Electronic Supplementary Information

For

[3+2] Cycloaddition Reaction of Metallacyclopropene with Nitrosonium Ion: Isolation of Aromatic Metallaisoxazole

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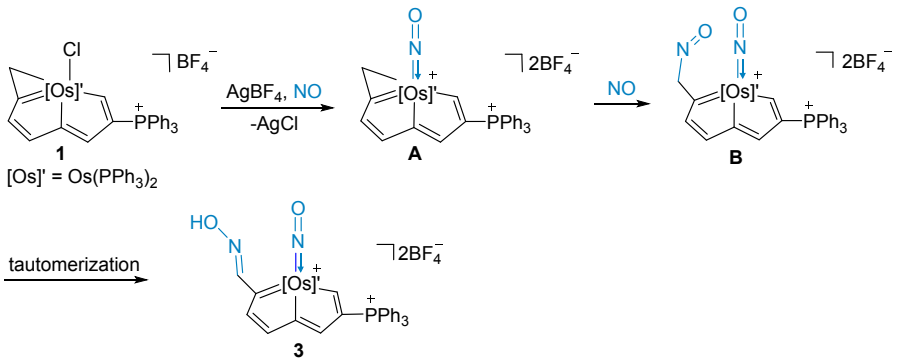
Contents

1. Experimental and calculated absorption spectral data for 1-5.

Table S1. Experimental and calculated absorption spectral data for 1-5.

Compound	Experimental (nm)	Calculated (nm)	*f*	Contribution (H = HOMO, L = LUMO)
1	436 nm	406 nm	0.1082	H−2→L (42%) H→L (31%)
2	602 nm	531 nm	0.0710	H→L (88%)
3	528 nm	471 nm	0.2659	H→L (86%)
4	500 nm	454 nm	0.3251	H−1→L (67%) H−1→L+1 (25%)
5	492 nm	493 nm	0.1408	H→L (32%) H→L+1 (33%) H→L+2 (29%)

2. A plausible mechanism for the formation of complex 3

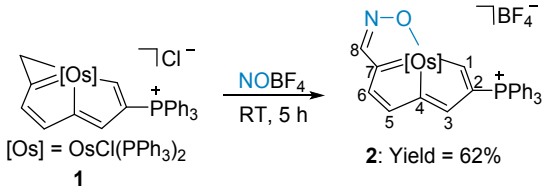


Scheme S1. A plausible mechanism for the formation of complex **3**.

3. Experimental Procedures and NMR Spectra

General Procedures: All syntheses were carried out under an inert atmosphere (N_2) by means of standard Schlenk techniques, unless otherwise stated. The metallacyclopropene was synthesized according to the previously published procedure.[1] Other reagents were used as received from commercial sources without further purification. Column chromatography was performed in air on silica gel (200-300 mesh). NMR spectroscopic experiments were performed on a Bruker AVII-600 (^{1}H 600.1 MHz; ^{31}P 242.9 MHz; ^{13}C 150.9 MHz) spectrometer and Bruker AVII-500 (^{1}H 500.1 MHz; ^{31}P 202.5 MHz; ^{13}C 102.8 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. Two-dimensional and one-dimensional NMR are abbreviated as heteronuclear single quantum coherence (HSQC), heteronuclear multiple bond correlation (HMBC), and distortionless enhancement by polarization transfer (DEPT). The absolute values of the coupling constants are given in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d) and broad (br). Elemental analyses were performed on a Vario EL III elemental analyzer.

Synthesis and characterization of complex 2:

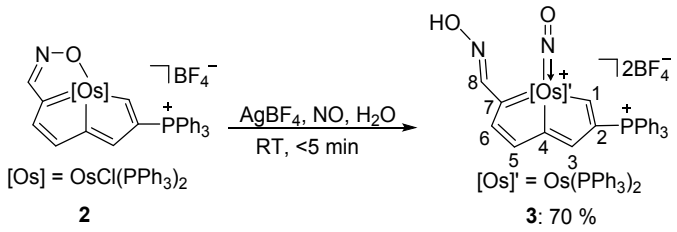


A solution of $NOBF_4$ (21 mg, 0.18 mmol) and compound **1** (200 mg, 0.17 mmol) in dichloromethane (10 mL) was stirred at RT for 5 h to give a green solution. The solution was reduced under vacuum to approximately 2 mL, and then purified by column chromatography (neutral alumina, eluent: dichloromethane/ acetone = 5:1) to give a green solution. The green solid of compound **2** (129 mg, 62%) was collected after the solvent was evaporated to dryness under vacuum and the resulting residue was washed with diethyl ether then dried under vacuum. ^{1}H NMR plus ^{1}H-^{13}C HSQC (500.1 MHz, CD_2Cl_2): δ = 14.35 (d, $J_{P\text{-}H}$ = 14.8 Hz, 1H, H1), 8.73 (s, 1H, H3), 8.47 (s,

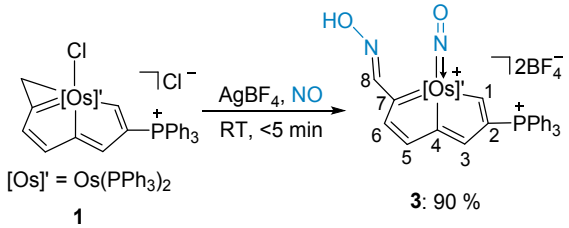
1H, H5), 7.72 (s, 1H, H8), 6.42 (s, 1H, H6), 7.94–7.00 ppm (m, 45H, other aromatic protons). ^{31}P NMR (202.5 MHz, CD_2Cl_2): δ = 11.14 (t, $J_{P\text{-}P}$ = 4.5 Hz, C*P*Ph$_3$), –21.58 (d, $J_{P\text{-}P}$ = 4.5 Hz, Os*P*Ph$_3$). ^{13}C NMR plus DEPT-135, ^{1}H-^{13}C HMBC and ^{1}H-^{13}C HSQC (125.8 MHz, CD_2Cl_2): δ = 236.4 (br, C7), 209.3 (br, C1), 191.2 (d, $J_{P\text{-}C}$ = 24.6 Hz, C4), 170.3 (s, C5), 157.9 (s, C8), 148.1 (s, C6), 144.0 (d, $J_{P\text{-}C}$ = 18.2 Hz, C3), 118.8 (d, $J_{P\text{-}C}$ = 89.6 Hz, C2), 135.1–127.4 ppm (m, other aromatic carbons). Elemental analysis calcd (%) for $C_{62}H_5BF_4ClNOOsP_3$: C 60.52, H 4.10, N 1.14; found C 60.87, H 3.72, N 1.33; HRMS (ESI): *m/z* calcd for $[C_{62}H_{50}ClNOOsP_3]^+$, 1144.2409; found 1144.2431.

Synthesis and characterization of complex 3:

Synthesis of NO gas: H_2SO_4 solution（1.36 M, 0.5 mL) was added to $NaNO_2$ (47 mg, 0.68 mmol) at room temperature, the yellow gas (NO and NO_2) formed immediately. The colorless NO gas was purified by injecting the yellow gas to the NaOH solution (10 M).



Method 1: The mixture of complex **2** (100 mg, 0.08 mmol), $AgBF_4$ (46 mg, 0.24 mmol) and H_2O (1.44 μL, 0.08 mmol) in dichloromethane (5 mL) was stirred under NO atmosphere at room temperature for 5 min to give a red solution. The solid suspension was removed through a filter. The red solid of **3** (73 mg, 70%) was collected after the solvent was evaporated to dryness under vacuum.

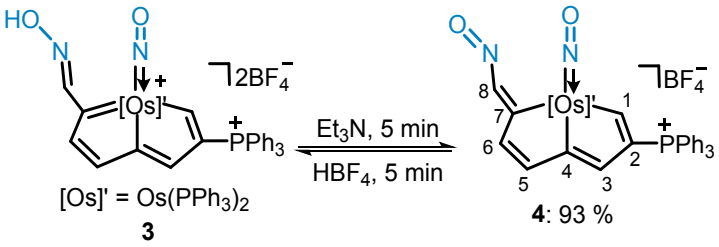


Method 2: The mixture of complex **1** (200 mg, 0.17 mmol) and $AgBF_4$ (99 mg, 0.51 mmol) in dichloromethane (10 mL) was stirred under NO atmosphere at room

temperature immediately to give a red solution. The solid suspension was removed through a filter. The red solid of **3** (201 mg, 90%) was collected after the solvent was evaporated to dryness under vacuum.

^{1}H-NMR plus ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 12.80 (dd, $J_{P\text{-}H}$ = 16.6 Hz, $J_{P\text{-}H}$ = 2.9 Hz, 1H, H7), 9.40 (s, 1H, H3), 8.69 (s, 1H, H5), 8.10 (s, 1H, H6), 7.91–6.05 ppm (45H, PPh_3), 6.92(m, 1H, H8). ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = 12.97 (s, C*P*Ph_3), 3.59 ppm (s, Os*P*Ph_3). ^{13}C-NMR plus DEPT-135 and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 232.03 (t, $J_{P\text{-}C}$ = 9.04 Hz, C7), 214.14 (m, C1), 194.29 (d, $J_{P\text{-}C}$ = 20.40 Hz, C4), 175.74 (s, C5), 168.03 (d, $J_{P\text{-}C}$ = 20.5 Hz, C3), 161.57 (s, C8), 159.53 (s, C6), 118.54 (d, $J_{P\text{-}C}$ = 20.40 Hz, C2), 139.7–127.2 ppm (m, Ph). Elemental analysis calcd (%) for $C_{62}H_{51}B_2F_8N_2O_2OsP_3$: C 56.72, H 3.92, N 2.13; found C 56.41, H 3.64, N 2.27; HRMS (ESI): *m/z* calcd for $[C_{62}H_{51}N_2O_2OsP_3]^{2+}$, 570.1384; found 570.1438.

Synthesis and characterization of complex 4:



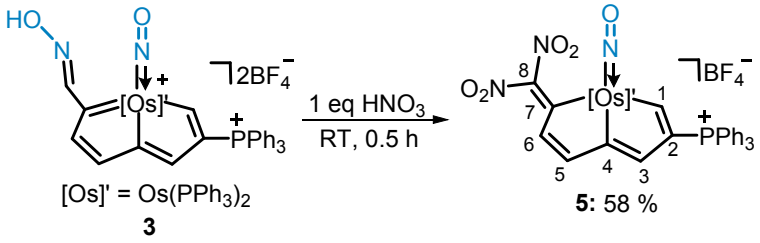
Et_3N (12 μL, 0.08 mmol) was added to a solution of compound **3** (100 mg, 0.08 mmol) in dichloromethane (5 mL). The mixture was stirred for 5 min to give an orange red solution. The solution was concentrated to ca. 2 mL, and then purified by column chromatography (silica gel, eluent: dichloromethane/acetone = 20:1) to give an orange red solution. The orange red solid of **4** (86 mg, 93%) was collected after the solvent was evaporated to dryness under vacuum.

$HBF_4 \cdot H_2O$ (11 μL, 0.08 mmol) was added to a solution of compound **4** (100 mg, 0.08 mmol) in dichloromethane (5 mL). The mixture was stirred for 5 min to give a red solution. The solid suspension was removed through a filter. The red solid of **3** (97 mg, 93%) was collected after the solvent was evaporated to dryness under vacuum.

^{1}H-NMR plus ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 10.79 (d, $J_{P\text{-}H}$ = 20.13 Hz, 1H,

H1), 7.50 (s, 1H, H3), 7.39 (s, 1H, H8), 6.60 (d, $J_{P\text{-}H}$ = 3.43 Hz, 1H, H5), 6.28 (s, 1H, H6), 7.89–6.92 ppm (m, 47H, Ph plus H3, H8). ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = 11.72 (s, C*P*Ph$_3$), 1.48 ppm (s, Os*P*Ph$_3$). ^{13}C-NMR plus DEPT-135 and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 214.18 (m, C7), 194.12 (s, C1), 190.48 (m, C4), 164.83 (s, C8), 157.97 (s, C5), 153.26 (s, C6), 148.23 (d, $J_{P\text{-}C}$ = 21.6 Hz, C3), 120.01 (d, $J_{P\text{-}C}$ = 89.0 Hz, C2), 135.6–128.9 ppm (m, Ph). Elemental analysis calcd (%) for $C_{62}H_{50}BF_4N_2O_2OsP_3$: C 60.79, H 4.11, N 2.29; found C 60.60, H 4.42, N 1.97; HRMS (ESI): m/z calcd for $[C_{62}H_{50}N_2O_2OsP_3]^+$, 1139.2694; found 1139.2798.

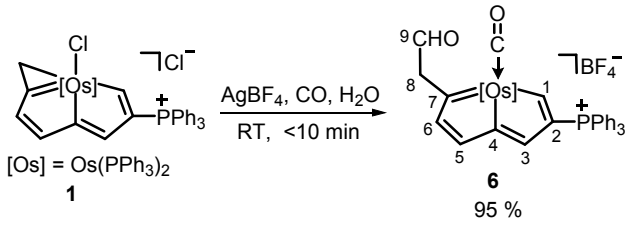
Synthesis and characterization of complex 5:



HNO_3 (7.75 μL, 0.08 mmol) was added to a solution of compound **3** (100 mg, 0.08 mmol) in dichloromethane (5 mL). The mixture was stirred for 0.5 h to give an orange solution. The solution was concentrated to ca. 2 mL, and then purified by column chromatography (silica gel, eluent: dichloromethane/acetone = 30:1) to give an orange solution. The orange solid of **4** (57 mg, 58%) was collected after the solvent was evaporated to dryness under vacuum.

^{1}H-NMR plus ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 12.80 (dd, $J_{P\text{-}H}$ = 19.8 Hz, $J_{P\text{-}H}$ = 2.6 Hz, 1H, H1), 7.15 (s, 1H, H3), 6.91 (s, 1H, H5), 5.84 (d, $J_{P\text{-}H}$ = 5.5 Hz, 1H, H6), 7.85–6.92 ppm (m, 46H, Ph plus H3). ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = 12.94 (s, C*P*Ph$_3$), –0.37 ppm (s, Os*P*Ph$_3$). ^{13}C-NMR plus DEPT-135 and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 190.28 (m, C4), 189.18 (s, C1), 172.32 (s, C7), 158.78 (s, C5), 152.23 (s, C8), 147.91 (d, $J_{P\text{-}C}$ = 22.6 Hz, C3), 144.08 (s, C6), 119.94 (d, $J_{P\text{-}C}$ = 88.6 Hz, C2), 135.81–128.35 ppm (m, Ph). Elemental analysis calcd (%) for $C_{62}H_{49}BF_4N_3O_5OsP_3$: C 57.90, H 3.84, N 3.27; found C 58.02, H 3.78, N 3.06; HRMS (ESI): *m/z* calcd for $[C_{62}H_{49}N_3O_5OsP_3]^+$, 1200.2494; found 1200.2555.

Reaction of complex 1 with CO:



The mixture of complex **1** (200 mg, 0.17 mmol) and $AgBF_4$ (99 mg, 0.51 mmol) in dichloromethane (10 mL) was stirred under CO atmosphere at room temperature immediately to give a red solution. The solid suspension was removed through a filter. The product (184 mg, 95%) was collected after the solvent was evaporated to dryness under vacuum.

^{1}H-NMR plus ^{1}H-^{13}C HSQC (600.1 MHz, CD_2Cl_2): δ = 14.54 (d, $J_{P\text{-}H}$ = 14.7 Hz, 1H, H1), 9.74 (s, 1H, H9), 8.74 (s, 1H, H3), 8.01 (s, 1H, H5), 7.76 (s, 1H, H6), 6.89–7.76 ppm (46H, H6 plus PPh_3), 2.97 (s, 2H, H8). ^{31}P-NMR (242.9 MHz, CD_2Cl_2): δ = 13.43 (s, C*P*Ph_3), -4.17 ppm (s, Os*P*Ph_3). ^{13}C-NMR plus DEPT-135 and ^{1}H-^{13}C HSQC (150.9 MHz, CD_2Cl_2): δ = 226.82 (s, C1), 220.20 (s, C7), 203.84 (s, C9), 201.92 (d, $J_{P\text{-}C}$ = 22.2 Hz, C4), 182.90 (br, Os(*C*O)), 179.60 (s, C3), 162.80 (d, $J_{P\text{-}H}$ = 18.8 Hz, C5), 144.36 (d, $J_{P\text{-}C}$ = 67.42 Hz, C2), 139.60 (s, C6), 135.43–117.64 ppm (m, Ph), 41.24 (s, C8). HRMS (ESI): *m/z* calcd for $[C_{64}H_{52}O_2OsP_3]^+$, 1137.2790; found 1137.2943.

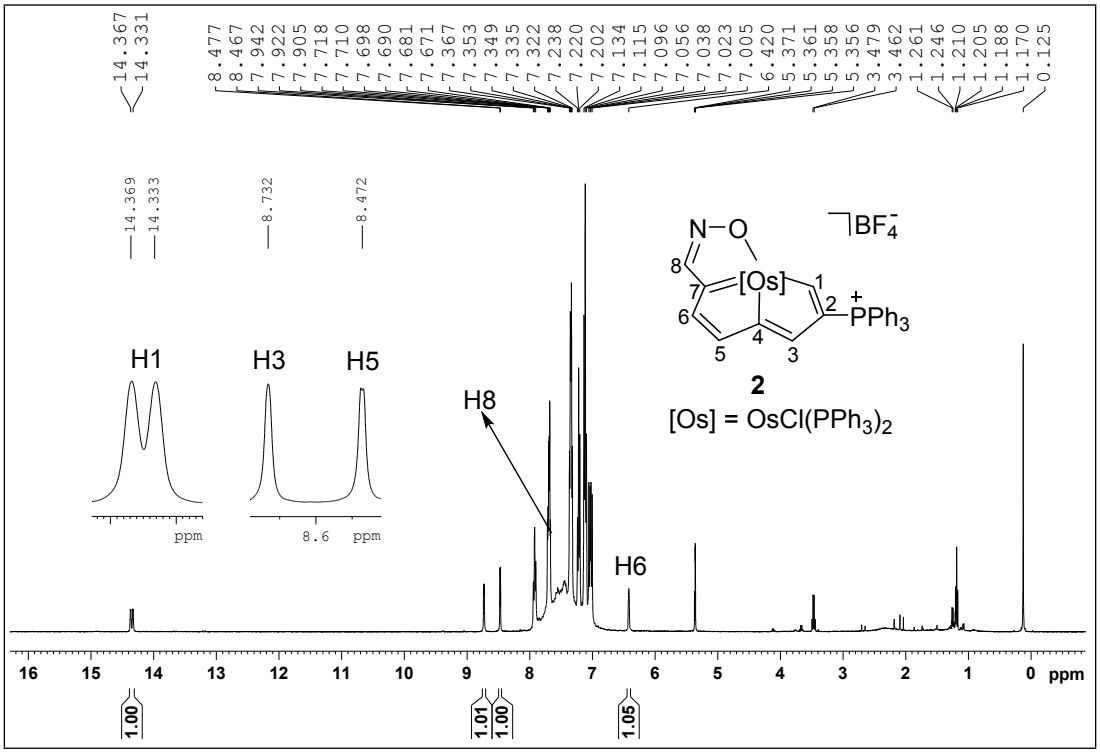


Figure S1. The ^{1}H NMR spectrum of complex **2** in CD_2Cl_2 at 500.1 MHz.

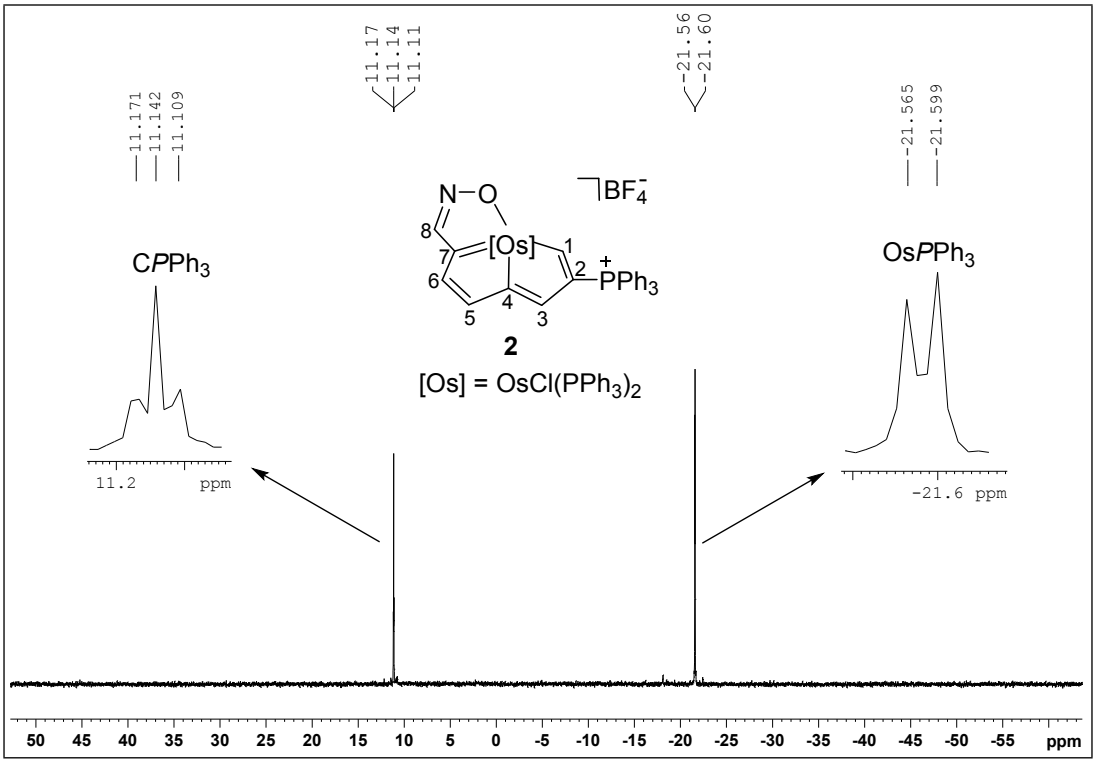


Figure S2. The $^{31}P\{^{1}H\}$ NMR spectrum of complex **2** in CD_2Cl_2 at 202.5 MHz.

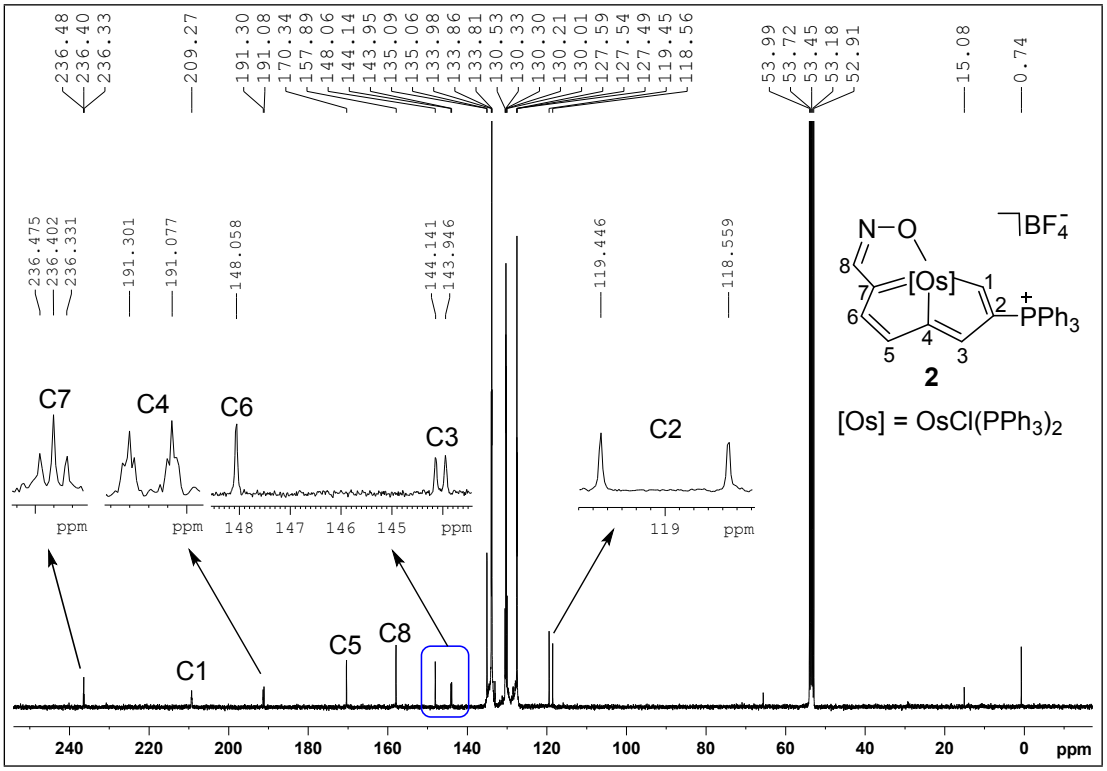


Figure S3. The $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** in CD_2Cl_2 at 125.8 MHz.

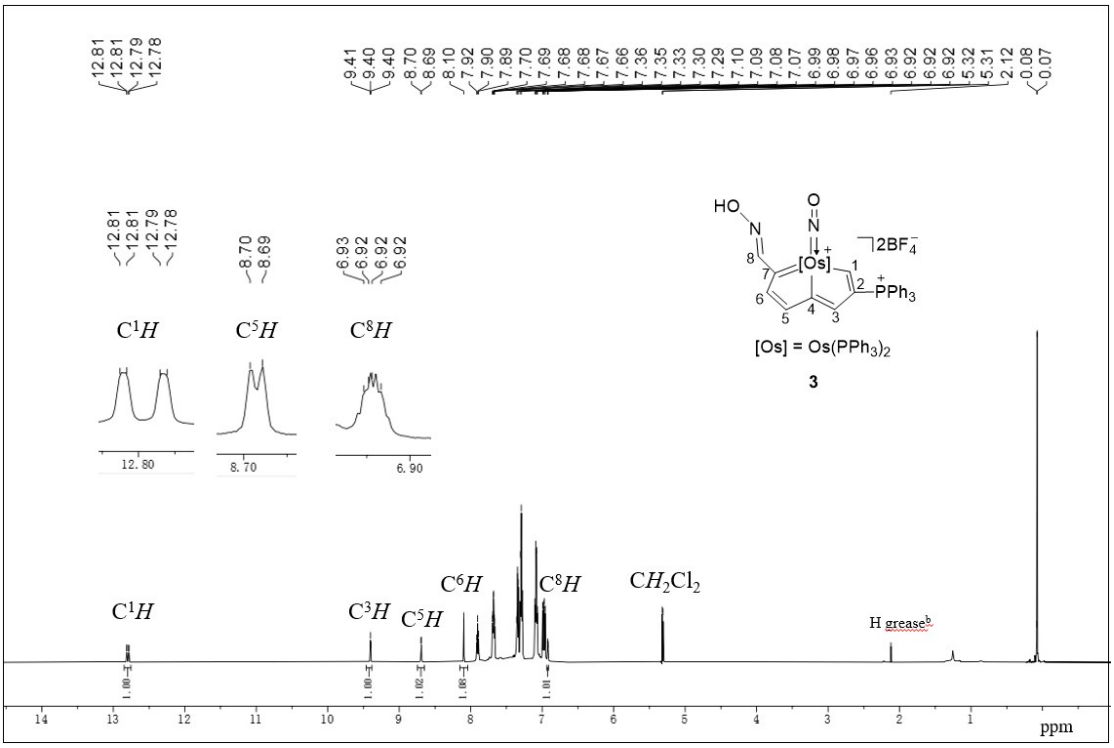


Figure S4. The ^{1}H NMR spectrum of complex **3** in CD_2Cl_2 at 600.1 MHz.

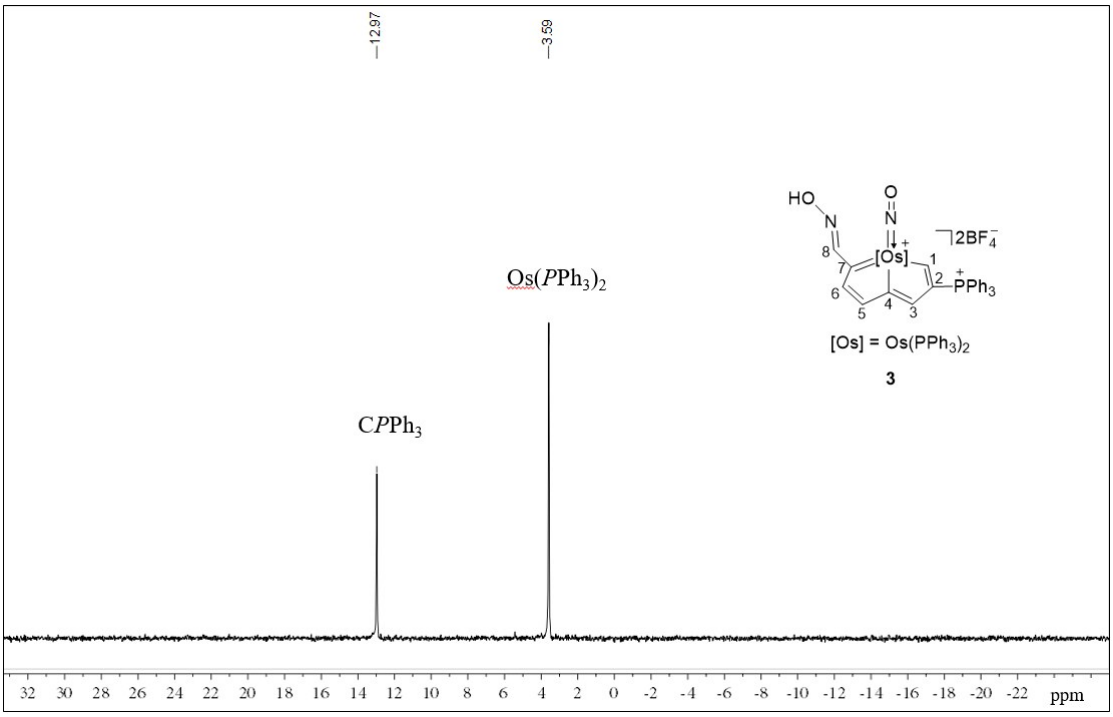


Figure S5. The $^{31}P\{^{1}H\}$ NMR spectrum of complex **3** in CD_2Cl_2 at 242.9 MHz.

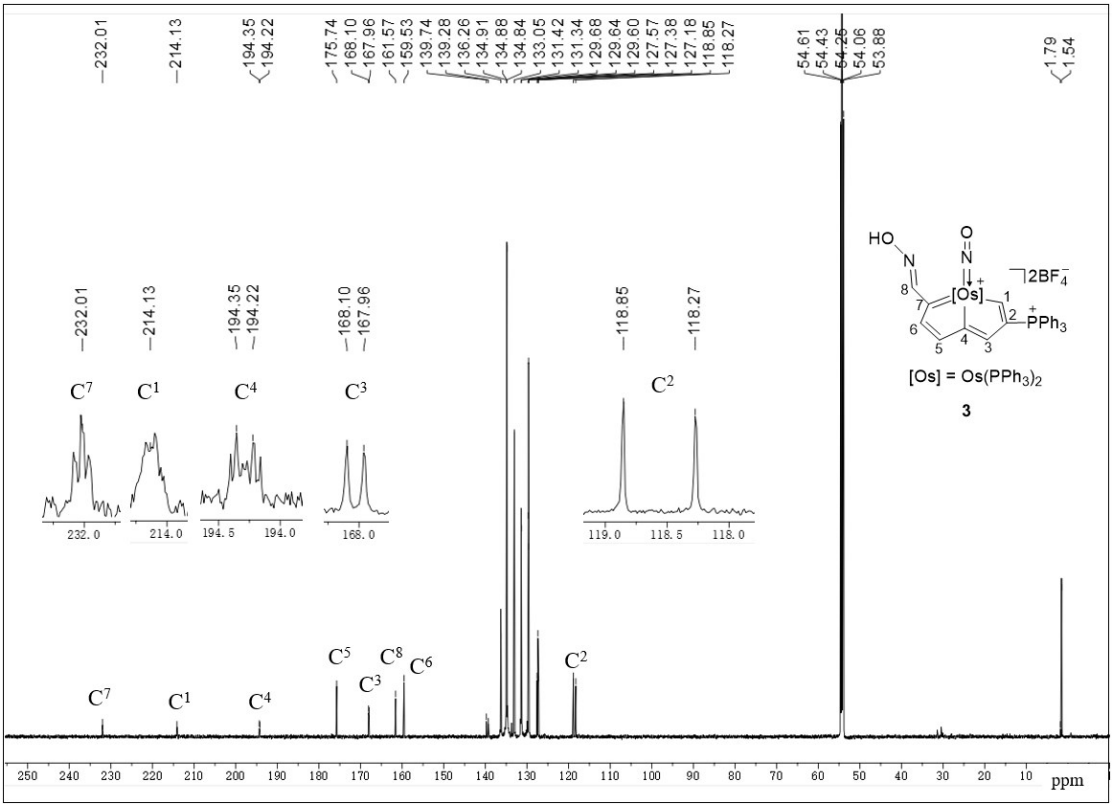


Figure S6. The $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** in CD_2Cl_2 at 150.9 MHz.

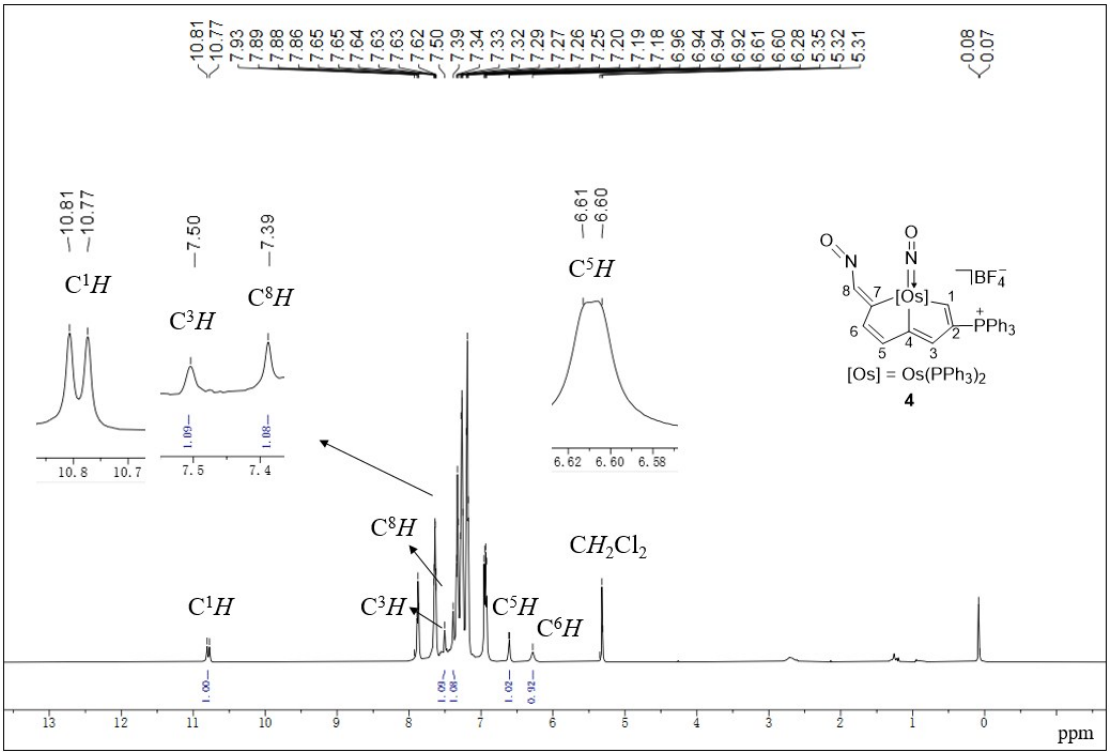


Figure S7. The ^{1}H NMR spectrum of complex **4** in CD_2Cl_2 at 600.1 MHz.

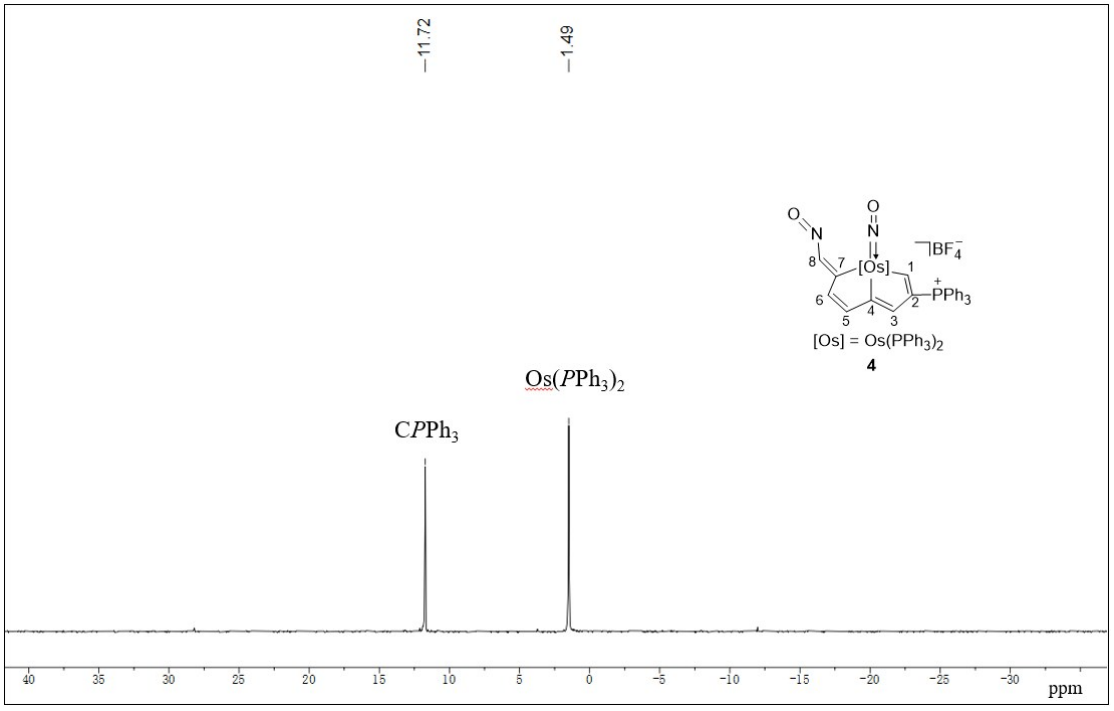


Figure S8. The $^{31}P\{^{1}H\}$ NMR spectrum of complex **4** in CD_2Cl_2 at 242.9 MHz.

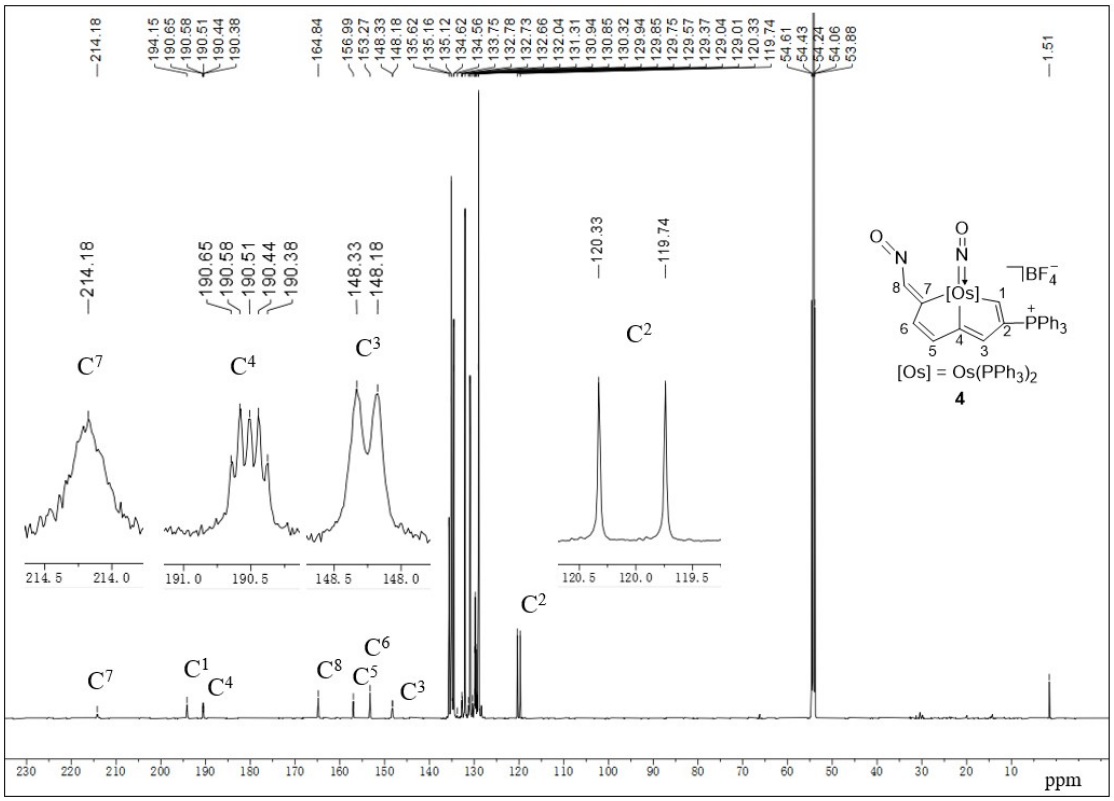


Figure S9. The $^{13}C\{^{1}H\}$ NMR spectrum of complex **4** in CD_2Cl_2 at 150.9 MHz.

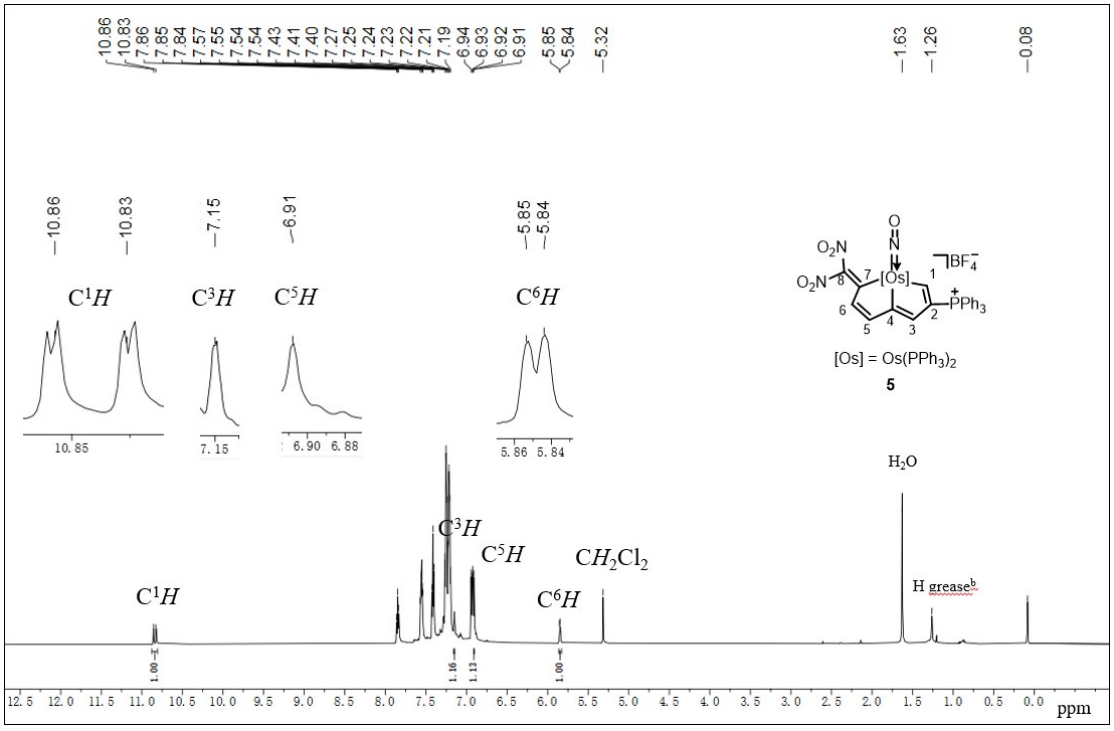


Figure S10. The ^{1}H NMR spectrum of complex **5** in CD_2Cl_2 at 600.1 MHz.

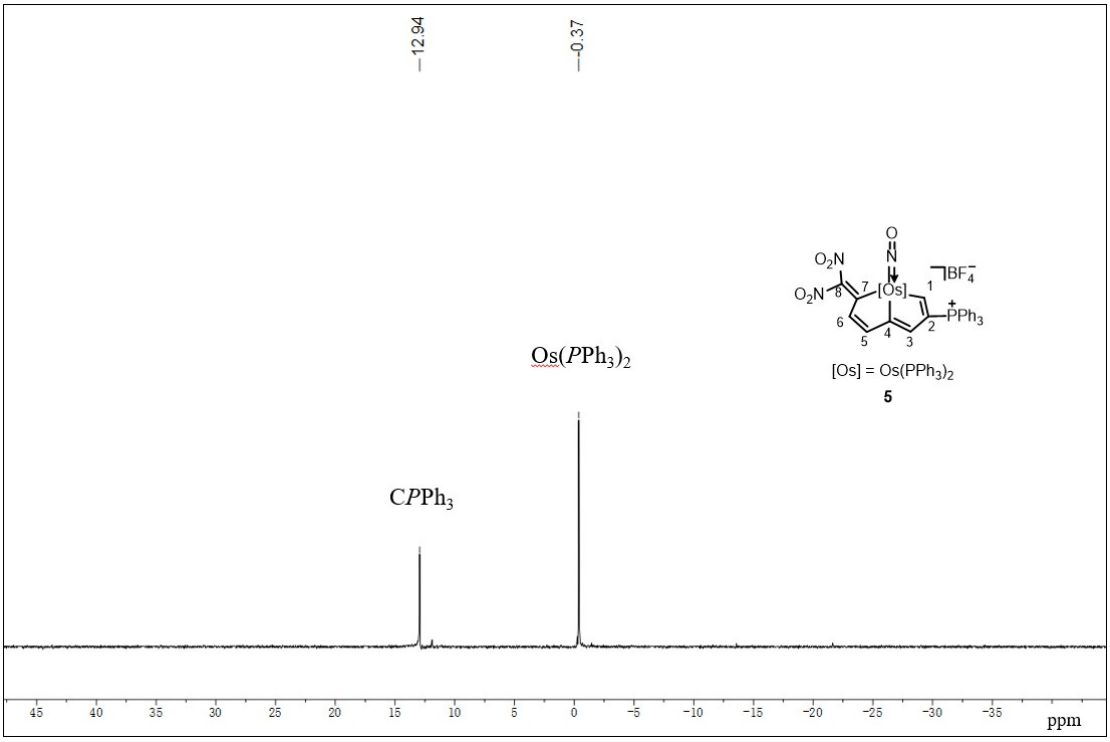


Figure S11. The $^{31}P\{^{1}H\}$ NMR spectrum of complex **5** in CD_2Cl_2 at 242.9 MHz.

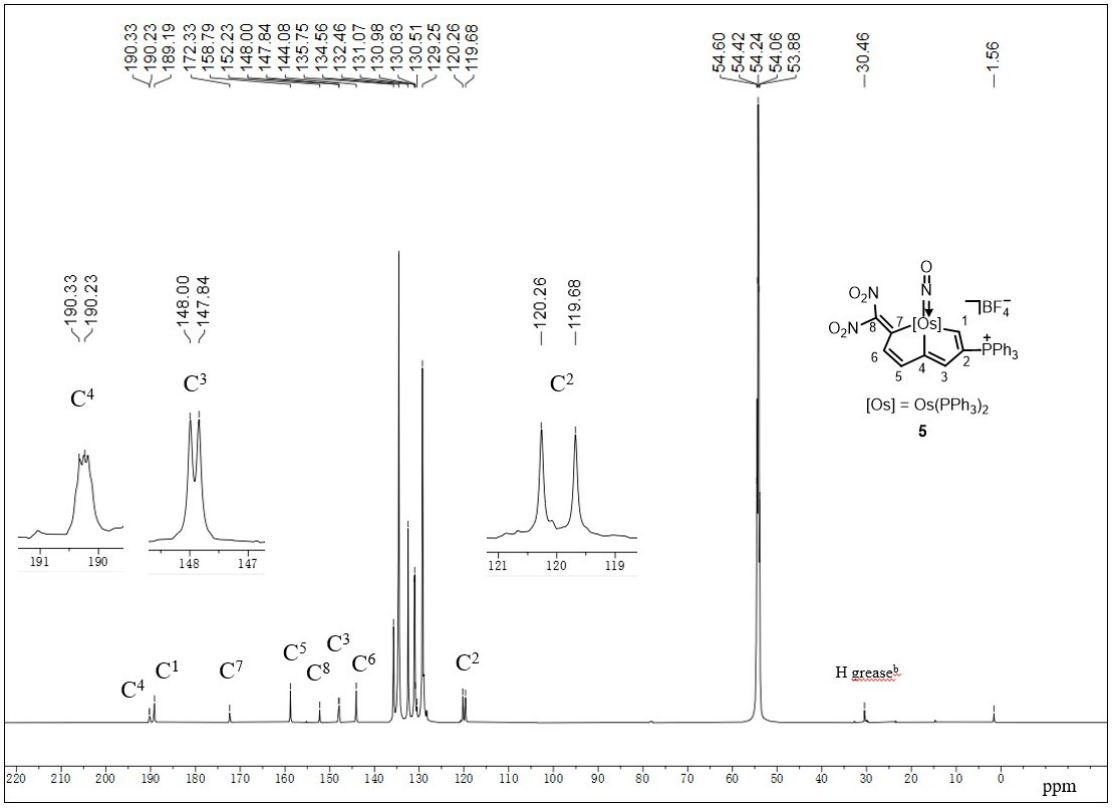


Figure S12. The $^{13}C\{^{1}H\}$ NMR spectrum of complex **5** in CD_2Cl_2 at 150.9 MHz.

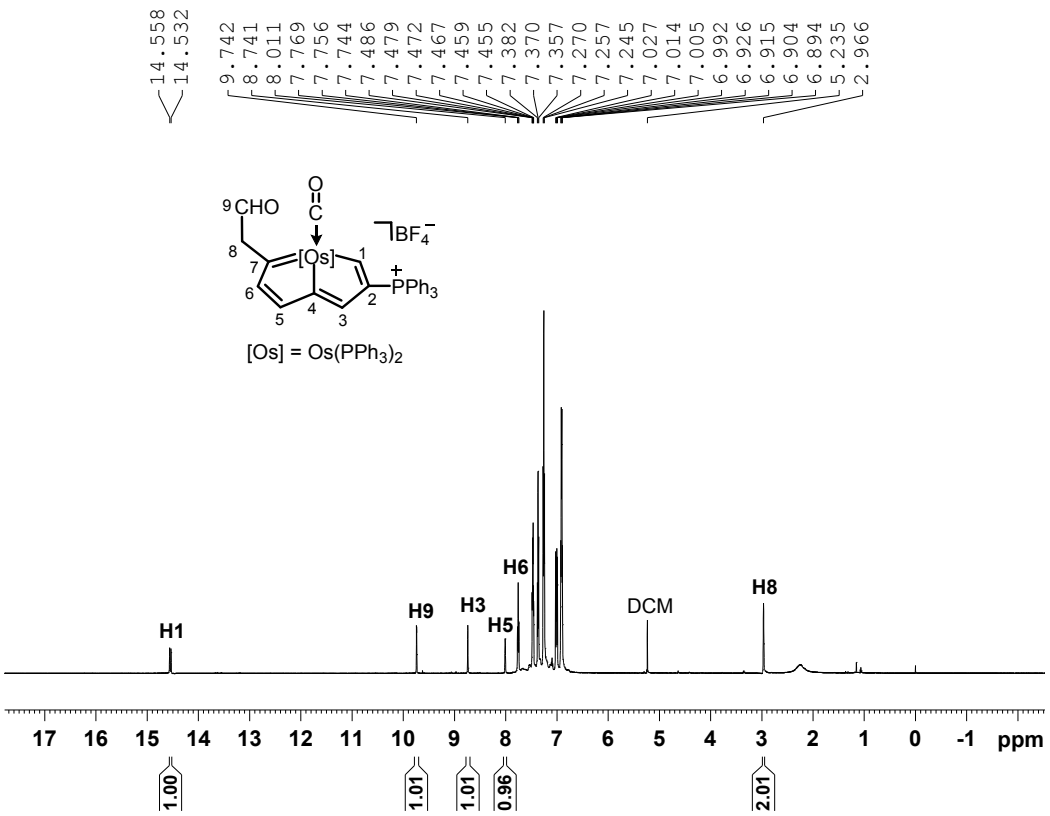


Figure S13. The ^{1}H NMR spectrum of complex **6** in CD_2Cl_2 at 600.1 MHz.

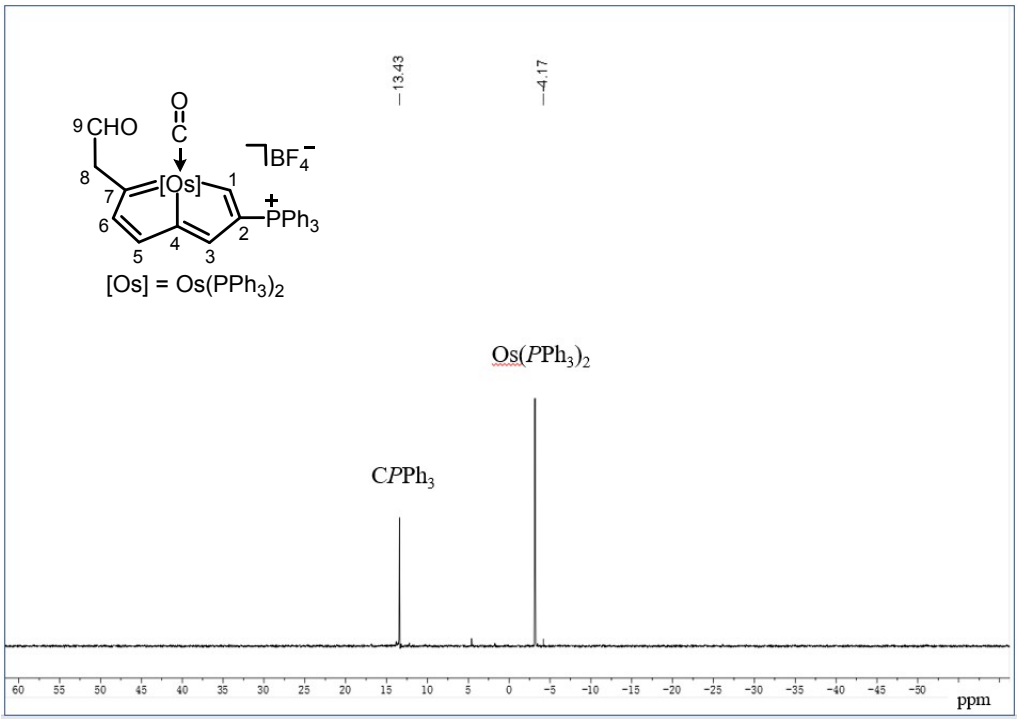


Figure S14. The $^{31}P\{^{1}H\}$ NMR spectrum of complex **6** in CD_2Cl_2 at 242.9 MHz.

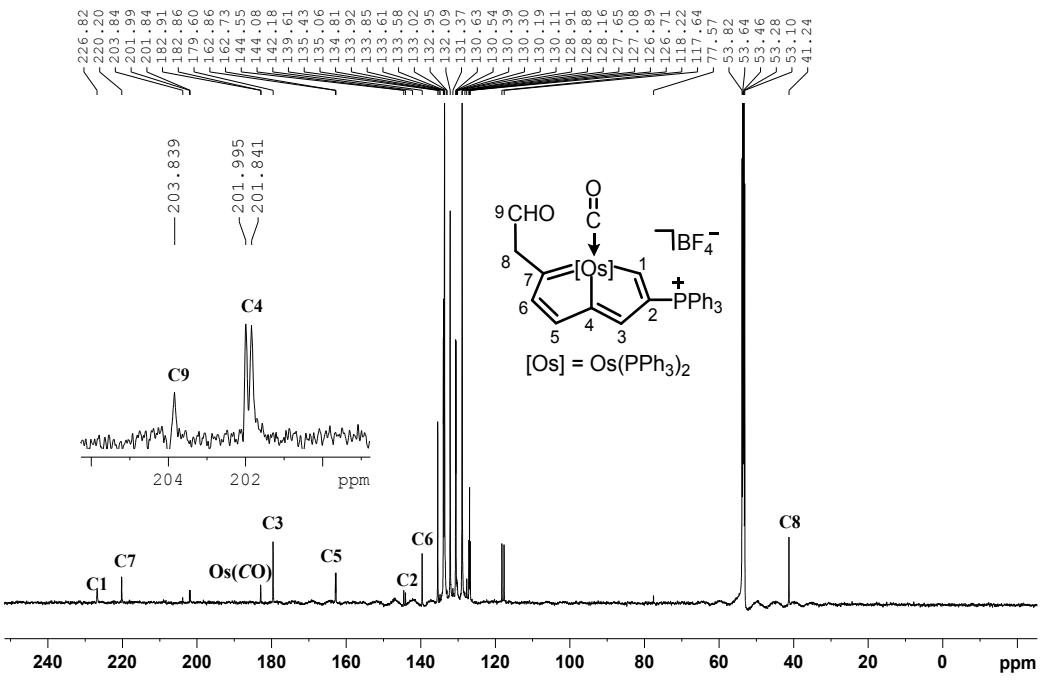


Figure S15. The $^{13}C\{^{1}H\}$ NMR spectrum of complex **6** in CD_2Cl_2 at 150.9 MHz.

4. X-ray Crystallographic Analysis

Crystals suitable for x-ray diffraction were grown from dichloromethane (**2**, **3**, **4** and **5**) solutions layered with hexane. Single-crystal X-ray diffraction data were collected on a XtaLAB Synergy, Dualflex, HyPlx CCD area detector using graphite-monochromatedm Mo Kα radiation (λ = 0.71073 Å) for **2** and Cu Kα radiation (λ = 1.54184 Å) for **3**, **4** and **5** Semi-empirical or multi-scan absorption corrections (SADABS) were applied.[2] All structures were solved by the Patterson function, completed by subsequent difference Fourier map calculations, and refined by full matrix least-squares on F^2 using the SHELXTL program package.[3] All non-hydrogen atoms were refined anisotropically unless otherwise stated. Hydrogen atoms were placed at idealized positions and assumed the riding model. X-ray crystal structures have been deposited in the Cambridge Crystallographic Database under the deposition numbers CCDC 1975099 (**2**), CCDC 1975095 (**3**), CCDC 1975096 (**4**), CCDC 1975097 (**5**). The data can be obtained free of charge from the CCDC (www.ccdc.cam.ac.uk/data_request/cif).

Crystal data for 2:

$[C_{62}H_{50}OClNOsP_3]BF_4 \cdot 2CH_2Cl_2$, M_r = 1400.25, crystal dimension 0.25 × 0.15 × 0.13 mm, Monoclinic, space group $P2_1/c$, a = 18.802(4) Å, b = 17.689(4) Å, c = 18.332(4) Å, β = 101.24(3)°, V = 5980(2) Å^3, Z = 4, T = 173 (2) K, ρ_{calcd} = 1.555 g·cm^{-3}, μ(Mo Kα) = 2.492 mm^{-1}, F(000) = 2800, θ_{max} = 25.00°, 43626 reflections, 10495 independent (R_{int} = 0.0499), R_1 = 0.0303, wR_2 = 0.0701 for 731 parameters and 9268 reflections with I > 2σ(I). GOF = 0.997. Residual electron density (e. Å^{-3}) max/min: 1.185/-1.116.

Crystal data for 3:

$[C_{62}H_{51.1}N_2O_2OsP_3]2BF_4 \cdot 1/2CH_2Cl_2 \cdot 1/2H_2O$ M_r = 1363.68, crystal dimension 0.20 × 0.10 × 0.10 mm, Triclinic, space group P-1 , a = 13.5628(2) Å, b = 19.3076(2) Å, c = 22.1482(2) Å, α = 89.75(10)°, β = 85.68(10)°, γ = 82.88(10)°, V = 5738(12) Å^3, Z = 4, T = 100(0) K, λ(Cu Kα) = 1.54184 Å, ρ_{calcd} = 1.578 g·cm^{-3}, μ(Cu Kα) = 6.036 mm^{-1},

F(000) = 2727, θ_{max} = 75.47°, 73611 reflections, 22928 independent (R_{int} = 0.0338), 1524 parameters, R_1 = 0.0414, wR_2 = 0.0890 for all data (R_1 = 0.0363 and wR_2 = 0.0851 for 51521 reflections with I > 2σ(I)). GOF = 1.039. Residual electron density (e. Å^{-3}) max/min: 1.14/–1.20.

Crystal data for 4:

$[C_{62}H_{50}N_2O_2OsP_3]BF_4 \cdot CH_2Cl_2$, Mr = 1309.88, crystal dimension 0.20 × 0.10 × 0.05 mm, Monoclinic, space group *P2(1)/n*, a = 15.7395(2) Å, b = 12.5093(2) Å, c = 29.0638(5) Å, α = 90°, β = 90.910(2)°, γ = 90°, V = 5721.65(15) Å^3, Z = 4, T = 100(10) K, λ(Cu Kα) = 1.54184 Å, ρ_{calcd} = 1.521 g·cm^{-3}, μ(Cu Kα) = 6.348 mm^{-1}, F(000) = 2624, θ_{max} = 75.56°, 43906 reflections, 11427 independent (R_{int} = 0.0509), 691 parameters, R_1 = 0.0622, wR_2 = 0.0.1507 for all data (R_1 = 0.0526 and wR_2 = 0.1383 for 19870 reflections with I >= 2σ(I)). GOF = 1.055. Residual electron density (e. Å^{-3}) max/min: 2.25/–2.17.

Crystal data for 5:

$[C_{62}H_{49}N_3O_5OsP_3]BF_4$, Mr = 1285.96, crystal dimension 0.3 × 0.05 × 0.05 mm, Triclinic, space group *P*-1 , a = 10.4930(10) Å, b = 16.0538(2) Å, c = 35.2150(4) Å, α = 90.7730(10)°, β = 90.8640(10)°, γ = 92.3780(10)°, V = 5925.68(11) Å^3, Z = 4, T = 100(10) K, λ(Cu Kα) = 1.54184 Å, ρ_{calcd} = 1.441 g·cm^{-3}, μ(Cu Kα) = 5.354 mm^{-1}, F(000) = 2576, θ_{max} = 68.55°, 59670 reflections, 19997 independent (R_{int} = 0.0514), 1423 parameters, R_1 = 0.0594, wR_2 = 0.1328 for all data (R_1 = 0.0527 and wR_2 = 0.1296 for 27834 reflections with I > 2σ(I)). GOF = 1.098. Residual electron density (e. Å^{-3}) max/min: 2.27/–1.73.

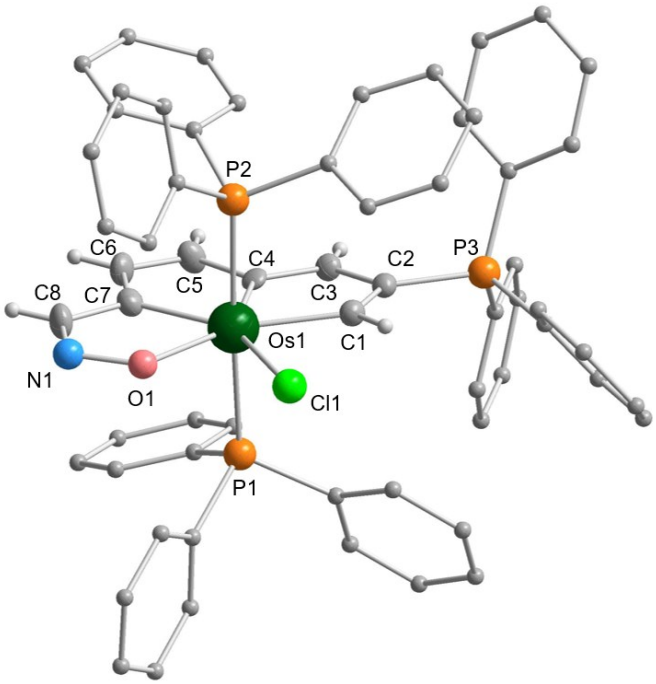


Figure S16. X-ray molecular structure for the cation of complex **2**. Selected bond distances (Å) and angles (deg): Os(1)−C(1) 2.087(4), Os(1)−C(4) 2.136(4), Os(1)−C(7) 2.050(4), Os(1)−N(1) 2.121(3), C(1)−C(2) 1.366(5), C(2)−C(3) 1.413(5), C(3)−C(4) 1.375 (5), C(4)−C(5) 1.406(5), C(5)−C(6) 1.353(5), C(6)−C(7) 1.398(6), C(7)−C(8) 1.435(5), C(8)−N(1) 1.292(5), N(1)−O(1) 1.334(4); Os(1)−C(1)−C(2) 123.1(3), C(1)−C(2)−C(3) 112.6(3), C(2)−C(3)−C(4) 112.0(3), C(3)−C(4)−Os(1) 121.1(3), C(4)−Os(1)−C(1) 71.03(14), Os(1)−C(4)−C(5) 120.2(3), C(4)−C(5)−C(6) 113.3(3), C(5)−C(6)−C(7) 111.1(3), C(6)−C(7)−Os(1) 125.1(3), C7(1)−Os(1)−C(4) 70.36(14), Os(1)−C(7)−C(8) 116.8(3), C(7)−C(8)−N(1) 118.2(4), C(8)−N(1)−O(1) 110.9(14), N(1)−O(1)−Os(1) 122.3(2), O(1)−Os(1)−C(7) 71.77(13).

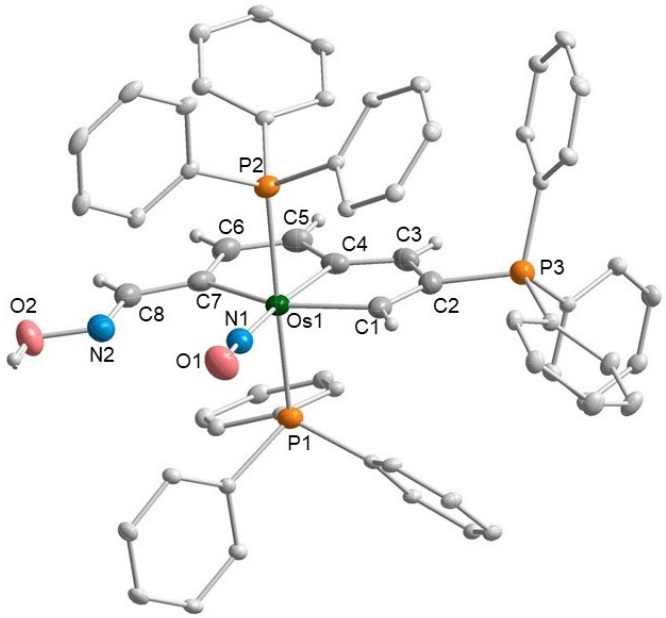


Figure S17. X-ray molecular structure for the cation of complex **3**. Selected bond distances (Å) and angles (deg): Os(1)−C(1) 2.056(3), Os(1)−C(4) 2.101(3), Os(1)−C(7) 2.097(3), Os(1)−N(1) 1.805(3), N(1)−O(1) 1.157(4), C(1)−C(2) 1.383(5), C(2)−C(3) 1.418(5), C(3)−C(4) 1.379(5), C(4)−C(5) 1.403(5), C(5)−C(6) 1.404(5), C(6)−C(7) 1.404(5), C(7)−C(8) 1.450(5), C(8)−N(2) 1.275(5) N(2)−O(2) 1.386(4); Os(1)−C(1)−C(2) 117.6(3), C(1)−C(2)−C(3) 115.5(3), C(2)−C(3)−C(4) 113.6(3), O(1)−N(1)−Os(1) 175.6(3), C(3)−C(4)−Os(1) 117.1(3), C(4)−Os(1)−C(1) 76.21(14), Os(1)−C(4)−C(5) 116.4(3), C(4)−C(5)−C(6) 115.2(3), C(5)−C(6)−C(7) 115.9(3), C(6)−C(7)−Os(1) 116.1(3), Os(1)−C(7)−C(8) 128.2(3), C(7)−C(8)−N(2) 120.4(3), C(7)−N(2)−O(2) 116.3(3), N(1)−C(7)−Os(1) 109.68(14), C(4)–Os(1)–C(7) 76.29(14).

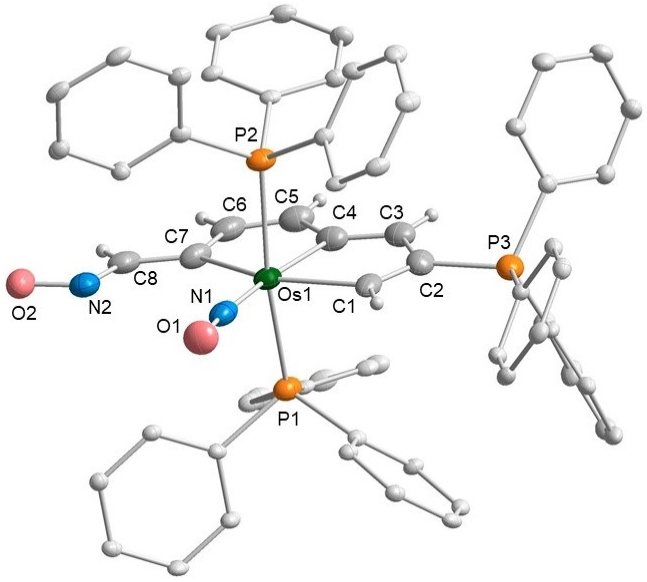


Figure S18. X-ray molecular structure for the cation of complex **4**. Selected bond distances (Å) and angles (deg): Os(1)−C(1) 2.114(5), Os(1)−C(4) 2.121(5), Os(1)−C(7) 2.143(5), Os(1)−N(1) 1.789(5), C(1)−C(2) 1.338(8), C(2)−C(3) 1.460(8), C(3)−C(4) 1.345(8), C(4)−C(5) 1.443(8), C(5)−C(6) 1.340(9), C(6)−C(7) 1.435(8), C(7)−C(8) 1.386(8), C(8)−N(2) 1.354(8), N(2)−O(2) 1.252(6), N(1)−O(1) 1.179(6); Os(1)−C(1)−C(2) 117.2(4), C(1)−C(2)−C(3) 115.6(5), C(2)−C(3)−C(4) 114.7(4), C(3)−C(4)−Os(1) 117.3(4), C(4)−Os(1)−C(1) 75.5(2), Os(1)−C(4)−C(5) 115.1(4), C(4)−C(5)−C(6) 115.5(5), C(5)−C(6)−C(7) 119.3(5), C(6)−C(7)−Os(1) 112.8(4), C(7)−Os(1)−N(1) 110.1(2), Os(1)−C(7)−C(8) 132.2(4), C(7)−C(8)−N(2) 123.3(5), C(8)−N(2)−O(2) 116.5(5), C(1)−Os(1)−N(1) 97.1(2), O(1)−N(1)−Os(1) 172.9(4), C(7)–Os(1)–C(4) 75.5(2).

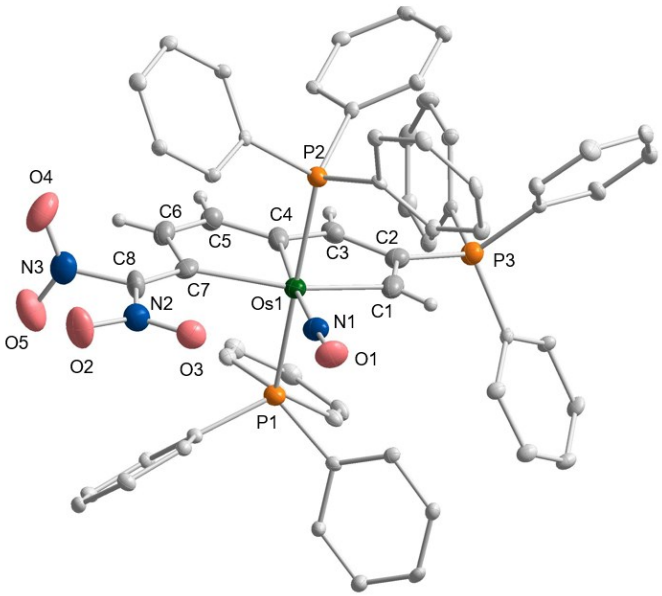


Figure S19. X-ray molecular structure for the cation of complex **5**. Selected bond distances (Å) and angles (deg): Os(1)−C(1) 2.115(6), Os(1)−C(4) 2.099(6), Os(1)−C(7) 2.163(6), Os(1)−N(1) 1.792(6), C(1)−C(2), 1.367(9), C(2)−C(3) 1.457(9), C(3)−C(4) 1.369(8), C(4)−C(5) 1.396(8), C(5)−C(6) 1.363(9), C(6)−C(7) 1.446(9), C(7)−C(8) 1.353(9), C(8)−N(2) 1.423(8), C(8)-N(3) 1.488(8), N(2)−O(2) 1.253(7), N(2)−O(3) 1.236(7), N(3)−O(4) 1.215(8), N(3)−O(5) 1.213(8), N(1)-O(1) 1.160(7); Os(1)−C(1)−C(2) 117.0(4), C(1)−C(2)−C(3) 114.6(5), C(2)−C(3)−C(4) 114.7(6), C(3)−C(4)−Os(1) 117.4(4), C(4)−Os(1)−C(1) 76.2(2), Os(1)−C(4)−C(5) 116.8(4), C(4)−C(5)−C(6) 116.3(6), C(5)−C(6)−C(7) 117.8(6), C(6)−C(7)−Os(1) 112.0(4), C(7)−Os(1)−N(1) 107.0(2), Os(1)−C(7)−C(8) 133.8(5), C(7)−C(8)−N(2) 131.5(6), C(7)−C(8)−N(3) 121.1(6), N(2)−C(8)−N(3) 107.4(5), Os(1)−N(1)−O(1) 177.5(5). C(7)-Os(1)-C(4) 77.1(2).

5. Thermal stability of 2-5

The solid thermal stability of the complex **2-5** was investigated. After heating the above compounds in an air atmosphere for 3 h, **2**, **3** and **5** are stable at 120 °C (Table S2).

Table S2 Thermal stability of **2-5** in different temperature

	80℃	100℃	120℃	140℃	160℃	180℃	200℃
2	●	●	●	▲	■		
3	●	●	●	■			
4	●	▲	■				
5	●	●	●	●	▲	■	

All thermal experiments were performed under air for 5 h.

● = Stable. ▲ = Partly decomposed. ■ = Completely decomposed.

6. Theoretical Calculations

All of the structures evaluated were optimized at the B3LYP/6-31G* level of DFT[4,6] with an SDD basis set[6] to describe P, Cl and Os atoms; single-point energy calculations were then performed on the energy using the def2-TZVP method[7] with the Solvation Model based on Density (SMD)[8] method in dichloromethane. TD-DFT calculations employed B3LYP/6-31G* with an SDD basis set to describe P, Cl and Os atoms (solvation with SMD, dichloromethane), with 10 states modelled. Frequency calculations were performed to confirm all stationary points as minima. All calculations were performed with the Gaussian 09 software package.[9]

7. References

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(9) Frisch, M. J. et al. Gaussian 09, revision E.01 (Gaussian, Inc., Wallingford CT, **2013**).

8. **Cartesian Coordinates**

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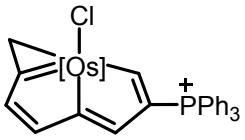

1^{+} [Os] = $Os(PPh_3)_2$

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P	-1.354355000	-2.575511000	-0.051555000
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C	0.585087000	0.076188000	-0.596756000
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C	1.101360000	0.007014000	1.710687000
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C	-2.715499000	-0.120285000	1.491992000
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H	-3.320013000	3.776929000	4.503758000
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C	5.446436000	4.026101000	1.530016000
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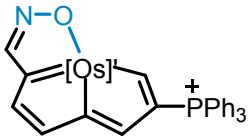

2^{+} [Os]' = $OsCl(PPh_3)_2$

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Cl	-1.253803000	-0.020057000	-2.638964000
P	3.502688000	-0.142343000	0.089494000
O	-3.324515000	0.156361000	-0.794431000
C	1.198473000	0.027371000	1.765209000
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C	-0.051439000	-3.464994000	-0.693785000
C	-2.886130000	-3.307783000	-1.046211000
C	-0.781605000	-3.166095000	2.642638000
H	0.218039000	-2.858469000	2.353908000

C	3.877426000	0.068316000	-1.708734000
C	-3.308610000	2.857913000	-2.107584000
H	-3.146790000	1.808952000	-2.313305000
C	0.789960000	2.920649000	-1.986554000
H	0.369828000	2.024160000	-2.431839000
C	-3.655608000	-2.607433000	-1.979532000
H	-3.520529000	-1.543517000	-2.114908000
C	1.810418000	5.285437000	-0.905816000
H	2.188027000	6.216119000	-0.490393000
C	-4.026222000	0.183785000	1.257976000
H	-4.810883000	0.223396000	2.008653000
C	0.761694000	4.620423000	-0.264345000
H	0.338746000	5.046738000	0.638590000
C	1.834709000	3.592463000	-2.625672000
H	2.235140000	3.193417000	-3.552975000
C	0.355141000	-3.192840000	-2.008833000
H	-0.110378000	-2.383996000	-2.564540000
C	4.245875000	-1.756892000	0.616949000
C	0.253148000	3.426717000	-0.795303000
C	-0.858277000	0.131752000	3.035608000
H	-0.325829000	0.158076000	3.984878000
C	3.755766000	2.503276000	0.992159000
H	2.859419000	2.693568000	0.409079000
C	-0.361848000	3.388529000	2.503065000
H	0.627796000	3.113791000	2.153101000
C	-4.438970000	4.940640000	-2.624783000
H	-5.152690000	5.500094000	-3.223109000
C	-1.019179000	-3.588815000	3.951696000
H	-0.198717000	-3.625514000	4.663534000
C	-0.521998000	3.840577000	3.814687000
H	0.345822000	3.925920000	4.463288000
C	-1.789199000	4.181884000	4.290628000
H	-1.912805000	4.536229000	5.310058000
C	-4.783621000	-4.665677000	-2.594200000
H	-5.522320000	-5.190471000	-3.193635000
C	-4.004280000	-5.368502000	-1.670797000
H	-4.130016000	-6.440876000	-1.550132000
C	-3.729228000	5.578807000	-1.604209000
H	-3.883940000	6.635865000	-1.406473000
C	5.442824000	-4.132954000	1.457834000
H	5.908288000	-5.057985000	1.785172000
C	5.516605000	3.311156000	2.443913000
H	5.984500000	4.126282000	2.988256000
C	3.644888000	-2.521476000	1.623070000

H	2.711665000	-2.200579000	2.073597000
C	-2.306185000	-3.958498000	4.346920000
H	-2.491522000	-4.287731000	5.365368000
C	-4.603659000	-3.292733000	-2.747215000
H	-5.199073000	-2.740346000	-3.468526000
C	5.443954000	-2.182858000	0.026331000
H	5.906150000	-1.599543000	-0.764182000
C	3.447852000	-0.916661000	-2.609635000
H	2.896518000	-1.785352000	-2.263214000
C	4.363627000	3.546809000	1.689943000
H	3.933597000	4.542505000	1.640269000
C	4.247024000	-3.709162000	2.040720000
H	3.779049000	-4.303680000	2.819656000
C	4.603625000	1.175978000	-2.160141000
H	4.940367000	1.936520000	-1.464429000
C	5.472194000	0.979129000	1.798747000
H	5.903940000	-0.015229000	1.843620000
C	0.532990000	-4.532796000	-0.003241000
H	0.209208000	-4.787621000	0.999344000
C	-3.352496000	-3.901499000	3.425564000
H	-4.358582000	-4.183156000	3.723195000
C	1.334573000	-3.980786000	-2.616061000
H	1.618070000	-3.779717000	-3.646253000
C	1.928582000	-5.036167000	-1.918544000
H	2.685835000	-5.651398000	-2.396463000
C	2.351352000	4.771943000	-2.086086000
H	3.157389000	5.298167000	-2.590127000
C	-4.223150000	3.586730000	-2.874537000
H	-4.765873000	3.083994000	-3.669925000
C	-3.055342000	-4.695365000	-0.904735000
H	-2.447202000	-5.255486000	-0.200659000
C	-2.895818000	4.066536000	3.448008000
H	-3.886809000	4.328202000	3.808139000
C	-2.813765000	4.861245000	-0.836533000
H	-2.265135000	5.372363000	-0.051683000
C	6.068518000	2.030165000	2.498661000
H	6.963229000	1.844826000	3.085372000
C	3.736651000	-0.778040000	-3.966647000
H	3.398144000	-1.535614000	-4.666967000
C	4.460904000	0.326797000	-4.422381000
H	4.688510000	0.426867000	-5.479589000
C	4.896541000	1.298425000	-3.520111000
H	5.466765000	2.153673000	-3.870330000
C	1.525828000	-5.307278000	-0.612001000

H	1.967784000	-6.135344000	-0.064636000
C	6.039489000	-3.370896000	0.450703000
H	6.966361000	-3.700924000	-0.008761000

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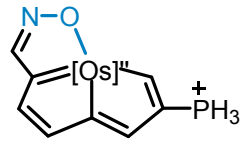

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P	0.437216295	-0.329392960	2.432111871
Cl	0.270524957	-2.689286119	-0.001079117
P	-4.430430137	-0.077321209	0.000010669
O	2.362641625	-0.920211100	-0.000261721
C	-2.163403729	1.682376651	0.000557832
H	-2.775627849	2.579139462	0.000793531
C	-0.790747854	1.701654906	0.000626145
N	3.386690096	-0.133687938	-0.000012870
C	-2.652492314	0.348311746	0.000080750
C	1.676011120	1.454953822	0.000529764
C	1.265065022	2.807928039	0.000939243
H	1.966877019	3.634852424	0.001155443
C	-1.699832478	-0.628456568	-0.000222348
H	-1.973977271	-1.677085376	-0.000564226
C	3.059924034	1.135232437	0.000406851
H	3.853760695	1.873878986	0.000641322
C	-0.091696821	2.939556784	0.000992045
H	-0.612572239	3.893312938	0.001274654
H	-5.153570776	0.393854740	1.112084134
H	-4.585209799	-1.472789577	-0.000659299
H	-5.153753634	0.394950932	-1.111478729
H	1.632360024	-0.906412935	2.907682830
H	0.348549939	0.835719628	3.224676962
H	-0.532949240	-1.150547721	3.039985074
H	0.347692399	0.839050359	-3.223648194
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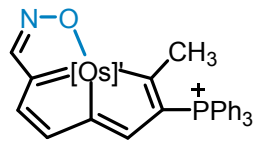
H	1.632726299	-0.902510793	-2.908601767

122



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P	0.915043000	-2.729430000	-0.097594000
Cl	1.570539000	-0.291900000	-2.602977000
P	-3.537762000	0.637647000	0.049728000
O	3.341897000	-0.695131000	-0.607098000
C	-1.295132000	0.019482000	1.578989000
H	-1.965691000	-0.012681000	2.435454000
C	0.918679000	-3.455923000	1.634973000
C	0.059897000	-0.162477000	1.700226000
C	2.112224000	-3.963840000	2.165738000
H	3.009113000	-3.996866000	1.556182000
N	4.308231000	-0.827721000	0.263671000
C	-4.378606000	-0.667022000	1.078424000
C	-1.706053000	0.320026000	0.256990000
C	2.239390000	2.885975000	1.713614000
C	2.492626000	-0.428022000	1.674655000
C	1.983402000	-0.403624000	2.984872000
H	2.609688000	-0.506266000	3.866536000
C	-0.693069000	0.384820000	-0.685089000
C	2.137535000	-3.852608000	-1.005963000
C	3.513603000	3.198736000	2.204813000
H	4.381624000	3.122678000	1.560384000
C	0.846946000	3.505064000	-0.879173000
C	3.591675000	2.772815000	-0.924267000
C	1.144259000	2.963135000	2.585454000
H	0.160000000	2.658267000	2.247719000
C	-4.275206000	0.535424000	-1.657711000
C	3.070595000	-3.370161000	-1.928056000
H	3.157911000	-2.309965000	-2.114681000
C	-1.039053000	-2.798410000	-2.137083000
H	-0.446012000	-1.996005000	-2.564319000
C	4.323416000	1.904125000	-1.738419000
H	4.016104000	0.874838000	-1.855102000
C	-2.498596000	-4.940056000	-1.098643000
H	-3.047629000	-5.788475000	-0.698552000
C	3.883883000	-0.688081000	1.488063000
H	4.591152000	-0.803774000	2.304645000

C	-1.411779000	-4.424649000	-0.385981000
H	-1.130995000	-4.885844000	0.554314000
C	-2.122320000	-3.320904000	-2.847741000
H	-2.377091000	-2.899848000	-3.816411000
C	0.897391000	3.579011000	-2.280045000
H	1.561323000	2.924050000	-2.835820000
C	-4.006063000	2.298310000	0.735756000
C	-0.682278000	-3.340954000	-0.895018000
C	0.618339000	-0.304929000	2.991425000
H	0.002084000	-0.315122000	3.888863000
C	-3.950593000	-1.996446000	0.952657000
H	-3.120701000	-2.252975000	0.301442000
C	-0.222463000	-3.417338000	2.447548000
H	-1.151109000	-3.004361000	2.068251000
C	3.791234000	-5.640194000	-2.393268000
H	4.435545000	-6.331539000	-2.929304000
C	1.309435000	3.393469000	3.902648000
H	0.446821000	3.457932000	4.560739000
C	-0.178500000	-3.905677000	3.755508000
H	-1.076288000	-3.882646000	4.367553000
C	1.011165000	-4.419153000	4.274196000
H	1.044826000	-4.800309000	5.290899000
C	5.853837000	3.703832000	-2.291555000
H	6.733105000	4.062354000	-2.819529000
C	5.112624000	4.578487000	-1.491248000
H	5.408378000	5.619582000	-1.396413000
C	2.849869000	-6.124025000	-1.480823000
H	2.754780000	-7.191849000	-1.304296000
C	-4.741020000	4.747192000	1.861238000
H	-5.027097000	5.698730000	2.299585000
C	-5.647205000	-2.681947000	2.537663000
H	-6.142524000	-3.465282000	3.103889000
C	-3.075703000	3.033981000	1.476155000
H	-2.067648000	2.657745000	1.607246000
C	2.579511000	3.724597000	4.377978000
H	2.710148000	4.057511000	5.403679000
C	5.453282000	2.375793000	-2.416669000
H	6.014994000	1.692056000	-3.046670000
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C	-4.432012000	1.700284000	-2.422524000
H	-4.113300000	2.662888000	-2.036032000
C	-4.592142000	-3.000027000	1.679023000
H	-4.262162000	-4.028666000	1.570234000

C	-3.446607000	4.257151000	2.038503000
H	-2.721703000	4.825761000	2.613540000
C	-4.687243000	-0.700325000	-2.168230000
H	-4.578088000	-1.608094000	-1.586486000
C	-5.432230000	-0.345501000	1.940506000
H	-5.760445000	0.681624000	2.055283000
C	0.006103000	4.377975000	-0.182421000
H	-0.015171000	4.378783000	0.900454000
C	3.680426000	3.613723000	3.528669000
H	4.676061000	3.854542000	3.890399000
C	0.106453000	4.498422000	-2.967858000
H	0.162413000	4.546021000	-4.051764000
C	-0.741463000	5.360144000	-2.267768000
H	-1.348804000	6.084534000	-2.803414000
C	-2.858569000	-4.388747000	-2.329687000
H	-3.692005000	-4.803658000	-2.890076000
C	3.894851000	-4.268672000	-2.614178000
H	4.619492000	-3.882545000	-3.325410000
C	3.983016000	4.119327000	-0.818225000
H	3.405137000	4.813131000	-0.214885000
C	2.156837000	-4.441014000	3.477321000
H	3.088846000	-4.836936000	3.870822000
C	2.023902000	-5.236639000	-0.794423000
H	1.295745000	-5.629810000	-0.092224000
C	-6.062420000	-1.356303000	2.669993000
H	-6.877479000	-1.103067000	3.341392000
C	-4.998817000	1.623311000	-3.693617000
H	-5.119604000	2.527855000	-4.282005000
C	-5.407719000	0.389926000	-4.206632000
H	-5.849622000	0.333390000	-5.197020000
C	-5.250077000	-0.767911000	-3.444520000
H	-5.570604000	-1.728434000	-3.836590000
C	-0.786360000	5.298935000	-0.875658000
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C	-5.669491000	4.015654000	1.115638000
H	-6.675929000	4.396570000	0.970306000
C	-1.066760000	0.893172000	-2.057567000
H	-1.427926000	0.078066000	-2.696002000
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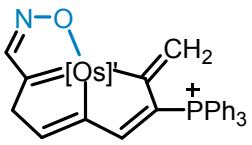

2a-1^{+} [Os]' = $OsCl(PPh_3)_2$

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Cl	1.587489000	-0.468100000	-2.596451000
P	-3.479752000	1.083245000	0.066756000
O	3.217265000	-1.292496000	-0.599990000
C	-1.327054000	0.223597000	1.526161000
H	-1.983297000	0.250073000	2.392770000
C	0.388447000	-3.531021000	1.609211000
C	0.067296000	-0.099118000	1.693008000
C	1.483882000	-4.268428000	2.081782000
H	2.323242000	-4.476718000	1.426913000
N	4.116849000	-1.583122000	0.272863000
C	-4.455526000	0.159514000	1.356980000
C	-1.710545000	0.516698000	0.266493000
C	2.657167000	2.540292000	1.689646000
C	2.421953000	-0.762803000	1.646938000
C	1.973020000	-0.533791000	3.063149000
H	2.564522000	0.270877000	3.529577000
C	-0.654355000	0.491313000	-0.747398000
C	1.417730000	-4.120151000	-1.075285000
C	3.948156000	2.569138000	2.235127000
H	4.803747000	2.298163000	1.626965000
C	1.463304000	3.360271000	-0.930176000
C	4.038837000	2.162799000	-0.899230000
C	1.569922000	2.881264000	2.507502000
H	0.559003000	2.826203000	2.118612000
C	-4.335379000	0.800429000	-1.567819000
C	2.406175000	-3.804414000	-2.011097000
H	2.685385000	-2.775772000	-2.185647000
C	-1.486094000	-2.550702000	-2.150661000
H	-0.759913000	-1.875563000	-2.591469000
C	4.627960000	1.173868000	-1.690777000
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C	-3.334196000	-4.333514000	-1.045625000
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H	4.383197000	-1.525254000	2.324082000

C	-2.174233000	-4.002665000	-0.337818000
H	-1.989191000	-4.470204000	0.623099000
C	-2.641364000	-2.892528000	-2.855413000
H	-2.810354000	-2.466996000	-3.840352000
C	1.331660000	3.272720000	-2.324153000
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C	-3.622731000	2.902698000	0.402206000
C	-1.247273000	-3.105771000	-0.885457000
C	0.537639000	-0.205506000	2.951896000
H	-0.090959000	-0.069855000	3.830879000
C	-4.324396000	-1.236122000	1.430315000
H	-3.636917000	-1.763600000	0.775578000
C	-0.681153000	-3.275075000	2.477811000
H	-1.528996000	-2.687123000	2.143055000
C	2.677301000	-6.159127000	-2.528125000
H	3.168918000	-6.948786000	-3.089498000
C	1.771162000	3.277828000	3.831000000
H	0.918316000	3.549714000	4.447073000
C	-0.669545000	-3.771989000	3.783019000
H	-1.513035000	-3.576153000	4.439617000
C	0.420827000	-4.511326000	4.244280000
H	0.428945000	-4.897995000	5.259394000
C	6.473688000	2.665422000	-2.192343000
H	7.418906000	2.858153000	-2.692111000
C	5.876187000	3.662575000	-1.415702000
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H	1.387987000	-7.509050000	-1.440645000
C	-3.864692000	5.622380000	0.976423000
H	-3.958931000	6.680680000	1.201473000
C	-5.944149000	-1.285789000	3.228931000
H	-6.524318000	-1.846972000	3.955528000
C	-2.507902000	3.622536000	0.840049000
H	-1.546765000	3.130537000	0.940020000
C	3.061421000	3.314378000	4.363643000
H	3.218997000	3.620718000	5.393820000
C	5.845593000	1.430020000	-2.331469000
H	6.294348000	0.653774000	-2.944636000
C	-4.859577000	3.546046000	0.235104000
H	-5.723120000	2.997381000	-0.128767000
C	-4.348303000	1.822245000	-2.529533000
H	-3.842328000	2.763959000	-2.343281000
C	-5.074258000	-1.953097000	2.362632000
H	-4.974873000	-3.033460000	2.411697000

C	-2.633201000	4.983987000	1.124308000
H	-1.763984000	5.543528000	1.455130000
C	-5.005360000	-0.401322000	-1.817956000
H	-5.016446000	-1.197298000	-1.083553000
C	-5.321572000	0.829029000	2.227464000
H	-5.417545000	1.908364000	2.191361000
C	1.056237000	4.527537000	-0.276224000
H	1.193997000	4.640645000	0.792927000
C	4.146746000	2.952105000	3.564192000
H	5.154487000	2.972155000	3.969452000
C	0.779921000	4.330257000	-3.045848000
H	0.690259000	4.250966000	-4.125752000
C	0.361078000	5.489993000	-2.388900000
H	-0.057651000	6.317938000	-2.954212000
C	-3.566943000	-3.783560000	-2.307069000
H	-4.456312000	-4.061500000	-2.866432000
C	3.032714000	-4.827564000	-2.730910000
H	3.801673000	-4.570578000	-3.453904000
C	4.661836000	3.416955000	-0.779090000
H	4.198981000	4.205977000	-0.194047000
C	1.499503000	-4.752771000	3.391562000
H	2.353374000	-5.327579000	3.738998000
C	1.048292000	-5.461723000	-0.883601000
H	0.269721000	-5.723758000	-0.174045000
C	-6.062741000	0.102525000	3.162879000
H	-6.730384000	0.627056000	3.839851000
C	-5.020626000	1.633496000	-3.735789000
H	-5.025839000	2.428144000	-4.475689000
C	-5.687530000	0.432029000	-3.986903000
H	-6.215602000	0.289236000	-4.925065000
C	-5.678576000	-0.580812000	-3.028211000
H	-6.199837000	-1.514962000	-3.214299000
C	0.505821000	5.586955000	-1.005976000
H	0.210723000	6.496200000	-0.488800000
C	-4.977116000	4.903798000	0.529033000
H	-5.934717000	5.400100000	0.403194000
C	-0.916382000	1.033453000	-1.951184000
H	-0.212979000	1.063672000	-2.766223000
H	-1.891450000	1.460871000	-2.168336000
H	2.162816000	-1.433589000	3.670405000

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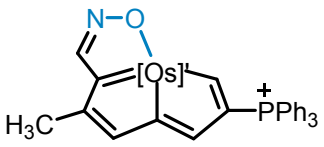

2b^{+} [Os]' = $OsCl(PPh_3)_2$

E = -4137.92606279 a.u.

Os	-1.274819000	-0.007254000	-0.135682000
P	-1.360943000	-2.547214000	-0.142301000
P	-1.339531000	2.537648000	-0.193034000
Cl	-1.091293000	-0.053453000	-2.734828000
P	3.546320000	-0.003610000	0.173316000
O	-3.238430000	0.019553000	-0.973699000
C	1.173070000	0.077201000	1.761126000
H	1.748170000	0.147707000	2.682741000
C	-1.661024000	3.235012000	1.519507000
C	-0.204984000	0.062595000	1.735875000
C	-2.970465000	3.540814000	1.914452000
H	-3.790080000	3.435661000	1.211342000
N	-4.311166000	0.012800000	-0.225591000
C	4.279233000	1.388293000	1.151842000
C	1.726369000	-0.002990000	0.455811000
C	-1.694396000	-3.214386000	1.580142000
C	-2.647216000	0.006398000	1.427689000
C	-2.298200000	0.035661000	2.802033000
C	0.777805000	-0.057403000	-0.532326000
H	1.083930000	-0.118302000	-1.569587000
C	-2.641797000	3.386215000	-1.262813000
C	-2.981419000	-3.637266000	1.938289000
H	-3.779643000	-3.637099000	1.203967000
C	0.168995000	-3.465615000	-0.758514000
C	-2.652935000	-3.416180000	-1.207467000
C	-0.685755000	-3.213865000	2.553491000
H	0.308363000	-2.858303000	2.303332000
C	3.976397000	0.214369000	-1.611672000
C	-3.294763000	2.714992000	-2.300982000
H	-3.110589000	1.664220000	-2.475121000
C	0.807707000	2.970399000	-1.981211000
H	0.446523000	2.062457000	-2.453930000
C	-3.405130000	-2.741867000	-2.173239000
H	-3.297284000	-1.674401000	-2.304624000
C	1.678969000	5.362304000	-0.832738000
H	1.998655000	6.302724000	-0.391416000
C	-4.023419000	0.003724000	1.049177000
H	-4.847838000	0.004043000	1.754978000

C	0.630589000	4.647663000	-0.245992000
H	0.150495000	5.046774000	0.640640000
C	1.851872000	3.691284000	-2.565179000
H	2.310778000	3.318919000	-3.476320000
C	0.601944000	-3.176919000	-2.061578000
H	0.121445000	-2.386771000	-2.631183000
C	4.328512000	-1.589123000	0.731781000
C	0.195168000	3.440921000	-0.811871000
C	-0.933568000	0.085264000	2.944905000
H	-0.433866000	0.130335000	3.912320000
C	3.662428000	2.646251000	1.090533000
H	2.768100000	2.797601000	0.493378000
C	-0.621228000	3.372302000	2.449023000
H	0.397157000	3.120507000	2.171394000
C	-4.436852000	4.766226000	-2.911213000
H	-5.137023000	5.299304000	-3.548380000
C	-0.948914000	-3.661116000	3.849525000
H	-0.152594000	-3.668329000	4.589117000
C	-0.882538000	3.833845000	3.741044000
H	-0.063710000	3.948440000	4.446322000
C	-2.187353000	4.148679000	4.124512000
H	-2.389355000	4.512373000	5.128011000
C	-4.441113000	-4.835286000	-2.828993000
H	-5.138102000	-5.383892000	-3.456413000
C	-3.676735000	-5.512320000	-1.874302000
H	-3.772018000	-6.588277000	-1.757597000
C	-3.772448000	5.440923000	-1.883458000
H	-3.949023000	6.500223000	-1.718723000
C	5.577862000	-3.920371000	1.621784000
H	6.063647000	-4.827853000	1.968171000
C	5.360402000	3.528092000	2.573732000
H	5.782026000	4.361676000	3.127851000
C	3.716407000	-2.376475000	1.713319000
H	2.754253000	-2.090581000	2.124829000
C	-2.230323000	-4.093751000	4.196090000
H	-2.435017000	-4.443717000	5.203862000
C	-4.298995000	-3.457414000	-2.977455000
H	-4.881968000	-2.924789000	-3.723371000
C	5.564153000	-1.970469000	0.190012000
H	6.036150000	-1.370403000	-0.581973000
C	3.629346000	-0.796315000	-2.519623000
H	3.111011000	-1.689979000	-2.186134000
C	4.210880000	3.713927000	1.801070000
H	3.737029000	4.689248000	1.746583000

C	4.344797000	-3.541415000	2.155710000
H	3.868111000	-4.153482000	2.915563000
C	4.660689000	1.354973000	-2.045989000
H	4.934603000	2.135438000	-1.344761000
C	5.431535000	1.198347000	1.922760000
H	5.906726000	0.224210000	1.973319000
C	0.774735000	-4.510270000	-0.051109000
H	0.432783000	-4.778612000	0.941841000
C	-3.245997000	-4.073171000	3.239233000
H	-4.247464000	-4.405362000	3.498128000
C	1.628101000	-3.925712000	-2.640344000
H	1.932825000	-3.712643000	-3.662006000
C	2.242479000	-4.957877000	-1.925898000
H	3.036179000	-5.543067000	-2.381911000
C	2.293410000	4.885323000	-1.992013000
H	3.098596000	5.450188000	-2.453846000
C	-4.192619000	3.410073000	-3.117802000
H	-4.699203000	2.878796000	-3.918465000
C	-2.781629000	-4.808633000	-1.071685000
H	-2.183902000	-5.348512000	-0.343337000
C	-3.230261000	3.995980000	3.209389000
H	-4.249424000	4.239772000	3.496374000
C	-2.874310000	4.757203000	-1.066444000
H	-2.361182000	5.297352000	-0.276927000
C	5.968203000	2.272853000	2.634980000
H	6.860260000	2.125985000	3.236452000
C	3.957888000	-0.650802000	-3.866820000
H	3.682985000	-1.428731000	-4.572664000
C	4.640231000	0.487071000	-4.305569000
H	4.898956000	0.592782000	-5.355040000
C	4.993996000	1.484740000	-3.395954000
H	5.531934000	2.365995000	-3.732553000
C	1.813648000	-5.245285000	-0.631143000
H	2.271563000	-6.056093000	-0.071202000
C	6.185780000	-3.135959000	0.638854000
H	7.141873000	-3.431128000	0.217073000
C	-3.279489000	0.028314000	3.944510000
H	-2.755184000	0.049393000	4.904219000
H	-3.943354000	0.899827000	3.907929000
H	-3.907484000	-0.869858000	3.925861000

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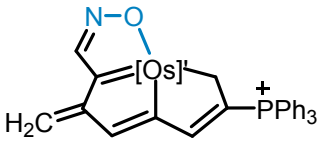

2b-1^{+} [Os]' = $OsCl(PPh_3)_2$

E = -4137.88753215 a.u.

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P	-1.266384000	2.616524000	-0.136463000
Cl	-1.150633000	-0.023744000	-2.593354000
P	3.548678000	-0.093850000	0.106472000
O	-3.282768000	0.349863000	-0.779568000
C	1.284567000	0.632530000	1.763383000
H	1.819457000	0.255673000	2.647681000
C	-1.217518000	3.373707000	1.582981000
C	-0.185858000	0.282733000	1.823731000
C	-2.361662000	3.285634000	2.389767000
H	-3.269680000	2.835617000	2.001067000
N	-4.320943000	0.261945000	-0.013115000
C	4.384223000	1.421260000	0.773371000
C	1.748665000	0.053335000	0.459756000
C	-1.643640000	-3.257725000	1.582245000
C	-2.615228000	-0.065268000	1.555961000
C	-2.188758000	-0.213939000	2.952321000
C	0.773937000	-0.267599000	-0.405347000
H	1.012442000	-0.670925000	-1.384750000
C	-2.758731000	3.424781000	-0.962073000
C	-2.844542000	-3.861826000	1.976762000
H	-3.675887000	-3.929133000	1.284326000
C	-0.013596000	-3.412664000	-0.927200000
C	-2.853690000	-3.253637000	-1.126999000
C	-0.594495000	-3.164978000	2.508177000
H	0.324666000	-2.657895000	2.236654000
C	3.915465000	-0.249455000	-1.700960000
C	-3.179396000	2.942805000	-2.208942000
H	-2.711209000	2.067560000	-2.644429000
C	0.891101000	2.785638000	-2.022529000
H	0.728810000	1.728123000	-2.187268000
C	-3.720256000	-2.487087000	-1.910052000
H	-3.623534000	-1.411329000	-1.943058000
C	1.233213000	5.542380000	-1.710023000
H	1.348001000	6.616617000	-1.594565000
C	-3.987786000	0.047259000	1.246814000
H	-4.792203000	0.000954000	1.973239000

C	0.282325000	4.864967000	-0.946864000
H	-0.339756000	5.424703000	-0.255829000
C	1.833616000	3.472136000	-2.796542000
H	2.414814000	2.925020000	-3.533467000
C	0.103876000	-3.319320000	-2.323015000
H	-0.561602000	-2.670951000	-2.882021000
C	4.283915000	-1.585148000	0.928095000
C	0.118788000	3.477126000	-1.083125000
C	-0.773402000	0.074461000	3.015210000
H	-0.240996000	0.128427000	3.964034000
C	3.877518000	2.679078000	0.412710000
H	3.017697000	2.761123000	-0.246176000
C	-0.059823000	3.957062000	2.111950000
H	0.836623000	4.044372000	1.507418000
C	-4.832726000	4.710450000	-2.335623000
H	-5.640747000	5.205671000	-2.866809000
C	-0.729265000	-3.702032000	3.788863000
H	0.095570000	-3.630574000	4.492933000
C	-0.047832000	4.447267000	3.420684000
H	0.857688000	4.901087000	3.814131000
C	-1.191917000	4.363954000	4.213747000
H	-1.183742000	4.751952000	5.228306000
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C	-3.946681000	-5.275807000	-1.904489000
H	-4.023962000	-6.359475000	-1.903785000
C	-4.406871000	5.195782000	-1.099549000
H	-4.877034000	6.072737000	-0.663138000
C	5.436215000	-3.797605000	2.179047000
H	5.884443000	-4.658674000	2.666023000
C	5.597568000	3.738224000	1.746079000
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C	3.603461000	-2.232213000	1.965237000
H	2.625917000	-1.883646000	2.280541000
C	-1.923409000	-4.316475000	4.170146000
H	-2.029121000	-4.733221000	5.167753000
C	-4.704581000	-3.118506000	-2.678542000
H	-5.372601000	-2.512900000	-3.284162000
C	5.539390000	-2.048702000	0.510748000
H	6.063175000	-1.559639000	-0.305299000
C	3.548379000	-1.429489000	-2.362555000
H	3.069745000	-2.244539000	-1.829254000
C	4.491654000	3.834213000	0.897154000
H	4.102663000	4.805970000	0.608056000

C	4.183385000	-3.338051000	2.589369000
H	3.654462000	-3.840897000	3.393603000
C	4.554338000	0.783997000	-2.396374000
H	4.851593000	1.693013000	-1.885478000
C	5.490468000	1.322861000	1.624372000
H	5.881215000	0.352832000	1.912715000
C	0.851728000	-4.257852000	-0.224047000
H	0.760193000	-4.377141000	0.848489000
C	-2.981588000	-4.386940000	3.263712000
H	-3.918051000	-4.855800000	3.552477000
C	1.066789000	-4.069415000	-2.999029000
H	1.127407000	-4.004404000	-4.082105000
C	1.929911000	-4.912879000	-2.293683000
H	2.668873000	-5.508568000	-2.822789000
C	2.014353000	4.845821000	-2.636386000
H	2.742974000	5.376883000	-3.242823000
C	-4.213634000	3.587602000	-2.888024000
H	-4.537030000	3.203745000	-3.851434000
C	-2.961135000	-4.655050000	-1.140391000
H	-2.275409000	-5.264384000	-0.559213000
C	-2.350237000	3.783274000	3.692817000
H	-3.248353000	3.714865000	4.300030000
C	-3.368672000	4.559820000	-0.414194000
H	-3.045592000	4.957963000	0.540890000
C	6.093388000	2.485356000	2.109780000
H	6.950642000	2.408019000	2.771809000
C	3.810330000	-1.561930000	-3.725835000
H	3.518742000	-2.473743000	-4.237091000
C	4.443464000	-0.531851000	-4.424865000
H	4.648989000	-0.642063000	-5.485549000
C	4.818567000	0.636550000	-3.759531000
H	5.322382000	1.434479000	-4.297034000
C	1.823004000	-4.998974000	-0.905518000
H	2.479714000	-5.659534000	-0.346049000
C	6.112661000	-3.154164000	1.139577000
H	7.084160000	-3.513932000	0.814196000
C	-2.993735000	-0.538230000	3.990601000
H	-2.599794000	-0.597468000	5.000774000
H	-4.043901000	-0.777672000	3.868129000
H	1.425840000	1.723501000	1.776373000

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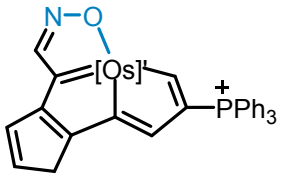

2c^{+} [Os]' = $OsCl(PPh_3)_2$

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P	-1.270006000	2.556263000	-0.321179000
Cl	-1.006832000	-0.051374000	-2.855000000
P	3.559590000	-0.064054000	0.151415000
O	-3.191043000	0.077212000	-1.159460000
C	1.167275000	0.040132000	1.701510000
H	1.736842000	0.093609000	2.627501000
C	-1.600316000	3.271545000	1.381582000
C	-0.210924000	0.050561000	1.660654000
C	-2.906153000	3.613440000	1.757765000
H	-3.720507000	3.517351000	1.047298000
N	-4.294090000	0.101162000	-0.453000000
C	4.294099000	1.317470000	1.143987000
C	1.734446000	-0.038409000	0.403285000
C	-1.771198000	-3.192178000	1.449563000
C	-2.693852000	0.055798000	1.250940000
C	-2.355919000	0.071600000	2.614258000
C	0.803814000	-0.068547000	-0.604195000
H	1.133117000	-0.124203000	-1.634443000
C	-2.535725000	3.427296000	-1.417579000
C	-3.073021000	-3.590034000	1.780608000
H	-3.857106000	-3.566907000	1.031564000
C	0.137159000	-3.476882000	-0.843854000
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C	-0.781302000	-3.219815000	2.442042000
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C	4.027656000	0.148508000	-1.624820000
C	-3.167294000	2.769704000	-2.477660000
H	-2.993052000	1.717159000	-2.651473000
C	0.908077000	2.941157000	-2.082398000
H	0.534408000	2.038512000	-2.555469000
C	-3.386943000	-2.689226000	-2.341546000
H	-3.254056000	-1.624537000	-2.472442000
C	1.810177000	5.321708000	-0.934966000
H	2.141663000	6.258502000	-0.494561000
C	-4.055029000	0.087915000	0.831420000

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H	0.257397000	5.043488000	0.520074000
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C	0.617090000	-3.189049000	-2.130593000
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C	-0.990382000	0.081796000	2.831673000
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H	-0.018053000	3.994706000	4.314607000
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H	-2.338165000	4.619101000	4.962539000
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H	-5.141974000	-5.299177000	-3.659997000
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H	5.967651000	-4.934082000	1.971954000
C	5.374084000	3.443343000	2.588466000
H	5.795618000	4.271513000	3.150726000
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H	-4.829951000	-2.846193000	-3.925962000
C	5.565601000	-2.040742000	0.227791000
H	6.075146000	-1.429521000	-0.511001000
C	3.680386000	-0.856158000	-2.539254000
H	3.138336000	-1.739351000	-2.215805000
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H	7.132398000	-3.511586000	0.298962000
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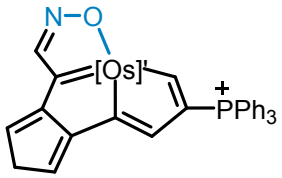

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Cl	0.992507000	0.102133000	-2.805679000
P	-3.567591000	-0.137990000	0.163259000
O	3.217043000	0.144535000	-1.163236000
C	-1.157825000	-0.116231000	1.717862000
H	-1.728170000	-0.206601000	2.640681000
C	1.941490000	-3.180711000	1.331581000
C	0.197881000	-0.046326000	1.687624000
C	3.280444000	-3.520485000	1.570613000
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C	-4.232273000	-1.543932000	1.171115000
C	-1.744411000	-0.067914000	0.403011000
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C	2.712331000	0.105836000	1.242230000
C	2.406356000	0.062172000	2.643180000
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C	2.666193000	-3.263798000	-1.523624000
C	2.950885000	3.924182000	1.574714000
H	3.641016000	4.009260000	0.742895000
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C	2.339921000	3.528019000	-1.479340000
C	0.827901000	3.220803000	2.488409000
H	-0.129419000	2.723521000	2.375894000
C	-4.036818000	-0.395012000	-1.606872000
C	3.305780000	-2.541958000	-2.534856000
H	3.139908000	-1.479583000	-2.637552000
C	-0.788106000	-3.040252000	-1.989297000
H	-0.483539000	-2.140102000	-2.514443000
C	3.133157000	2.885848000	-2.433361000
H	3.146387000	1.807676000	-2.498955000
C	-1.528233000	-5.405024000	-0.700252000
H	-1.797421000	-6.333850000	-0.204055000

C	4.064094000	0.168029000	0.829460000
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C	-0.880168000	3.182675000	-2.052699000
H	-0.356677000	2.483059000	-2.698130000
C	-4.404710000	1.414567000	0.736646000
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C	0.983201000	-0.035254000	2.909399000
C	-3.542009000	-2.763736000	1.156673000
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H	0.668219000	-3.901351000	4.409428000
C	2.737125000	-4.143385000	3.846676000
H	3.042537000	-4.528326000	4.815701000
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H	4.486160000	5.621327000	-3.955864000
C	3.081063000	5.681579000	-2.319217000
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H	-5.594023000	-4.545516000	3.206399000
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C	2.442876000	4.333896000	3.907127000
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H	4.517191000	3.136441000	-4.058109000
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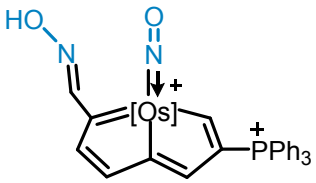

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H	6.531417000	0.527232000	-0.696292000
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N	4.821649000	0.401421000	0.051356000
C	-0.765480000	-0.066059000	-0.683646000
H	-1.112138000	-0.064208000	-1.716531000
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H	3.530298000	-5.913406000	-3.046626000
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H	-5.987496000	-0.458858000	1.724767000
C	-2.703727000	4.470540000	-2.201778000
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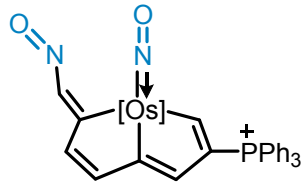
C	-4.957746000	-2.182189000	-3.313395000
H	-5.487842000	-3.101756000	-3.542219000
C	-4.030448000	2.015540000	1.647515000
H	-3.213581000	1.664775000	2.270231000
C	-4.398428000	1.318222000	0.488593000
C	-1.397480000	4.235983000	-0.173862000
H	-1.209027000	4.539088000	0.849583000
C	-4.730400000	3.163804000	2.016253000
H	-4.449214000	3.699444000	2.918006000
C	-2.470567000	4.804739000	-0.868812000
H	-3.110795000	5.523333000	-0.366115000
C	-4.625478000	-1.889444000	-1.988605000
H	-4.893600000	-2.582688000	-1.198864000
C	-5.795583000	3.618009000	1.233438000
H	-6.342674000	4.509026000	1.526657000
C	4.412656000	3.749104000	-2.191143000
H	5.330134000	3.280418000	-2.535219000
C	2.983077000	5.687853000	-2.028082000
H	2.783346000	6.733366000	-2.242957000
C	1.380822000	4.425567000	4.275820000
H	1.472375000	4.839305000	5.275589000
C	2.427500000	4.560068000	3.363090000
H	3.337894000	5.078643000	3.648521000
C	-5.950684000	-2.395748000	2.663073000
H	-6.895711000	-2.243297000	3.175140000
C	4.165723000	5.091414000	-2.474063000
H	4.888568000	5.672315000	-3.039012000

120



4^{+} [Os] = $Os(PPh_3)_2$

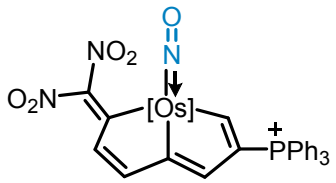
E = -3766.97696775 a.u.

Os	-1.223790000	0.073674000	-0.139953000
P	-1.126824000	2.597871000	-0.011053000
P	-1.481085000	-2.450111000	-0.044172000
P	3.545084000	-0.192985000	0.069756000
O	-6.049784000	0.385619000	-0.038415000
O	-1.901757000	0.158817000	-3.026073000
N	-4.809952000	0.304537000	-0.054804000
N	-1.780906000	0.131839000	-1.859049000
C	1.221890000	4.296532000	-0.115506000
H	1.015183000	4.572877000	0.912128000
C	-1.915154000	-3.153385000	1.634249000
C	-3.584391000	2.849689000	-1.480578000
H	-3.757070000	1.800600000	-1.270133000
C	-4.547420000	3.564500000	-2.200645000
H	-5.439155000	3.048940000	-2.544713000
C	-2.836966000	0.175809000	1.327857000
C	4.047925000	0.319582000	-3.985456000
H	3.860263000	1.105455000	-4.711161000
C	-3.224624000	-3.569840000	1.899461000
H	-3.985061000	-3.510671000	1.128427000
C	2.284447000	4.909493000	-0.788966000
H	2.899657000	5.636729000	-0.266848000
C	-0.260909000	3.226779000	2.637625000
H	0.654677000	2.707586000	2.376649000
C	4.243438000	-1.573614000	1.091030000
C	-0.183987000	-0.029779000	1.712073000
C	-4.367084000	4.921052000	-2.463290000
H	-5.116229000	5.473642000	-3.023298000
C	0.809225000	-0.032932000	-0.689920000
H	1.158180000	-0.016385000	-1.722222000
C	3.731867000	0.530833000	-2.643405000
H	3.309018000	1.481586000	-2.333745000
C	-1.002544000	0.014890000	2.892830000
H	-0.570737000	-0.033808000	3.892884000
C	-3.871129000	-2.317418000	-1.622622000
H	-3.935664000	-1.276754000	-1.326003000
C	-2.437189000	3.497653000	-1.017487000

C	1.178453000	-0.125686000	1.674661000
H	1.807420000	-0.214971000	2.561370000
C	4.409794000	1.367623000	0.585391000
C	-2.343979000	0.127383000	2.692371000
H	-3.042131000	0.170326000	3.528026000
C	3.973568000	-0.484736000	-1.706550000
C	-1.295460000	3.339310000	1.698258000
C	2.540836000	4.605301000	-2.124652000
H	3.353567000	5.097408000	-2.651379000
C	0.419313000	3.359441000	-0.772112000
C	1.719943000	-0.112236000	0.325544000
C	-4.875880000	-2.855595000	-2.432521000
H	-5.690186000	-2.215468000	-2.759021000
C	1.732462000	3.676757000	-2.788558000
H	1.906489000	3.451309000	-3.837532000
C	0.601015000	-3.110606000	-1.839452000
H	0.281339000	-2.216979000	-2.365528000
C	0.397420000	-4.640721000	0.019535000
H	-0.078765000	-4.949547000	0.943350000
C	-0.947123000	-3.233932000	2.645789000
H	0.067413000	-2.896580000	2.459316000
C	-3.560405000	-4.065480000	3.161849000
H	-4.580263000	-4.384253000	3.356689000
C	4.610890000	-0.892641000	-4.393195000
H	4.862198000	-1.049886000	-5.438040000
C	-0.408183000	3.766994000	3.915371000
H	0.403403000	3.682145000	4.633064000
C	-2.820536000	-3.127159000	-1.181828000
C	0.684244000	3.050714000	-2.114613000
H	0.053171000	2.345859000	-2.648627000
C	5.610784000	1.736836000	-0.035589000
H	6.011781000	1.147271000	-0.853846000
C	-2.592272000	-4.157069000	4.161857000
H	-2.854000000	-4.549607000	5.140335000
C	4.857993000	-1.897703000	-3.456739000
H	5.305047000	-2.837065000	-3.768467000
C	-4.204398000	0.269603000	1.186050000
H	-4.881309000	0.314555000	2.045613000
C	3.528730000	-2.775814000	1.178182000
H	2.575133000	-2.887985000	0.672024000
C	-0.005873000	-3.464946000	-0.627068000
C	4.537913000	-1.699366000	-2.111693000
H	4.730126000	-2.485210000	-1.389397000
C	1.597345000	-3.914360000	-2.394377000

H	2.050851000	-3.630038000	-3.339217000
C	5.472280000	-1.429393000	1.746281000
H	6.024179000	-0.497263000	1.683889000
C	2.002112000	-5.081813000	-1.742093000
H	2.771254000	-5.713116000	-2.178229000
C	1.400670000	-5.442166000	-0.536000000
H	1.694372000	-6.358633000	-0.031222000
C	-2.783254000	-4.479850000	-1.555676000
H	-1.976861000	-5.123762000	-1.221314000
C	-2.488026000	3.974697000	2.064590000
H	-3.303103000	4.060120000	1.354576000
C	6.293247000	2.875478000	0.395869000
H	7.222847000	3.159586000	-0.088323000
C	-1.284068000	-3.742761000	3.900165000
H	-0.524989000	-3.809974000	4.674810000
C	-3.218648000	5.570965000	-2.000971000
H	-3.070580000	6.628544000	-2.200598000
C	-4.834603000	-4.197117000	-2.808533000
H	-5.615180000	-4.612157000	-3.439918000
C	3.897196000	2.138842000	1.635362000
H	2.966590000	1.858302000	2.116846000
C	-3.786255000	-5.008757000	-2.366643000
H	-3.747087000	-6.056121000	-2.652599000
C	-2.256346000	4.865469000	-1.281308000
H	-1.368591000	5.382287000	-0.930375000
C	-1.597358000	4.405124000	4.274903000
H	-1.712900000	4.821756000	5.271390000
C	5.782720000	3.643832000	1.444069000
H	6.317125000	4.527958000	1.779268000
C	5.985780000	-2.492913000	2.490162000
H	6.937008000	-2.380663000	3.001766000
C	4.585805000	3.275053000	2.061712000
H	4.186167000	3.871096000	2.876903000
C	-2.636836000	4.501406000	3.349817000
H	-3.567802000	4.990101000	3.622135000
C	4.052570000	-3.833953000	1.921582000
H	3.499781000	-4.766194000	1.986271000
C	5.277740000	-3.693214000	2.577947000
H	5.679919000	-4.518052000	3.158982000

123



5^{+} [Os] = Os(PPh$_3$)$_2$

E = -4046.65523186 a.u.

Os	0.970994000	-0.130885000	0.264117000
P	0.701874000	-2.678418000	0.151468000
P	1.341565000	2.380445000	0.138187000
P	-3.758186000	0.380021000	-0.188125000
O	4.140436000	-0.677595000	1.402840000
O	1.721791000	-0.297121000	3.130674000
O	5.872031000	0.211932000	0.418606000
N	1.522036000	-0.228493000	1.982401000
O	4.949245000	0.844334000	-2.717955000
C	-1.926982000	0.186957000	-0.370696000
N	4.721670000	-0.229383000	0.400343000
O	5.801496000	-1.062522000	-2.087571000
C	2.685139000	-0.257659000	-1.094844000
C	0.046192000	-0.027704000	-1.633281000
C	0.308512000	3.402669000	1.337264000
C	-1.080172000	0.088830000	0.702410000
H	-1.499164000	0.124906000	1.708837000
N	5.017748000	-0.129289000	-1.965254000
C	1.364378000	-4.521833000	2.242512000
H	2.022466000	-4.992207000	1.520907000
C	-0.216261000	2.820046000	2.496191000
H	-0.120226000	1.753849000	2.662201000
C	0.925325000	-0.162072000	-2.758016000
H	0.556415000	-0.143413000	-3.784671000
C	-1.309501000	0.128517000	-1.680062000
H	-1.881375000	0.176790000	-2.604258000
C	2.113822000	-3.610898000	-0.657557000
C	-0.828318000	-3.398352000	-0.672178000
C	-0.330878000	-3.335823000	4.119667000
H	-0.987400000	-2.865956000	4.846841000
C	4.030982000	-0.211230000	-0.858903000
C	3.631203000	4.107693000	-0.005831000
H	3.149983000	4.574323000	-0.857258000
C	1.020526000	3.102894000	-1.554144000
C	3.687080000	2.435440000	1.740458000
H	3.260716000	1.583738000	2.253925000
C	0.622704000	-3.388495000	1.888721000

C	1.263340000	-5.050888000	3.531664000
H	1.849207000	-5.926090000	3.797071000
C	-0.225699000	-2.799305000	2.836043000
H	-0.806733000	-1.921398000	2.573436000
C	2.254200000	-0.292375000	-2.489696000
H	2.969190000	-0.387529000	-3.301424000
C	0.417654000	-4.461281000	4.471511000
H	0.344650000	-4.873421000	5.473798000
C	-4.624068000	0.149340000	-2.863013000
H	-4.087516000	1.079274000	-3.027074000
C	3.415202000	-3.361699000	-0.201735000
H	3.588014000	-2.633775000	0.583901000
C	-4.667327000	-0.435711000	-1.588039000
C	-5.387924000	-1.616432000	-1.382304000
H	-5.433308000	-2.069772000	-0.398306000
C	-1.077651000	-3.149279000	-2.029873000
H	-0.415681000	-2.504843000	-2.594804000
C	-1.676548000	-4.267617000	0.027014000
H	-1.483062000	-4.499598000	1.068232000
C	-2.159399000	-3.754209000	-2.671455000
H	-2.333413000	-3.559751000	-3.726007000
C	2.010842000	3.015165000	-2.543962000
H	2.971646000	2.556338000	-2.333652000
C	5.483670000	4.044857000	1.552354000
H	6.432114000	4.441566000	1.902283000
C	-0.219655000	3.673410000	-1.868371000
H	-1.000402000	3.737999000	-1.118748000
C	3.052852000	2.999506000	0.627854000
C	-0.964410000	4.986550000	3.275155000
H	-1.450705000	5.600583000	4.027776000
C	4.900977000	2.952534000	2.194782000
H	5.392102000	2.487564000	3.043864000
C	4.844237000	4.622188000	0.455101000
H	5.288206000	5.474551000	-0.051226000
C	-4.304562000	-0.371543000	1.414061000
C	-0.851031000	3.608696000	3.460361000
H	-1.245749000	3.143113000	4.359063000
C	-4.286905000	2.159085000	-0.187388000
C	4.495244000	-4.044697000	-0.761169000
H	5.500850000	-3.829576000	-0.413657000
C	1.901031000	-4.563404000	-1.661594000
H	0.901167000	-4.787249000	-2.013702000
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H	-1.420360000	4.626058000	-3.377279000

C	-3.006686000	-4.611987000	-1.967224000
H	-3.842357000	-5.088532000	-2.471691000
C	4.284206000	-4.982295000	-1.774335000
H	5.127219000	-5.506755000	-2.214743000
C	-6.060036000	-2.212540000	-2.451913000
H	-6.626333000	-3.124254000	-2.286685000
C	1.766495000	3.522436000	-3.821830000
H	2.545342000	3.458679000	-4.576130000
C	-5.293108000	-0.455222000	-3.926289000
H	-5.259789000	0.001010000	-4.911143000
C	-6.011787000	-1.636275000	-3.721485000
H	-6.538752000	-2.100657000	-4.549856000
C	-3.846433000	-1.649106000	1.768517000
H	-3.162015000	-2.189217000	1.122015000
C	0.207390000	4.791038000	1.164203000
H	0.635758000	5.266295000	0.287707000
C	-3.436907000	3.126230000	0.360541000
H	-2.458768000	2.848377000	0.739472000
C	-2.762480000	-4.867238000	-0.617700000
H	-3.403131000	-5.548787000	-0.064751000
C	2.987723000	-5.242561000	-2.218487000
H	2.814020000	-5.977048000	-2.999863000
C	-5.555950000	2.518778000	-0.662142000
H	-6.220705000	1.771924000	-1.083991000
C	-0.432306000	5.576018000	2.124862000
H	-0.497717000	6.651080000	1.981435000
C	-3.855092000	4.456950000	0.423602000
H	-3.191419000	5.202462000	0.849915000
C	-5.187858000	0.318922000	2.252387000
H	-5.542437000	1.308178000	1.983771000
C	0.535208000	4.104592000	-4.127177000
H	0.351900000	4.503137000	-5.121043000
C	-5.115606000	4.819778000	-0.055649000
H	-5.437405000	5.855998000	-0.007059000
C	-5.965213000	3.851461000	-0.595570000
H	-6.946974000	4.130257000	-0.966587000
C	-5.611034000	-0.269643000	3.445704000
H	-6.293846000	0.268608000	4.096154000
C	-5.157484000	-1.541019000	3.800889000
H	-5.489033000	-1.995425000	4.729964000
C	-4.277218000	-2.229517000	2.961972000
H	-3.919536000	-3.217637000	3.235994000