-1.81481700	-2.65102800	-0.58568000
C	4.73351900	3.43345600	-0.96743300
H	5.44491600	4.04749700	-0.42384200
C	0.91958900	3.92174000	1.78912000
H	1.32635800	3.02484700	2.23210500
C	-3.69146000	-2.26912300	2.93139700
H	-4.60077000	-1.67974400	2.87811500
C	5.13050000	2.74424100	-2.11213600
H	6.15343000	2.82005000	-2.46871500
C	2.89444800	1.85245900	-2.34208500
H	2.19286500	1.23171000	-2.88470200
C	1.11760700	-4.29938100	-0.09788600
H	1.95802400	-4.36482600	0.57983000
C	5.47316300	-3.26578700	-1.63868700
H	5.40066000	-4.31900400	-1.89281500
C	-0.61724200	3.49130000	-4.37840300
H	-0.19204600	3.74896900	-5.34380300
C	4.20645600	1.95170700	-2.79782200
H	4.50727500	1.40604200	-3.68704100
C	5.65824200	-0.56156700	-0.95603300
H	5.72771000	0.48739800	-0.69970400
C	1.21096300	-2.01042300	3.93459100
H	0.21166900	-1.72265300	4.24016000
C	-1.34521400	-3.78418300	2.97429600
H	-0.43865400	-4.38140600	2.98406200
C	-3.66717000	-3.49809500	3.58897900
H	-4.56129100	-3.87267900	4.07861000
C	-2.38125700	0.37860200	-0.20958400
C	1.01914000	-5.21875800	-1.14670400
H	1.80053700	-5.96129600	-1.27985700
C	3.79852100	-2.71649400	3.16710200
H	4.80501100	-2.97666400	2.85479300
C	-2.00052100	3.49031600	-4.19786000
H	-2.65874800	3.73575400	-5.02609000
C	-0.08018000	-5.19782700	-2.00437100
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C	0.02294700	5.11553100	-0.11385000
H	-0.25722900	5.15095700	-1.15971000
C	2.38913700	-1.64156100	-3.17150200
H	3.36212000	-1.18602200	-3.37168700
H	2.53122200	-2.72765000	-3.07142900
C	-2.53180900	3.18810000	-2.94265000
H	-3.60304400	3.17949800	-2.77120100
C	-1.10251600	-4.26940700	-1.79053500
H	-1.98469200	-4.26103000	-2.42469800
C	6.66593800	-2.57210300	-1.85082000
H	7.52508200	-3.08309500	-2.27460900
C	-0.15154700	6.24723200	0.68246700
H	-0.55926300	7.15312800	0.24367200
C	0.16273600	-1.25939700	-3.77583100

H	-0.34951500	-2.23202100	-3.85856900
H	-0.37423300	-0.52503400	-4.38277900
C	0.20385400	6.21927800	2.03287000
H	0.06503500	7.10101700	2.65133400
C	2.23159300	-2.06716100	4.88211700
H	2.01152200	-1.83090300	5.91884300
C	-2.49025100	-4.25405300	3.61135400
H	-2.46782900	-5.21385300	4.11878500
C	6.75232600	-1.21948100	-1.51147400
H	7.67797600	-0.67611900	-1.67551900
C	-4.67879200	-0.94197700	-1.33064900
C	3.52632500	-2.42616400	4.50352100
H	4.31908500	-2.47070300	5.24395100
C	0.75012200	5.05746900	2.58066500
H	1.04036600	5.02876900	3.62655700
C	-4.96687700	-0.68119100	-2.66979200
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C	-5.20959000	-3.07254700	-3.05802400
C	-4.64437600	-2.24883800	-0.83689700
H	-4.41399300	-2.43337400	0.20705200
C	-4.90990200	-3.30322900	-1.70539900
H	-4.89088500	-4.32244600	-1.32884100
C	-5.23611800	-1.75032700	-3.52319900
H	-5.46813200	-1.55640900	-4.56684100
C	-5.52722700	-4.22113200	-3.98167100
H	-5.01220100	-5.13715000	-3.67547000
H	-5.24579100	-3.99518700	-5.01479400
H	-6.60352900	-4.43567100	-3.97608100
C	2.06517400	0.59161000	1.45376800
H	1.97453200	1.07099000	2.42156700
H	-2.53156500	1.62300000	1.41896900
C	-3.60711000	1.82993900	3.21443600
H	-3.58773700	0.74775100	3.13700300
O	-3.15492100	2.28563500	1.87245400
C	-2.69122800	3.68949100	1.71919600
H	-1.71894800	3.61086100	1.24265200
H	-2.55054200	4.07441400	2.72992700
H	-2.85254300	2.16884700	3.92612300
C	-3.69361900	4.46764400	0.89935000
H	-3.26881500	5.45438700	0.68705700
H	-3.90086400	3.95486200	-0.04210800
H	-4.63820700	4.60023600	1.43280600
C	-4.99630000	2.36059100	3.47079300
H	-5.67372600	2.02162600	2.68411100
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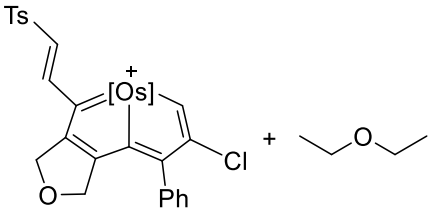

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Int 4A

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Cl	-1.40709100	1.09165300	-1.96549200
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P	0.14978400	2.53181400	0.74990700
S	-4.20954300	-0.95108800	1.17679100
Cl	4.26183700	1.93442300	-2.22097800
O	-4.66040300	-0.74966800	2.56454700
C	2.19750400	-0.03270300	0.55008800
C	-0.10716700	-0.53667100	1.31209700
O	2.20459300	-1.08202000	4.09526500
C	0.83659600	-0.85955400	2.25949600

C	-1.07384100	-2.13320400	-2.64319500
C	2.13472400	-0.56914300	1.83900100
C	0.11699600	4.09375500	-0.21665400
C	0.93283700	-3.30233200	-1.00265400
O	-4.14913000	-2.32020400	0.62877200
C	3.37745700	0.39430400	-0.06812900
C	3.06670200	1.18623100	-1.19927300
C	-1.41206000	2.67486600	1.70043900
C	1.74740100	-1.40437700	-3.02421500
C	1.82025700	-3.36419900	0.07915700
H	2.17896600	-2.44854500	0.51887700
C	1.61165400	2.80411400	1.82846400
C	-1.16465800	-2.20626700	-4.03776100
H	-0.30529600	-1.98316400	-4.65830400
C	4.73309500	0.03761200	0.38121000
C	-2.50616000	3.25149700	1.02797700
H	-2.36660800	3.70926500	0.05586900
C	-2.18978300	-2.46704900	-1.86159900
H	-2.13837800	-2.44394600	-0.78077500
C	-1.49685500	-0.97875700	1.29506400
C	5.69771600	1.01954800	0.65580200
H	5.44283600	2.06508800	0.53762000
C	0.01831600	4.15803700	-1.61005100
H	-0.07162100	3.25514800	-2.19566900
C	1.76378200	2.22312800	3.09560400
H	0.98466700	1.61814900	3.53244900
C	2.25179100	-4.59261200	0.57877200
H	2.93653600	-4.62004200	1.42143300
C	1.54183100	-0.40690700	-3.99315400
H	0.59446700	0.12303100	-4.03244200
C	-3.78192400	3.21109900	1.58818600
H	-4.61877400	3.63393300	1.04187500
C	1.80196900	-5.77910000	-0.00171900
H	2.13548400	-6.73694100	0.38539600
C	0.48228100	-4.50077500	-1.58019400
H	-0.20173700	-4.47764000	-2.42010700
C	2.68764800	3.53290600	1.29132900
H	2.60429100	3.98372100	0.30965800
C	6.96261200	0.65131800	1.10727900
H	7.69724800	1.41842300	1.33254600
C	-3.38515900	-2.84987900	-2.46418100
H	-4.23371700	-3.09433300	-1.83426700
C	0.91674300	-5.72844200	-1.08032200
H	0.56191800	-6.64690200	-1.53780600
C	5.07261900	-1.31727300	0.53170500
H	4.34370600	-2.08017300	0.27930200
C	0.15244600	5.29067800	0.52318400
H	0.21800100	5.25684300	1.60614500
C	-1.63144000	2.06419500	2.94435600
H	-0.82948600	1.56518500	3.46865600
C	-3.98545800	2.60797000	2.83004300
H	-4.98070700	2.55967100	3.25896400
C	-2.57849100	-0.23064600	1.02873000
C	3.86532500	3.69798600	2.01763000
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C	-0.02175600	5.39662200	-2.25594700
H	2.38065900	0.67226400	-5.65047400
C	-3.47836300	-2.90030000	-3.85757000
H	-0.09999900	5.43119300	-3.33834500
C	4.00021400	3.12546800	3.28349300
H	4.91906700	3.25409200	3.84721900
C	2.97912800	-2.06500400	-2.96745700
H	-4.41071500	-3.19394400	-4.33058100
C	3.07073400	-0.93576900	2.96192900

H	3.81749400	-0.16933800	3.18184100
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H	3.15239600	-2.83583600	-2.22512800
C	2.94578900	2.38627000	3.81801900
H	-2.42910800	-2.63558000	-5.72238300
C	7.28932300	-0.69778200	1.26459200
H	8.27895200	-0.98072200	1.61005300
C	3.99350700	-1.73415500	-3.86904100
H	3.03568700	1.92085500	4.79459700
C	0.88490900	-1.43480600	3.64709200
H	0.73192400	-2.52367000	3.62950900
H	0.16042600	-0.99992000	4.34267600
C	3.78179900	-0.75302300	-4.83577500
H	4.94857000	-2.24733700	-3.81210400
C	0.11014600	6.52138800	-0.12355600
H	4.57196400	-0.49744900	-5.53483500
C	-2.90638400	2.04315800	3.50868000
H	-3.06149900	1.55263200	4.46381500
C	6.34478700	-1.68187400	0.96643000
H	6.59996700	-2.73234200	1.06886800
C	-5.15688100	0.10980600	0.10761800
C	0.02815400	6.57712600	-1.51814200
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C	2.55086100	-0.09351100	-4.89970200
H	-0.00321200	7.53787900	-2.02301600
C	-6.22035600	0.83458200	0.64191300
H	-6.47847900	0.71697400	1.68826500
C	-6.56358300	1.86827500	-1.53529500
C	-4.77929100	0.24056300	-1.23038200
H	-3.94699000	-0.32515600	-1.63313000
C	-5.48282500	1.12807400	-2.03869800
H	-5.18776700	1.24748900	-3.07735000
C	-6.92203000	1.70512700	-0.18912800
H	-7.75762200	2.27119400	0.21329500
C	-7.33774100	2.80098200	-2.43158700
H	-6.69088900	3.25758800	-3.18732400
H	-7.81827700	3.60055000	-1.85985400
H	-8.12891500	2.25794700	-2.96425500
C	1.72811500	1.27229000	-1.46620700
H	1.36208100	1.81676200	-2.32964900
H	-2.58052600	0.82302200	0.79470700
H	-1.62172800	-2.03993300	1.54664200
C	-0.46971800	-5.93264800	2.76450000
H	-0.29171600	-6.81933400	2.14646000
H	0.49876200	-5.55363400	3.10819400
H	-1.04815100	-6.24700800	3.63951400
C	-1.19903700	-4.87277400	1.94900600
H	-2.17479300	-5.24275200	1.61120700
H	-0.62022200	-4.61439900	1.06025200
O	-1.35636300	-3.63457700	2.64484400
C	-2.22928000	-3.63657400	3.78450800
H	-1.74061100	-4.15717100	4.61978500
H	-2.31164700	-2.57881600	4.05545500
C	-3.61685700	-4.20982900	3.52638000
H	-3.59615700	-5.29634200	3.39335000
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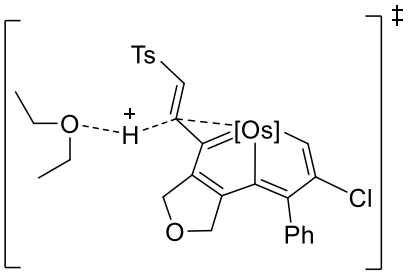

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P	0.01909400	-2.53876000	-0.23110400
S	-4.14954700	0.96728300	-1.03624300
Cl	4.39740700	-1.66816300	2.31798900
O	-4.24775700	0.59403500	-2.46472200
C	2.18901600	-0.15229800	-0.64057600
C	-0.13414800	0.41702400	-1.30277000
O	2.01536500	0.52677400	-4.29103400
C	0.75792500	0.55491900	-2.34977800
C	-0.63646700	2.73610900	2.34684000
C	2.06400700	0.21967200	-1.98399400
C	0.46352700	-3.88515500	0.93403600
C	1.24052100	3.43088700	0.33124900
O	-4.23615300	2.41396900	-0.70478700
C	3.39287000	-0.56282600	-0.02218300
C	3.14508500	-1.04254100	1.27445300
C	-1.70904400	-3.00970900	-0.64646900
C	2.16890400	1.95068900	2.62804200
C	2.12601600	3.23748400	-0.73842800
H	2.49367300	2.24475300	-0.94467800
C	1.01674900	-2.85796700	-1.72935500
C	-0.53766200	3.23342000	3.65081700
H	0.39974500	3.17637300	4.19127300
C	4.72511800	-0.48680100	-0.65037200
C	-2.69752700	-2.73052700	0.31032500
H	-2.43056800	-2.21391000	1.22383200
C	-1.85319800	2.85477600	1.66043900
H	-1.94698500	2.48441200	0.65017700
C	-1.48502200	0.53236800	-1.04994400
C	5.50047400	-1.64093800	-0.83978600
H	5.12150200	-2.59965700	-0.50380600
C	0.35105200	-3.69094200	2.31702500
H	0.03601300	-2.73076000	2.70558000
C	0.55955300	-2.44559200	-2.99023500
H	-0.43482700	-2.02637200	-3.09534300
C	2.55120000	4.31193500	-1.51985400
H	3.24201900	4.13981300	-2.34052200
C	1.99831300	1.20852900	3.81010900
H	1.03092400	0.77093100	4.03847600
C	-4.01611000	-3.12333600	0.09935600
H	-4.76974700	-2.88547600	0.84262400
C	2.09889700	5.60223900	-1.23929900
H	2.43335400	6.44190400	-1.84126800
C	0.78819600	4.73257800	0.60399300
H	0.11415100	4.91112600	1.43299700
C	2.32568600	-3.34974700	-1.61121100
H	2.70517300	-3.64870400	-0.64044600
C	6.74436400	-1.55791100	-1.46130400
H	7.33196500	-2.45845600	-1.61244900
C	-2.95979300	3.44103800	2.26724400
H	-3.88690700	3.51887400	1.70770000
C	1.21711400	5.80748300	-0.17644900
H	0.86810600	6.80924800	0.05660900
C	5.23658400	0.75384400	-1.06007200
H	4.66015800	1.65489700	-0.87475400

C	0.77883200	-5.16248300	0.44352400
H	0.83032500	-5.34041200	-0.62521800
C	-2.05772500	-3.73407100	-1.79420800
H	-1.30492900	-4.01560400	-2.51987500
C	-4.36612700	-3.80595100	-1.06653900
H	-5.39733300	-4.10131200	-1.23540300
C	-2.61067900	0.35394200	-0.36819000
C	3.14110300	-3.46303600	-2.73613700
H	4.14963600	-3.85034200	-2.63144000
C	0.59770700	-4.74652500	3.19564200
H	2.92602700	0.45518700	5.59475500
C	-2.86207400	3.91575200	3.57837900
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C	2.66686000	-3.07685700	-3.99136900
H	3.30260500	-3.16808800	-4.86674800
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H	-3.72306500	4.36951600	4.06026500
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H	3.57075900	3.07201000	1.42793300
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H	-1.56576700	4.19115500	5.27825600
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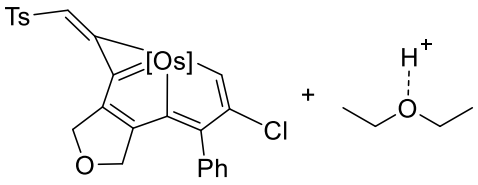
H	8.21209200	-0.25776800	-2.35820800
C	4.49678700	2.29368000	3.20403900
H	1.00919800	-2.23837600	-5.08289500
C	0.73081800	0.91987600	-3.80736900
H	0.57297300	1.99933800	-3.95555600
H	-0.03759600	0.38365200	-4.37750100
C	4.32233600	1.56241200	4.37757700
H	5.46893400	2.71177600	2.96103400
C	1.02966200	-6.21123800	1.32572300
H	5.15878900	1.40658200	5.05174600
C	-3.38312200	-4.12021600	-2.00431000
H	-3.64081500	-4.67614300	-2.90103600
C	6.48767900	0.83652500	-1.66861200
H	6.87766400	1.80321200	-1.97316500
C	-5.37834400	0.07586900	-0.11693500
C	0.94871700	-6.00362500	2.70437300
H	1.28320700	-7.19219100	0.93496600
C	3.06847600	1.02572900	4.68197200
H	1.14553000	-6.82214200	3.39023700
C	-6.24900400	-0.77205000	-0.79756100
H	-6.16860700	-0.87266400	-1.87373000
C	-7.26954600	-1.37514300	1.32827700
C	-5.42932500	0.21844000	1.27269100
H	-4.74789100	0.88780300	1.78911500
C	-6.36866400	-0.52016300	1.98487800
H	-6.41081500	-0.42848400	3.06648400
C	-7.19782200	-1.48422600	-0.06726300
H	-7.88746500	-2.14352300	-0.58691200
C	-8.30724300	-2.13913800	2.11060300
H	-7.91662900	-2.46727200	3.07905600
H	-8.65418200	-3.01997500	1.56260900
H	-9.18321700	-1.50863500	2.30948300
C	1.83018300	-0.93509400	1.70343500
H	1.59101700	-1.22121100	2.72268000
H	-2.71759400	-0.04085900	0.63990400
H	-1.77887500	1.67394100	-2.26449100
C	-0.90717200	4.81400700	-3.00112100
H	-0.76477800	5.71123900	-2.39239800
H	0.08025700	4.46102900	-3.30887900

H	-1.48540300	5.09382900	-3.88589900
C	-1.61015900	3.77801800	-2.15539400
H	-2.60523200	4.06408400	-1.81580000
H	-1.00551100	3.48679000	-1.29757200
O	-1.74908200	2.51443100	-2.91519700
C	-2.61978600	2.44218000	-4.12755500
H	-1.95968600	2.72857300	-4.94773600
H	-2.86666700	1.38431900	-4.18156100
C	-3.86359300	3.29779500	-4.04077000
H	-3.64022700	4.36794700	-4.05653200
H	-4.46976100	3.07404400	-4.92540500
H	-4.45285200	3.05454000	-3.15654200



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P	-1.65825300	1.84082700	-1.12652300
P	0.40919200	-2.54273000	-0.49475300
S	3.81710200	1.70640500	-0.04162600
Cl	-4.67518100	-2.31764900	-0.54752500
O	3.23187300	1.96845000	1.34963100
C	-1.53009800	-0.48039900	1.10471400
C	0.75977200	0.36859600	0.66993100
O	0.27832800	0.14489600	4.30312700
C	0.47208400	0.33758400	2.01294700
C	-0.73776400	3.22825400	-1.91141500
C	-0.82601100	-0.11674300	2.26559900
C	-0.44283700	-3.89844400	-1.38986000
C	-2.23226700	2.66907700	0.41453500
O	4.51820900	2.83615400	-0.67513200
C	-2.81513200	-1.05874400	1.08332600
C	-3.15155500	-1.51109000	-0.21405600
C	2.16229900	-2.80845500	-0.97029300
C	-3.11500400	1.64255100	-2.21030700
C	-1.24932600	2.97107700	1.37150400
H	-0.21679400	2.70842700	1.18293300
C	0.34465900	-3.02736500	1.26930500
C	-1.22673300	4.53822100	-1.76801500
H	-2.11184300	4.72656300	-1.16990000
C	-3.69641500	-1.13586200	2.26219500
C	2.75619800	-1.99445400	-1.94202200
H	2.18486400	-1.19090600	-2.38684100
C	0.39459200	3.00299700	-2.70331400
H	0.73151600	1.99019500	-2.86894800
C	1.39870800	0.63051600	-0.48890700
C	-4.21923800	-2.35689800	2.71667600
H	-3.98999500	-3.27146700	2.18087300
C	-0.92699100	-3.66928400	-2.68629100
H	-0.82954200	-2.68824300	-3.13608200
C	1.41158400	-2.71839300	2.12360500
H	2.33182300	-2.32621700	1.70780700
C	-1.58640500	3.59795600	2.56775600
H	-0.81186600	3.81130600	3.29899300
C	-3.00708700	1.96756100	-3.56923500
H	-2.09546200	2.40990700	-3.95277100
C	4.06241200	-2.24832000	-2.36430800
H	4.51700100	-1.60833900	-3.11466700
C	-2.91628500	3.94606700	2.82517700
H	-3.18349000	4.43065300	3.75938700
C	-3.55509300	3.05124400	0.66494000

H	-4.32521700	2.87252000	-0.07483900
C	-0.84029700	-3.53526200	1.82294100
H	-1.68009700	-3.76814000	1.17793200
C	-5.02326800	-2.39643100	3.85344400
H	-5.41363400	-3.34727200	4.20373300
C	1.04976700	4.07519100	-3.31345300
H	1.93139400	3.88852800	-3.91931000
C	-3.89364700	3.68174900	1.86665200
H	-4.92564200	3.96767600	2.04646500
C	-4.02331500	0.04545300	2.94707800
H	-3.64534100	0.99349500	2.57981500
C	-0.51471700	-5.19096300	-0.84812200
H	-0.12178100	-5.39432800	0.14157400
C	2.87752600	-3.90274900	-0.45606100
H	2.41996400	-4.55684700	0.27869600
C	4.77426000	-3.32464100	-1.83869700
H	5.78847500	-3.52211500	-2.17282900
C	2.50080800	1.15297000	-1.04619700
C	-0.94555600	-3.74483400	3.19669100
H	-1.86832700	-4.13967300	3.60987200
C	-1.50846400	-4.71039800	-3.40945400
H	-3.96822500	1.95683000	-5.49053100
C	0.56441700	5.37407800	-3.16322700
H	-1.88263100	-4.51972300	-4.41088800
C	0.12406900	-3.43442300	4.03949200
H	0.03787200	-3.58867700	5.11062200
C	-4.29531800	1.04256300	-1.73989600
H	1.06699100	6.20446700	-3.65063800
C	-1.03225100	-0.09255900	3.75755300
H	-1.41231400	-1.03360500	4.16248000
H	-1.71616000	0.71301000	4.05672300
C	-0.58487400	5.60132500	-2.39973000
H	-4.39310800	0.76146700	-0.69915400
C	1.30212300	-2.91890000	3.49958100
H	-0.98361100	6.60678300	-2.29832200
C	-5.33613300	-1.21746500	4.53513300
H	-5.96977100	-1.25132900	5.41626000
C	-5.35257100	0.79074800	-2.61132900
H	2.13424400	-2.66736700	4.15001500
C	1.15285900	0.67377500	3.30643100
H	1.27896600	1.76402300	3.42739500
H	2.13937500	0.21298800	3.42091300
C	-5.23928400	1.11957600	-3.96353000
H	-6.25754900	0.32708800	-2.23173200
C	-1.09972100	-6.22620100	-1.57582800
H	-6.06116400	0.91648200	-4.64340700
C	4.17584300	-4.15751000	-0.88933400
H	4.71787700	-5.01080300	-0.49131000
C	-4.84214700	0.00399000	4.07374800
H	-5.09526600	0.92589600	4.58911300
C	4.93900700	0.36269000	0.22774000
C	-1.60507600	-5.98693100	-2.85466200
H	-1.15789200	-7.22017600	-1.14211600
C	-4.06585000	1.70529000	-4.43887900
H	-2.06292500	-6.79410600	-3.41866500
C	4.55947700	-0.68038200	1.07825800
H	3.61797200	-0.63281700	1.61156300
C	6.64051100	-1.81731600	0.54278400
C	6.14223700	0.33838800	-0.47206700
H	6.41253900	1.16458000	-1.12046900
C	6.98911400	-0.75678300	-0.30055400
H	7.93505500	-0.78609600	-0.83325300
C	5.41622000	-1.75954500	1.23102200
H	5.13210000	-2.57858500	1.88514900

C	7.54007600	-3.01406300	0.70434700
H	8.48313400	-2.88590300	0.16650100
H	7.04995900	-3.91694600	0.32029700
H	7.77175900	-3.19708200	1.75964000
C	-2.25685900	-1.20366900	-1.22677700
H	-2.53289700	-1.43845100	-2.25120600
H	2.72446700	1.19146800	-2.10565100
H	2.53799000	3.08777500	1.44897500
C	0.99305700	6.06253500	0.70129800
H	0.74021500	6.52927000	-0.25321500
H	0.06054600	5.83386700	1.22551000
H	1.57331500	6.78302600	1.28527400
C	1.76612600	4.79770300	0.41009700
H	2.72120900	4.96890200	-0.08984500
H	1.17969100	4.09286400	-0.17872300
O	2.03863300	4.05728600	1.66697400
C	2.85177100	4.72810800	2.70387000
H	2.22174100	5.51860200	3.11184800
H	2.97255500	3.94827200	3.45771700
C	4.18390200	5.23228700	2.18528600
H	4.06804300	6.07449200	1.49740000
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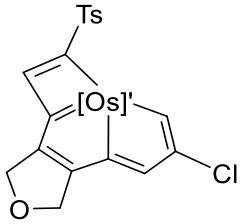
H	4.73979500	4.43787900	1.67987800

Part 2: NICS and AICD



[Os] = $OsCl(PH_3)_2$

2a'

E = -1067.53319139 a.u.

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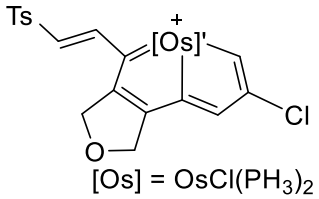
Cl	-0.84965420	2.34486181	-0.41497587
Cl	4.48102132	1.44343070	0.05647497
S	-3.54955979	0.70397969	0.73907029
O	-4.09366812	1.58476953	-0.34137297
O	1.17187447	-5.03574347	-0.19767601
O	-3.14356848	1.28196913	2.06334958
C	1.64389014	-1.35638405	-0.01953578
C	1.35443894	-2.72356325	-0.01120272
C	-2.21571258	-1.65103681	0.11952110
H	-3.04695637	-2.34587390	0.22421256
C	-0.80801307	-1.91613096	0.00293821
C	1.72179772	1.14032547	0.05524651
H	1.64469292	2.21983730	0.14313068
C	2.96051839	0.54621356	0.00745096
C	-2.16230617	-0.29827850	0.19837125
C	2.14719424	-3.99469646	-0.01419735
H	2.87220352	-4.05007621	-0.83358676
H	2.68346881	-4.13171206	0.93778001
C	-0.16079123	-4.53306009	-0.01159355
H	-0.58509184	-4.91987083	0.93003052
H	-0.78898568	-4.90138928	-0.83319056
C	0.00000000	-3.03869611	0.00000000
C	-4.80517683	-0.55709560	1.06068260
C	-6.65499182	-2.58650820	1.53578015
C	-5.59400875	-1.01669515	0.00734753
H	-5.47546892	-0.59055758	-0.98258685
C	-4.91830311	-1.08516531	2.34211527
H	-4.28657511	-0.70756624	3.13593536
C	-7.67604128	-3.66605936	1.79813280
H	-7.82454305	-4.29987561	0.91766317
H	-8.65080490	-3.23027306	2.05373359
H	-7.37606161	-4.30604022	2.63428475
C	-5.84545263	-2.09933098	2.57083793

H	-5.93666544	-2.52213554	3.56804314
C	-6.51360469	-2.03355437	0.25393418
H	-7.13207231	-2.40577657	-0.55897511
C	2.93626014	-0.85477042	-0.04316168
H	3.83127621	-1.47079908	-0.04846461
P	-0.05571251	-0.12424018	-2.43409468
H	-1.31116959	-0.40755202	-2.84160168
H	0.32960357	1.06051199	-2.95408873
H	0.78357741	-1.09447917	-2.85448584
P	0.09291420	-0.00944662	2.46208932
H	-0.22607843	1.21635696	2.92915387
H	-0.78449943	-0.91624746	2.94204510
H	1.34023011	-0.33362537	2.86409822



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Cl	4.37630857	-1.51326480	0.01691644
O	-5.45840319	2.01731031	-1.10720589
C	1.66866556	1.38485364	0.01690660
C	-0.73552526	1.84570354	-0.01433528
O	1.08533064	5.05042813	-0.06903603
C	0.00000000	3.00775153	0.00000000
C	1.36360091	2.74704626	0.00268395
O	-4.82359104	1.08546973	1.25093588
C	2.93568366	-0.53961704	0.00000000
C	-2.16243427	1.65486862	0.20539952
C	-3.01272548	1.10971291	-0.68315818
C	2.10503966	4.04943428	0.03010840
H	2.79667880	4.15882109	-0.81255399
H	2.67624853	4.17354690	0.96220635
C	-0.23128816	4.48727483	0.05021298
H	-0.69257831	4.79436693	0.99921888
H	-0.84953092	4.85640490	-0.77562334
C	-5.25512278	-0.62987202	-0.78191848
C	-6.22565798	-0.73739299	-1.77540852
H	-6.63981851	0.15872222	-2.22343384
C	-6.08994178	-3.16130499	-1.58538718
C	-4.68809320	-1.75311727	-0.17669916
H	-3.93670310	-1.65536531	0.59709400
C	-5.09998470	-3.01298854	-0.59991632
H	-4.65553249	-3.89557813	-0.14891174
C	-6.64376617	-2.00863527	-2.16244166
H	-7.40856612	-2.10851243	-2.92743833
C	-6.56331792	-4.53253900	-1.99488006
H	-7.35672339	-4.88296253	-1.32251451
H	-5.75209205	-5.26587619	-1.95091791
H	-6.97235507	-4.52972354	-3.00949702
C	1.67406840	-1.07790594	-0.03061468
H	1.53121456	-2.14964778	-0.07740793
H	-2.76454071	0.80997579	-1.69334174
H	-2.55365261	1.95077743	1.18052489
C	2.94897923	0.86074555	0.02636954
H	3.85813823	1.45543664	0.03461832
P	0.02979674	0.01107357	2.48073634
H	-0.83708791	0.93994330	2.93703893
H	-0.33124861	-1.20577713	2.94054130
H	1.27394065	0.30508025	2.91451741
P	0.09764445	-0.00529076	-2.47748088
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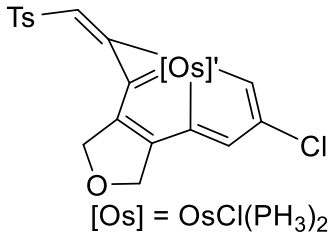

3a'

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O -0.11849116 -5.13604822 -0.15568989

O -4.01707934 -2.67997617 -1.23259156

O -5.88534975 -0.98685969 -0.53495540

C 2.94847047 -0.08173986 0.00000000

C 1.86677784 0.78588612 0.00850480

H 2.06836302 1.85226235 0.00690644

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H -3.24434726 -3.93444048 5.65842194

H -4.50463434 -5.12153369 5.29771569

H -4.93329434 -3.55251777 6.00583233

C -4.32803455 -3.71385749 1.48746702

H -4.21995585 -4.32472881 0.59886032

C -3.35818614 -0.27274916 -0.19182068

H -3.79889078 0.71310800 -0.26069529

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H -1.78731043 -4.53617861 0.94308856

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P -0.03907657 -0.03369537 2.43439323

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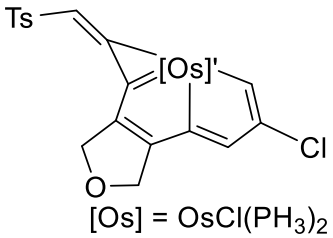
H -0.05734756 -1.30728182 -2.88040687

Part 3: isodesmic reactions



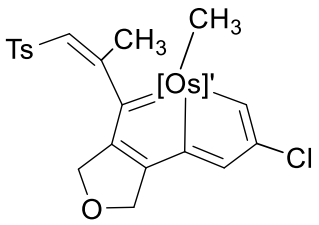
3a'

E = -3016.28802050 a.u.

Os -1.29477000 -0.53300300 -0.27051200

Cl -5.41514600 -0.53305100 1.90212300

Cl	-1.03862700	-2.92070400	-0.98128700
S	3.18044600	0.28155700	-1.82590100
P	-2.41552900	-0.14378200	-2.30971500
P	-0.21982800	-1.15916000	1.73718300
O	-0.15064800	4.41285700	0.50110900
O	2.76723000	1.69832700	-1.84102900
O	4.04693300	-0.27719500	-2.87519200
C	-3.85386700	-0.18327000	1.16136100
C	-3.07179000	-1.14884300	0.54426500
H	-3.41854900	-2.18137500	0.52020000
C	-1.33399700	2.41131100	0.41324200
C	0.63444100	-0.19390000	-1.14789700
C	-2.10260600	1.23838400	0.54944900
C	-0.11357400	2.22242900	-0.23836400
C	-1.44898400	3.86929300	0.76733900
H	-2.21691700	4.36942200	0.15321300
H	-1.69475500	4.05083600	1.82044800
C	5.46470300	-1.30108800	1.12965700
H	6.21690500	-2.07972500	1.22542300
C	5.66817600	-0.88603400	3.61686300
H	5.98153200	-1.93169300	3.69767500
H	4.96663900	-0.67442300	4.43031600
H	6.55760800	-0.26438700	3.78313600
C	3.53749300	0.70222300	0.87915800
H	2.79588700	1.48532500	0.76542800
C	1.72180300	-0.73627500	-1.68889000
H	1.83541300	-1.78059300	-1.95911400
C	4.92303800	-1.02164900	-0.12424700
H	5.24049900	-1.56240100	-1.00939100
C	0.62060200	3.52803300	-0.33307800
H	1.64656000	3.49160800	0.04387500
H	0.66237300	3.89615300	-1.36865600
C	3.96126600	-0.02002000	-0.23860000
C	4.08530700	0.40765500	2.12446400
H	3.76568000	0.97040100	2.99815400
C	5.05544800	-0.59649400	2.26914700
C	0.07808700	0.91297000	-0.61948000
H	-1.74362400	0.59421000	-3.30900000
H	-3.63778500	0.56170200	-2.27501500
H	-2.79247700	-1.28776900	-3.03822400
H	-0.27906700	-2.52546400	2.06908100
H	-0.64432200	-0.57651500	2.95171500
H	1.16949900	-0.92416800	1.83070100
C	-3.34031000	1.12914600	1.17747400
H	-3.87072300	1.95495200	1.64686800



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

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E = -3096.12614928 a.u.

Os	1.81539400	-0.53865600	0.06773800
Cl	5.06198800	2.19274000	-1.97482600
Cl	3.56929400	-2.43366500	0.23233300
S	-2.66683900	-0.78381800	-0.76539300
P	2.68977400	-0.35607700	2.24196800
P	1.03313300	-0.69403800	-2.15026600
O	-1.02515000	3.40944600	1.83777900
O	-2.60248500	-2.00799000	-1.58666700
O	-1.89159000	0.40355600	-1.17920000
C	3.68001700	1.52028700	-1.11224300
C	3.51416000	0.17134400	-0.88103300
H	4.25802600	-0.51749900	-1.27119600

C	0.57946500	2.19595400	0.67027900
C	1.66283800	1.61851200	0.02169200
C	-0.33185700	1.28577400	1.18978100
C	0.08465900	3.58720100	0.94837800
H	0.82360100	4.23258600	1.43758000
H	-0.23630000	4.08514300	0.01837000
C	-6.04465400	1.42041900	-0.41416000
H	-6.30707300	2.47239200	-0.34177100
C	-8.50530100	0.85659100	-0.24241300
H	-8.80673500	0.82477200	0.81275100
H	-9.16986700	0.18166300	-0.79122900
H	-8.67850300	1.87559600	-0.60178600
C	-5.37175600	-1.28165400	-0.63937500
H	-5.09825100	-2.32443500	-0.76205700
C	-2.26613400	-1.23475500	0.90469100
H	-3.00935500	-1.89325800	1.34449700
C	-4.70553200	1.05461100	-0.52924300
H	-3.91926000	1.80044600	-0.56397200
C	-1.47218500	2.04523900	1.81502400
H	-2.39153100	1.94767400	1.21886500
H	-1.70498900	1.74402900	2.84337000
C	-4.38181100	-0.29782900	-0.63432700
C	-6.70435300	-0.89710700	-0.51964300
H	-7.48299000	-1.65512700	-0.53086900
C	-7.06016600	0.45440900	-0.39939100
C	-0.06336700	-0.05477500	0.96306500
C	-1.10699300	-0.94704100	1.51843300
C	-0.83899500	-1.47934400	2.90599100
H	0.07678400	-2.07803700	2.90635600
H	-0.68493900	-0.64560500	3.60226100
H	-1.66327200	-2.09731400	3.27234700
H	2.60031800	-1.46196400	3.11325900
H	4.06392000	-0.07243000	2.36093500
H	2.15651800	0.65187600	3.08027000
H	-0.20760000	-1.29786100	-2.41310700
H	0.90885100	0.50593500	-2.87788200
H	1.85671700	-1.42570600	-3.03408800
C	2.66150500	2.34518900	-0.61332300
H	2.65139200	3.42593000	-0.73626900
C	0.74516100	-2.50322700	0.10960900
H	0.81311400	-2.96130900	1.09830000
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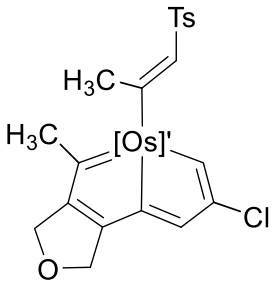
H	1.27510700	-3.15333800	-0.58597100



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

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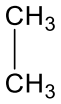
Os	1.03200300	0.28894200	-0.05539200
Cl	4.21922200	3.75078900	-0.59025600
Cl	-0.80134700	2.07397600	-0.05852600
S	-3.27619800	-1.62177000	-1.13791400
P	1.15912000	0.09032300	-2.38351100
P	1.17653800	0.68647200	2.26702100
O	4.55714600	-3.26662300	1.25455200
O	-3.31571500	-2.87750000	-0.35541600
O	-3.62170000	-1.64806700	-2.57169500
C	3.34684300	2.24669000	-0.31318800
C	1.98220300	2.12978200	-0.39968200
H	1.39945600	3.00638300	-0.66313400
C	3.58746000	-1.28851300	0.53368400

C	3.16152400	-0.00732800	0.19710700
C	2.59672900	-2.25839900	0.50276300
C	4.90436500	-1.94144100	0.84612600
H	5.56027600	-1.95821900	-0.04124000
H	5.45655000	-1.45771700	1.66007600
C	-5.08916200	1.80168800	0.06340400
H	-4.99486500	2.86585100	-0.13640400
C	-6.99555800	2.33005500	1.63672200
H	-6.46664900	3.23617700	1.95193900
H	-7.47510700	1.89078900	2.51694300
H	-7.79162400	2.64289300	0.94859200
C	-5.29599100	-0.92909100	0.60264600
H	-5.34602900	-1.99175600	0.81386700
C	-1.65303700	-0.89014100	-1.06203600
H	-1.33084800	-0.67440600	-2.07369700
C	-4.23729500	0.90927000	-0.57927900
H	-3.47529500	1.27042700	-1.26058700
C	3.23859200	-3.59716000	0.79330100
H	2.73879500	-4.17111500	1.58067600
H	3.29277600	-4.23170100	-0.10649200
C	-4.34792000	-0.45390900	-0.30005800
C	-6.14875600	-0.02169000	1.22995000
H	-6.89025000	-0.38492200	1.93689500
C	-6.06030400	1.35146400	0.97027300
H	0.81261300	-1.12015300	-3.02343500
H	2.43970100	0.28326300	-2.94300300
H	0.41302700	0.99418600	-3.17002100
H	0.06867100	1.19666300	2.97048400
H	2.15442900	1.63331000	2.63379100
H	1.54935000	-0.37918400	3.11617400
C	1.31961500	-1.84778500	0.13129000
C	-0.95613800	-0.62269400	0.04928700
C	-1.53245600	-0.87275500	1.42243100
H	-1.83559300	0.08756300	1.85396000
H	-2.40502200	-1.52835800	1.40770100
H	-0.78988600	-1.32790100	2.08751800
C	4.02361900	1.06332400	0.03434700
H	5.10522500	0.99813200	0.13074700
C	0.37827900	-2.99148000	-0.16445900
H	-0.51623200	-3.01496900	0.46219400
H	-0.00536800	-2.91493600	-1.18728800
H	0.88653700	-3.95630900	-0.06048900



E = -79.8715342272 a.u.

C	0.00000000	0.00000000	0.76506000
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H	0.51092500	0.88403600	1.16371100
H	-1.02106000	0.00045600	1.16371100
C	0.00000000	0.00000000	-0.76506000
H	1.02106000	0.00045600	-1.16371100
H	-0.51013500	-0.88449200	-1.16371100
H	-0.51092500	0.88403600	-1.16371100

7. NMR Spectra and ESI-MS Spectra

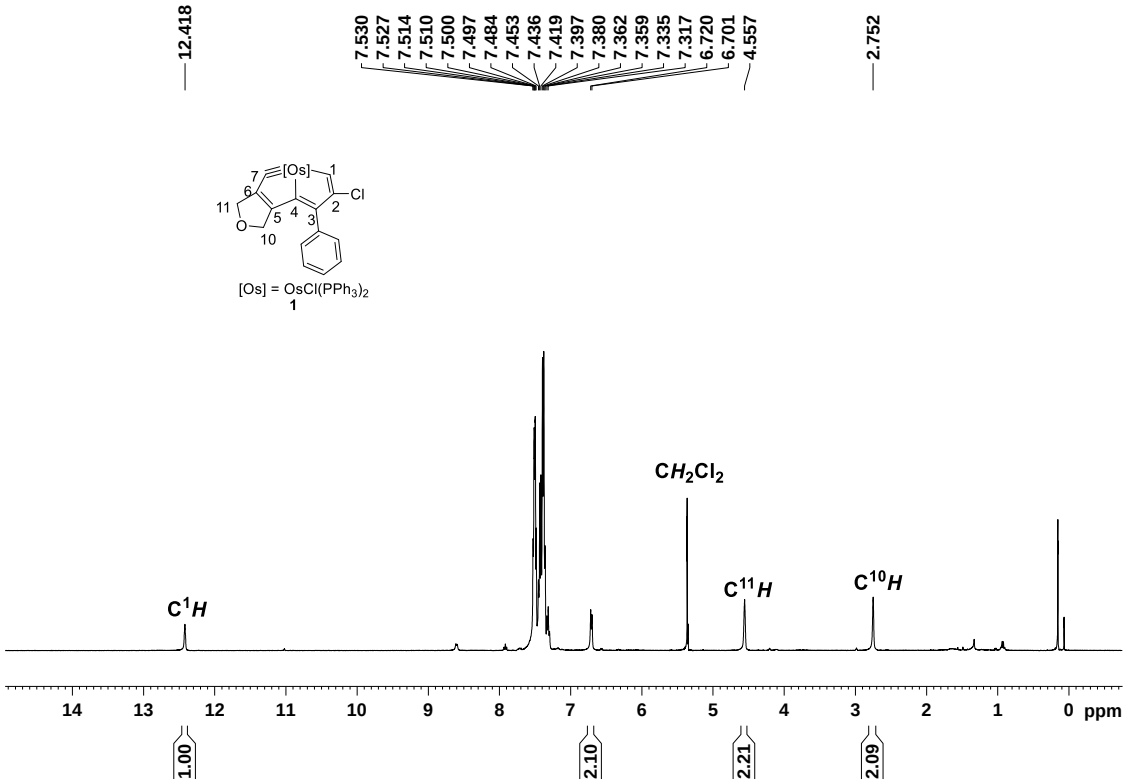

Fig. S15. The ^{1}H-NMR (400.0 MHz) spectrum for complex **1** in CD_2Cl_2.

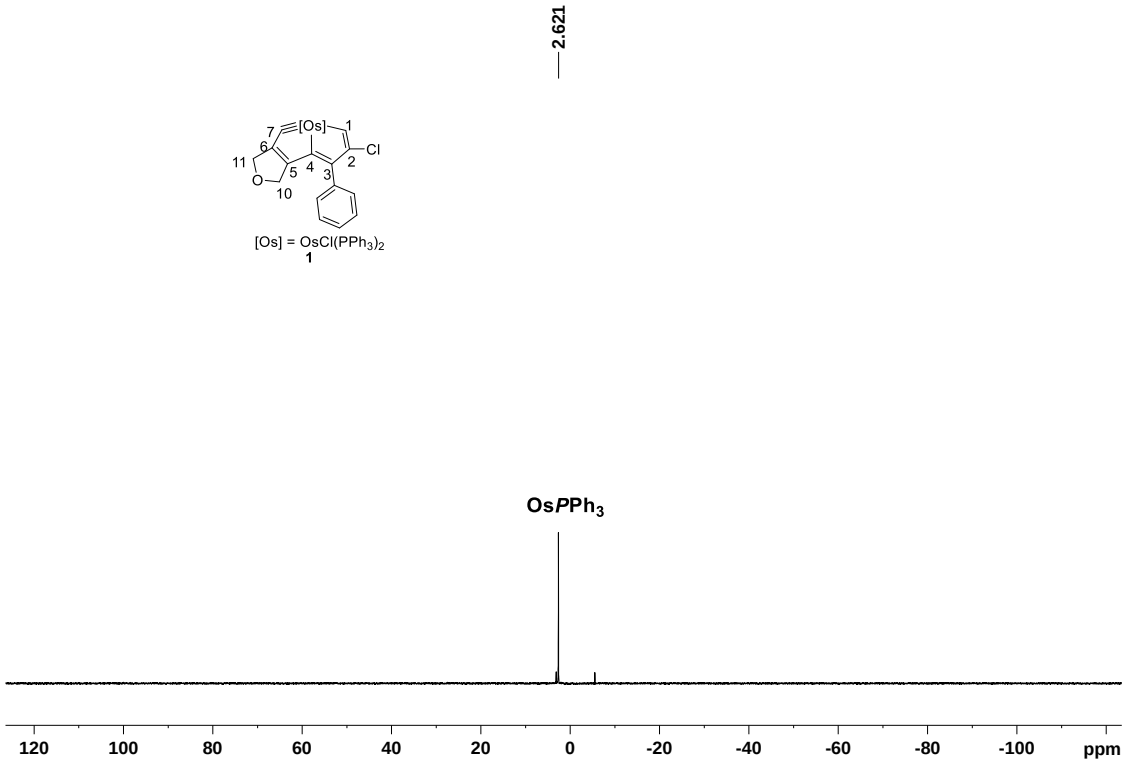

Fig. S16. The ^{31}P-NMR (161.9 MHz) spectrum for complex **1** in CD_2Cl_2.

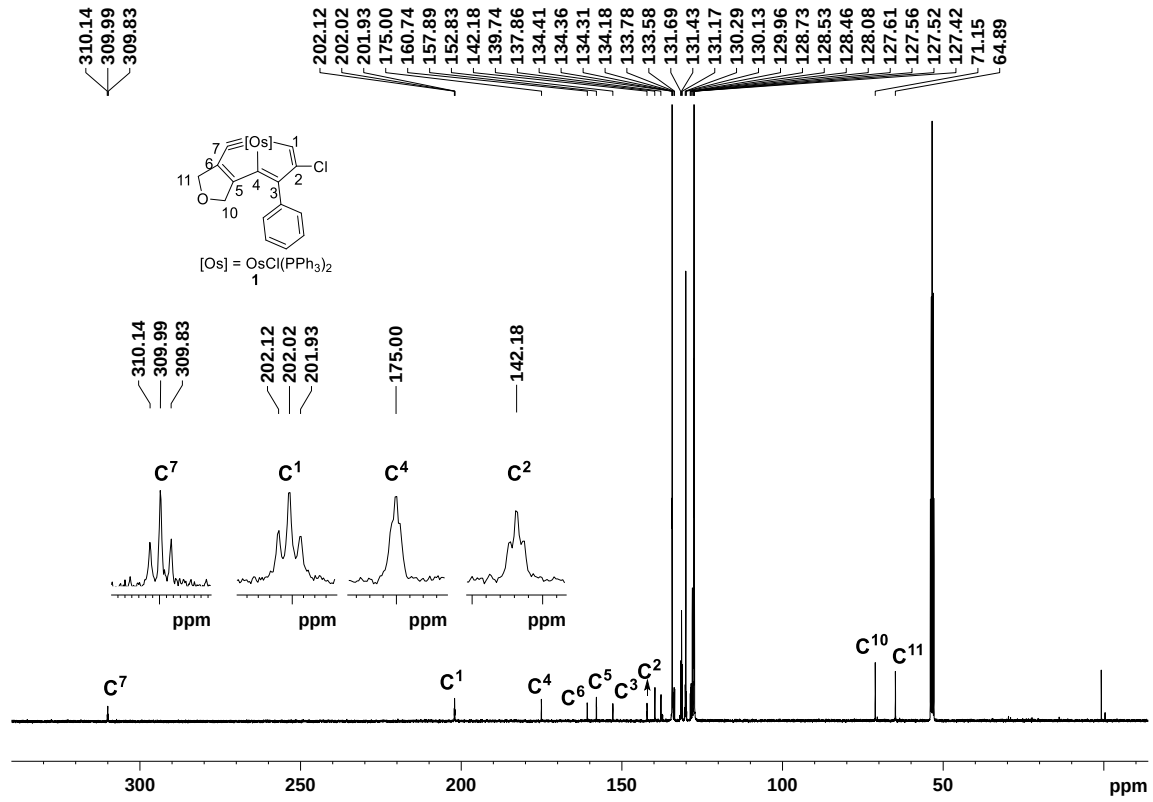

Fig. S17. The ^{13}C-NMR (100.6 MHz) spectrum for complex **1** in CD_2Cl_2.

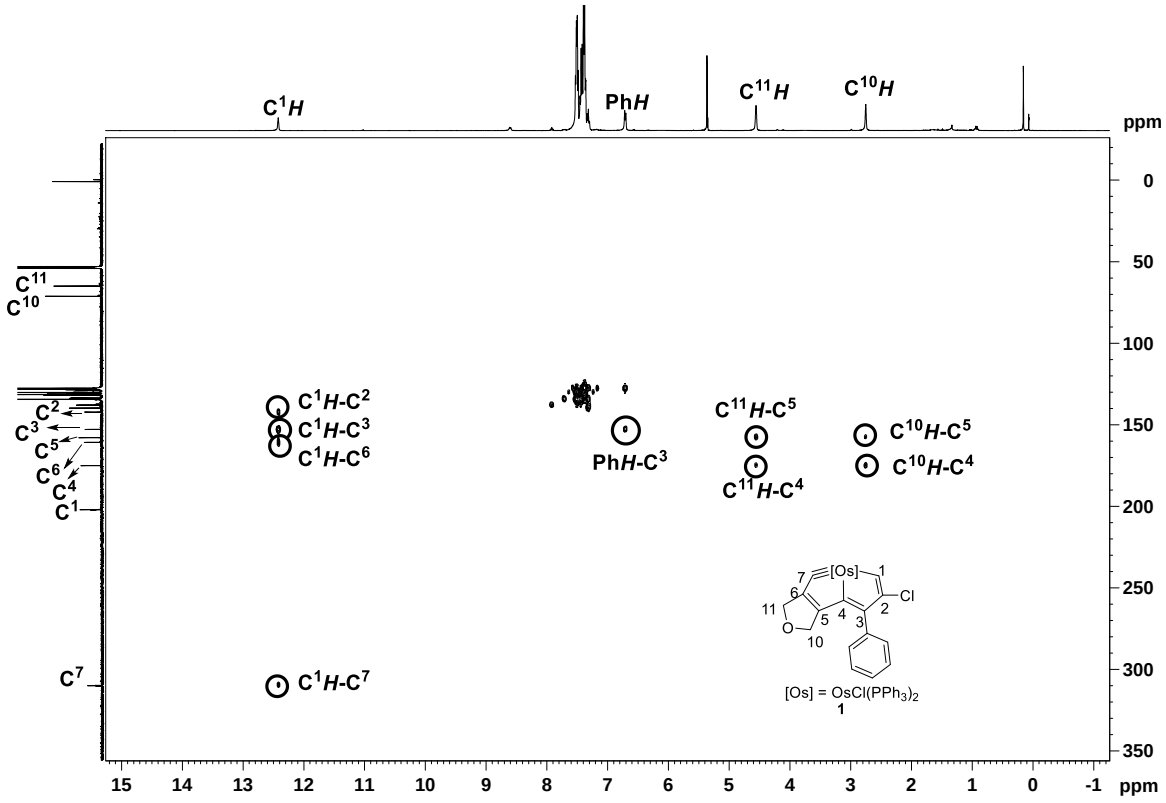

Fig. S18. The ^{1}H-^{13}C HMBC (100.6 MHz) spectrum for complex **1** in CD_2Cl_2.

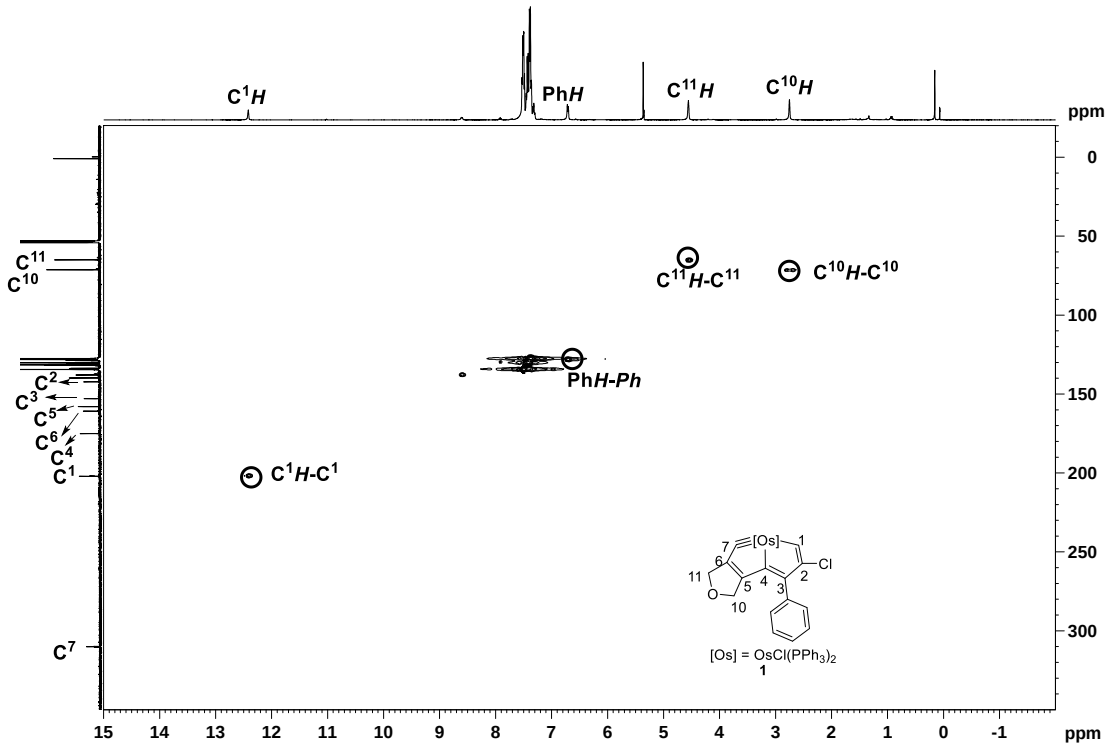

Fig. S19. The ^{1}H-^{13}C HSQC (100.6 MHz) spectrum for complex **1** in CD_2Cl_2.

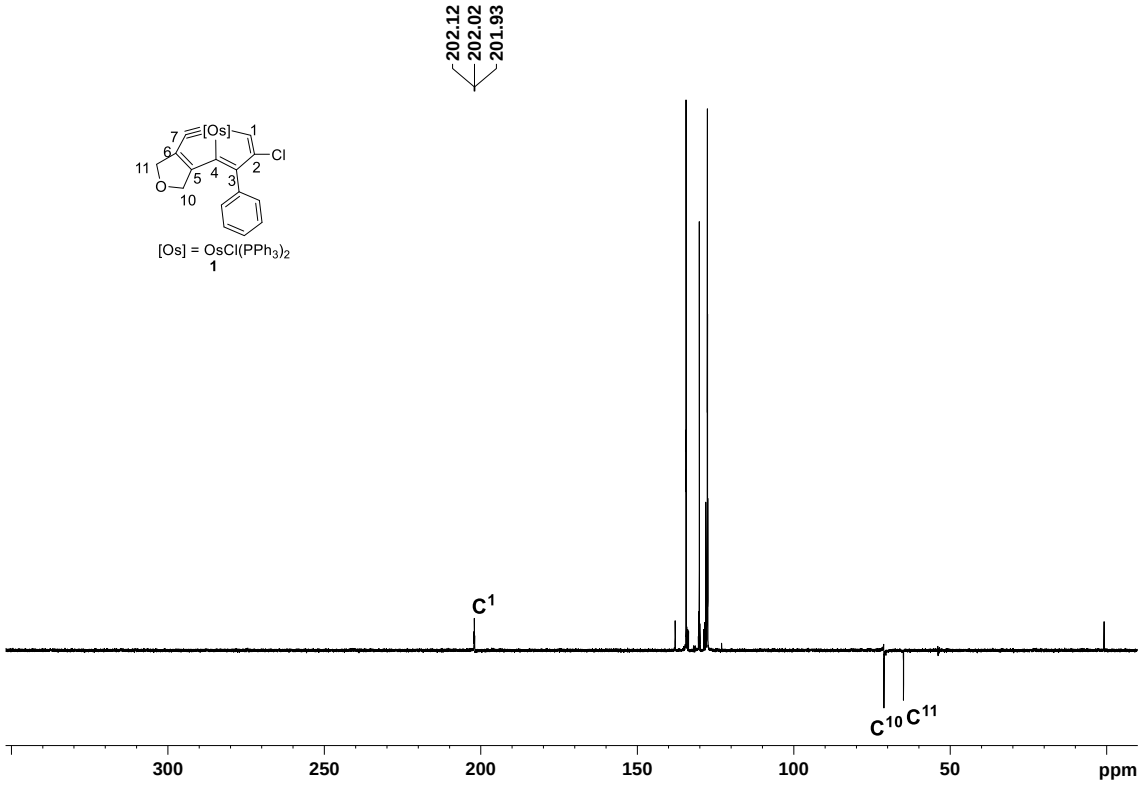

Fig. S20. The DEPT-135 (100.6 MHz) spectrum for complex **1** in CD_2Cl_2.

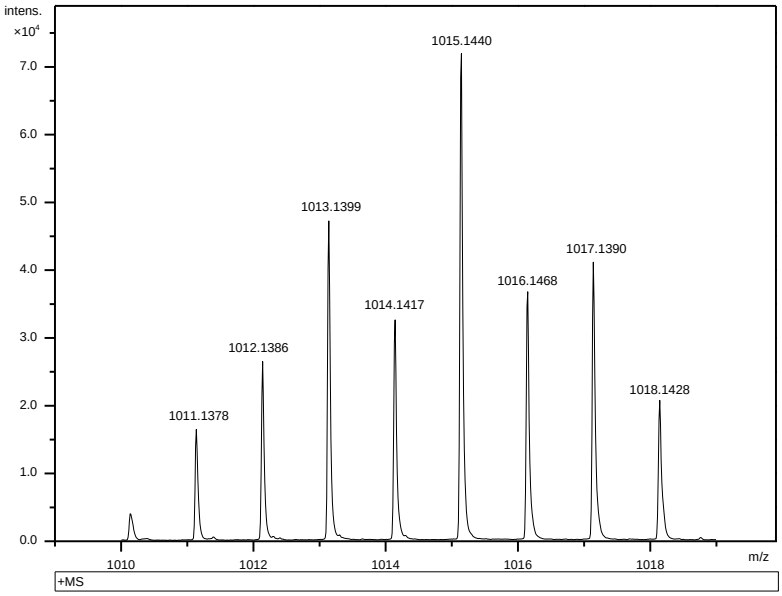

Fig. S21. Positive-ion ESI-MS spectrum of **[1+Na$^+$]$^+$** measured in MeOH.

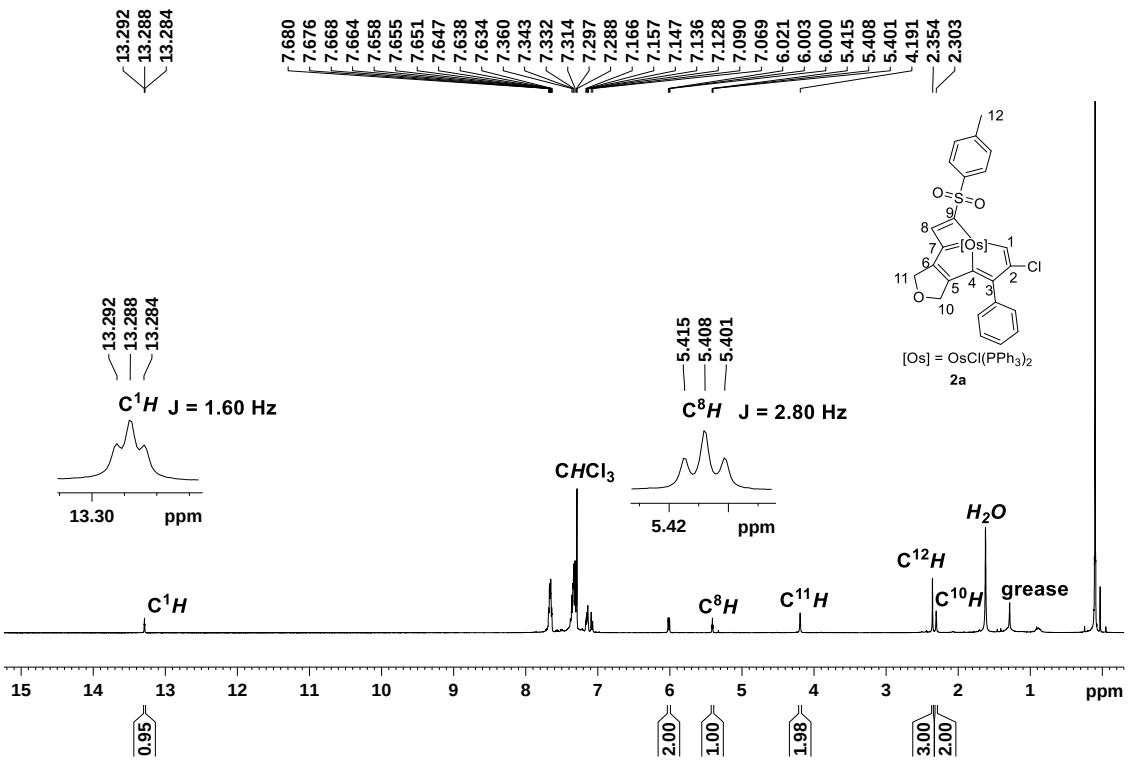

Fig. S22. The ^{1}H-NMR (400.0 MHz) spectrum for complex **2a** in $CDCl_3$.

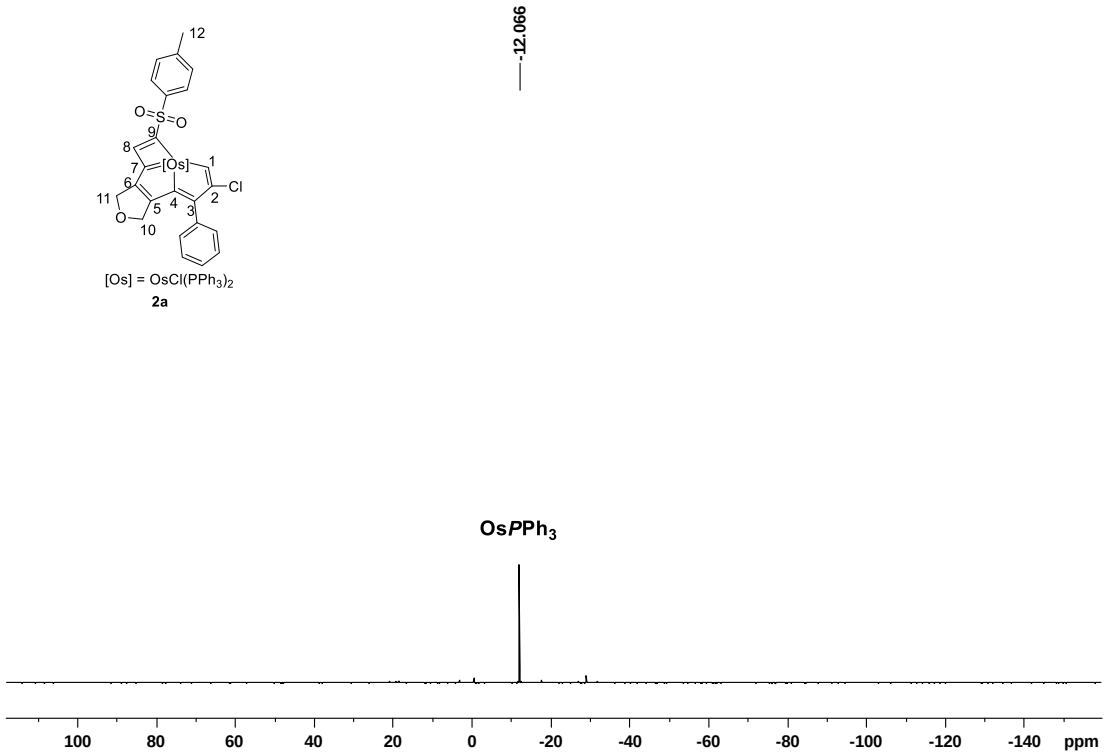

Fig. S23. The ^{31}P-NMR (242.9 MHz) spectrum for complex **2a** in CD_2Cl_2.

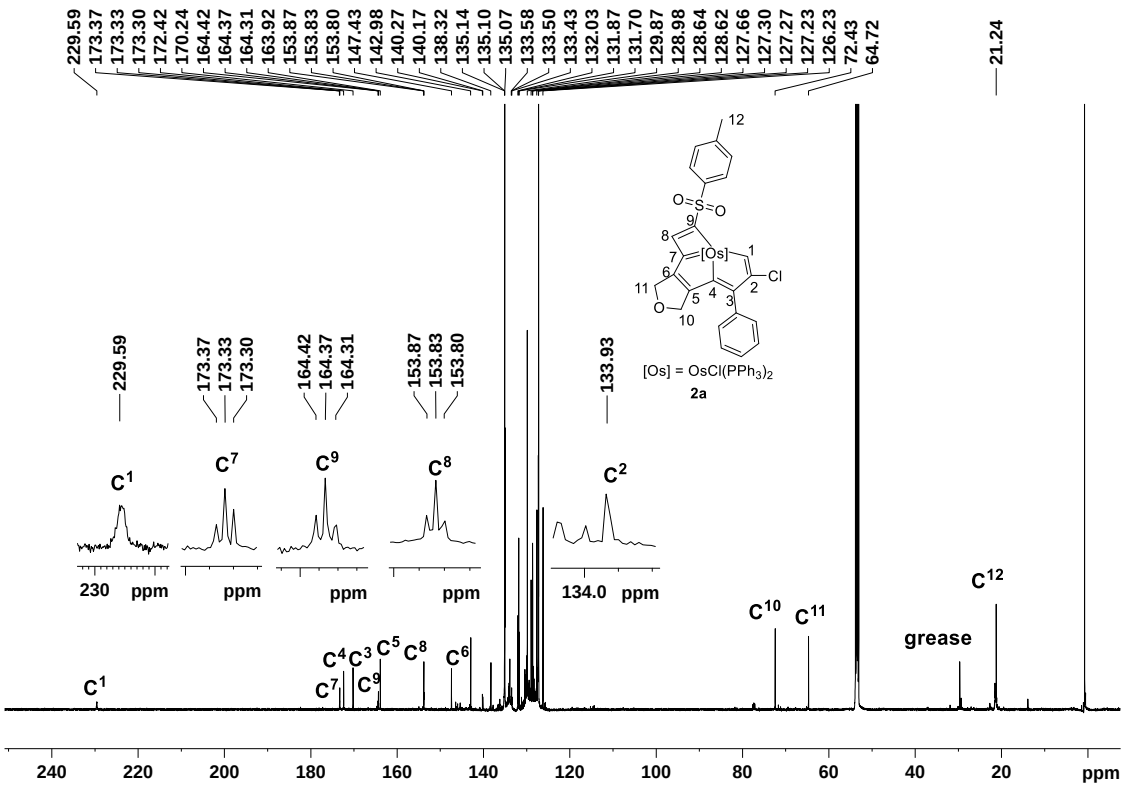

Fig. S24. The ^{13}C-NMR (150.9 MHz) spectrum for complex **2a** in CD_2Cl_2.

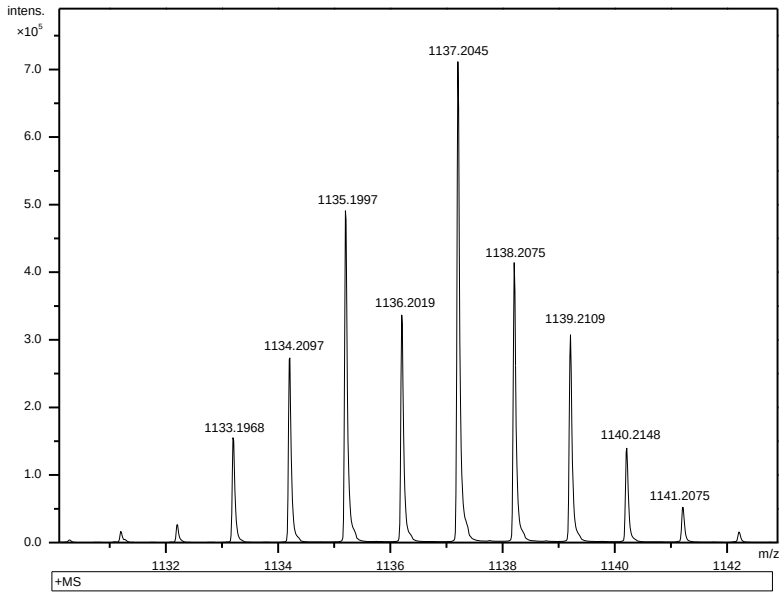

Fig. S25. Positive-ion ESI-MS spectrum of **[2a-Cl$^-$]$^+$** measured in MeOH.

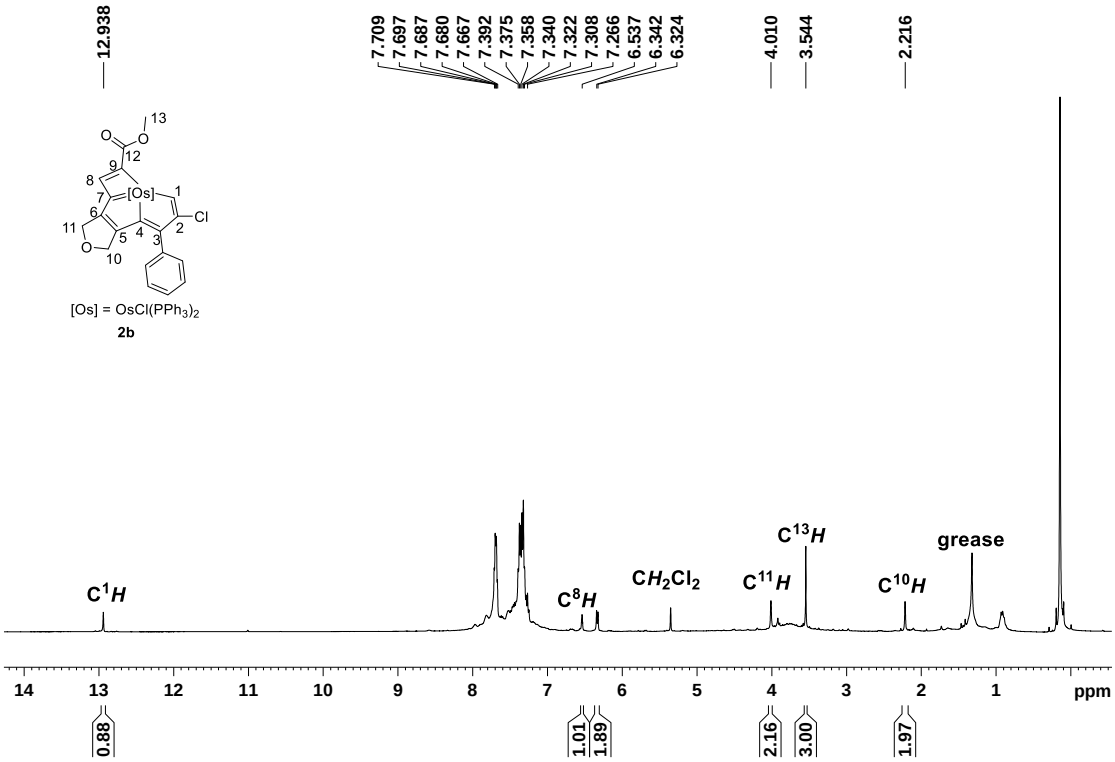

Fig. S26. The ^{1}H-NMR (400.0 MHz) spectrum for complex **2b** in CD_2Cl_2.

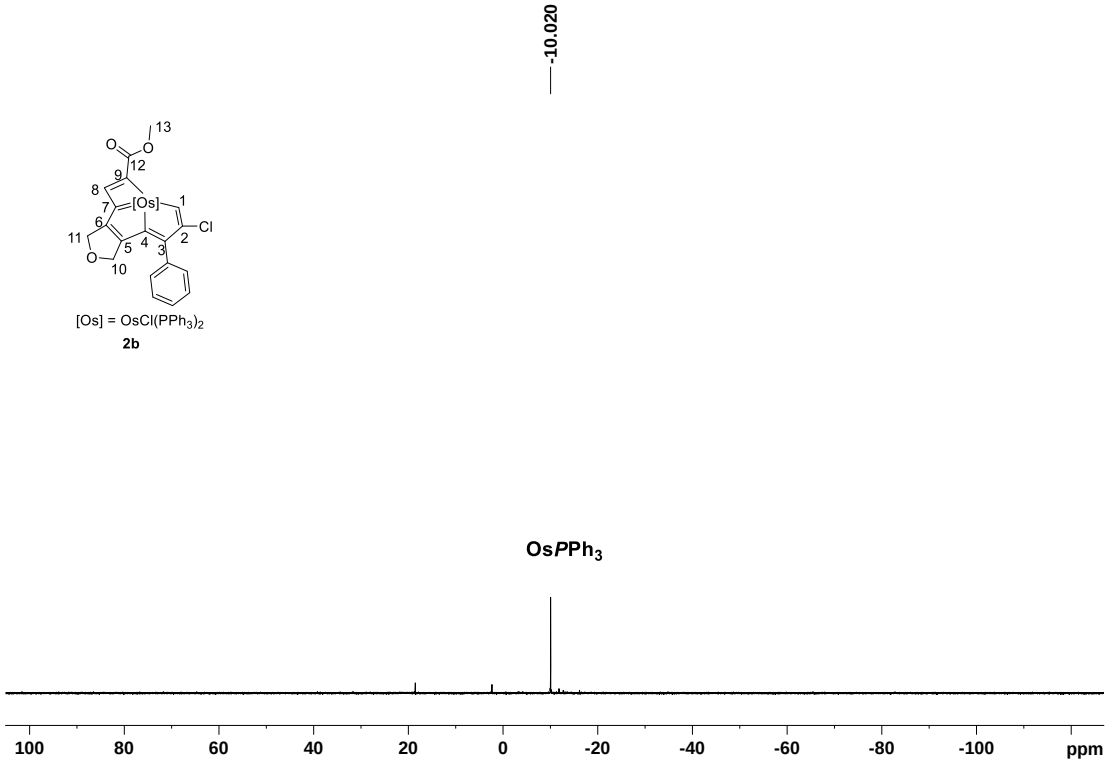

Fig. S27. The ^{31}P-NMR (161.9 MHz) spectrum for complex **2b** in CD_2Cl_2.

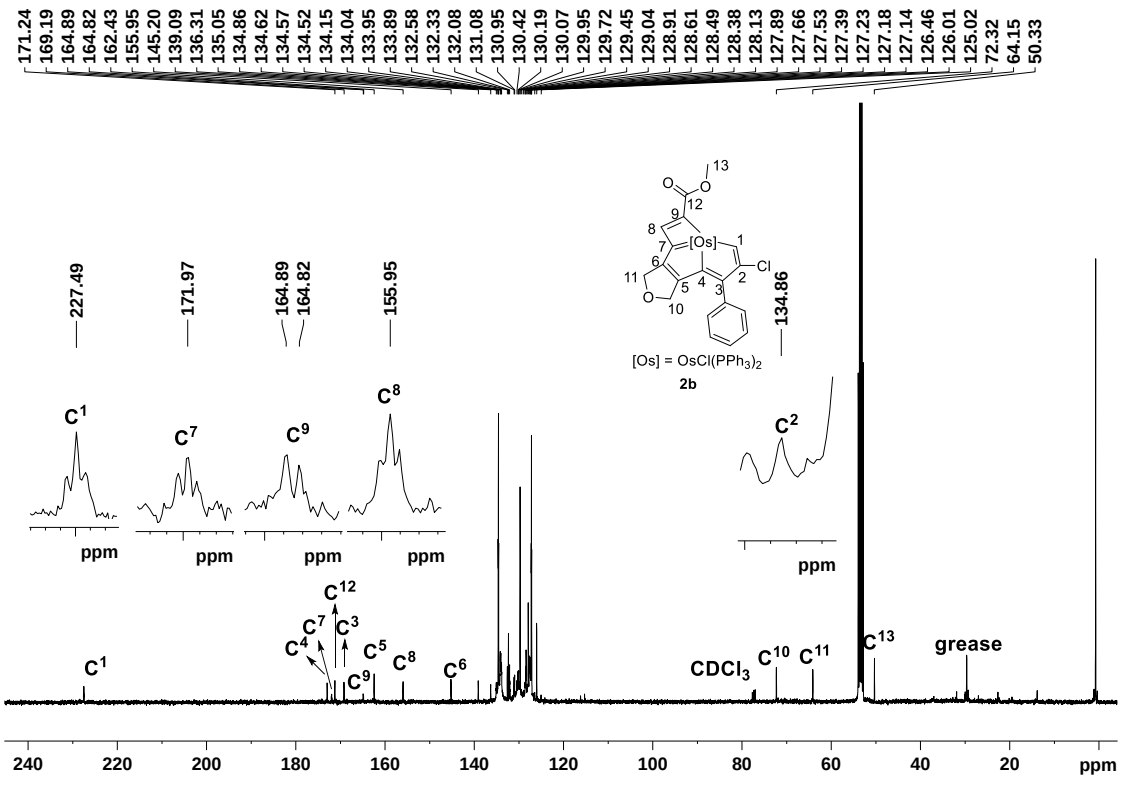

Fig. S28. The ^{13}C-NMR (100.6 MHz) spectrum for complex **2b** in CD_2Cl_2.

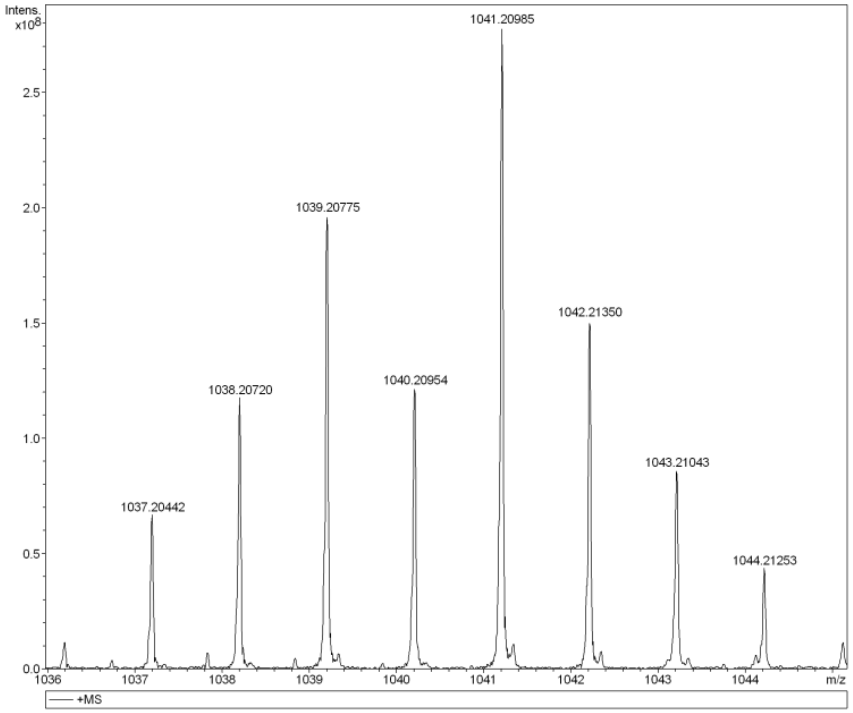

Fig. S29. Positive-ion ESI-MS spectrum of **[2b-Cl$^-$]$^+$** measured in MeOH.

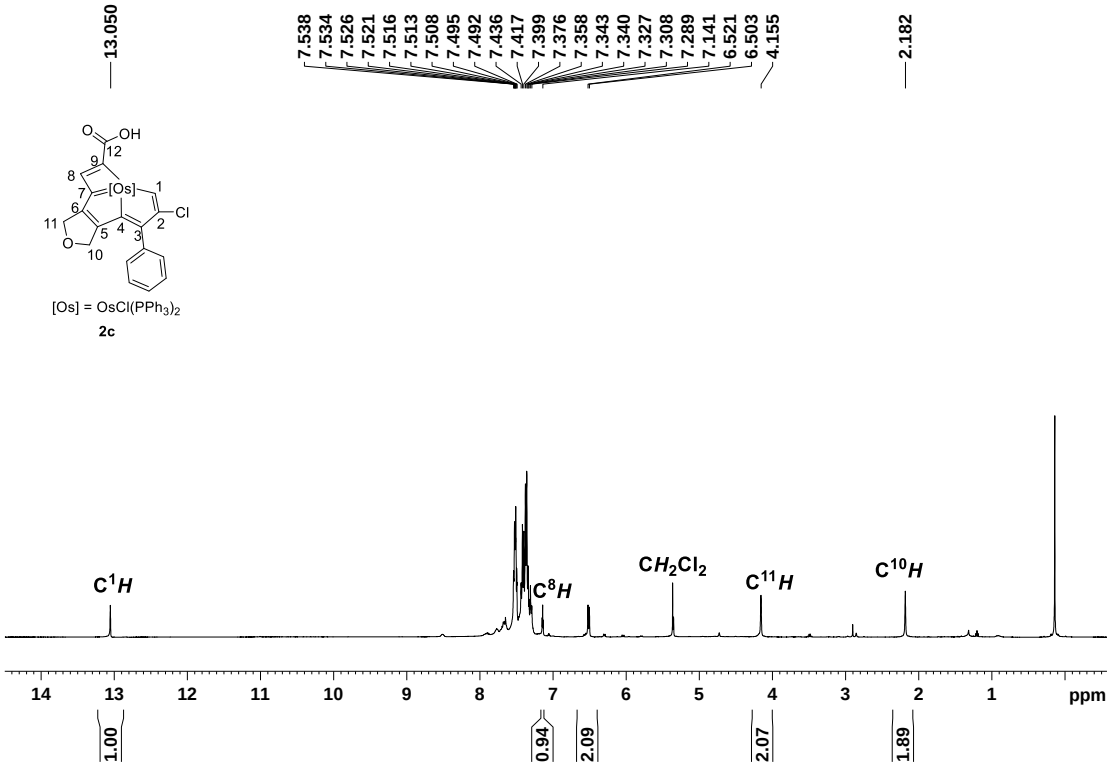

Fig. S30. The ^{1}H-NMR (400.0 MHz) spectrum for complex **2c** in CD_2Cl_2.

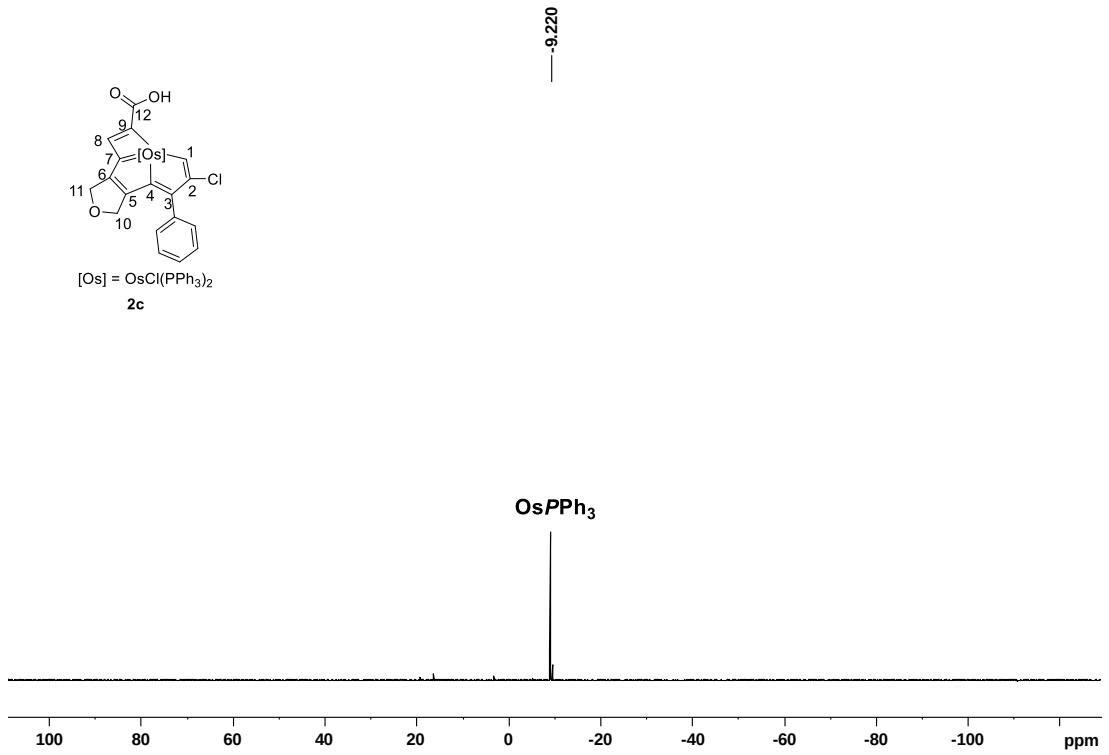

Fig. S31. The ^{31}P-NMR (161.9 MHz) spectrum for complex **2c** in CD_2Cl_2.

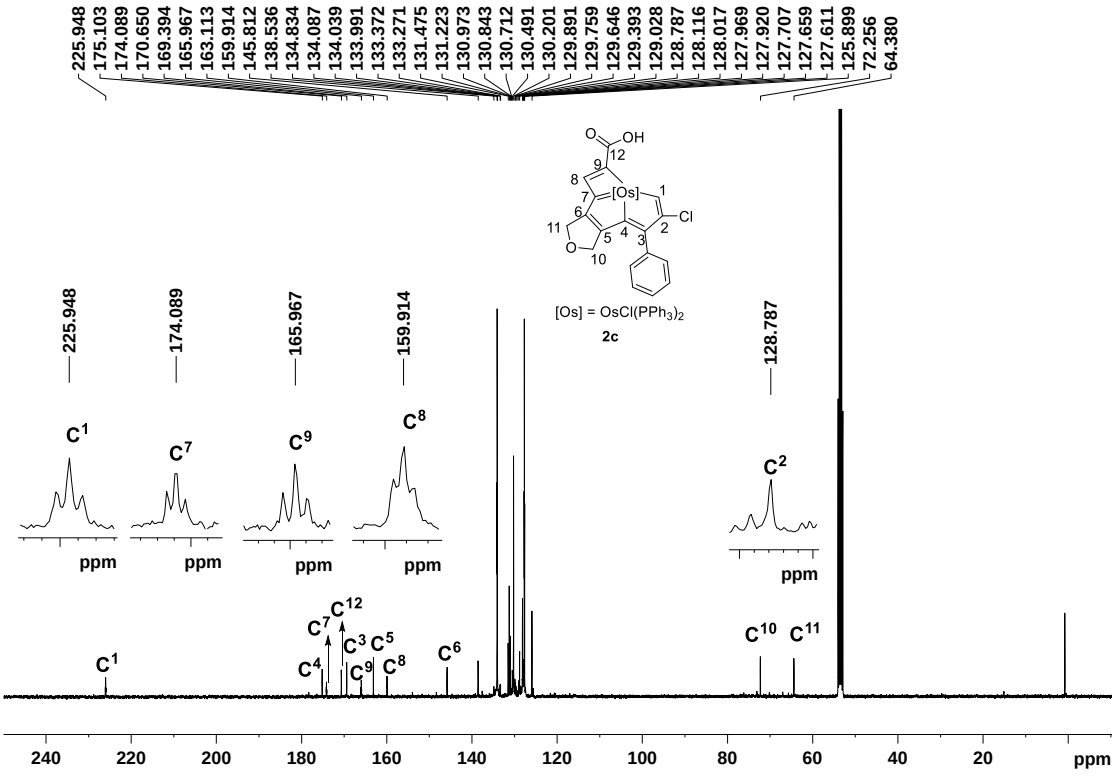

Fig. S32. The ^{13}C-NMR (100.6 MHz) spectrum for complex **2c** in CD_2Cl_2.

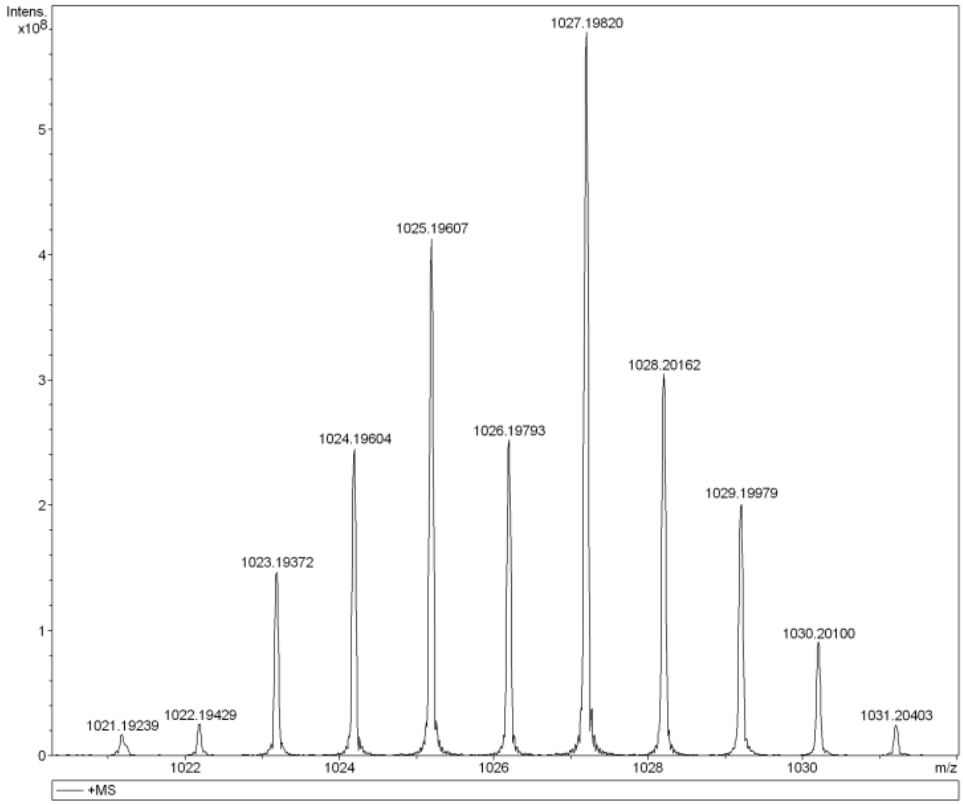

Fig. S33. Positive-ion ESI-MS spectrum of **[2c-Cl$^-$]$^+$** measured in MeOH.

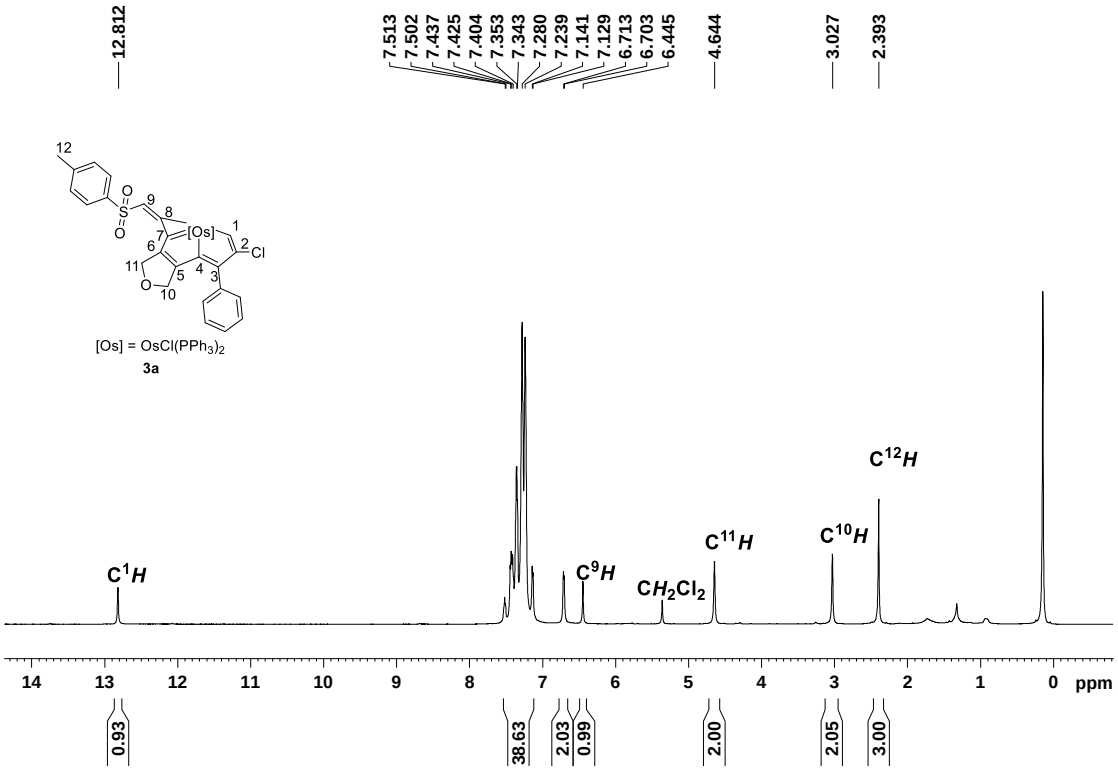

Fig. S34. The ^{1}H-NMR (600.1 MHz) spectrum for complex **3a** in CD_2Cl_2.

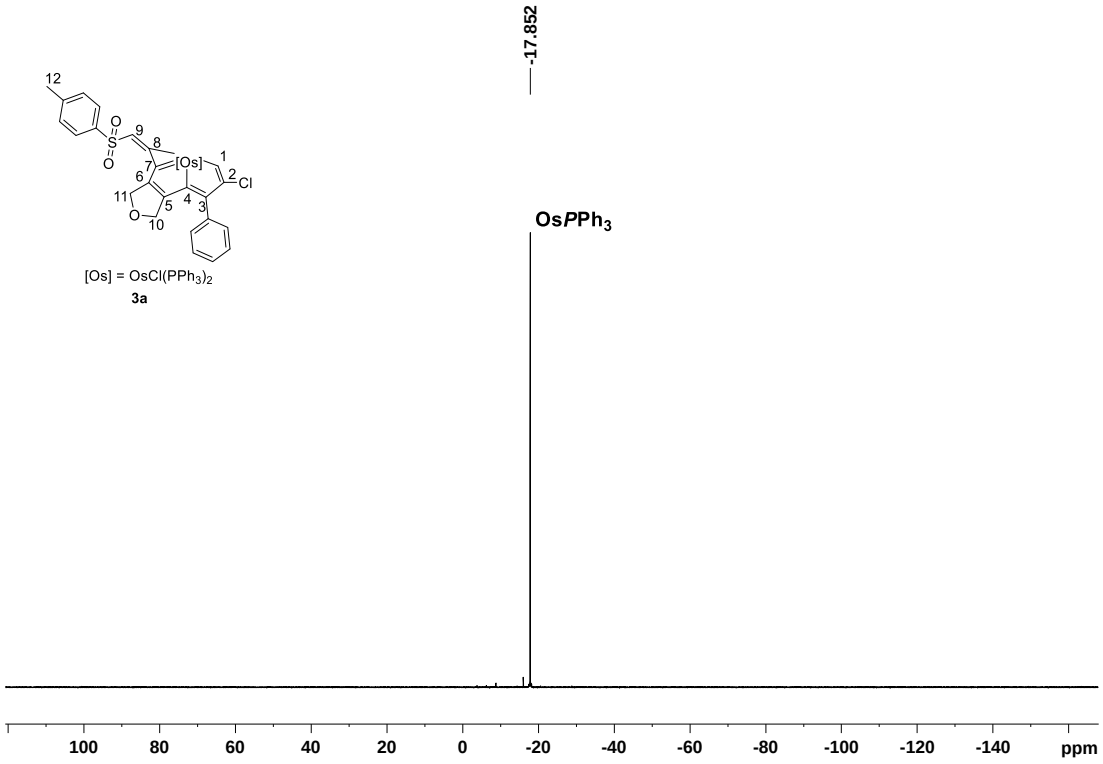

Fig. S35. The ^{31}P-NMR (242.9 MHz) spectrum for complex **3a** in CD_2Cl_2.

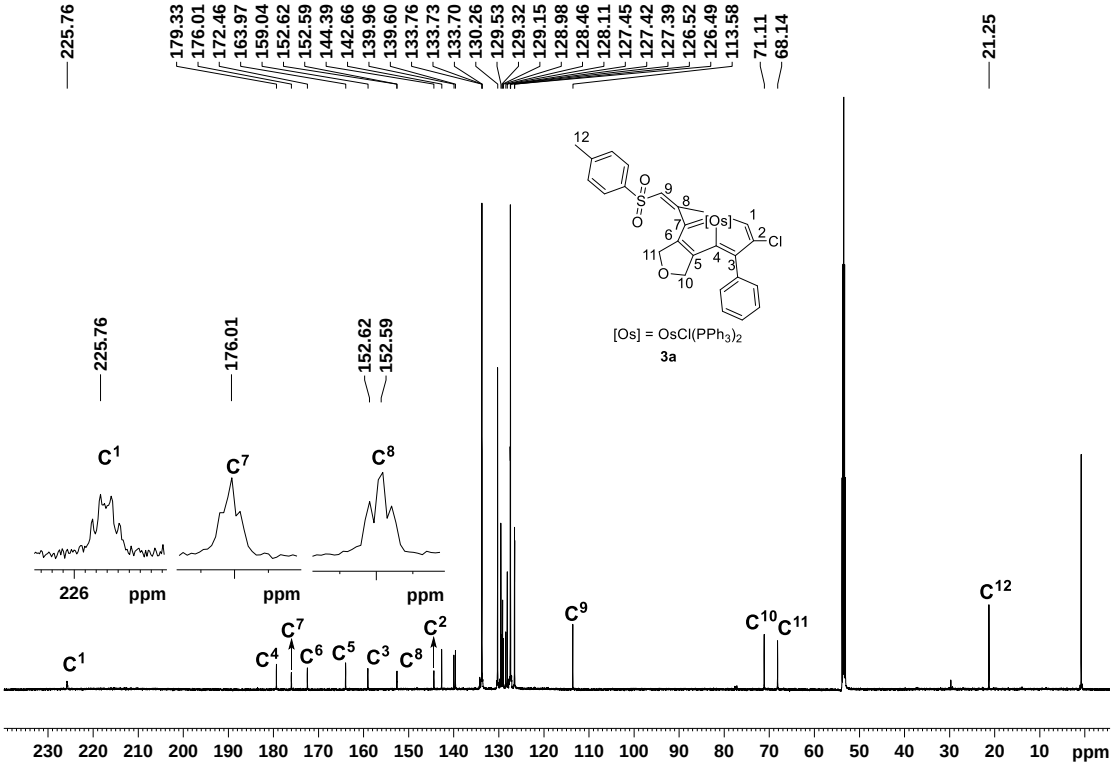

Fig. S36. The ^{13}C-NMR (150.9 MHz) spectrum for complex **3a** in CD_2Cl_2.

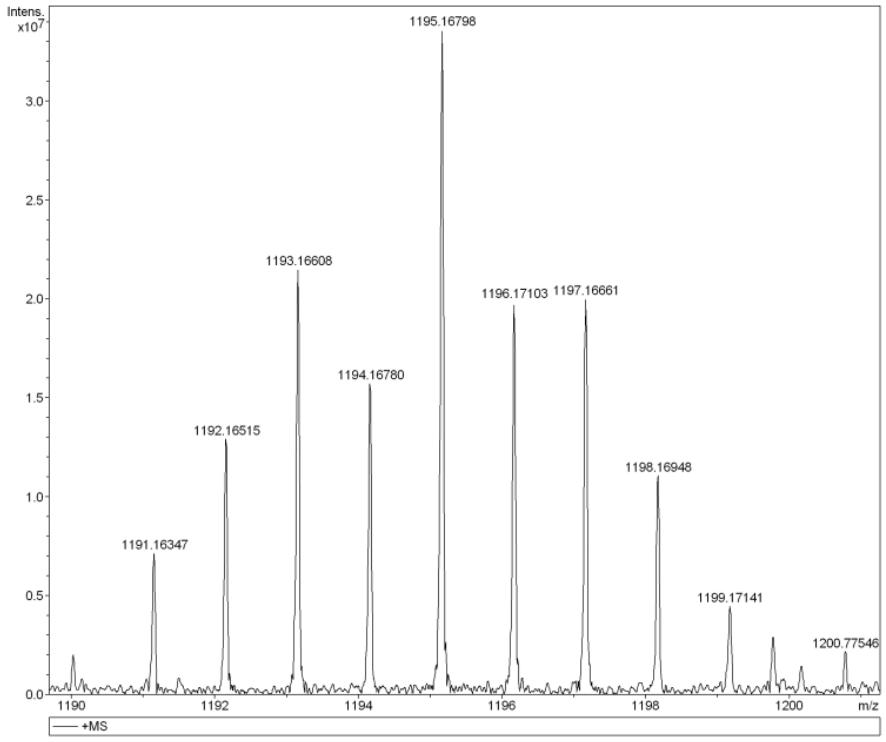

Fig. S37. Positive-ion ESI-MS spectrum of **[3a+Na$^+$]$^+$** measured in MeOH.

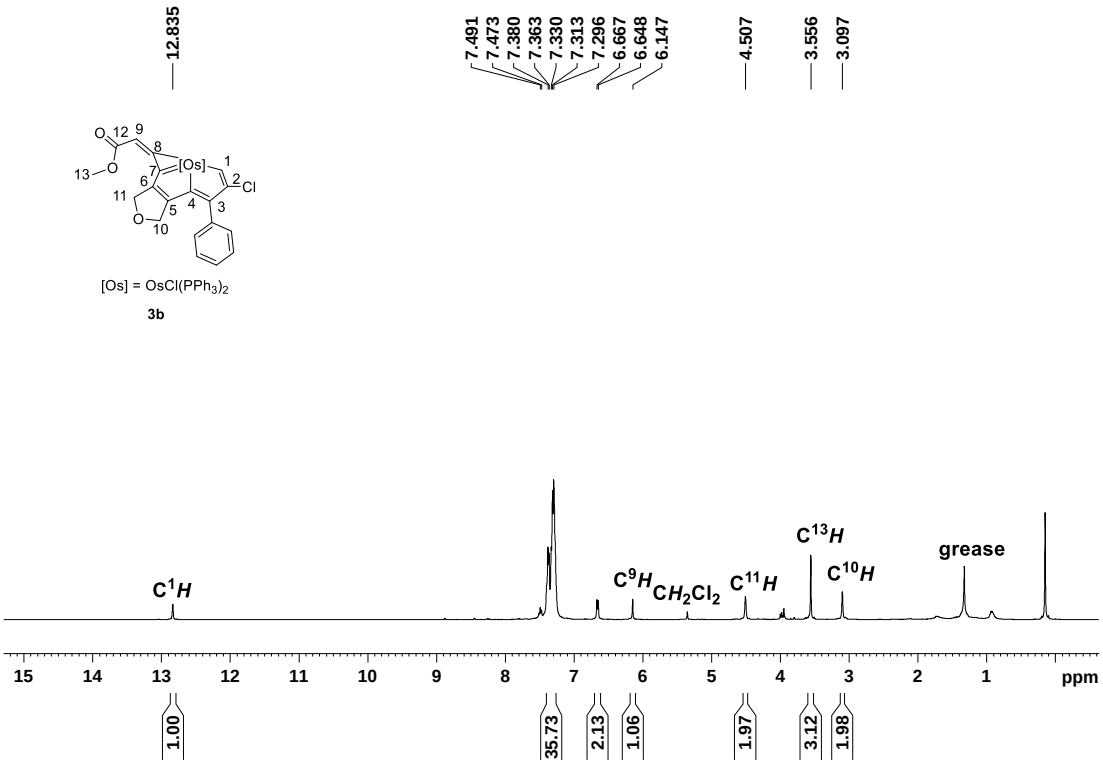

Fig. S38. The ^{1}H-NMR (400.0 MHz) spectrum for complex **3b** in CD_2Cl_2.

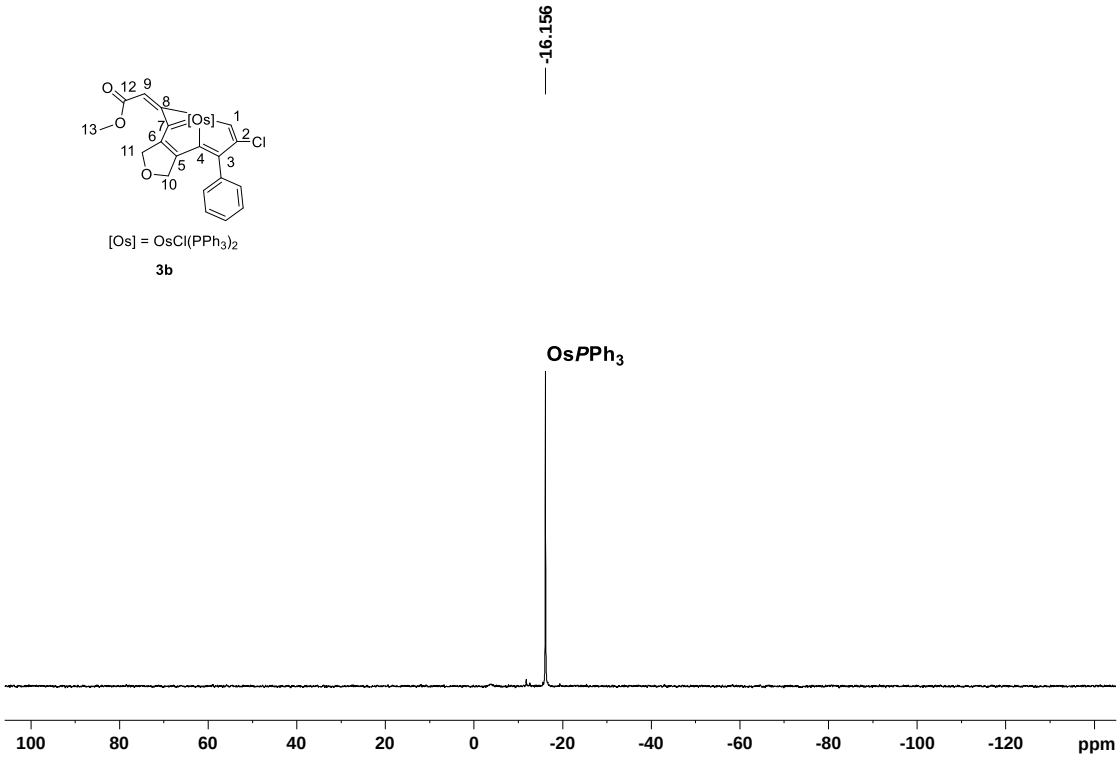

Fig. S39. The ^{31}P-NMR (161.9 MHz) spectrum for complex **3b** in CD_2Cl_2.

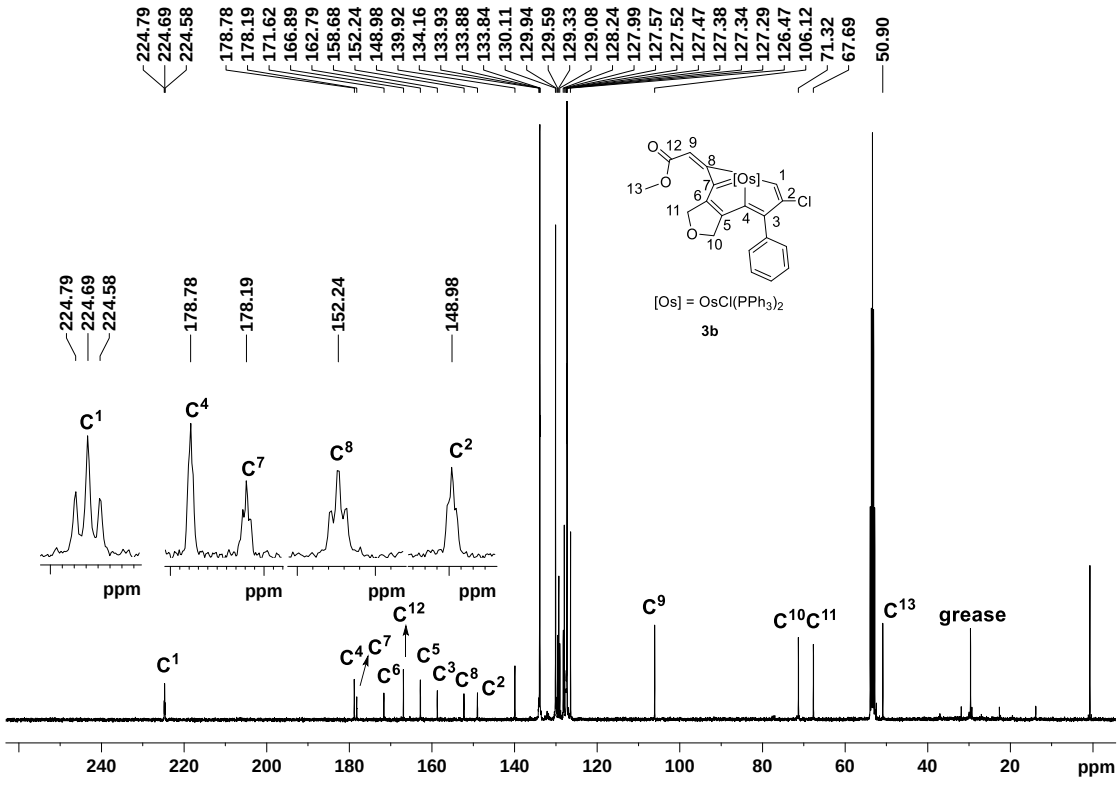

Fig. S40. The ^{13}C-NMR (100.6 MHz) spectrum for complex **3b** in CD_2Cl_2.

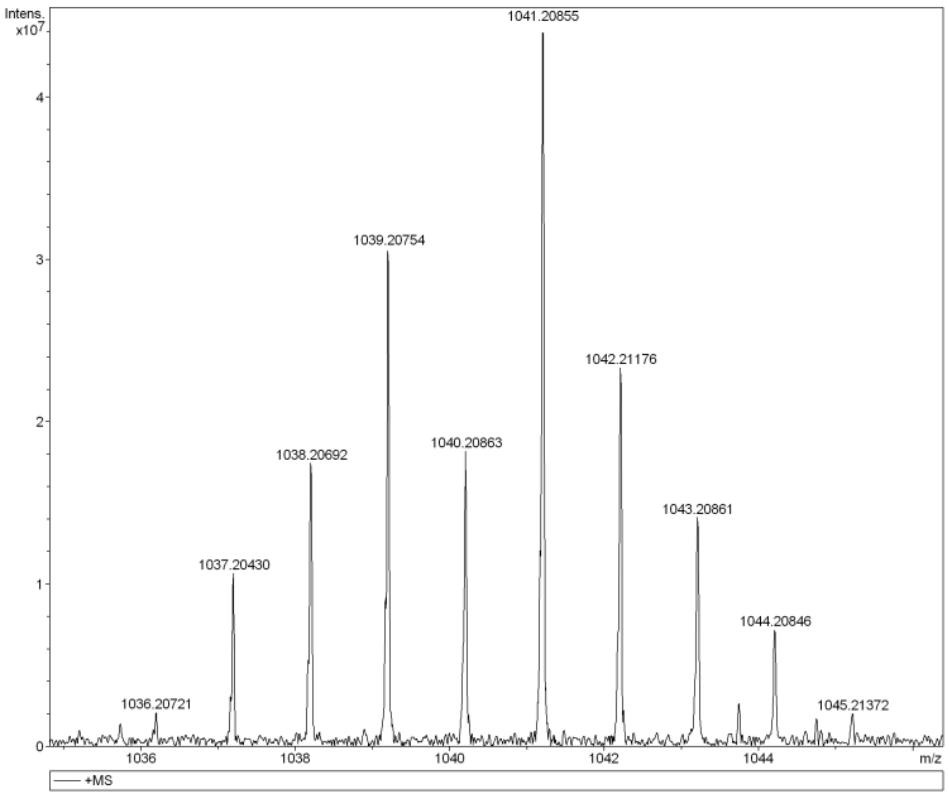

Fig. S41. Positive-ion ESI-MS spectrum of **[3b-Cl$^-$]$^+$** measured in MeOH.

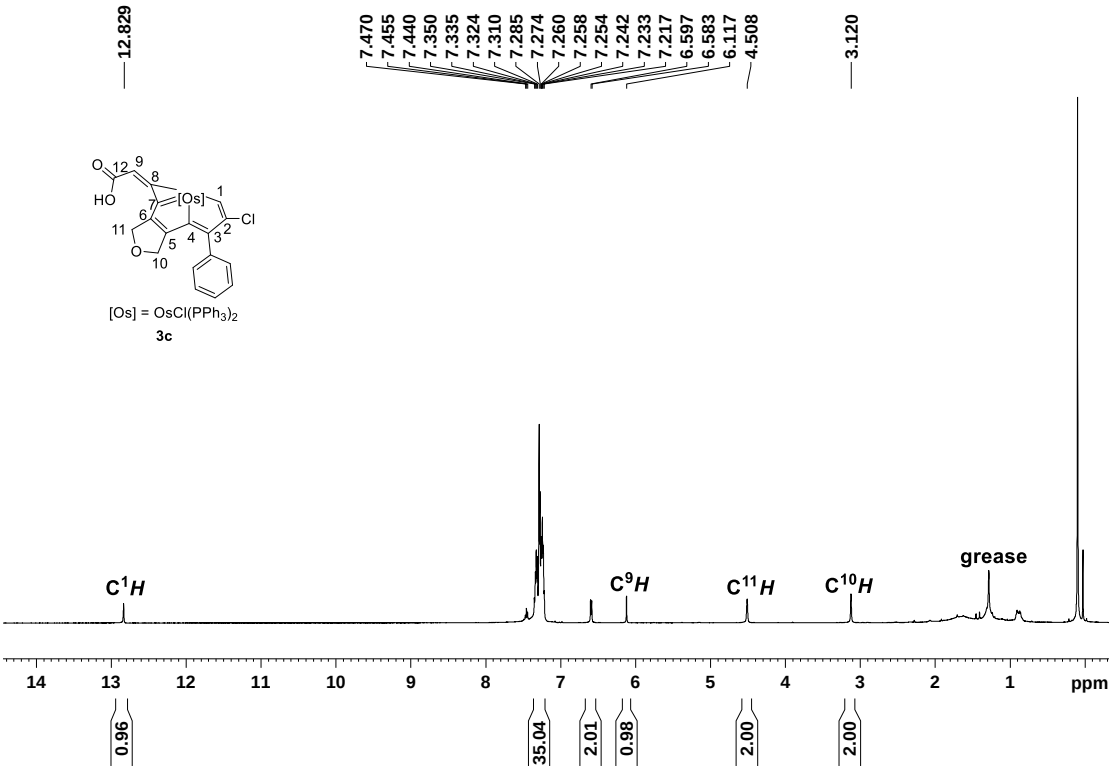

Fig. S42. The ^{1}H-NMR (400.0 MHz) spectrum for complex **3c** in CD_2Cl_2.

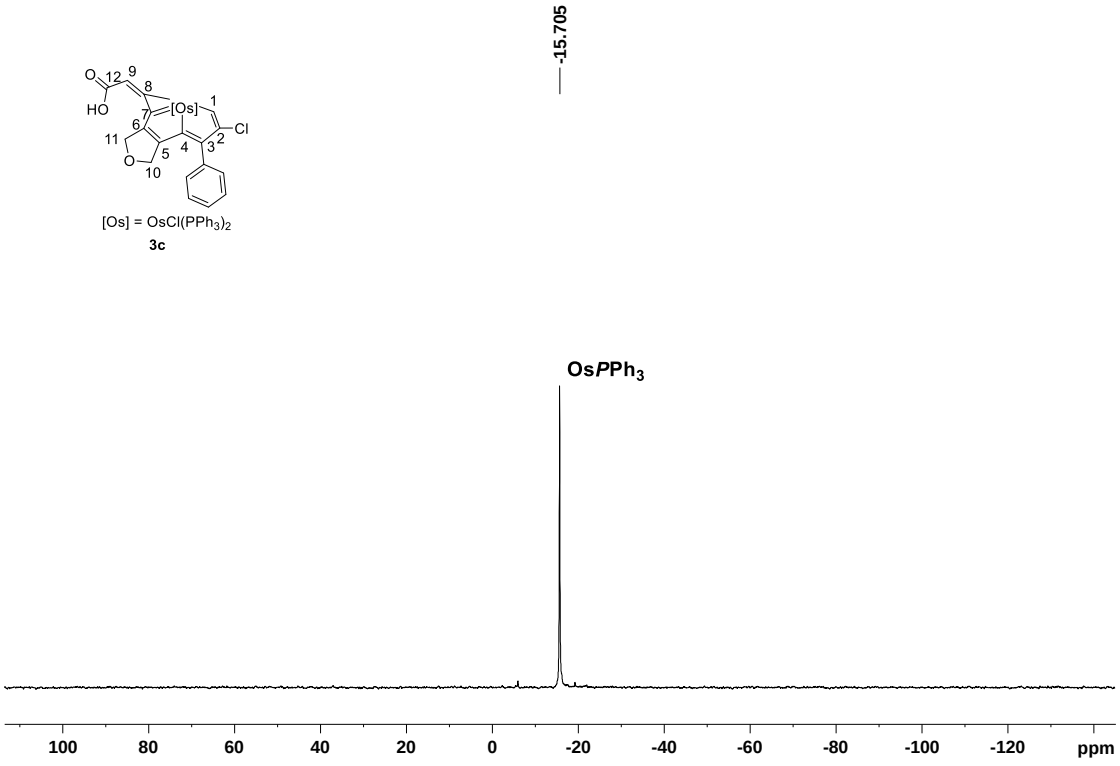

Fig. S43. The ^{31}P-NMR (161.9 MHz) spectrum for complex **3c** in CF_3COOD:CD_2Cl_2 = 1:100, v/v.

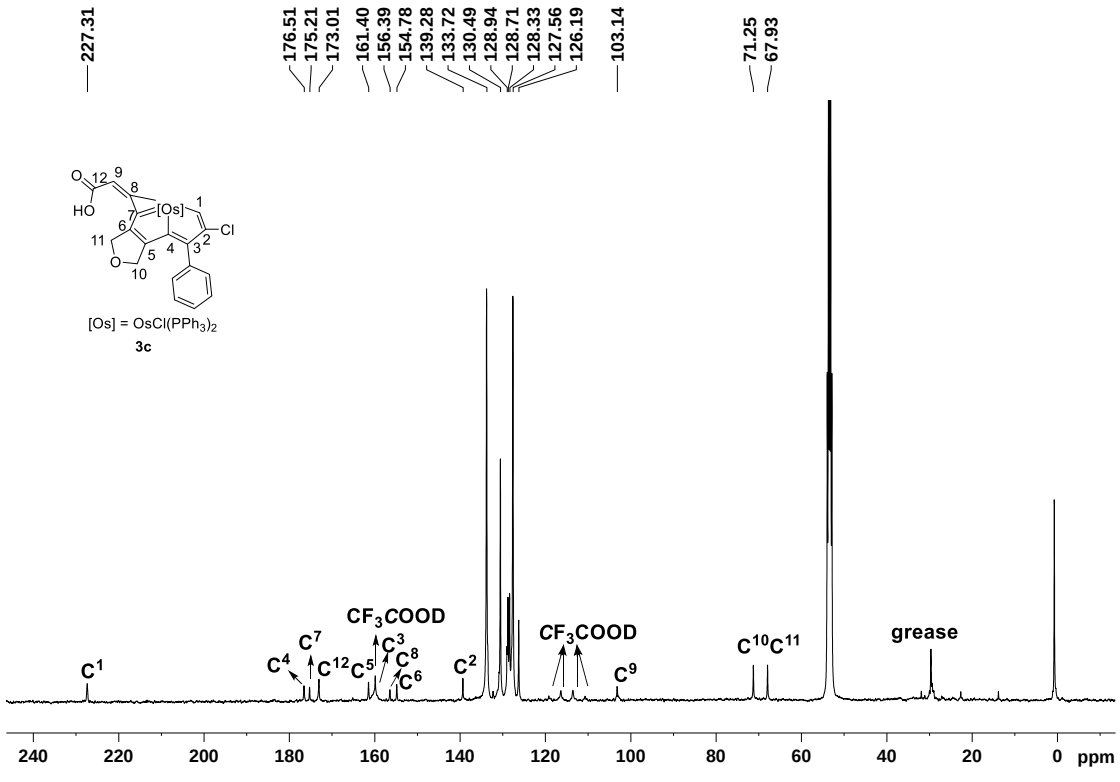

Fig. S44. The ^{13}C-NMR (100.6 MHz) spectrum for complex **3c** in CF_3COOD:CD_2Cl_2 = 1:100, v/v.

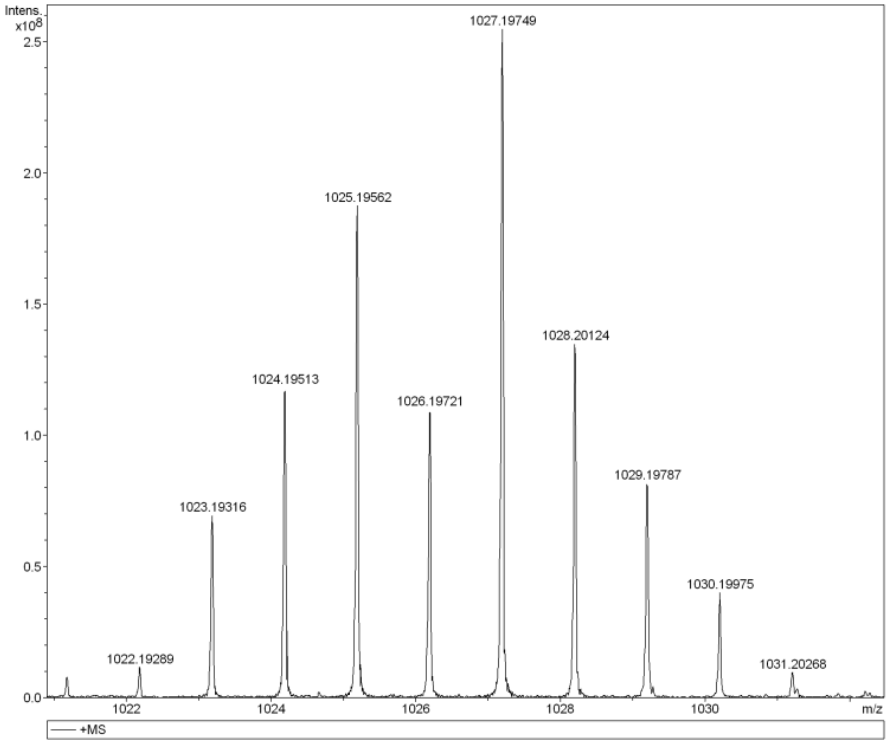

Fig. S45. Positive-ion ESI-MS spectrum of **[3c-Cl$^-$]$^+$** measured in MeOH.

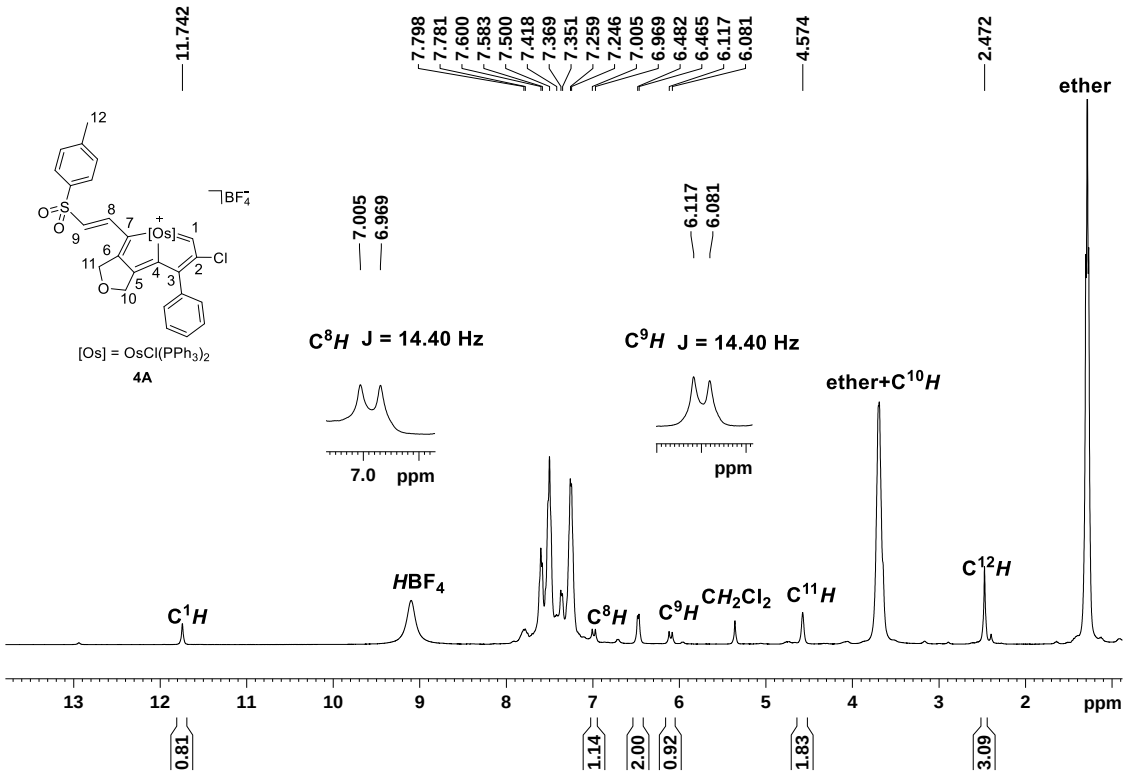

Fig. S46. The ^{1}H-NMR (400.0 MHz) spectrum for complex **4A** in CD_2Cl_2.

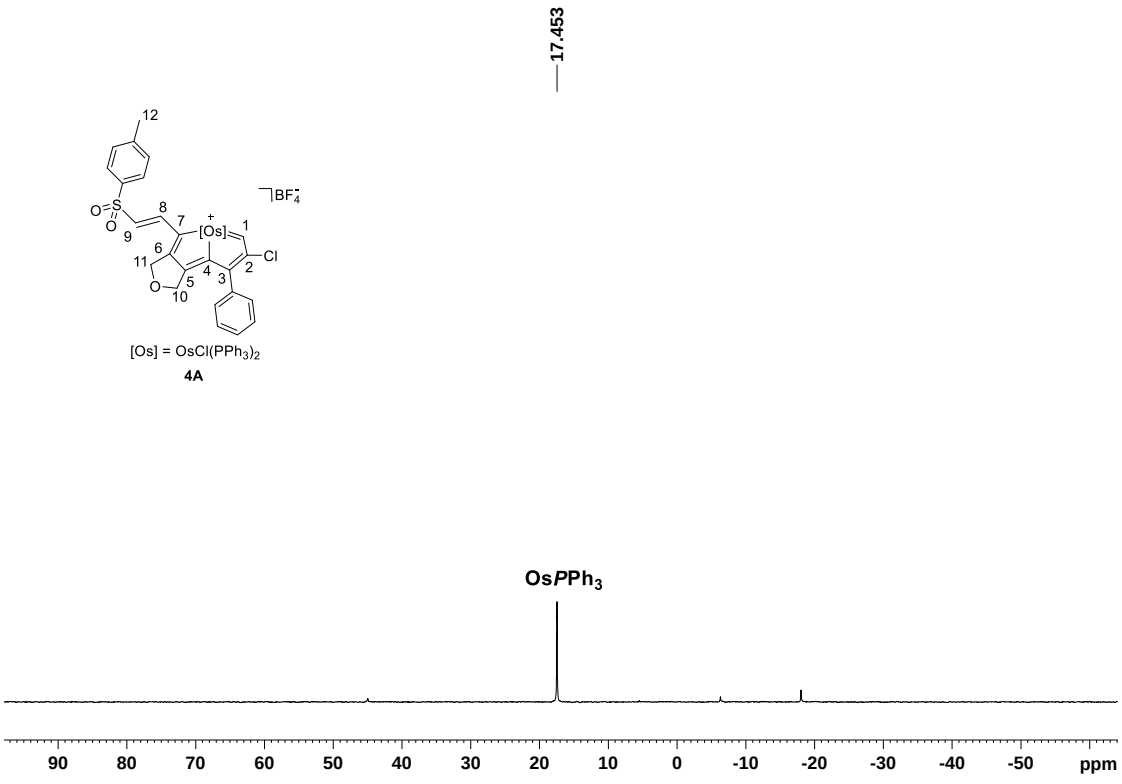

Fig. S47. The ^{31}P-NMR (161.9 MHz) spectrum for complex **4A** in CD_2Cl_2.

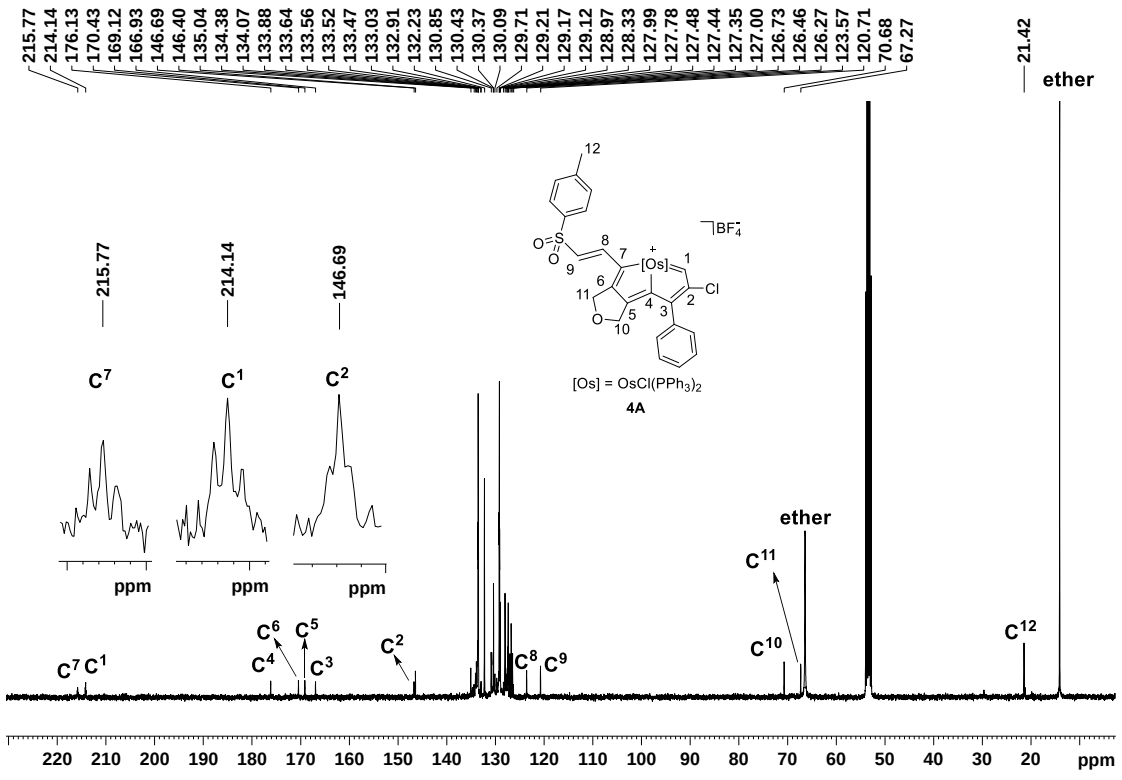

Fig. S48. The ^{13}C-NMR (100.6 MHz) spectrum for complex **4A** in CD_2Cl_2.

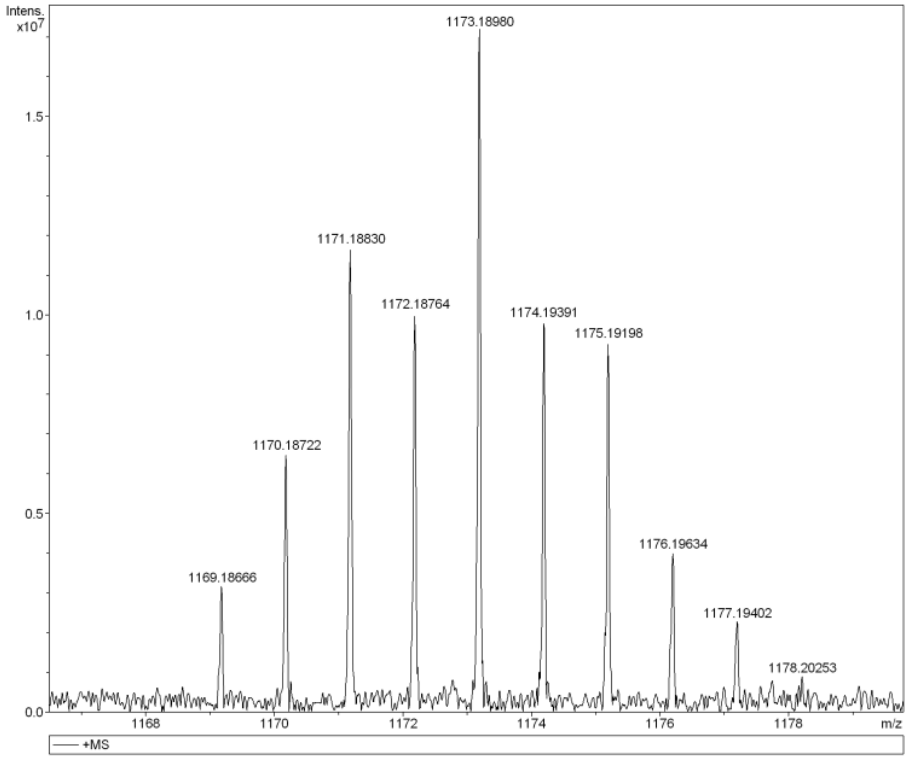

Fig. S49. Positive-ion ESI-MS spectrum of **[4A]**$^{+}$ measured in MeOH.

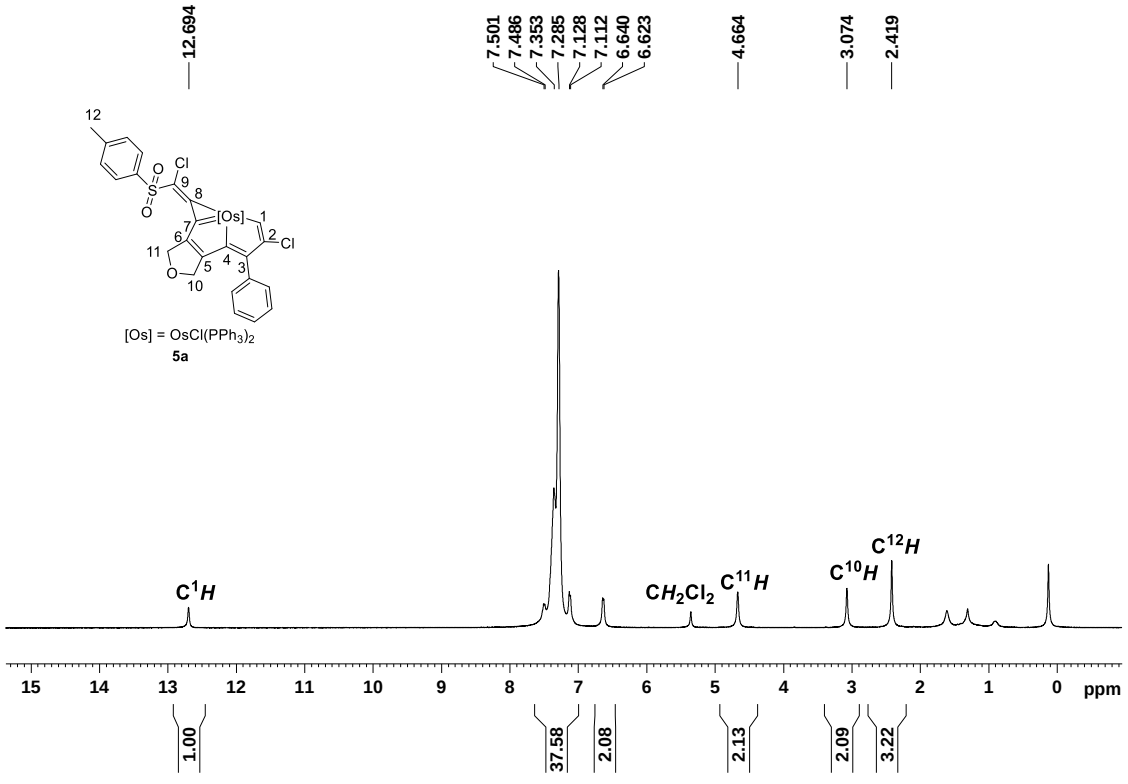

Fig. S50. The ^{1}H-NMR (400.0 MHz) spectrum for complex **5a** in CD_2Cl_2.

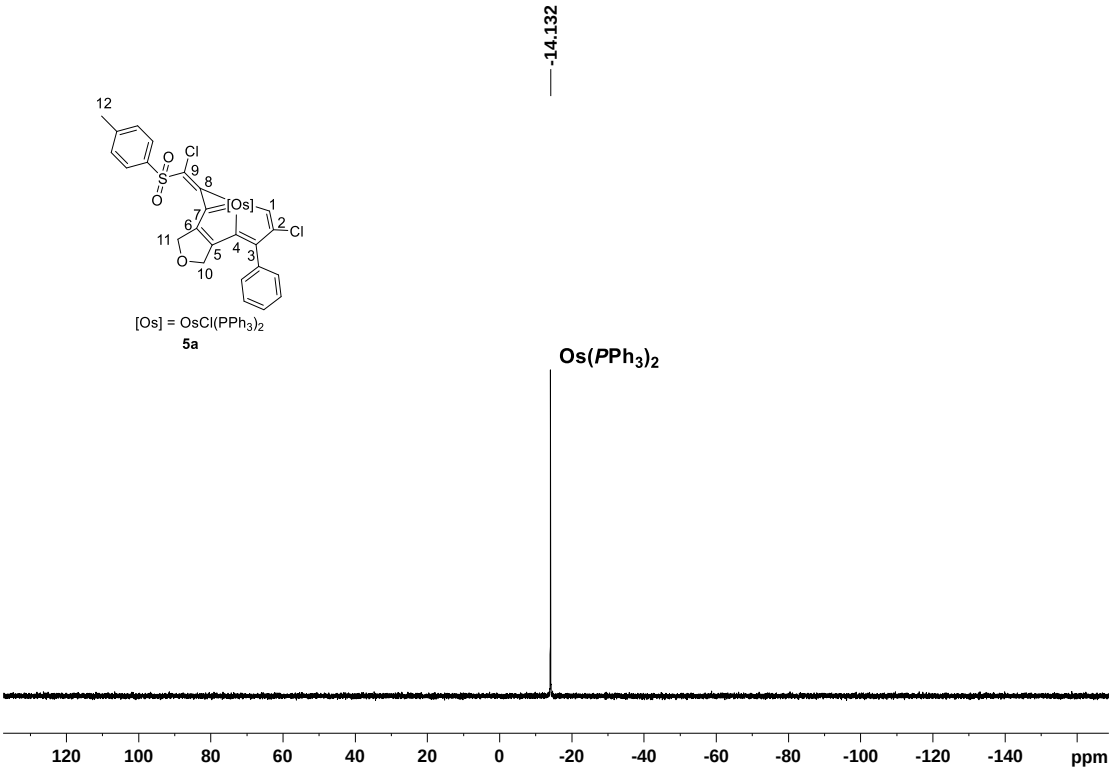

Fig. S51. The ^{31}P-NMR (161.9 MHz) spectrum for complex **5a** in CD_2Cl_2.

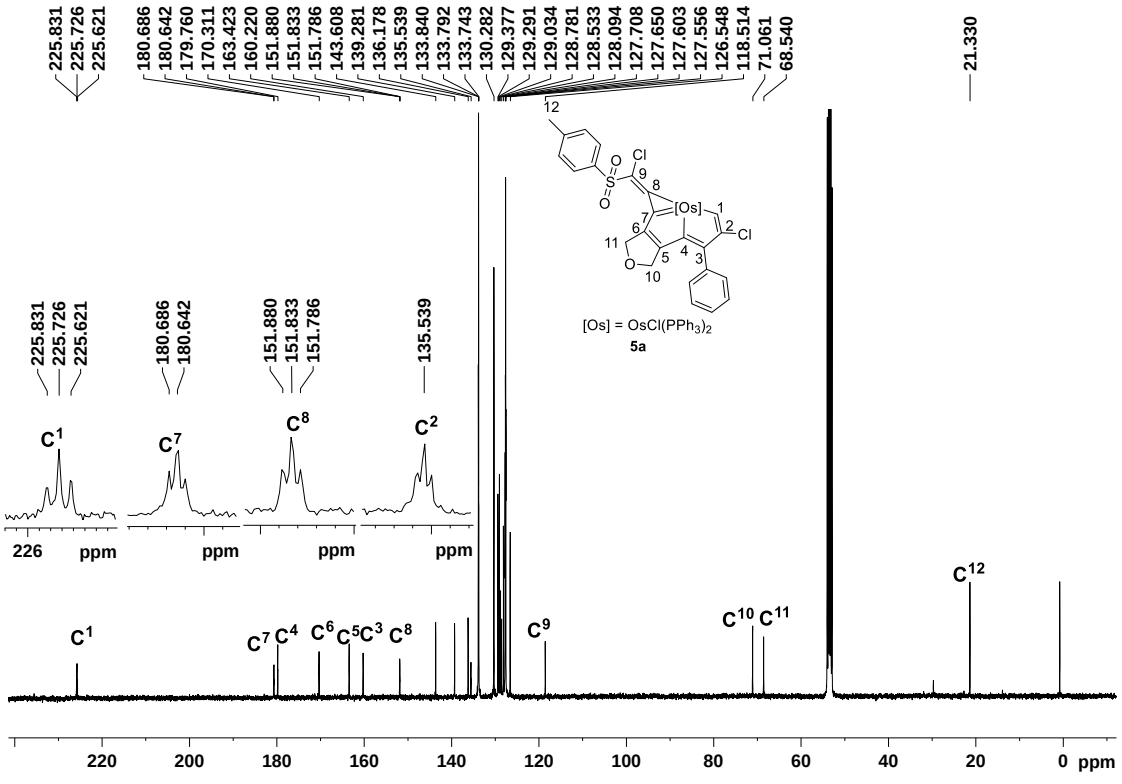

Fig. S52. The ^{13}C-NMR (100.6 MHz) spectrum for complex **5a** in CD_2Cl_2.

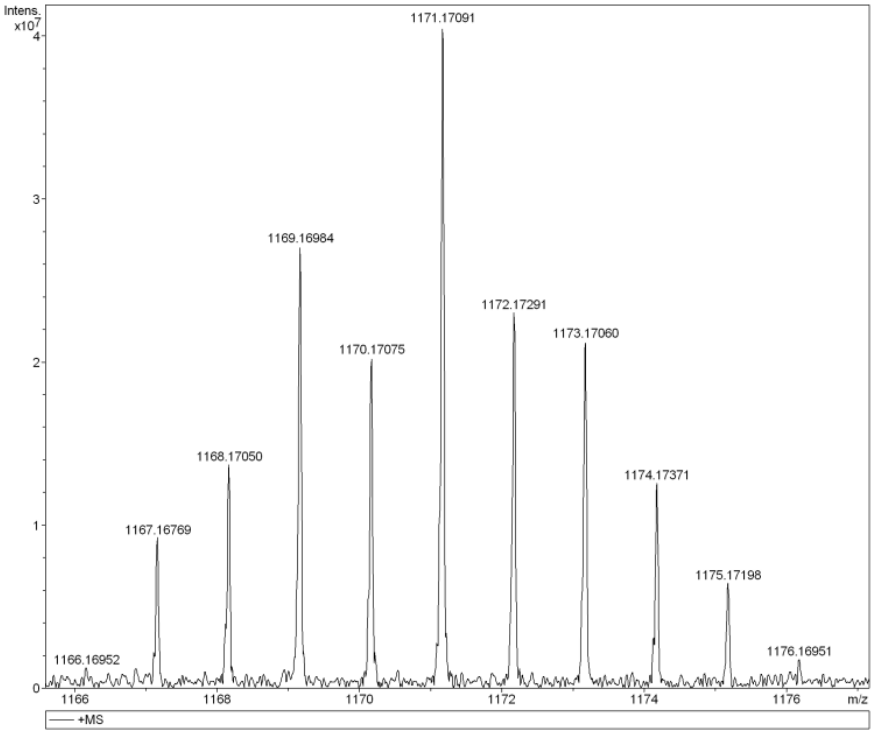

Fig. S53. Positive-ion ESI-MS spectrum of **[5a-Cl$^-$]$^+$** measured in MeOH.

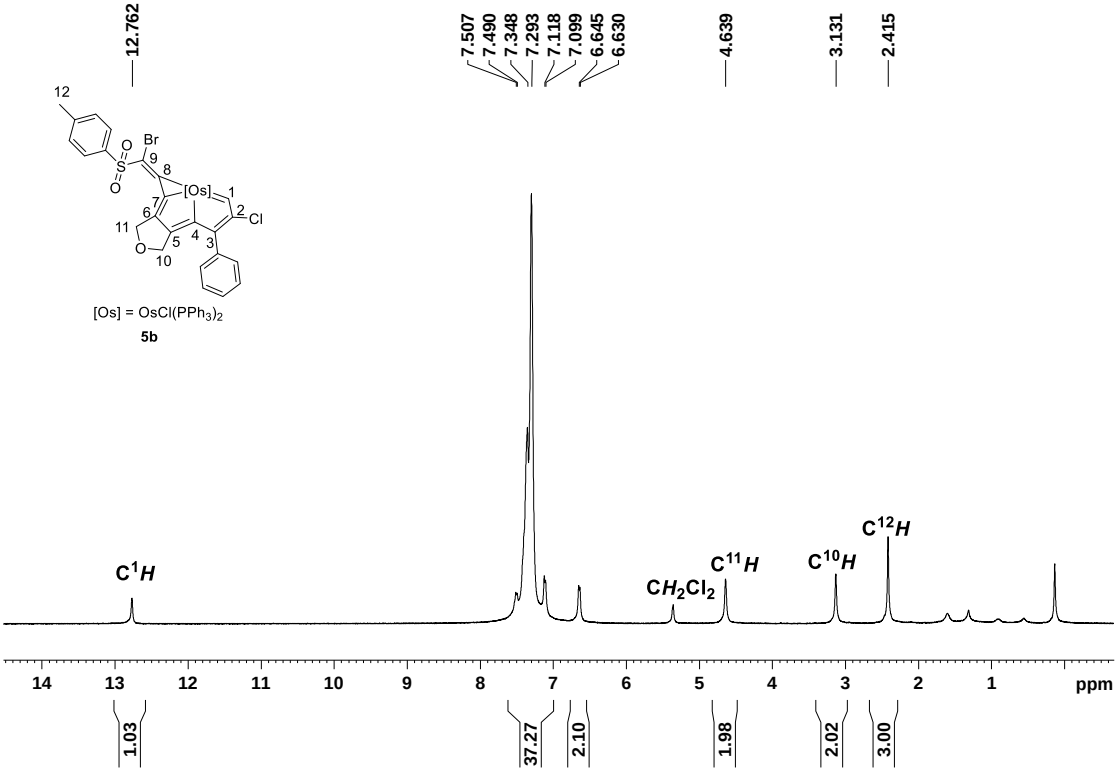

Fig. S54. The ^{1}H-NMR (400.0 MHz) spectrum for complex **5b** in CD_2Cl_2.

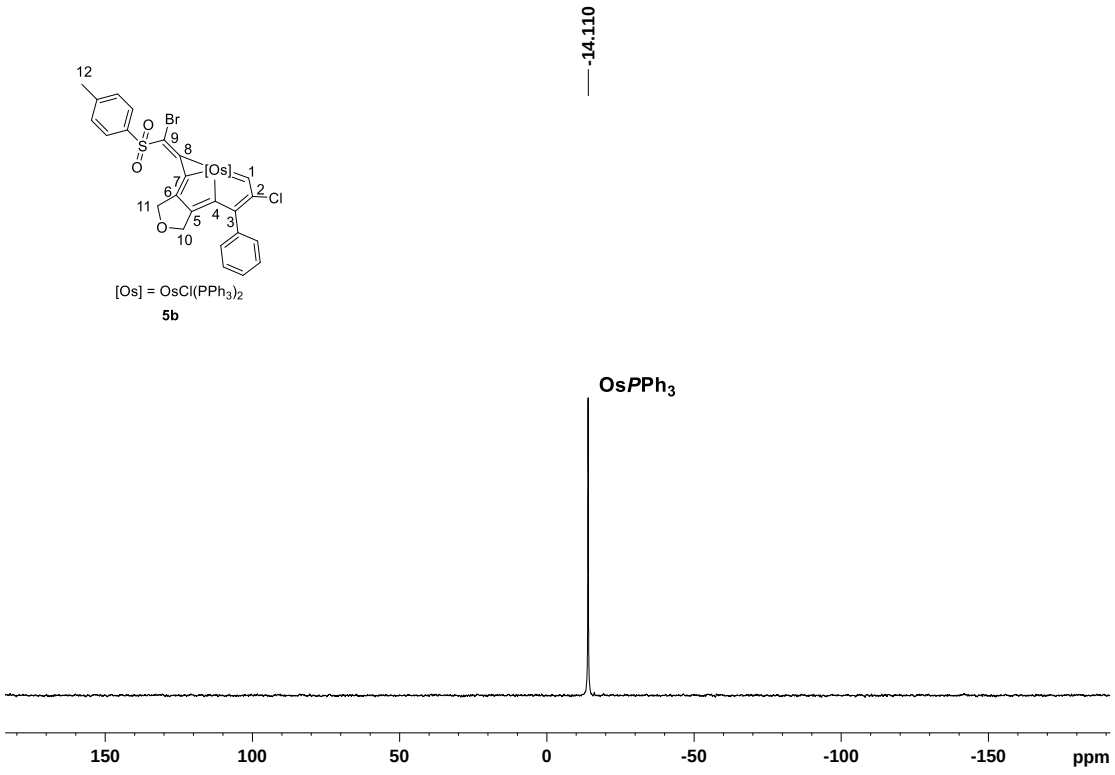

Fig. S55. The ^{31}P-NMR (161.9 MHz) spectrum for complex **5b** in CD_2Cl_2.

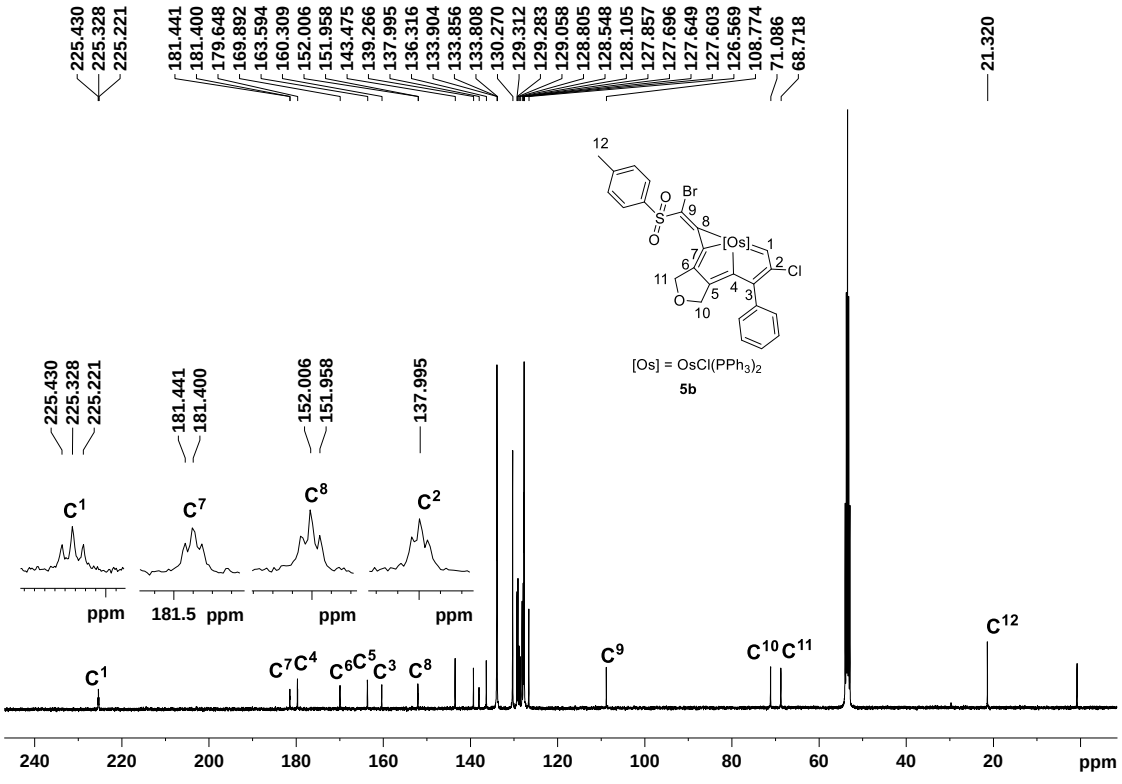

Fig. S56. The ^{13}C-NMR (100.6 MHz) spectrum for complex **5b** in CD_2Cl_2.

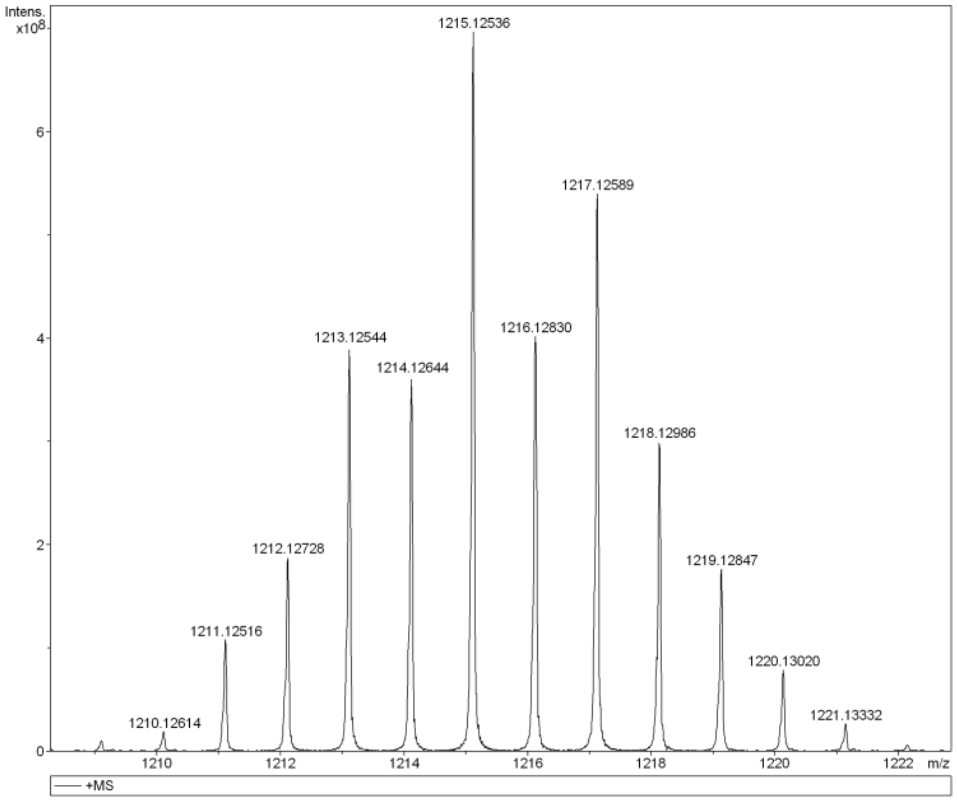

Fig. S57. Positive-ion ESI-MS spectrum of **[5b-Cl$^-$]$^+$** measured in MeOH.

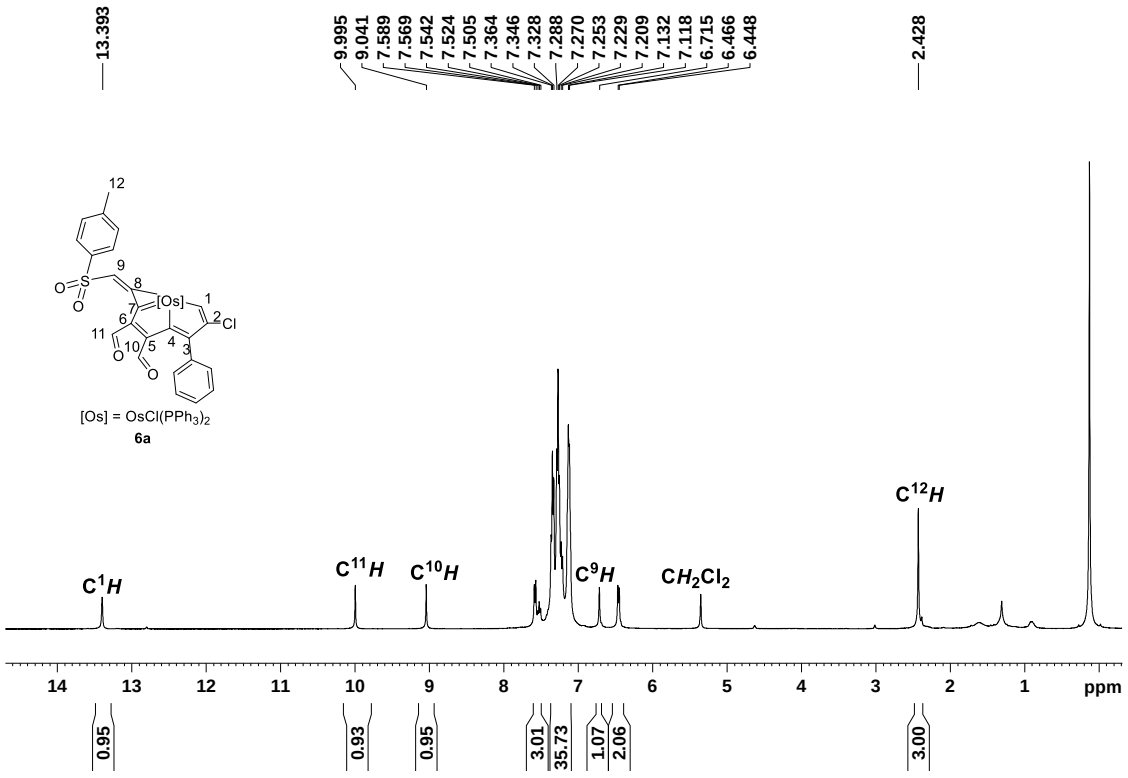

Fig. S58. The ^{1}H-NMR (400.0 MHz) spectrum for complex **6a** in CD_2Cl_2.

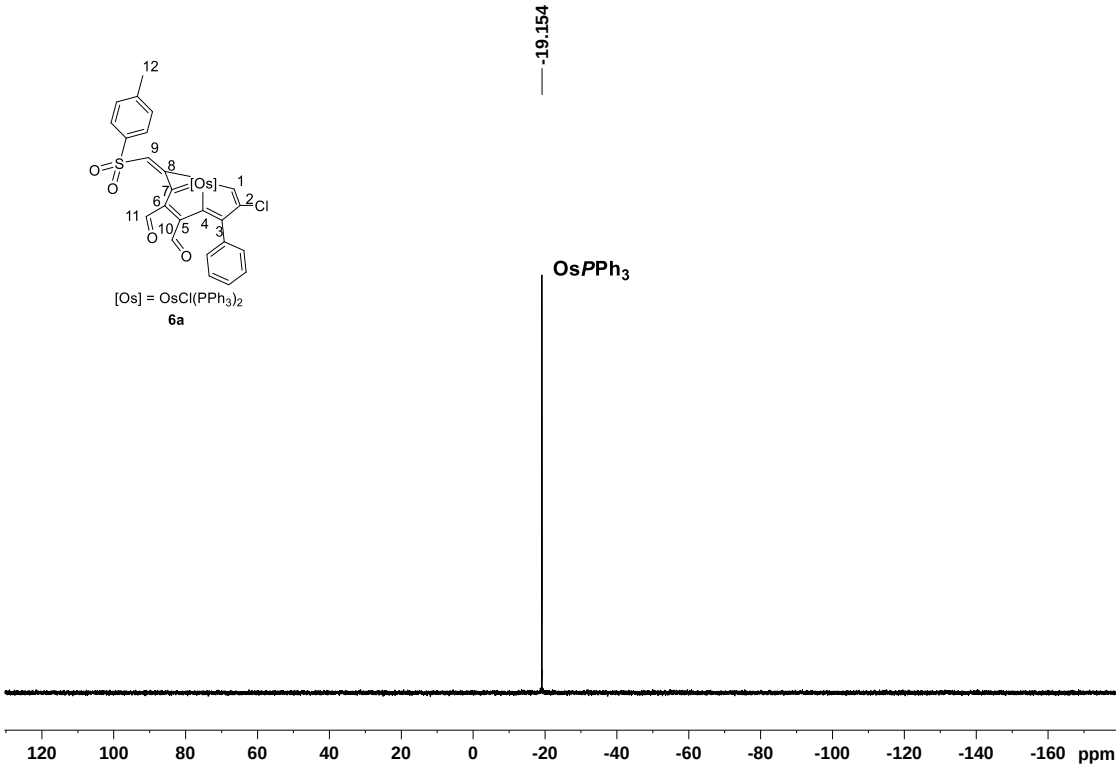

Fig. S59. The ^{31}P-NMR (161.9 MHz) spectrum for complex **6a** in CD_2Cl_2.

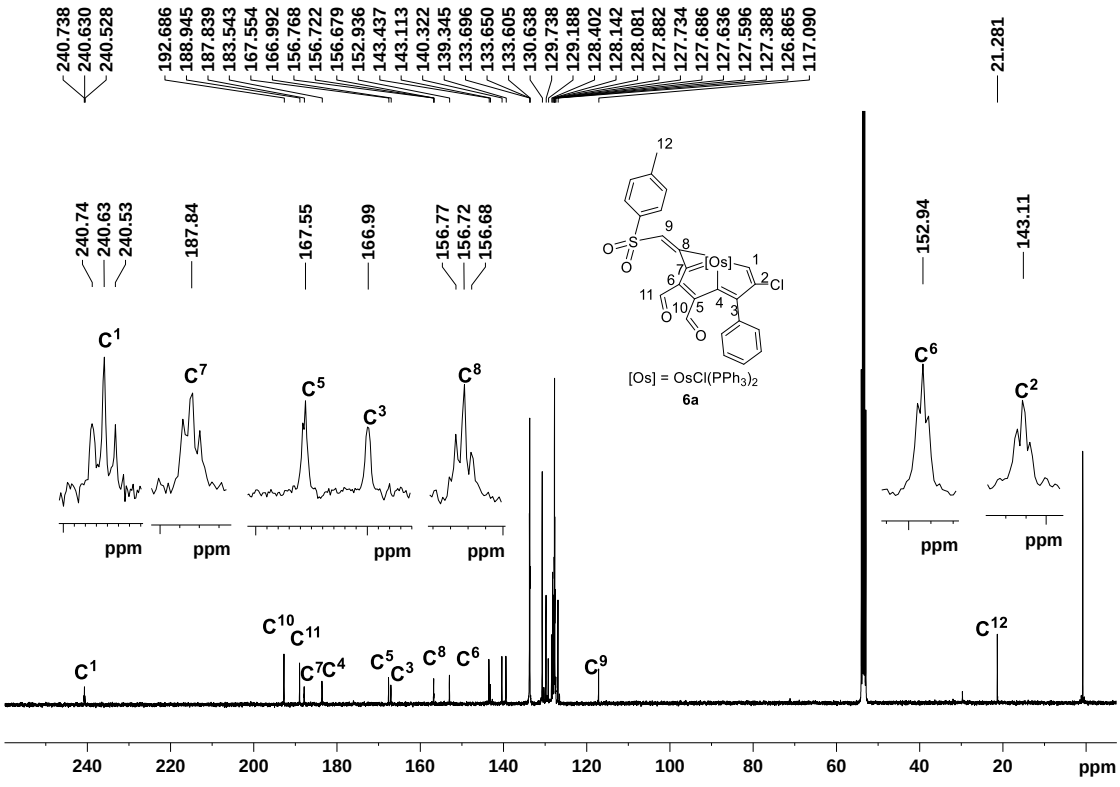

Fig. S60. The ^{13}C-NMR (100.6 MHz) spectrum for complex **6a** in CD_2Cl_2.

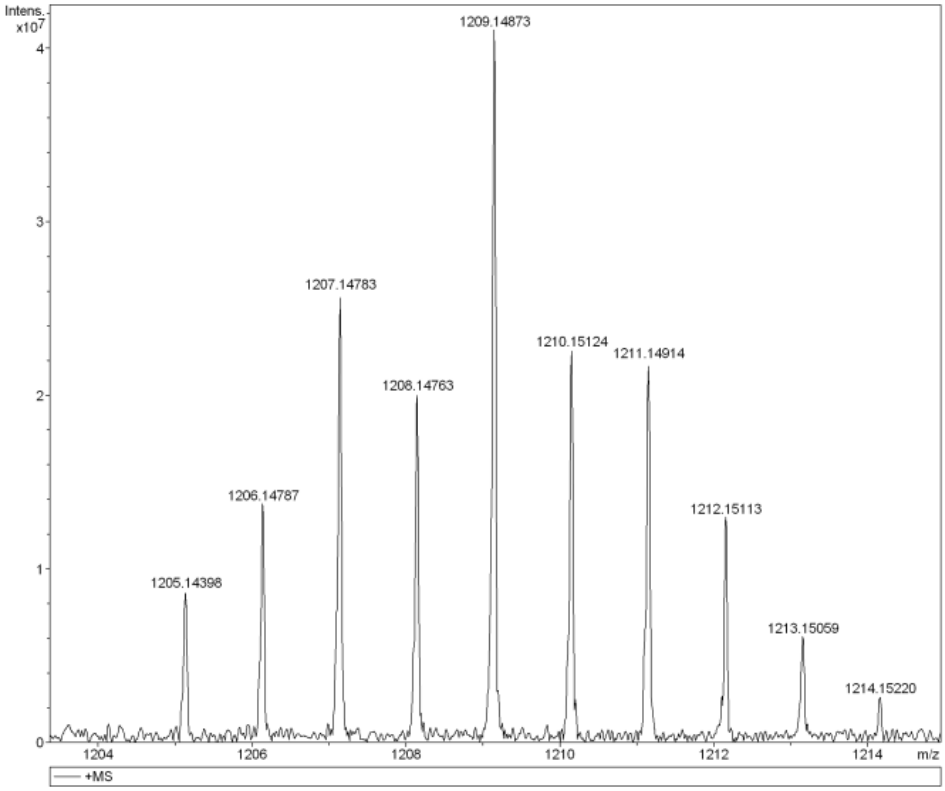

Fig. S61. Positive-ion ESI-MS spectrum of **[6a+Na$^+$]$^+$** measured in MeOH.

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