

Electronic Supplementary Information

For

Tuning the reactivity of an osmium–peroxo unit by modulating metallacycle aromaticity

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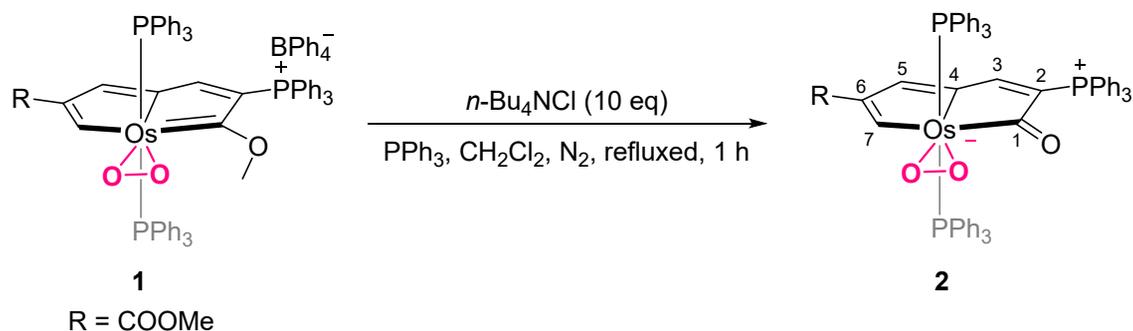
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1. General Considerations

Unless otherwise stated, all manipulations were carried out under nitrogen atmosphere using standard Schlenk techniques or a glovebox. Solvents were purified by an Mbraun SPS-5 solvent purification system and dried over molecular sieves in a glovebox. All other reagents were used as received from commercial sources without further purification. NMR spectroscopic experimentals were recorded on a Bruker Advance III 400, 500, or 600 MHz spectrometer. The ^1H and ^{13}C NMR chemical shifts were referenced to the residual protons in the solvent, and the ^{31}P NMR chemical shifts were relative to 85% H_3PO_4 . HRMS measurements were conducted using a Bruker En Apex-Ultra 7.0 T FT-MS. GC-MS analysis was performed on a SHIMADZU QP-2010 Plus GC-MS spectrometer.

2. Synthetic Details and Characterizations

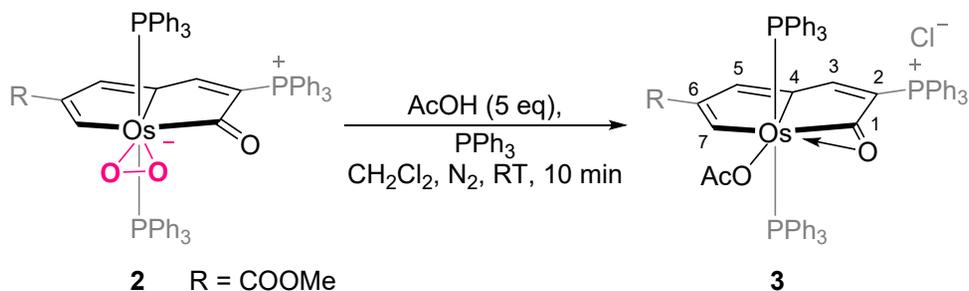
Synthesis and characterization of compound 2



Compound **1** was prepared according to the previous report.¹ Under nitrogen atmosphere, **1** (150 mg, 0.1 mmol), *n*-Bu₄NCl (278 mg, 1 mmol), and PPh₃ (262 mg, 1 mmol, the addition of excess triphenylphosphine can inhibit the substitution of triphenylphosphines at the metal center by chloride ions) were placed in a dried Schlenk flask (50 mL), and then dichloromethane (15 mL) was injected via syringe. The reaction mixture was refluxed for 1 h, and the ³¹P NMR spectra indicated that **1** was completely converted into **2**. After the reaction mixture was cooled to RT, the solvent was evaporated under vacuum to a volume of approximately 2 mL and then washed with diethyl ether (3 × 20 mL) to give **2** as a brown solid (NMR yield: 93%; tetrabutylammonium chloride is present in product **2**).

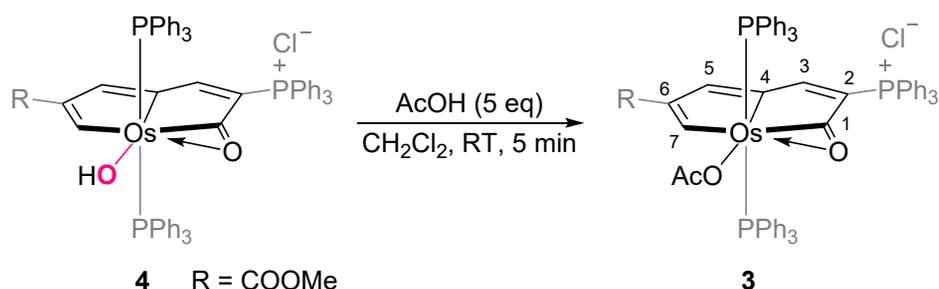
¹H-NMR (600.1 MHz, CD₂Cl₂): δ (ppm) = 12.21 (b, 1H, H7), 7.71 (s, 1H, H5), 7.41 (s, 1H, H3), 3.42 (s, 3H, COOCH₃), 6.78-7.56 (m, Ph). ³¹P-NMR (161.9 MHz, CD₂Cl₂): δ (ppm) = 11.99 (s, C₃PPh₃), -11.84 (s, OsPPh₃). ¹³C-NMR (150.9 MHz, CD₂Cl₂): δ (ppm) = 239.09 (t, *J*_{P-C} = 7.1 Hz, C1), 207.40 (m, C7), 185.33 (d, *J*_{P-C} = 28.0 Hz, C4), 169.31 (d, *J*_{P-C} = 16.3 Hz, C3), 163.51 (s, COOCH₃), 150.83 (s, C5), 142.13 (s, C6), 121.88 (d, *J*_{P-C} = 89.6 Hz, C2), 50.09 (s, COOCH₃), 121.75-135.92 (m, Ph). HRMS (ESI): *m/z* calcd. for [C₆₃H₅₁O₅OsP₃ - H]⁺, 1171.2486; found, 1171.2544.

Synthesis and characterization of compound 3



Method A: Compound **2** was prepared *in situ* in 93% NMR yield and used in the next step without purification. Under a nitrogen atmosphere, **2** (0.1 mmol) and triphenylphosphine (304

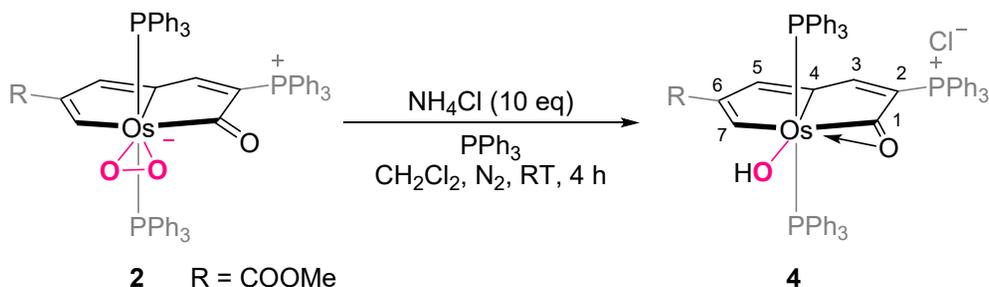
mg, 1 mmol) were placed in a Schlenk flask (50 mL), then dichloromethane (15 mL) and AcOH (29 μ L, 0.5 mmol) were injected sequentially via syringe. The reaction mixture was stirred at room temperature for 10 min. The solvent was evaporated under vacuum to a volume of approximately 2 mL and then washed with diethyl ether (3×20 mL) to remove the AcOH. The resulting residue was purified by flash chromatography on silica gel (dichloromethane/acetone, 20/1) to yield **3** as a red solid (99 mg, 79% yield).



Method B: Compound **4** (119 mg, 0.1 mmol) was placed in a Schlenk flask (50 mL), and then dichloromethane (15 mL) and AcOH (29 μ L, 0.5 mmol) were injected sequentially via syringe. The reaction mixture was stirred at room temperature for 5 min. The solvent was evaporated under vacuum to a volume of approximately 2 mL and then washed with diethyl ether (3×20 mL) to remove the AcOH. The resulting residue was purified by flash chromatography on silica gel (dichloromethane/acetone, 20/1) to yield **3** as a red solid (120 mg, 95% yield).

$^1\text{H-NMR}$ (600.1 MHz, CH_2Cl_2): δ (ppm) = 13.32 (s, 1H, H7), 8.52 (d, $J_{\text{P-H}} = 3.9$ Hz, 1H, H3), 8.04 (s, 1H, H5), 3.59 (s, 3H, COOCH_3), 1.34 (s, 3H, CH_3COO), 7.74-6.86 (m, Ph). $^{31}\text{P-NMR}$ (161.9 MHz, CD_2Cl_2): δ (ppm) = 10.20 (s, $\text{C}(\text{PPh}_3)$), 5.19 (s, $\text{Os}(\text{PPh}_3)$). $^{13}\text{C-NMR}$ (150.9 MHz, CD_2Cl_2): δ (ppm) = 232.60 (m, C7), 223.62 (m, C1), 179.31 (dt, $J_{\text{P-C}} = 23.6, 3.9$ Hz, C4), 177.36 (s, CH_3COO), 170.21 (d, $J_{\text{P-C}} = 14.3$ Hz, C3), 162.21 (s, COOCH_3), 159.89 (s, C5), 146.12 (s, C6), 105.83 (d, $J_{\text{P-C}} = 87.1$ Hz, C2), 51.22 (s, COOCH_3), 23.99 (s, CH_3COO), 118.18-136.07 (m, Ph). HRMS (ESI): m/z calcd. for $[\text{C}_{65}\text{H}_{54}\text{O}_5\text{OsP}_3]^+$, 1199.2793; found, 1199.2766.

Synthesis and characterization of compound 4



Compound **2** was prepared *in situ* in 93% NMR yield and used in the next step without purification. Under a nitrogen atmosphere, **2** (0.1 mmol), NH_4Cl (53 mg, 1 mmol), and

triphenylphosphine (304 mg, 1 mmol) were placed in a dried Schlenk flask (50 mL), and then dichloromethane (15 mL) was injected via syringe. The reaction mixture was stirred at room temperature for 4 h, and the solvent was removed under reduced pressure. The resulting residue was purified by flash chromatography on silica gel (dichloromethane/acetone, 30/1) to yield **4** as a red solid (97 mg, 81% yield).

$^1\text{H-NMR}$ (600.1 MHz, CH_2Cl_2): δ (ppm) = 12.31 (d, $J_{\text{P-H}} = 1.7$ Hz, 1H, H7), 8.11 (d, $J_{\text{P-H}} = 4.7$ Hz, 1H, H3), 8.05 (d, $J_{\text{P-H}} = 1.7$ Hz, 1H, H5), 5.65 (t, $J_{\text{P-H}} = 7.2$ Hz, 1H, Os-OH), 3.55 (s, 3H, COOCH_3), 7.73-6.91 (m, Ph). $^{31}\text{P-NMR}$ (202.4 MHz, CD_2Cl_2): δ (ppm) = 9.96 (s, CPh_3), 7.85 (s, OsPPh_3). $^{13}\text{C-NMR}$ (150.9 MHz, CD_2Cl_2): δ (ppm) = 233.82 (m, C1), 222.87 (t, $J_{\text{P-C}} = 9.4$ Hz, C7), 180.25 (d, $J_{\text{P-C}} = 24.9$ Hz, C4), 172.20 (d, $J_{\text{P-C}} = 14.3$ Hz, C3), 162.24 (s, COOCH_3), 156.77 (s, C5), 144.98 (s, C6), 118.93 (d, $J_{\text{P-C}} = 90.5$ Hz, C2), 50.92 (s, COOCH_3), 121.69-135.94 (m, Ph). HRMS (ESI): m/z calcd. for $[\text{C}_{63}\text{H}_{52}\text{O}_4\text{OsP}_3]^+$, 1157.2688; found, 1157.2704.

3. Supplementary Figures for Experiments

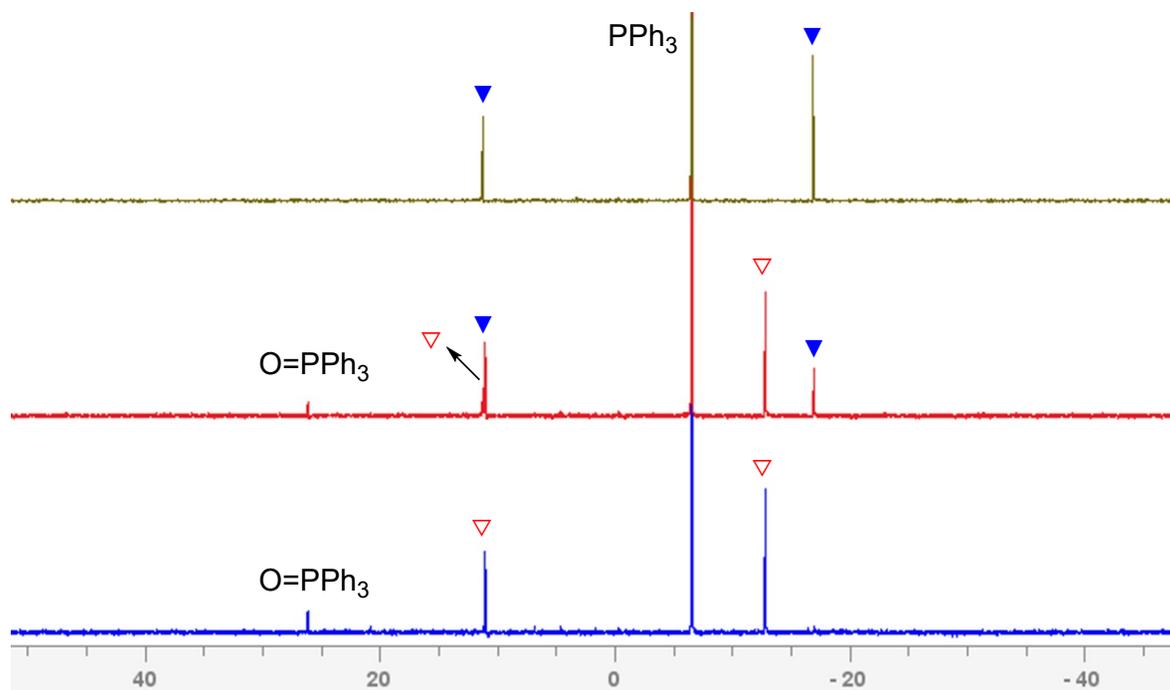
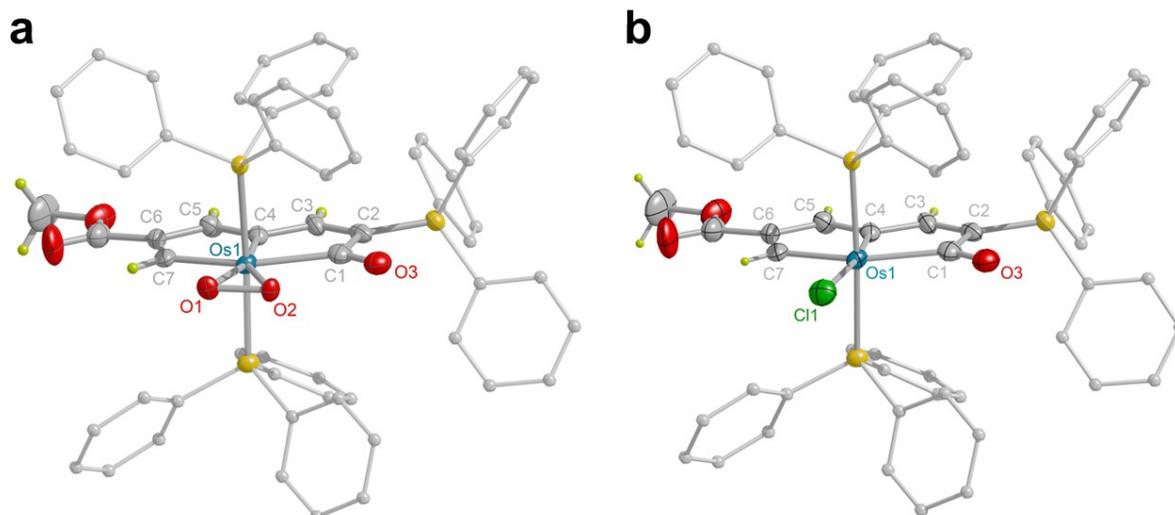


Fig. S1 The $^{31}\text{P}\{^1\text{H}\}$ NMR monitoring of the reaction of **1** with $n\text{-Bu}_4\text{NCl}$.

The $^{31}\text{P}\{^1\text{H}\}$ NMR spectra observed at 0 min (a), 20 min (b), and 60 min (c) for the reaction of **1** with $n\text{-Bu}_4\text{NCl}$ (10 equiv.) in the presence of triphenylphosphine (10 equiv.) in CH_2Cl_2 (refluxed, N_2). The peaks marked with ▼ and ▽ denote **1** and **2**, respectively.



Bond Distances (Å) in a					
Os1–O1	2.016(8)	Os1–O2	2.043(5)	O1–O2	1.441(10)
Os1–C1	2.182(8)	Os1–C4	2.070(7)	Os1–C7	2.034(7)
C1–C2	1.482(10)	C2–C3	1.372(10)	C3–C4	1.427(9)
C4–C5	1.370(9)	C5–C6	1.431(10)	C6–C7	1.407(10)
C1–O3	1.196(9)				
Bond Angles (°) in a					
Os1–O1–O2	70.2(4)	Os1–O2–O1	68.2(4)		
O1–Os1–O2	41.6(3)	Os1–C1–C2	117.0(5)		
C1–C2–C3	111.4(6)	C2–C3–C4	117.2(6)		
Os1–C4–C3	120.1(5)	C4–Os1–C1	74.3(3)		
C4–Os1–C7	74.3(3)	Os1–C4–C5	120.7(5)		
C4–C5–C6	112.4(6)	C5–C6–C7	111.9(6)		
Os1–C7–C6	120.8(5)	Os1–C1–O3	127.3(6)		

Fig. S2 Molecular structures of compounds 2 (a) and 2-Cl (b).

Thermal ellipsoids are set at 50% probability level. Hydrogen atoms in phenyl groups and counter anions are omitted for clarity. **2** co-crystallizes with **2-Cl** that is formed by replacing the peroxo unit with chloride ion during crystallization (–20 °C in glovebox). The occupancy of **2** in the co-crystal was refined to about 0.75. Chloride ion in **2-Cl** is probably derived from the residual tetrabutylammonium chloride, which could not be removed by precipitation with diethyl ether. Also, the product **2** could not be purified by column chromatography due to the high reactivity, which prevent us from obtaining single-component crystals of **2**.

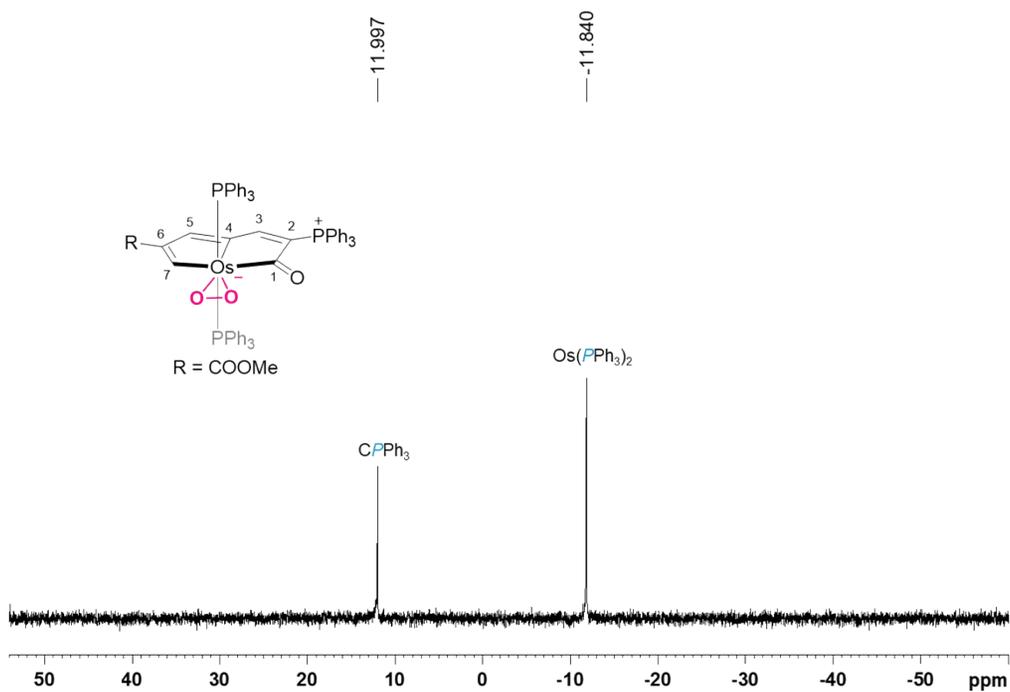


Fig. S3 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.9 MHz, CD_2Cl_2) for compound **2**.

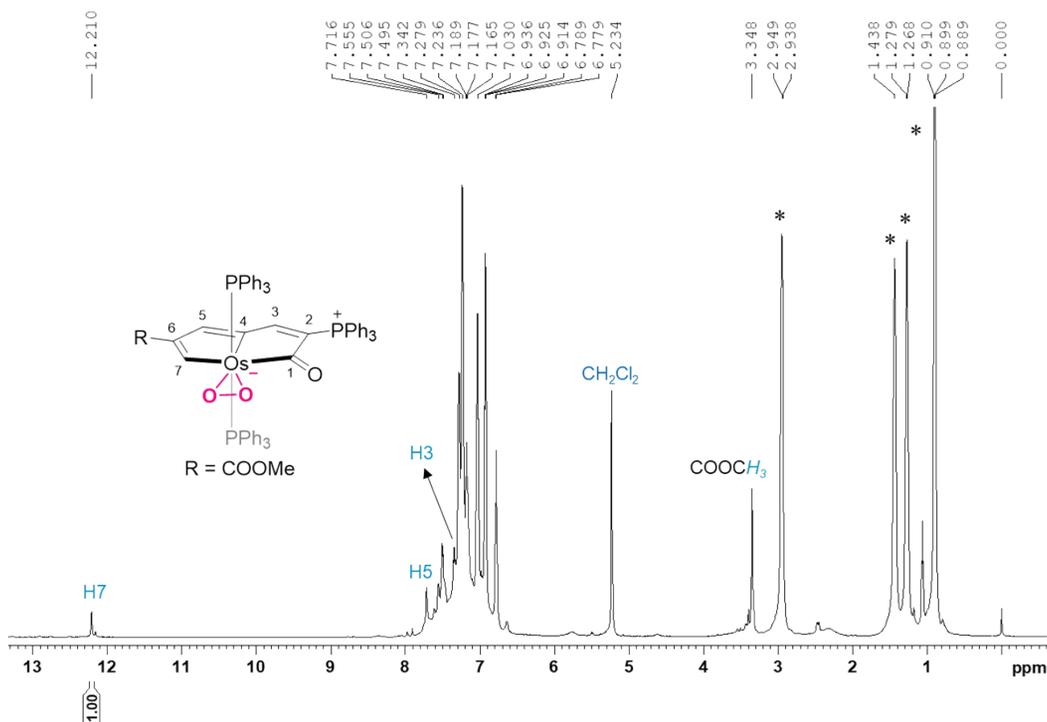


Fig. S4 The ^1H NMR spectrum (600.1 MHz, CD_2Cl_2) for compound **2**.

The peaks marked with asterisk originate from residual tetrabutylammonium chloride, which could not be removed by washing with diethyl ether. Also, the product **2** could not be purified by column chromatography or aqueous washing due to its high reactivity.

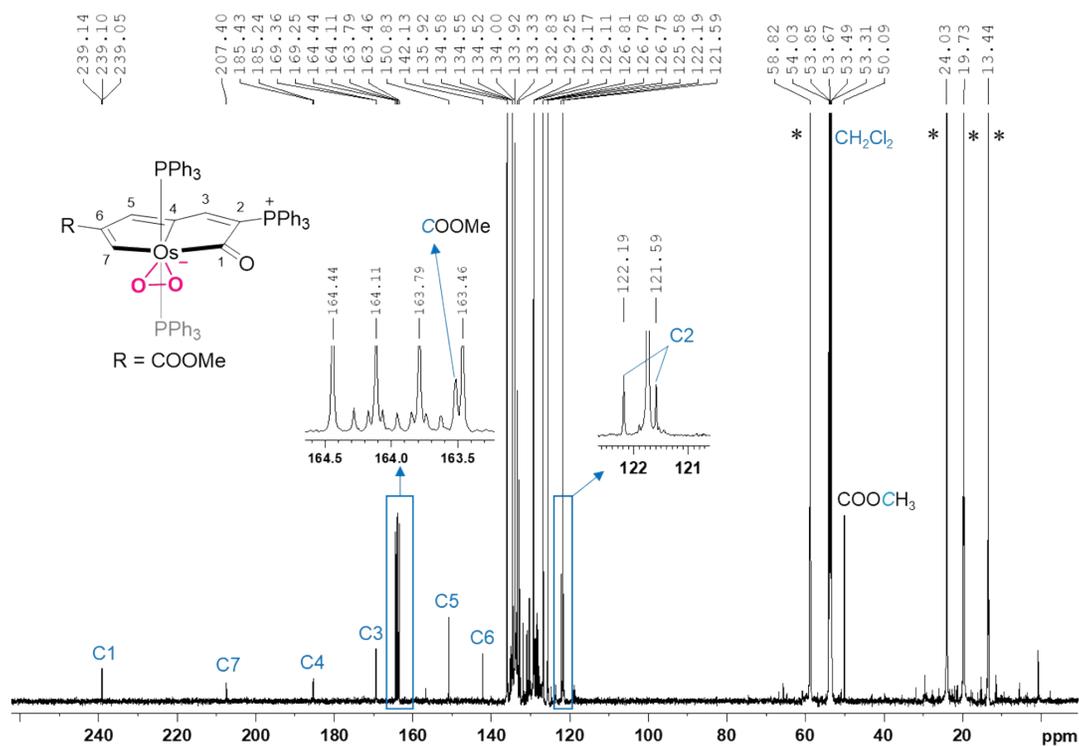


Fig. S5 The $^{13}\text{C}\{^1\text{H}\}$ NMR (150.9 MHz, CD_2Cl_2) spectrum for compound 2.

The peaks marked with asterisk originate from residual tetrabutylammonium chloride.

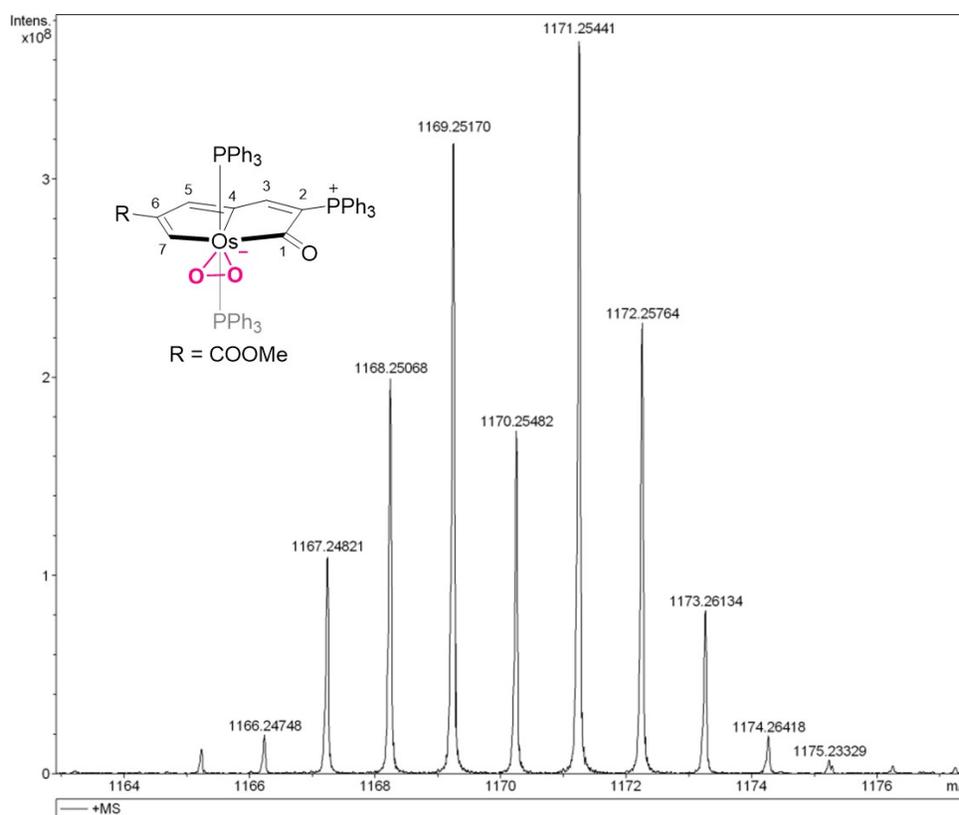


Fig. S6 Positive-ion ESI-MS spectrum for compound 2 measured in DCM.

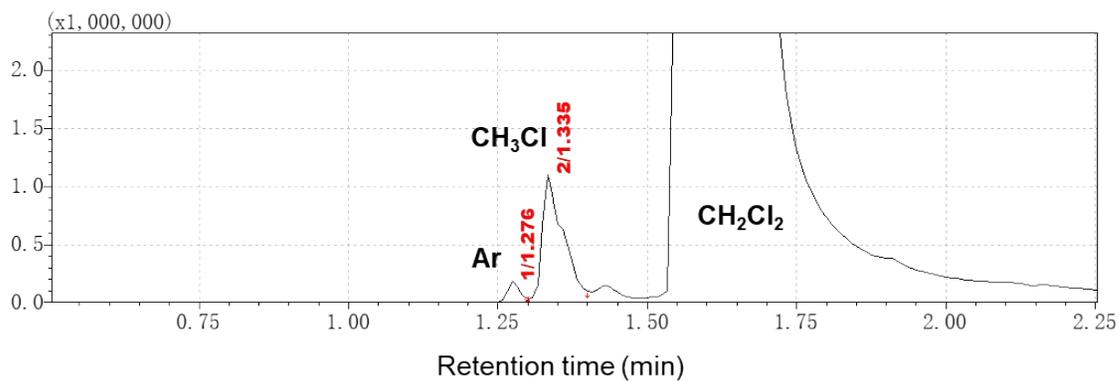


Fig. S7 GC-MS analysis of the reaction mixture of **1** + PPh₃ (10 equiv.) + n-Bu₄NCl (10 equiv.) in CH₂Cl₂ (refluxed, Ar).

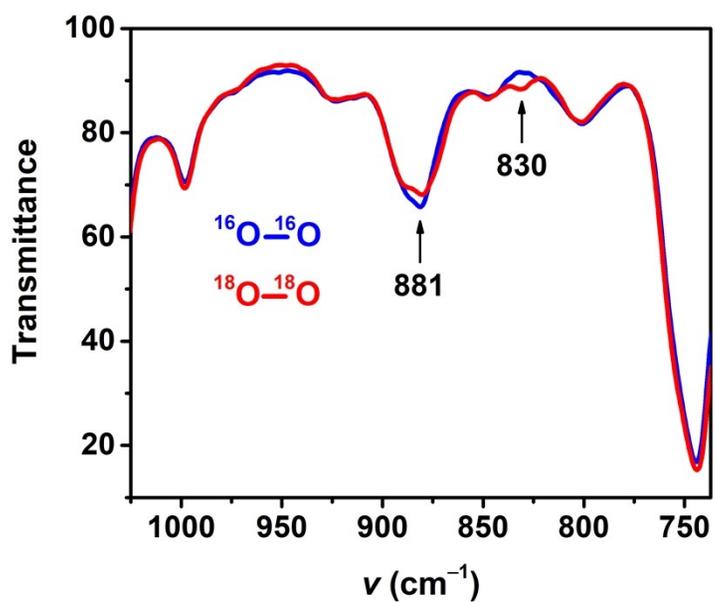


Fig. S8 Fourier transform infrared spectra of 2(¹⁶O₂) (blue line) and 2(¹⁸O₂) (red line).

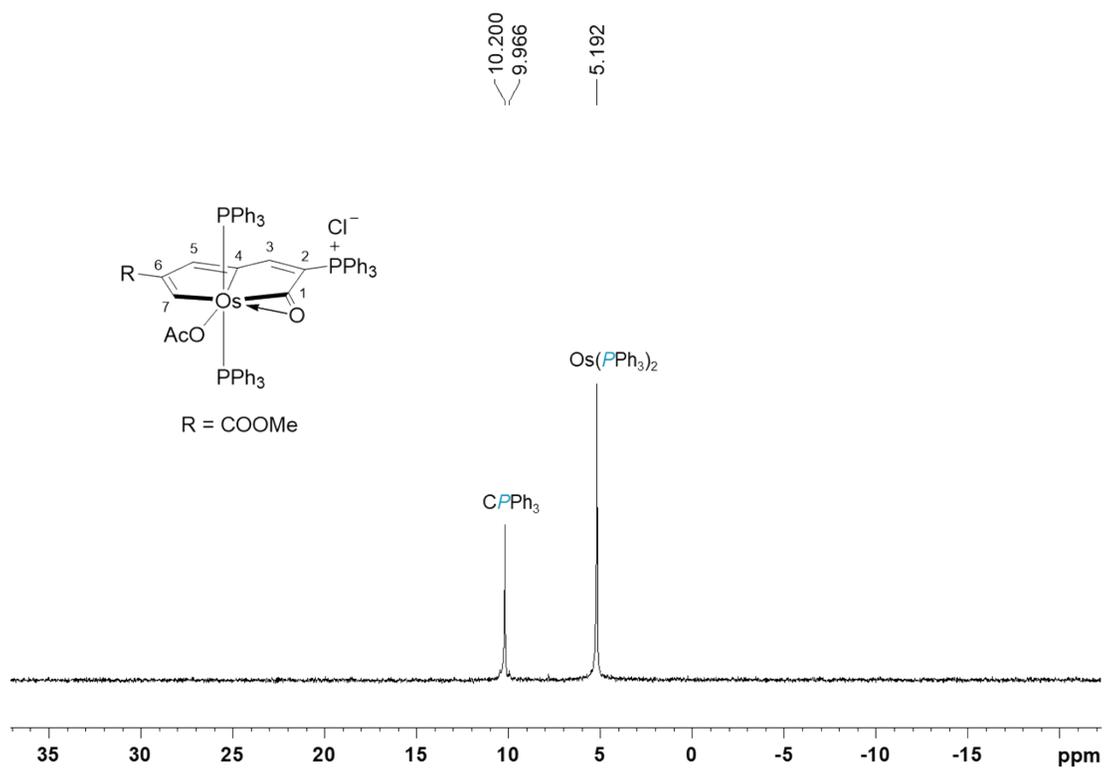


Fig. S9 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (161.9 MHz, CD_2Cl_2) for compound 3.

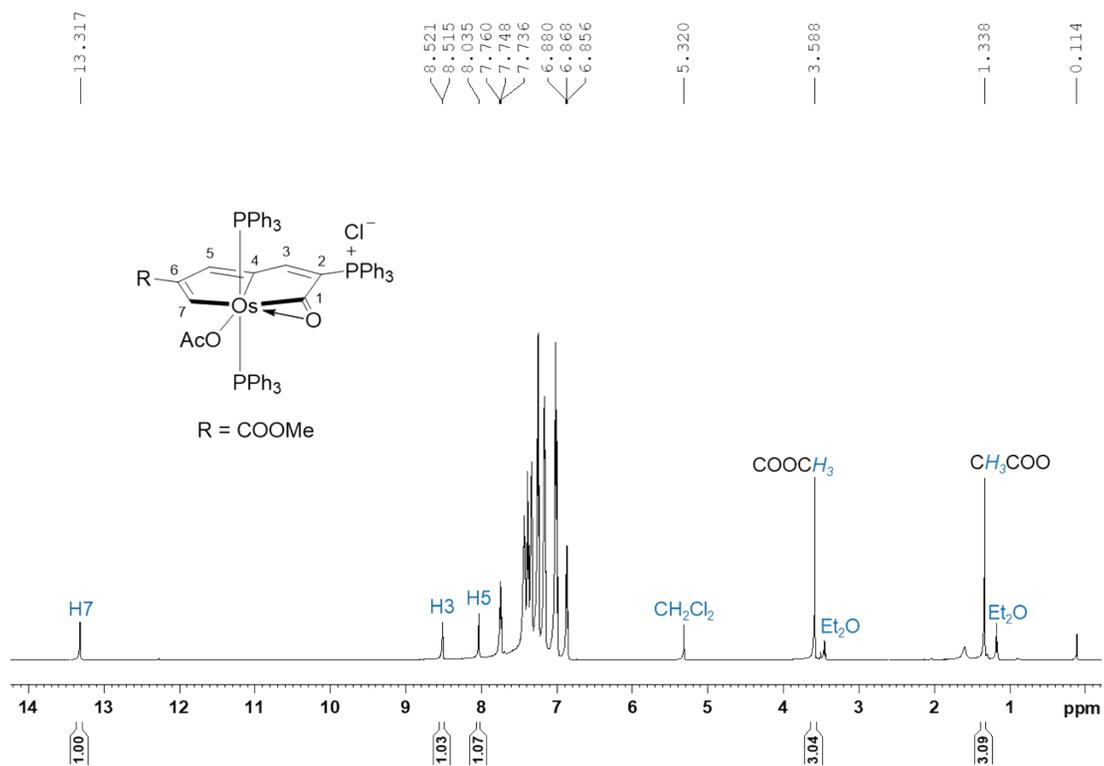
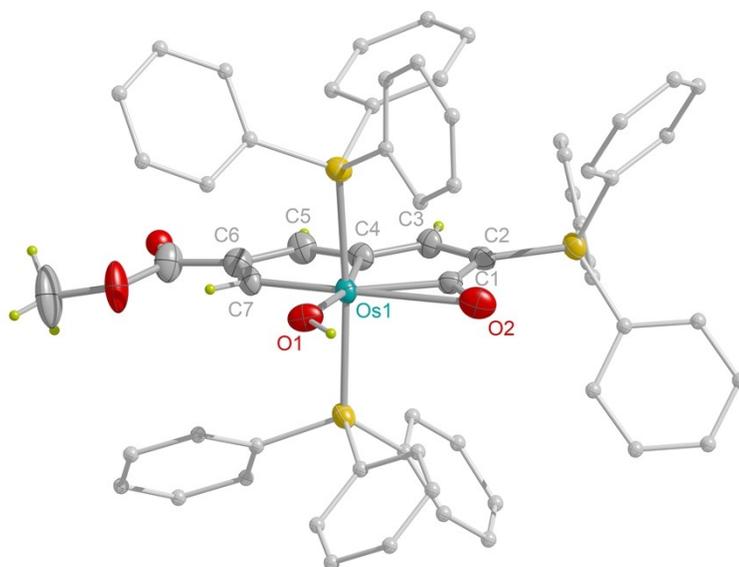


Fig. S10 The ^1H NMR spectrum (600.1 MHz, CD_2Cl_2) for compound 3.



Bond Distances (Å)					
Os1–O1	2.027(3)	Os1–O2	2.586(4)	Os1–C1	1.997(4)
Os1–C7	1.998(4)	C1–O2	1.228(5)	C1–C2	1.442(6)
C2–C3	1.378(6)	C3–C4	1.404(6)	C4–C5	1.371(6)
C5–C6	1.418(6)	C6–C7	1.370(6)	Os1–C4	2.127(4)
Bond Angles (°)					
O1–Os1–O2	95.83(12)	O2–Os1–C1	27.43(14)		
Os1–C1–O2	104.1(3)	Os1–O2–C1	48.5(2)		
Os1–C1–C2	125.9(3)	C1–C2–C3	108.7(4)		
C2–C3–C4	114.2(4)	Os1–C4–C3	119.4(3)		
C4–Os1–C1	71.66(17)	Os1–C4–C5	118.7(3)		
C4–C5–C6	112.7(4)	C5–C6–C7	111.6(4)		
Os1–C7–C6	124.1(3)	C7–Os1–C4	72.84(17)		
O1–Os1–C7	92.35(15)				

Fig. S13 Molecular structure of compound **4**. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms in phenyl groups and counter anion are omitted for clarity.

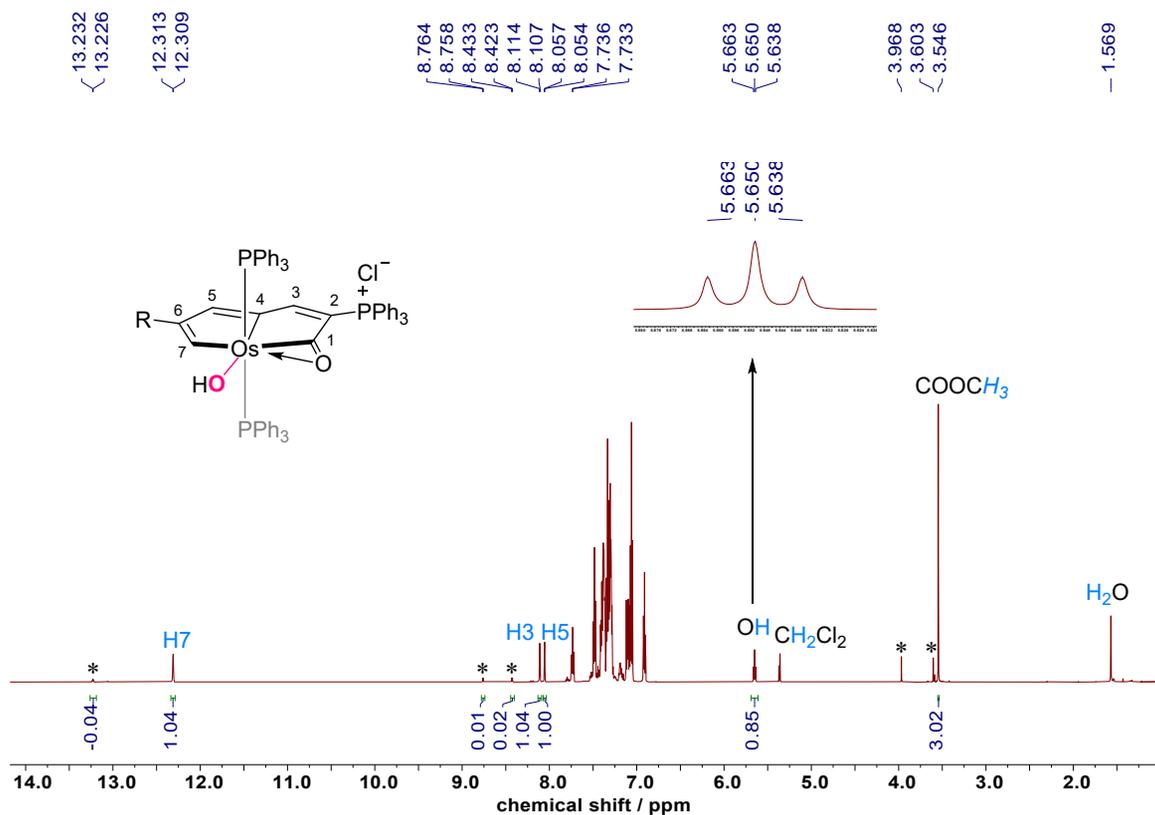


Fig. S14 The ^1H NMR spectrum (600.1 MHz, CD_2Cl_2) for compound 4.

The peaks marked with asterisk originate from complex 1. Based on the ^1H NMR integrations, the ratio of complex 4 to complex 1 is approximately 1:0.03.

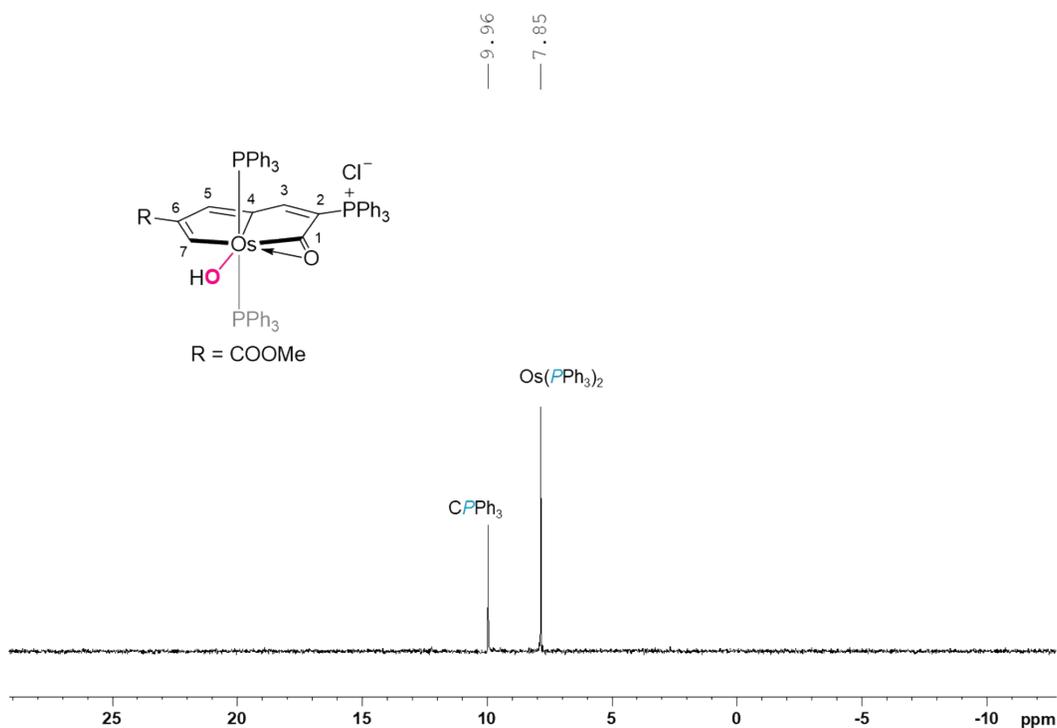


Fig. S15 The $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum (202.4 MHz, CD_2Cl_2) for compound 4.

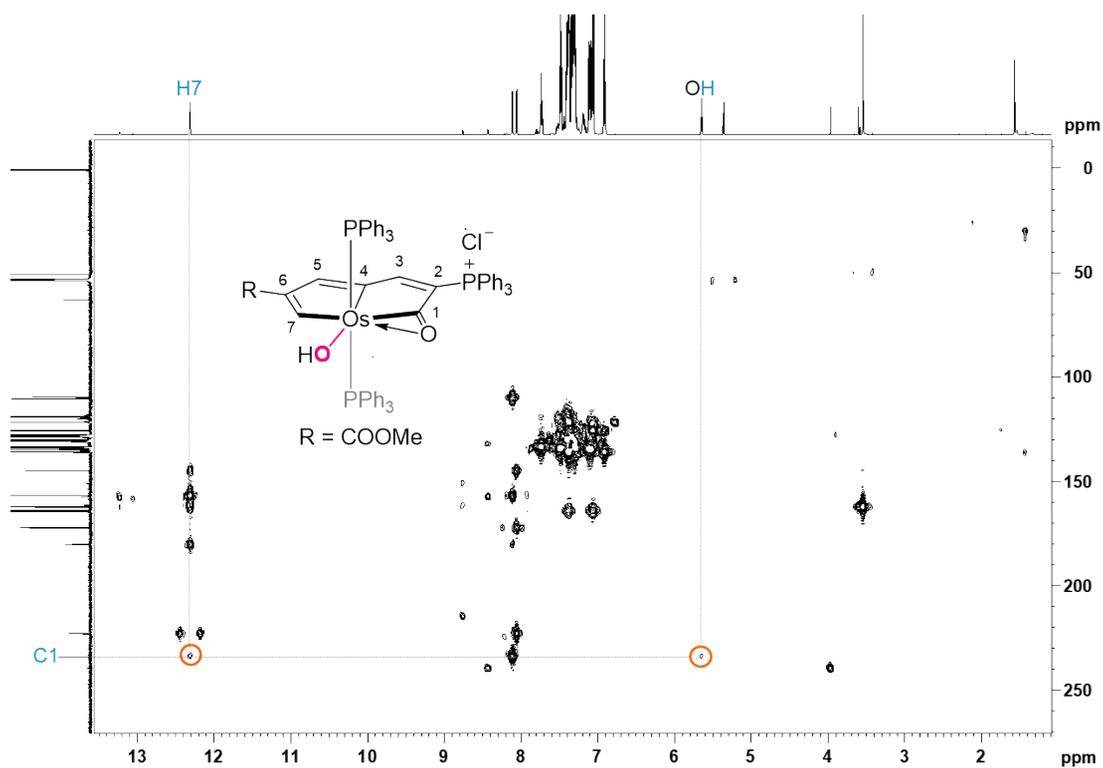


Fig. S18 Two-dimensional ^1H - ^{13}C HMBC spectrum for compound **4** in CD_2Cl_2 .

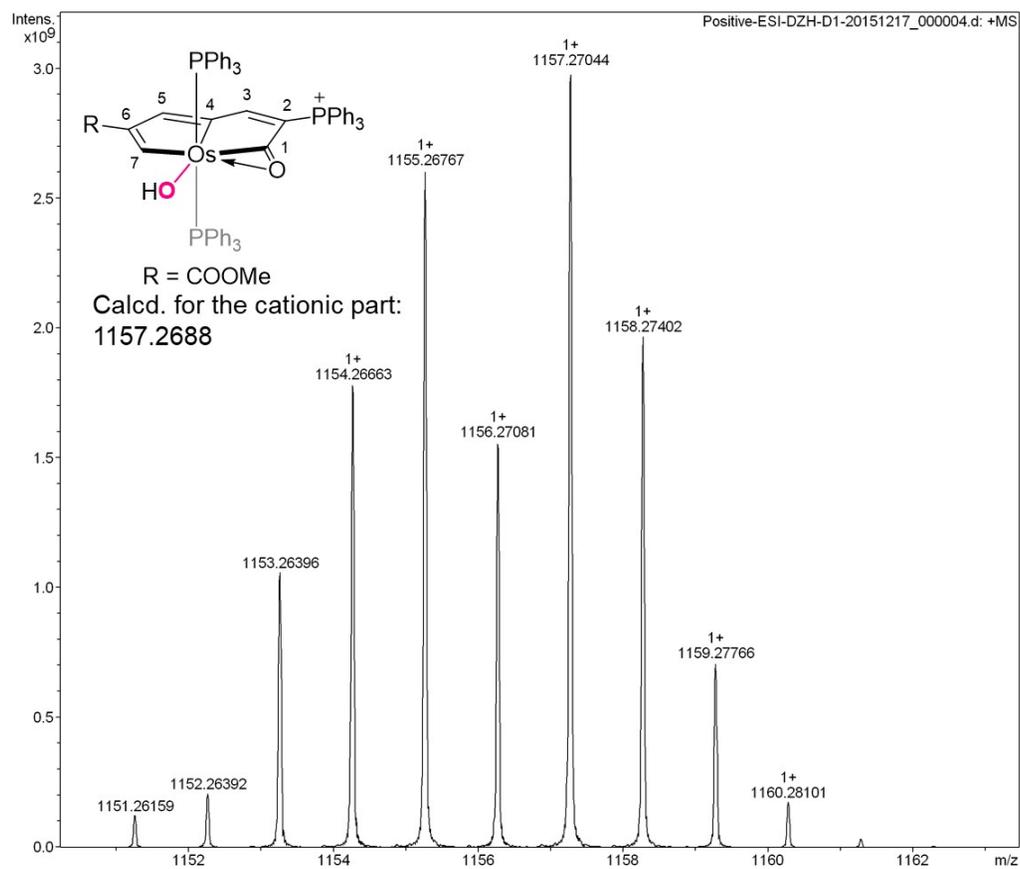


Fig. S19 Positive-ion ESI-MS spectrum for compound **4** measured in methanol.

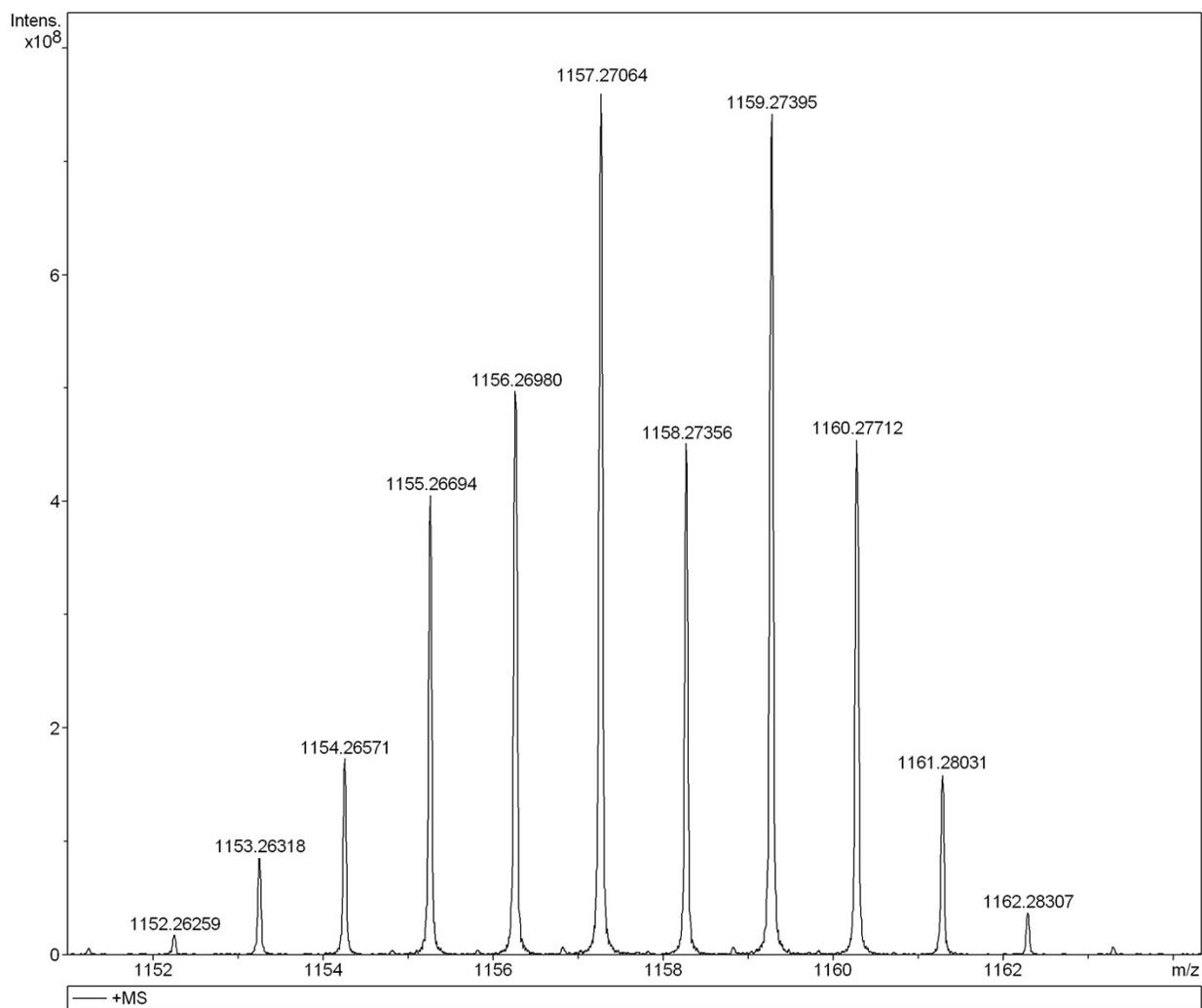
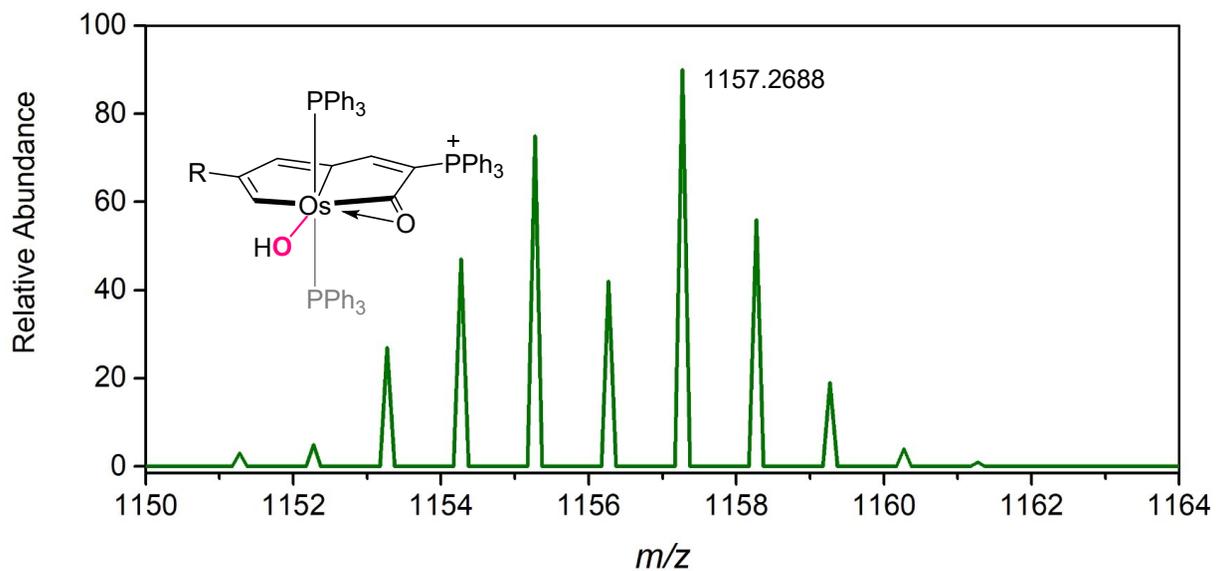


Fig. S20 High-resolution ESI-MS spectrum (Positive-ion mode) of compound 4 obtained from the reaction of $2(^{18}\text{O}_2)$ with NH_4Cl in the presence of triphenylphosphine.

A) Simulated for $C_{63}H_{52}O_4OsP_3^+$: 1157.2688



B) Simulated for $C_{63}H_{52}O_3^{18}O OsP_3^+$: 1159.2730

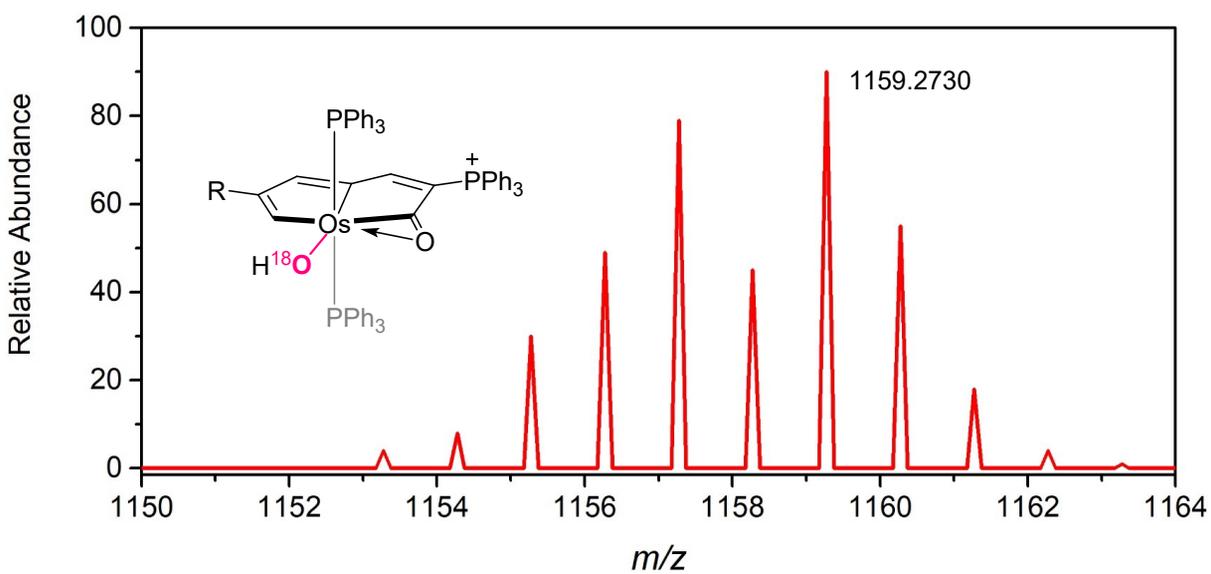


Fig. S21 Simulated isotope distribution patterns for 4(^{16}O) (A) and 4(^{18}O) (B). R = COOMe.

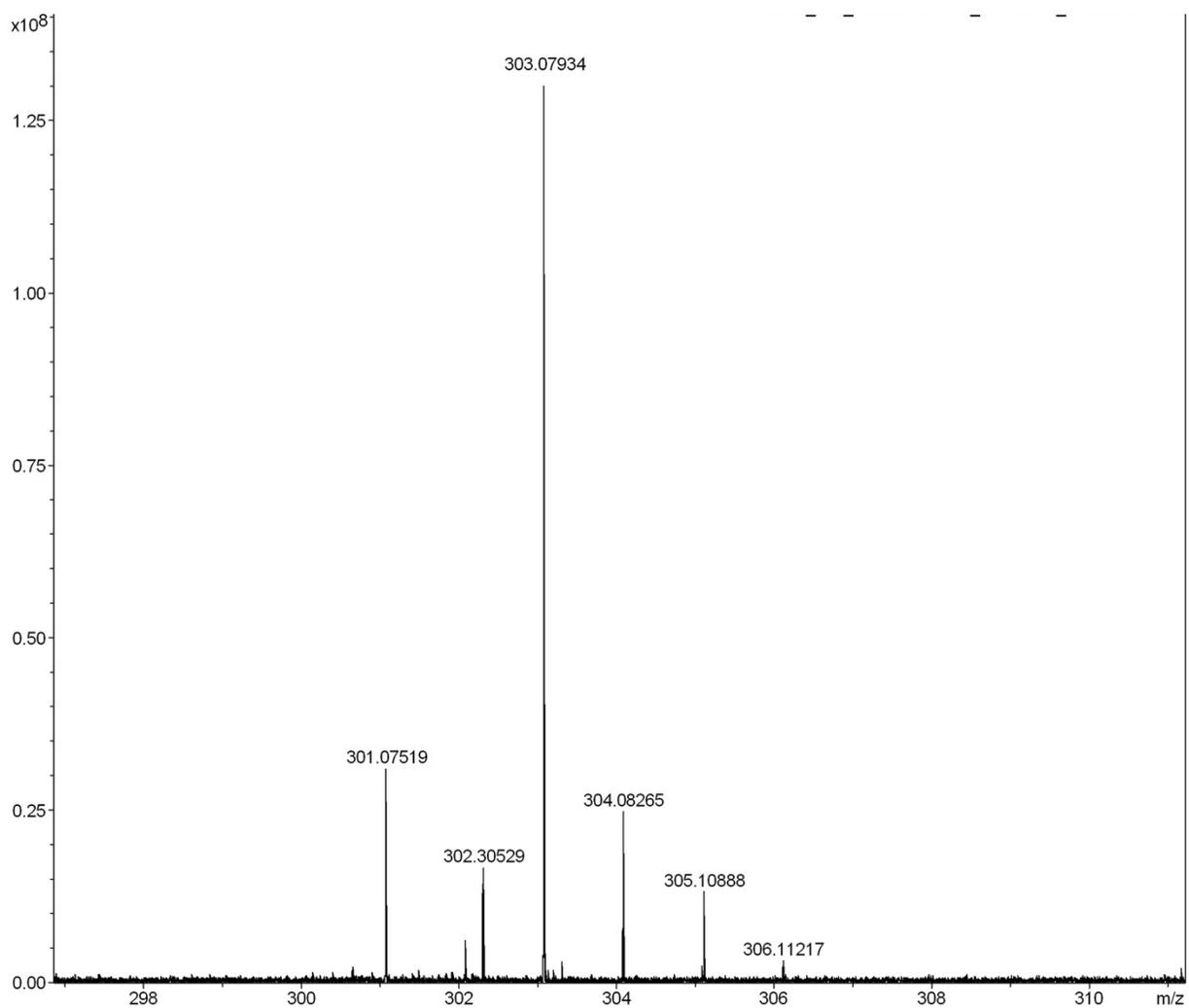
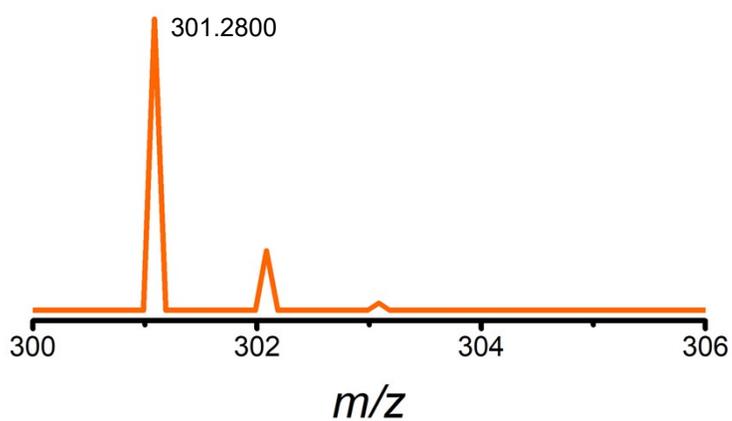


Fig. S22 High-resolution ESI-MS spectrum (Positive-ion mode) of triphenylphosphine oxide obtained from the reaction of $2(^{18}\text{O}_2)$ with NH_4Cl in the presence of triphenylphosphine.

A) Simulated for $[\text{O}=\text{PPh}_3+\text{Na}]^+$: 301.2800



B) Simulated for $[\text{}^{18}\text{O}=\text{PPh}_3+\text{Na}]^+$: 303.2801

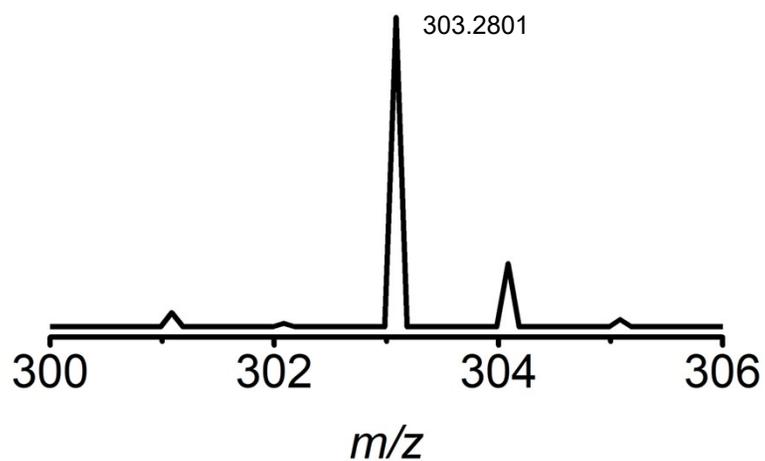


Fig. S23 Simulated isotope distribution patterns for $[\text{O}=\text{PPh}_3+\text{Na}]^+$ (A) and $[\text{}^{18}\text{O}=\text{PPh}_3+\text{Na}]^+$ (B).

4. X-ray Crystallographic Studies

Single-crystal X-ray diffraction data were collected using a Bruker APEX-II CCD diffractometer with Mo K α ($\lambda = 0.71073 \text{ \AA}$). Data reduction, scaling and absorption corrections were performed using SAINT (Bruker, V8.38A, after 2013). All data were corrected for absorption effects using the multi-scan technique. The structure was solved with the ShelXT 2014/5 (Sheldrick, 2014)² solution program using dual methods or the olex2.solve 1.3 (Bourhis et al., 2015)³ solution program using iterative methods and by using Olex2 (Dolomanov et al., 2009)⁴ as the graphical interface. The model was refined with ShelXL 2018/3 (Sheldrick, 2015)⁵ using full matrix least squares minimisation on F^2 . All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Single crystals suitable for X-ray diffraction were grown from a solution of CH₂Cl₂ layered with hexane. Some of the solvent molecules and counterions were disordered and refined with suitable restraints. Further details on the crystal data, data collection, and refinements are provided in the following Tables. The X-ray crystallographic coordinates for structures reported in this study have been deposited at the Cambridge Crystallographic Data Centre (CCDC), under deposition numbers 1892842 (2) and 1892836 (4). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S1. Crystal Data and Structure Refinement for Compound 2.

Empirical formula	C ₆₆ H ₅₇ Cl _{6.25} O _{4.5} OsP ₃
Formula weight	1426.79
Temperature/K	172.95(10)
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	13.0692(3)
b/Å	23.4824(6)
c/Å	20.1169(5)
α/°	90
β/°	96.239(3)
γ/°	90
Volume/Å ³	6137.3(3)
Z	4
ρ _{calc} /cm ³	1.544
μ/mm ⁻¹	2.477
F(000)	2865.0
Crystal size/mm ³	0.6 × 0.4 × 0.4
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	4.428 to 50.054
Index ranges	-15 ≤ h ≤ 15, -27 ≤ k ≤ 25, -23 ≤ l ≤ 16
Reflections collected	26259
Independent reflections	10818 [R _{int} = 0.0354, R _{sigma} = 0.0472]
Data/restraints/parameters	10818/52/758
Goodness-of-fit on F ²	1.172
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0571, wR ₂ = 0.1163
Final R indexes [all data]	R ₁ = 0.0655, wR ₂ = 0.1199
Largest diff. peak/hole / e Å ⁻³	2.00/-1.63

Table S2. Crystal Data and Structure Refinement for Compound 4.

Empirical formula	C _{88.5} H ₇₅ BCl ₃ O ₄ OsP ₃
Formula weight	1602.75
Temperature/K	181(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	13.0065(3)
b/Å	24.5208(5)
c/Å	23.9619(5)
α/°	90
β/°	96.580(2)
γ/°	90
Volume/Å ³	7591.9(3)
Z	4
ρ _{calc} /cm ³	1.402
μ/mm ⁻¹	1.900
F(000)	3260.0
Crystal size/mm ³	0.3 × 0.2 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.38 to 54.998
Index ranges	-16 ≤ h ≤ 16, -31 ≤ k ≤ 28, -31 ≤ l ≤ 31
Reflections collected	46781
Independent reflections	17402 [R _{int} = 0.0404, R _{sigma} = 0.0486]
Data/restraints/parameters	17402/105/948
Goodness-of-fit on F ²	1.098
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0479, wR ₂ = 0.0977
Final R indexes [all data]	R ₁ = 0.0625, wR ₂ = 0.1022
Largest diff. peak/hole / e Å ⁻³	1.51/-1.34

5. Theoretical Calculations

All the optimizations were performed with the Gaussian 16 software package.⁶ All of these structures evaluated were optimized at the B3LYP level^{7,8} of density functional theory with a SDD basis set and the related Stuttgart relativistic energy-consistent pseudopotentials to describe Os⁹ and the standard 6-31G* basis set was used for the C, O, P, and H atoms for all the complexes. Grimme's D3(BJ) empirical dispersion correction D3(BJ) was implemented to take the dispersion correction into account.¹⁰⁻¹² Frequency analyses have been performed to validate the stationary points as intermediate with zero imaginary frequency. Natural bond orbital (NBO) calculations were carried out using NBO 7.0 program¹³ at the B3LYP-D3(BJ)/def2-TZVP level of theory. Optimized structures were visualized by the IBOview program.¹⁴ To estimate the aromaticity of these systems, the nucleus-independent chemical shifts^{15,16} using the GIAO method were calculated.¹⁷

6 The Calculated Cartesian Coordinates

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Os	1.11157000	0.08609500	-0.43239900
P	1.09425600	2.54296800	-0.43352000
P	-3.53604200	-0.21458000	0.51690300
P	1.36501500	-2.35650100	-0.49039000
O	2.55228800	0.41463100	-1.88242900
O	1.32181100	0.20659300	-2.51326300
O	-1.81270100	-0.00988200	-1.70048400
C	-0.98213500	-0.03662800	-0.64825100
C	0.37523800	-0.08705600	1.53684800
C	-1.74964000	-0.15639300	0.55303000
C	3.06555300	-3.01216600	-0.72369700
C	-1.00209200	-0.19518300	1.73103200
H	-1.44824500	-0.29318000	2.71651000
C	2.75341900	0.08388700	0.80917300
H	3.75738900	0.14244100	0.39653100
C	0.81876900	3.17201500	-2.13661800
C	-4.16930900	-1.79615900	-0.10964100
C	-0.17201600	3.46189900	0.55194700
C	0.81964800	-3.08253300	1.10665300
C	1.27382700	-0.13185700	2.59721400
H	0.98856500	-0.25915300	3.63846000
C	2.68250400	3.26367000	0.14972700
C	2.61852800	-0.03044700	2.18369400
C	-3.55407300	2.39805100	-0.42869200
H	-2.67998700	2.54365600	0.19681900
C	-4.19368600	1.14950300	-0.48378700
O	4.93607900	0.07561100	2.59209900
C	3.36053400	-4.34519100	-0.38985200
H	2.59976600	-4.97992400	0.05385900
C	1.84957000	3.68521500	-2.93013600
H	2.85591600	3.76616800	-2.53743600
C	-0.50106600	3.02855700	1.84544100

H	-0.01284400	2.15797100	2.25666400
C	0.44144100	-3.27927600	-1.79101100
C	4.05239700	-2.21115100	-1.31367500
H	3.80606200	-1.19798900	-1.61180300
C	3.72755600	-0.11705400	3.16286900
C	-0.77009500	4.63958000	0.06929900
H	-0.50678300	5.02449800	-0.90855500
C	-0.11148200	-4.55245400	-1.57999700
H	-0.08193100	-5.00990700	-0.59744800
C	-1.44576800	0.05797100	-3.09103000
H	-0.48743500	0.54953000	-3.22322500
H	-2.24400800	0.62863600	-3.56808700
H	-1.42493800	-0.95767800	-3.48867700
C	-0.47868700	3.08989900	-2.66826600
H	-1.29004300	2.69546600	-2.06486900
C	-3.39091300	-2.59512900	-0.96270900
H	-2.39415600	-2.28901600	-1.25347600
C	-4.03360700	3.45251100	-1.20389000
H	-3.52903900	4.41141300	-1.16086400
C	0.42909700	-2.73149200	-3.08390400
H	0.88343600	-1.75869900	-3.24942100
C	-4.77989000	1.37718200	4.08031400
H	-5.05841700	2.35363800	4.46398500
C	-5.19301900	-4.20445700	-1.09109500
H	-5.59004800	-5.14120000	-1.47014300
C	1.73517800	-3.21088500	2.16216500
H	2.78790900	-3.01549600	1.99350900
O	3.56906400	-0.34934200	4.34754700
C	-5.30682100	0.96218900	-1.31404500
H	-5.79357800	-0.00539300	-1.37397300
C	-5.77888900	2.02511500	-2.08534800
H	-6.63855900	1.87858800	-2.73166500
C	4.63616800	-4.85728700	-0.61485500
H	4.85891700	-5.88559300	-0.34610000
C	-4.10566800	-0.02973400	2.23087400

C	2.72284800	4.24464800	1.15075200
H	1.80625500	4.63198600	1.58031200
C	-5.46383200	-2.21023900	0.25014800
H	-6.06684400	-1.60682300	0.92178800
C	-5.97170100	-3.41098600	-0.24466000
H	-6.97097300	-3.72831600	0.03628100
C	1.30112200	-3.56868300	3.43929000
H	2.02268000	-3.64232700	4.24683100
C	-1.71104300	5.32567000	0.83921700
H	-2.16004300	6.23475900	0.44969400
C	5.10920600	3.28062600	0.06715400
H	6.03394400	2.90345600	-0.35927500
C	5.62428000	-4.05031500	-1.18723200
H	6.61796300	-4.45203400	-1.36234000
C	5.32806000	-2.73414200	-1.54075400
H	6.08831300	-2.10841200	-1.99902300
C	-4.45824700	1.23270900	2.73039000
H	-4.48007900	2.09713100	2.07587700
C	-0.69961700	-5.24797500	-2.63847700
H	-1.12106900	-6.23380100	-2.46315500
C	-0.53959900	-3.32831100	1.35733800
H	-1.26902100	-3.22218800	0.56381000
C	3.89002700	2.78468400	-0.39040300
H	3.86269200	2.02594400	-1.16387100
C	-0.96889100	-3.70477700	2.62963800
H	-2.02144400	-3.91433000	2.80039000
C	-5.14343100	3.26738000	-2.03270500
H	-5.51072100	4.08991100	-2.63880100
C	1.58640100	4.10427600	-4.23693200
H	2.39533900	4.49801600	-4.84475000
C	-3.90509600	-3.79780200	-1.44627500
H	-3.28925600	-4.40940500	-2.09710000
C	-4.74919900	0.27146800	4.93241300
H	-5.00112200	0.38859900	5.98186400
C	-1.45110700	3.70872400	2.60954800

H	-1.70128800	3.34312300	3.60115000
C	-0.73127700	-4.68808000	-3.91796900
H	-1.18383000	-5.23403000	-4.74051800
C	-2.06941200	4.85328500	2.10378500
H	-2.80829900	5.38515800	2.69580300
C	-4.07545700	-1.14179800	3.08976800
H	-3.80055700	-2.11997200	2.70838100
C	-0.74094400	3.52141900	-3.96549500
H	-1.75220000	3.46086400	-4.35817400
C	-0.05174100	-3.81694100	3.67716600
H	-0.38712800	-4.10219000	4.66979500
C	0.29497600	4.02554200	-4.75727900
H	0.09431900	4.35799700	-5.77131100
C	-4.39756200	-0.98724300	4.43668300
H	-4.37473700	-1.84754700	5.09809000
C	-0.15871800	-3.43329400	-4.13799900
H	-0.15976100	-3.00098600	-5.13455900
C	3.94922700	4.72959300	1.61092600
H	3.96653900	5.48492400	2.39089800
C	5.14304600	4.24974800	1.07280000
H	6.09455000	4.62926100	1.43304700
C	6.05692600	-0.00250000	3.48961600
H	6.10559600	-0.98826400	3.95980700
H	5.97443700	0.75625100	4.27223100
H	6.93886800	0.17366100	2.87448100

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Os	1.25064200	-0.03265000	-0.57433600
P	1.19872500	2.38488500	-0.64567900
P	1.29647100	-2.45298500	-0.51362200
P	-3.41145900	0.00896600	0.45483400
C	2.90370100	0.09399000	0.65324200
H	3.91282400	0.13060000	0.24254400
O	-1.50765500	0.05113000	-1.86829100

C	0.52039500	0.00978000	1.40665400
C	0.47175800	3.07320800	0.90289700
C	2.82625700	3.23450100	-0.79367000
O	3.56617100	0.34465700	4.23856800
C	1.41427300	0.10184200	2.45682100
H	1.11721600	0.14160800	3.50206700
C	2.77238700	0.15369700	2.03143100
C	-0.90955000	3.29445000	0.99339400
H	-1.53586000	3.18035000	0.11803500
O	5.10447100	0.32810300	2.57791300
C	0.20278100	3.20859800	-1.96443600
C	-1.63849300	-0.04334100	0.47619600
C	-0.88294300	-0.00222900	-0.79011200
C	0.75478100	-3.33716000	-2.03593100
C	-0.86871300	-0.03432700	1.62532300
H	-1.28366600	-0.05253300	2.62917500
C	0.20500700	-3.20893000	0.77232000
C	-0.16559000	2.48653700	-3.10747600
H	0.13089100	1.44777400	-3.19414500
C	1.25712100	3.22402800	2.05631800
H	2.32433600	3.03802600	2.00984400
C	2.95740500	-3.17017500	-0.16897300
C	-4.16877500	-1.22480800	-0.64244600
C	3.84395700	2.57833000	-1.50216300
H	3.64775000	1.58829800	-1.90768900
C	5.30700600	4.48150900	-1.17334900
H	6.27114800	4.96245700	-1.31385800
C	4.05132700	-2.59407200	-0.83598400
H	3.87357400	-1.75761000	-1.50614000
C	4.29215200	5.14160400	-0.47616700
H	4.46333700	6.13657500	-0.07437600
C	-4.07610200	1.63666100	-0.03934400
C	-3.97830700	-0.34387800	2.14749400
C	3.93780900	0.27842400	2.92345900
C	-5.55753400	-1.19472000	-0.84445300

H	-6.16306500	-0.42206400	-0.37882700
C	0.67237800	3.59233800	3.26801500
H	1.29527400	3.69785100	4.15158900
C	-0.15504300	4.56386400	-1.85793200
H	0.12593300	5.13462700	-0.97856700
C	-6.15991200	-2.15499600	-1.65594500
H	-7.23428500	-2.13197700	-1.81166900
C	-3.39051300	-2.20450300	-1.26776500
H	-2.32031400	-2.20709000	-1.13553000
C	5.07788600	3.20473800	-1.68813800
H	5.86203800	2.68831500	-2.23456100
C	-1.49405900	3.66646900	2.20507500
H	-2.56478100	3.85178400	2.24367300
C	-0.18721600	-2.74157300	-2.88840900
H	-0.50178800	-1.71963300	-2.72614900
C	0.50419100	-3.02158900	2.13264500
H	1.42518000	-2.52596100	2.41563800
C	-0.70492800	3.81241700	3.34815000
H	-1.15686000	4.10390800	4.29245200
C	-0.70765600	-3.46527500	-3.96484500
H	-1.43564200	-2.99290800	-4.61857600
C	-3.74637500	0.59666900	3.16729200
H	-3.29135000	1.55447900	2.93363400
C	-3.54647700	2.25736100	-1.18565700
H	-2.77342400	1.75976000	-1.76185000
C	-0.88538800	5.18306800	-2.86988500
H	-1.15705600	6.23098000	-2.77584300
C	-1.26332800	4.45573600	-4.00398000
H	-1.83053100	4.93885300	-4.79549800
C	3.05519700	4.52487400	-0.29073900
H	2.27810200	5.04487700	0.26016500
C	-0.90154000	3.11311100	-4.11814700
H	-1.18740000	2.54333900	-4.99772500
C	-5.00763600	4.15427600	-0.82623400
H	-5.36130700	5.13712900	-1.12424400

C	3.16801700	-4.26386600	0.68228400
H	2.33263900	-4.72775200	1.19582000
C	-0.97727400	-3.87957200	0.43306000
H	-1.20579500	-4.07780500	-0.60741300
C	5.33520000	-3.09871100	-0.63650500
H	6.17588400	-2.64136100	-1.15022000
C	1.18244900	-4.64962500	-2.29127100
H	1.91796000	-5.11711100	-1.64430600
C	-5.37995100	-3.13581800	-2.27622200
H	-5.85149600	-3.87633600	-2.91585700
C	-5.55151600	3.52977100	0.29767400
H	-6.33288600	4.01938500	0.87154600
C	-4.53023200	-1.59209300	2.46633200
H	-4.69432200	-2.32919500	1.68822100
C	-5.08971200	2.27318300	0.69432100
H	-5.51438800	1.80132200	1.57366400
C	-3.99695200	-3.15709800	-2.08528900
H	-3.37777000	-3.89705500	-2.58373800
C	-4.07818900	0.29046200	4.48545700
H	-3.89514200	1.01987000	5.26860200
C	-0.28557700	-4.77334700	-4.20965900
H	-0.68773200	-5.32901500	-5.05262100
C	5.54345200	-4.17823500	0.22577600
H	6.54680700	-4.56290100	0.38601500
C	-4.01093000	3.51499100	-1.56778500
H	-3.57347900	3.99317200	-2.43791500
C	4.65394800	0.46787700	5.16097400
H	5.23054600	1.37735400	4.96652500
H	5.33041300	-0.38874900	5.08440900
H	4.20150000	0.50833100	6.15314200
C	-1.57747500	-4.08126500	2.76824700
H	-2.27264600	-4.40185700	3.53912600
C	0.66621100	-5.36242800	-3.37350800
H	1.00709400	-6.37660700	-3.56227300
C	-1.86916400	-4.30143500	1.42228200

H	-2.78844000	-4.80361400	1.13341100
C	-0.37744000	-3.45740000	3.12035900
H	-0.13053500	-3.29876400	4.16636200
C	4.45835900	-4.76135400	0.88083300
H	4.61190300	-5.60430100	1.54903300
C	-4.85724800	-1.89164600	3.78960800
H	-5.28344000	-2.86086100	4.03036600
C	-4.63502700	-0.95300800	4.79791900
H	-4.88984200	-1.18991600	5.82667000
O	1.27676200	-0.17371100	-2.64487400
O	2.60678300	-0.16129500	-2.16358700

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Os	-0.00115500	0.05428200	-0.09578600
P	2.43124100	0.05235900	-0.16142300
P	-2.41627800	0.00410900	-0.08781200
O	-0.00960400	0.33588100	-2.15744900
O	0.15404600	1.58443600	-1.52142800
O	-0.16229700	2.82050400	1.48606800
C	-0.03477900	1.47406800	1.48635400
C	0.05147600	-1.07695600	1.69655100
C	0.13899500	0.99409500	2.80631100
C	-3.22880600	-1.24124400	-1.17972600
C	0.15657600	-0.37984300	2.91417600
H	0.23080600	-0.89416500	3.87080700
C	0.00302400	-1.95127500	-0.63776200
H	0.02244400	-2.21393000	-1.69528200
C	3.20336200	1.60926900	-0.77279300
C	3.23692100	-0.22465500	1.46993600
C	-3.04217200	-0.31892900	1.60658900
C	0.03243400	-2.45717500	1.61906100
H	0.06198800	-3.09457500	2.50387500
C	3.16977100	-1.21657600	-1.27295300
C	0.00106800	-2.96608900	0.29325700

C	-4.48128100	-1.80179700	-0.88947000
H	-4.98437000	-1.56625600	0.04243100
C	4.33519700	1.59585000	-1.59966700
H	4.76125700	0.65390300	-1.92662700
C	3.20880800	-1.50840900	2.03986700
H	2.77030400	-2.33172300	1.48731700
C	-3.29300500	1.50992500	-0.69273300
C	-2.62298500	-1.51955000	-2.41434200
H	-1.68470500	-1.03649000	-2.66293300
C	3.78938000	0.83152200	2.20567200
H	3.82255600	1.83009100	1.78440200
C	-4.43490300	2.05526500	-0.08953100
H	-4.84478300	1.61357500	0.81188400
C	-0.78226400	3.54502500	0.41066300
H	-0.61415700	3.06569000	-0.55067000
H	-0.35130500	4.54822600	0.43368500
H	-1.85815800	3.60723800	0.60303600
C	2.66896900	2.84171600	-0.36931600
H	1.79414500	2.86592900	0.26429800
C	-2.81121300	2.06944900	-1.88851500
H	-1.93538800	1.64451200	-2.36402000
C	-3.24269700	-1.63418900	2.05549200
H	-3.12709600	-2.46372900	1.36697600
C	-5.09283400	-2.66720400	-1.79772400
H	-6.05789800	-3.10407100	-1.55659300
C	4.32056200	-1.95242200	-0.95828500
H	4.80841100	-1.82371100	0.00148600
C	-3.57130100	-1.88617900	3.38674800
H	-3.72731500	-2.90962700	3.71570900
C	4.30252900	0.60916900	3.48554400
H	4.72579500	1.43911200	4.04414600
C	3.11438800	-2.27432200	-3.45543300
H	2.64609700	-2.39076700	-4.42886800
C	-4.47237700	-2.96292500	-3.01290200
H	-4.95043600	-3.63628000	-3.71881400

C	-3.24341100	-2.37722400	-3.32300600
H	-2.76432800	-2.58557900	-4.27554600
C	-5.05948700	3.17287300	-0.64810300
H	-5.93922600	3.59189600	-0.16753500
C	-3.13161400	0.73069500	2.53378900
H	-2.92594800	1.74930100	2.22335700
C	2.57504100	-1.37575800	-2.53611200
H	1.69652300	-0.78436400	-2.77957400
C	-3.46405500	0.47686700	3.86478000
H	-3.53380500	1.30295600	4.56647300
C	4.91941600	2.79416200	-2.01538400
H	5.79258700	2.76891200	-2.66123200
C	3.73244000	-1.72994200	3.31202900
H	3.70812700	-2.72985400	3.73616000
C	-4.56162500	3.74240500	-1.82092100
H	-5.04749700	4.61308200	-2.25244000
C	4.27649100	-0.66969800	4.04161500
H	4.67949200	-0.84152900	5.03572400
C	3.26213900	4.03590600	-0.77537500
H	2.83698900	4.98236600	-0.45333900
C	-3.68970600	-0.83121000	4.29423000
H	-3.94762100	-1.02876700	5.33078200
C	4.38626900	4.01599100	-1.60419900
H	4.84154400	4.94725900	-1.92942000
C	-3.44400000	3.18096300	-2.44359900
H	-3.05748800	3.61166200	-3.36290400
C	4.85138900	-2.85680800	-1.88161800
H	5.73985400	-3.42662900	-1.62412000
C	4.24857700	-3.02254100	-3.12902800
H	4.66388700	-3.72596700	-3.84539800
H	0.17634500	1.67822400	3.64903800
C	-0.01049200	-4.43865300	-0.03233400
H	0.86004900	-4.95254700	0.39429000
H	-0.90318700	-4.93198200	0.37258600
H	0.00038800	-4.60225500	-1.11341600

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Os	0.03047700	0.00467800	-0.10053800
P	2.46364300	0.02364500	-0.15560000
P	-2.39036700	0.04053500	-0.07629500
O	-0.10650200	0.50346700	-2.09844000
O	0.24755500	1.67461700	-1.39075800
O	0.00878000	2.45638300	1.85532700
C	0.07140700	1.14549200	1.64920600
C	0.01780700	-1.40569900	1.48667000
C	0.17148700	0.46462300	2.92060200
C	-3.25271100	-1.14587600	-1.19852600
C	0.14829600	-0.89055900	2.82245000
H	0.18230200	-1.54790200	3.68958900
C	0.00612300	-2.01629900	-1.03649400
H	1.04474500	-2.23479200	-1.31041300
C	3.08477100	1.73681700	0.11126300
C	3.35372100	-1.01846200	1.08256600
C	-3.03181800	-0.26792400	1.62038100
C	-0.23017000	-2.72852400	1.27155400
H	-0.31594600	-3.45443100	2.08159000
C	3.30672100	-0.49828100	-1.71001900
C	-0.49586600	-3.08658000	-0.10598900
C	-4.34524700	-1.94031700	-0.82808500
H	-4.72207700	-1.92006800	0.18787100
C	3.49178800	2.52291500	-0.97595900
H	3.52218300	2.09438300	-1.97121700
C	3.04791600	-2.39001800	1.09616000
H	2.29065500	-2.78008600	0.42899700
C	-3.28120900	1.57442200	-0.59859900
C	-2.82460100	-1.15268700	-2.53701400
H	-2.00352000	-0.50731300	-2.83348800
C	4.36382000	-0.54832800	1.93378600
H	4.65449600	0.49509200	1.91619200

C	-4.63629400	1.75646900	-0.27278000
H	-5.14658500	1.03390000	0.35668500
C	-0.06739700	3.41587800	0.78277000
H	0.73680400	3.25565900	0.06808200
H	0.03636100	4.38641900	1.26886400
H	-1.03290800	3.33715800	0.28540900
C	3.03405400	2.31926200	1.38850500
H	2.69500500	1.73665600	2.23813700
C	-2.64550500	2.49904000	-1.43871800
H	-1.59946200	2.35527400	-1.69275300
C	-3.11909700	-1.57073100	2.13523900
H	-2.90118100	-2.41965500	1.49752400
C	-4.96823900	-2.76406700	-1.76799800
H	-5.80941800	-3.38132800	-1.46484000
C	4.64465800	-0.92688500	-1.69971900
H	5.18939800	-0.99625400	-0.76373300
C	-3.46242700	-1.78307000	3.47095200
H	-3.53212100	-2.79862900	3.85049800
C	5.02448100	-1.42115100	2.80266400
H	5.80206100	-1.03699200	3.45691200
C	3.26104300	-0.76430700	-4.11788500
H	2.71866000	-0.70113200	-5.05721300
C	-4.51805800	-2.79191300	-3.08809500
H	-5.00248900	-3.43634700	-3.81630200
C	-3.45166300	-1.97504300	-3.47167500
H	-3.10555000	-1.97625800	-4.50143200
C	-5.33379800	2.86345900	-0.75134700
H	-6.37871300	2.99801500	-0.48581700
C	-3.26454900	0.81491500	2.48303200
H	-3.18268800	1.83099300	2.11132900
C	2.61553200	-0.41690800	-2.92820700
H	1.58077000	-0.08366000	-2.92446300
C	-3.60079600	0.60048300	3.81964200
H	-3.77916300	1.45125100	4.47100900
C	3.84473400	3.86003300	-0.78729900

H	4.15155400	4.45789100	-1.64066800
C	3.71192900	-3.25981900	1.95820000
H	3.45726100	-4.31574000	1.95352400
C	-4.69247600	3.79283100	-1.57601500
H	-5.23811000	4.65445000	-1.95088700
C	4.69702400	-2.77648500	2.82267000
H	5.21209400	-3.45359000	3.49819500
C	3.39967400	3.65192900	1.57615700
H	3.35678300	4.08455900	2.57157800
C	-3.70457400	-0.69962700	4.31707300
H	-3.96895500	-0.86724600	5.35730700
C	3.80319400	4.42762600	0.48740400
H	4.08055600	5.46796800	0.63151400
C	-3.35417400	3.60489400	-1.91948200
H	-2.85167000	4.31900300	-2.56617200
C	5.27994600	-1.27234500	-2.89142400
H	6.31390200	-1.60551100	-2.87310200
C	4.58871700	-1.19289600	-4.10351900
H	5.08514000	-1.46568600	-5.03084600
H	0.20572900	1.02670600	3.84885000
C	-1.16816700	-4.19582500	-0.47804500
H	-1.50003900	-4.92834700	0.25362400
H	-1.42223500	-4.38246600	-1.51668000
H	-0.55772500	-1.98870700	-1.96933300

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Os	0.00191000	-0.22213200	-0.03577400
P	-2.42948800	-0.25793500	0.00054800
P	2.41709300	-0.19151100	-0.06731400
O	0.02031500	-2.11540000	0.82476000
O	-0.15671700	-1.15108000	1.83946300
O	0.19530000	2.09395200	2.14041900
C	0.04298400	1.70835100	0.85280700
C	-0.05123300	1.16330000	-1.63656800

C	-0.13953800	2.84908800	0.01979200
C	3.25685400	-1.53775100	-1.00515700
C	-0.15596000	2.52860100	-1.32327600
H	-0.23384800	3.29257900	-2.09599100
C	-0.01228000	-1.33490000	-1.79070100
H	-0.03481600	-2.42212200	-1.73286200
C	-3.19171100	-0.37076200	1.67510200
C	-3.19923000	1.24429800	-0.73310900
C	3.01906300	1.39331100	-0.77203400
C	-0.04074300	0.68809300	-2.93715500
H	-0.07264200	1.34835500	-3.80383200
C	-3.20323500	-1.67710700	-0.87719800
C	-0.01540400	-0.72493500	-3.02276600
C	4.49259900	-1.37028000	-1.64575700
H	4.96960900	-0.39623300	-1.67081000
C	-4.32598000	-1.15776400	1.91795500
H	-4.76215000	-1.74813400	1.12006800
C	-3.20605800	1.40196300	-2.12876300
H	-2.83165700	0.60513400	-2.76174300
C	3.28616200	-0.40084200	1.54642400
C	2.68503700	-2.81769800	-0.93989200
H	1.75794900	-2.95604500	-0.39420300
C	-3.65873400	2.29606300	0.07018800
H	-3.66145700	2.19617000	1.14991000
C	4.43437600	0.31372200	1.91675300
H	4.84753400	1.06969700	1.25821300
C	0.79035700	1.26235100	3.15068000
H	0.61746700	0.20582200	2.96069700
H	0.34605000	1.57269100	4.09892800
H	1.86730100	1.45628300	3.17372900
C	-2.64472100	0.37667200	2.72839100
H	-1.76800200	0.98365500	2.55596800
C	2.79964900	-1.41059100	2.39389300
H	1.92170300	-1.97559500	2.10511900
C	3.20647100	1.53413400	-2.15581200

H	3.10330300	0.67249300	-2.80578800
C	5.12180100	-2.45730800	-2.25489300
H	6.07369800	-2.31351600	-2.75843900
C	-4.37230200	-1.57563200	-1.64387600
H	-4.85100700	-0.61341100	-1.78877200
C	3.49999800	2.78099500	-2.70772800
H	3.64547100	2.87082500	-3.78043800
C	-4.11457100	3.48199200	-0.50937800
H	-4.46431700	4.28943200	0.12758100
C	-3.18765900	-4.07340600	-1.25112400
H	-2.72780000	-5.04441000	-1.08982100
C	4.53611400	-3.72362500	-2.20972500
H	5.02812400	-4.56832000	-2.68369000
C	3.32357900	-3.90257400	-1.54040600
H	2.87153500	-4.88880800	-1.48407800
C	5.06022000	0.05552400	3.13827500
H	5.94478400	0.62093200	3.41816700
C	3.08826900	2.53834800	0.03705100
H	2.89242600	2.46538700	1.10129800
C	-2.61843100	-2.93862100	-0.67484800
H	-1.72525500	-3.01093400	-0.05972400
C	3.38367400	3.78435200	-0.51612200
H	3.43561000	4.65770600	0.12743900
C	-4.89999600	-1.19498600	3.19053100
H	-5.77533000	-1.81421400	3.36524900
C	-3.67433800	2.58133700	-2.70519500
H	-3.67738700	2.68583100	-3.78654600
C	4.55729400	-0.92913900	3.99015100
H	5.04412300	-1.12709900	4.94104600
C	-4.12441700	3.62803700	-1.89668200
H	-4.48218500	4.54994800	-2.34642800
C	-3.22721500	0.34758800	3.99421200
H	-2.79163700	0.93360000	4.79870000
C	3.59424300	3.90877100	-1.88991300
H	3.82215500	4.87910400	-2.32173800

C	-4.35427400	-0.44279000	4.23084200
H	-4.80168700	-0.47404400	5.22033500
C	3.43391900	-1.66694700	3.60913900
H	3.04398600	-2.44330100	4.26125900
C	-4.93249400	-2.71588400	-2.22507800
H	-5.83481100	-2.62502200	-2.82333200
C	-4.34065500	-3.96497000	-2.03307400
H	-4.77898400	-4.85021800	-2.48546000
H	-0.01887300	-1.26789800	-3.96577200
C	-0.20581900	4.24764700	0.56418300
H	0.72195700	4.50997700	1.08567400
H	-0.36768100	4.97075500	-0.23965700
H	-1.01769200	4.35076800	1.29206000

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Os	-0.00840900	-0.16797900	-0.11150900
P	-2.43183900	-0.25464200	-0.04243200
P	2.42834300	-0.14000500	-0.11276500
O	0.14361300	-2.16945900	0.36213600
O	-0.14489200	-1.47457200	1.55352400
O	0.16321600	1.63809000	2.39858500
C	-0.01122100	1.50515600	1.09239100
C	0.07531900	1.43267200	-1.49832300
C	-0.23222100	2.84176800	0.48842900
C	3.31551800	-1.23527600	-1.29823300
C	0.00430500	2.85202100	-0.99242400
H	0.94118200	3.38502100	-1.20361700
C	-0.05961300	-1.04228600	-2.06068400
H	-0.20223400	-2.11821400	-2.14898300
C	-3.01188100	-0.12292000	1.70158100
C	-3.31624900	1.06961400	-0.96343100
C	3.04107000	1.56432300	-0.42525500
C	0.19296800	1.15903000	-2.82203000
H	0.25929900	1.93644300	-3.58405100

C	-3.26452100	-1.77243500	-0.66539700
C	0.10391700	-0.24922000	-3.14300400
C	4.60067200	-0.93644300	-1.77493400
H	5.07816800	0.00196200	-1.51331400
C	-3.42891400	-1.25949100	2.40775500
H	-3.48891400	-2.21783300	1.90468600
C	-3.00733100	1.18262000	-2.32910300
H	-2.27268200	0.51686600	-2.76401600
C	3.26004300	-0.68741700	1.44433600
C	2.74329800	-2.47786500	-1.60522300
H	1.77499000	-2.73175500	-1.19473000
C	-4.29619400	1.90740000	-0.41392800
H	-4.58248500	1.81106700	0.62655500
C	4.37573800	-0.04533100	2.00168200
H	4.77764200	0.85314900	1.54725700
C	0.30334800	0.52988000	3.31439800
H	-0.59472200	-0.08436700	3.29723700
H	0.43326100	0.99891300	4.29043800
H	1.16940200	-0.07072700	3.04765000
C	-2.92481700	1.10399300	2.38068000
H	-2.58660500	1.99252500	1.85985300
C	2.79321000	-1.87972700	2.02526500
H	1.94805800	-2.39228800	1.58343900
C	3.32919200	2.00067600	-1.72820700
H	3.27985800	1.30283800	-2.55534800
C	5.27979700	-1.84535900	-2.58703000
H	6.26999200	-1.59757100	-2.95900700
C	-4.57884600	-1.72538700	-1.15649200
H	-5.10582700	-0.77882700	-1.21722000
C	3.64789300	3.33671500	-1.97063700
H	3.86599700	3.65886900	-2.98467500
C	-4.92649300	2.86950600	-1.20778600
H	-5.68088800	3.51573900	-0.76789800
C	-3.23940000	-4.17005500	-1.01377500
H	-2.71454500	-5.11975300	-0.95781200

C	4.69349400	-3.07018700	-2.91151000
H	5.22351400	-3.77720700	-3.54354700
C	3.43070300	-3.38792700	-2.40856000
H	2.97530600	-4.34615500	-2.64180200
C	4.98803300	-0.56148600	3.14552400
H	5.84822300	-0.05090700	3.56964700
C	3.04208000	2.50356600	0.61828400
H	2.77514800	2.19911900	1.62455600
C	-2.59573900	-3.00390000	-0.59407900
H	-1.57862400	-3.02818500	-0.21436700
C	3.36414000	3.83928200	0.37361400
H	3.35815900	4.55055200	1.19404100
C	-3.75403800	-1.16952700	3.76218700
H	-4.06914600	-2.06094100	4.29691100
C	-3.64196800	2.14015800	-3.11767200
H	-3.38708300	2.22017400	-4.17054000
C	4.50390100	-1.73012000	3.73490700
H	4.98059900	-2.12910100	4.62596700
C	-4.59606900	2.99356100	-2.55741300
H	-5.08633200	3.74341500	-3.17206200
C	-3.26147000	1.19278500	3.73115000
H	-3.19155400	2.15072700	4.23884300
C	3.67258900	4.25883700	-0.92082300
H	3.91943300	5.29885000	-1.11377600
C	-3.67385500	0.05484400	4.42768100
H	-3.92916200	0.12191700	5.48139700
C	3.41264000	-2.39050800	3.16604000
H	3.03724400	-3.30773700	3.61078700
C	-5.21256300	-2.89445500	-1.57676900
H	-6.22818400	-2.84756400	-1.95970400
C	-4.54416400	-4.11910400	-1.50702700
H	-5.03945300	-5.02828800	-1.83680900
H	0.12393900	-0.62105200	-4.16719200
C	-0.66460800	3.89152000	1.20968900
H	-0.88925900	4.84065100	0.73207300

H	-0.81313200	3.82020400	2.28113300
H	-0.79274900	3.40209800	-1.50837800

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Os	0.01300200	0.13127200	0.11386500
P	-2.36307300	0.16666700	0.12405700
P	2.38953500	0.09122600	0.11680600
C	-0.16086600	-1.81192600	0.91311500
H	-0.24794400	-1.94220500	1.99538200
O	0.13908700	2.64331700	-1.60233900
C	-0.02042000	-1.20705300	-1.53206400
C	-3.09095900	-1.08228200	-1.02030700
C	-3.23073500	-0.19577300	1.72076100
C	-0.11152000	-2.55328900	-1.29435500
H	-0.15993500	-3.29488400	-2.09560500
C	-0.20211500	-2.90823200	0.09890300
C	-3.23476900	-0.78868300	-2.38437400
H	-3.00125700	0.20672700	-2.74620300
C	-3.20940500	1.73836600	-0.36054600
C	0.04961800	0.70262100	-2.93410600
C	0.06444900	1.40502300	-1.64103500
C	3.23056700	1.63822000	0.67232100
C	0.01811800	-0.65086700	-2.85313700
H	0.01767200	-1.29761200	-3.73171800
C	3.17241600	-0.23717200	-1.52069100
C	-2.53158800	2.94601100	-0.13798800
H	-1.52266200	2.92162700	0.25737800
C	-3.34616200	-2.38873100	-0.58001400
H	-3.20654200	-2.64016700	0.46505000
C	3.14967200	-1.16844600	1.23908800
C	-2.51911000	-0.01533000	2.91533800
H	-1.47388600	0.29527700	2.85919400
C	-4.49611400	-0.61034600	4.19087100
H	-4.98554400	-0.77484100	5.14814800

C	2.58449000	-1.28538600	2.52026700
H	1.73928600	-0.65226400	2.77180900
C	-5.21026500	-0.78283900	3.00152500
H	-6.25566500	-1.08111200	3.02960900
C	-3.75191900	-3.37457500	-1.48028700
H	-3.94058900	-4.38331500	-1.12170200
C	-4.51603200	1.76819700	-0.87495700
H	-5.04908700	0.84089300	-1.06050400
C	-3.15640100	-0.22292200	4.14239100
H	-2.59748800	-0.07967700	5.06399600
C	-3.64524700	-1.77319700	-3.28262600
H	-3.74999000	-1.52816900	-4.33646100
C	2.65172800	2.87552400	0.34351900
H	1.70617700	2.91204100	-0.18526700
C	3.09221900	-1.52472200	-2.07730900
H	2.61894000	-2.32135200	-1.51531100
C	-3.90472800	-3.07013800	-2.83394800
H	-4.21978200	-3.83874900	-3.53549000
C	3.29798600	4.05998100	0.70706200
H	2.84177500	5.01211300	0.44878500
C	-5.13300800	2.98316100	-1.17090600
H	-6.14268500	2.99190500	-1.57481500
C	-4.45275800	4.18395700	-0.94955300
H	-4.93203000	5.13198600	-1.18289800
C	-4.58285700	-0.57126000	1.77437800
H	-5.14452600	-0.71229600	0.85610100
C	-3.15693200	4.15981500	-0.43324100
H	-2.61734000	5.08820000	-0.26678600
C	4.25981500	-1.95690700	0.91106000
H	4.72017100	-1.86864200	-0.06714800
C	3.74343400	0.79243900	-2.27960700
H	3.80088600	1.79582700	-1.87190700
C	3.11564100	-2.18348300	3.44397300
H	2.66717500	-2.26499700	4.43080500
C	4.44553700	1.61127200	1.37376200

H	4.89874700	0.66177200	1.63958300
C	4.50555100	4.02808000	1.40604600
H	4.99741300	4.95516600	1.69203900
C	4.21233200	-2.98140600	3.10428400
H	4.61964800	-3.68742600	3.82401600
C	4.15450500	-0.74236300	-4.10628000
H	4.53224700	-0.93697800	-5.10707100
C	5.07926400	2.79930200	1.74026100
H	6.01913900	2.76306900	2.28601000
C	4.22808900	0.54142600	-3.56506800
H	4.66106500	1.35415700	-4.14255500
C	3.58742200	-1.77546400	-3.35618500
H	3.51615100	-2.77744100	-3.77176100
C	4.78392600	-2.86390700	1.83754500
H	5.64155500	-3.47453600	1.56561000
O	0.07539300	1.90224400	1.23791700
O	0.24409400	0.78447500	2.10324600
H	0.08776300	1.27518600	-3.85903100
C	-0.36990500	-4.33673700	0.55372300
H	-1.29130700	-4.77968800	0.14744500
H	0.46026400	-4.97437900	0.21858600
H	-0.41926100	-4.40030100	1.64574200

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Os	0.02831600	0.02774300	-0.10316400
P	2.40599000	0.02468300	-0.15290600
P	-2.34876200	0.12471700	-0.14873900
C	-0.01197500	-2.17863700	-0.45127200
H	1.02472400	-2.49984300	-0.60193400
O	0.07294600	2.86633200	1.00774500
C	-0.01358300	-0.89511300	1.80898600
C	3.19754000	-0.27213200	1.48532100
C	3.18749100	-1.24920000	-1.24817700
C	-0.27126300	-2.22491500	1.95614400

H	-0.38747500	-2.70106800	2.93290700
C	-0.55801100	-2.93872800	0.72507900
C	3.81195000	0.75800800	2.20928700
H	3.90593100	1.74445900	1.76748700
C	3.28796600	1.54392900	-0.74220300
C	0.16205300	1.28270700	2.73618400
C	0.09016200	1.66080900	1.30168700
C	-3.11111100	1.62701100	-0.92237600
C	0.11529000	-0.04086400	2.97652600
H	0.14167600	-0.46858100	3.97909200
C	-3.15560400	0.10377900	1.51112800
C	2.61522300	2.77202300	-0.80759100
H	1.56600000	2.82932200	-0.55261200
C	3.06638500	-1.53674300	2.08318500
H	2.56064700	-2.33267500	1.54839000
C	-3.20283300	-1.20540700	-1.11152500
C	2.61074900	-1.39966300	-2.52147500
H	1.72014600	-0.81680100	-2.75852400
C	4.27707900	-3.06641200	-3.08900800
H	4.69734200	-3.77280400	-3.80096900
C	-2.68334100	-1.45687800	-2.39350800
H	-1.81064300	-0.89264100	-2.71699800
C	4.84943700	-2.92356400	-1.82452200
H	5.71802700	-3.51613400	-1.54728600
C	3.55911100	-1.76758200	3.36680200
H	3.44896700	-2.75185800	3.81441600
C	4.65038400	1.48962200	-1.08199800
H	5.18160400	0.54365800	-1.04334000
C	3.15849300	-2.30169800	-3.43289400
H	2.70258000	-2.41457900	-4.41329800
C	4.29625300	0.52751200	3.49857000
H	4.76686400	1.33868600	4.04824200
C	-2.40627900	2.84018200	-0.92931500
H	-1.40142300	2.88648100	-0.53036900
C	-3.23471300	-1.09209700	2.24448400

H	-2.89418000	-2.02033700	1.79955500
C	4.17414100	-0.73539600	4.07978400
H	4.55140700	-0.91431900	5.08360900
C	-3.00668800	3.98975900	-1.45104700
H	-2.45006600	4.92335900	-1.45131500
C	5.33156100	2.64009600	-1.47702200
H	6.38534700	2.58098500	-1.73860400
C	4.65723000	3.86275400	-1.53853300
H	5.18531100	4.76144600	-1.84916400
C	4.30910900	-2.01709400	-0.90773000
H	4.76306100	-1.91335200	0.07253300
C	3.30500600	3.92259800	-1.20227100
H	2.77168500	4.86838500	-1.24925200
C	-4.33083300	-1.91667000	-0.68247800
H	-4.75976500	-1.72286200	0.29437500
C	-3.57463900	1.29683500	2.11705900
H	-3.50556200	2.23210300	1.57179200
C	-3.27421200	-2.41637700	-3.21455900
H	-2.85792000	-2.60623700	-4.20068500
C	-4.41262100	1.58752700	-1.44796400
H	-4.96773200	0.65491500	-1.45326100
C	-4.29881500	3.94400100	-1.97520600
H	-4.75621800	4.84155400	-2.38549900
C	-4.38892200	-3.13506100	-2.77409600
H	-4.84453500	-3.88666000	-3.41439100
C	-4.16013600	0.10076000	4.13827300
H	-4.54826300	0.09934900	5.15394000
C	-5.00299900	2.73744200	-1.97219100
H	-6.01069000	2.68941600	-2.37811000
C	-4.07169400	1.29495700	3.42140600
H	-4.38775200	2.23043700	3.87588800
C	-3.74242000	-1.09180600	3.54375300
H	-3.79924000	-2.02691300	4.09532500
C	-4.91728300	-2.87929300	-1.50845300
H	-5.78863900	-3.42769500	-1.15873800

O	0.07606900	1.44745100	-1.65537100
O	-0.02650600	0.13367700	-2.19359700
H	0.22630900	2.06170900	3.49301000
C	-1.28237000	-4.07810900	0.65767600
H	-1.65568800	-4.56620300	1.55633100
H	-1.53509000	-4.53387500	-0.29522200
H	-0.54889500	-2.40720500	-1.37593500

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Os	0.00010700	0.23374400	0.00090600
P	2.37327300	0.21381200	0.06317200
P	-2.37307900	0.21424700	0.06314700
C	0.00018900	1.54166200	-1.65017100
H	0.00020300	2.61920700	-1.47694700
O	-0.00002000	-2.13593900	1.92698000
C	0.00002500	-0.98354500	-1.74206600
C	3.13028000	-1.22200300	-0.80781600
C	3.19694300	1.69924900	-0.66405900
C	0.00016500	-0.38196400	-2.97683200
H	0.00013400	-0.94905200	-3.91078300
C	0.00025800	1.05289600	-2.92465200
C	3.56840200	-2.34762000	-0.09776700
H	3.55612200	-2.33968600	0.98705800
C	3.18484400	0.14077100	1.72481400
C	-0.00032400	-2.87184400	-0.30144400
C	-0.00010200	-1.80870900	0.72312200
C	-3.18490500	0.14056800	1.72464600
C	-0.00016500	-2.40360700	-1.57540000
H	-0.00018200	-3.06948000	-2.44049600
C	-3.13044100	-1.22111200	-0.80834900
C	2.50803500	-0.46071600	2.79712500
H	1.50067800	-0.83494300	2.66322200
C	3.12714100	-1.26217900	-2.21156800
H	2.74903400	-0.41349700	-2.76994500

C	-3.19645500	1.70013900	-0.66351500
C	2.63684600	2.93800900	-0.30753900
H	1.75144600	2.94180000	0.32673800
C	4.34459600	4.08922300	-1.58410400
H	4.78670900	5.01503600	-1.94454800
C	-2.63612200	2.93864700	-0.30648700
H	-1.75072000	2.94200100	0.32779300
C	4.90605500	2.86189800	-1.93715500
H	5.78874400	2.82665500	-2.57126700
C	3.57624700	-2.39699000	-2.88626000
H	3.56692100	-2.41341200	-3.97314400
C	4.48823900	0.62483400	1.91996200
H	5.02059200	1.09838100	1.10124600
C	3.21248200	4.12250500	-0.76398900
H	2.77064400	5.07556600	-0.48423200
C	4.00491900	-3.48746900	-0.77569000
H	4.33357300	-4.35535100	-0.20987000
C	-2.50799400	-0.46057900	2.79706900
H	-1.50036000	-0.83410800	2.66337400
C	-3.12715900	-1.26092700	-2.21211300
H	-2.74863500	-0.41225800	-2.77022600
C	4.01340700	-3.51434700	-2.17098100
H	4.35281100	-4.40227800	-2.69873600
C	-3.14046700	-0.57888000	4.03784800
H	-2.60649800	-1.04658200	4.86094700
C	5.10941700	0.51025800	3.16385300
H	6.11797600	0.89319100	3.30049800
C	4.43475000	-0.09335700	4.22772100
H	4.91651400	-0.18202400	5.19890200
C	4.33890100	1.67059100	-1.47408200
H	4.78888200	0.72180100	-1.74755400
C	3.14022500	-0.57840500	4.03810100
H	2.60634500	-1.04637100	4.86110900
C	-4.33837900	1.67203800	-1.47361600
H	-4.78852900	0.72345100	-1.74750100

C	-3.56911100	-2.34674200	-0.09865900
H	-3.55699000	-2.33910000	0.98616800
C	-3.21148500	4.12344200	-0.76252000
H	-2.76945500	5.07630400	-0.48239000
C	-4.48873500	0.62361100	1.91944400
H	-5.02119100	1.09685900	1.10061900
C	-4.43541300	-0.09483200	4.22712800
H	-4.91741300	-0.18399100	5.19814600
C	-4.34356100	4.09071400	-1.58270500
H	-4.78546200	5.01675700	-1.94282000
C	-4.01437700	-3.51273300	-2.17223800
H	-4.35410000	-4.40038100	-2.70026400
C	-5.11021400	0.50839900	3.16311900
H	-6.11910900	0.89054400	3.29949600
C	-4.00601600	-3.48623300	-0.77694100
H	-4.33511800	-4.35412100	-0.21138600
C	-3.57667900	-2.39536000	-2.88716600
H	-3.56726400	-2.41147800	-3.97405400
C	-4.90526200	2.86364300	-1.93625300
H	-5.78792500	2.82883800	-2.57042300
O	0.00018500	0.86336300	2.00070500
O	0.00040800	1.99842400	1.14088900
H	0.00031000	1.67604200	-3.82020600
C	-0.00084500	-4.30977400	0.12138400
H	-0.88030000	-4.53156400	0.73845300
H	0.00187200	-4.98346200	-0.74195300
H	0.87518200	-4.53053300	0.74358700

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Os	-0.02393900	0.12672500	0.00466200
P	2.36166800	0.21941300	0.03230200
P	-2.39129200	0.17386700	0.07530400
C	-0.08928500	1.35567900	-1.74526500
H	-0.13725500	2.43927100	-1.63182900

O	0.18579800	-2.01934300	2.11797100
C	-0.03422700	-1.19308500	-1.66267700
C	3.23180900	-1.31786400	-0.50239600
C	3.10769800	1.55758900	-0.99842200
C	-0.01061100	-0.67462800	-2.91818100
H	-0.01679100	-1.29622500	-3.81771400
C	-0.05061400	0.77731500	-2.96710500
C	3.94017800	-2.11974400	0.40209800
H	4.04734200	-1.80597900	1.43437900
C	3.13016700	0.56292800	1.67673900
C	0.28280900	-3.00029600	-0.03527000
C	0.12497800	-1.81357000	0.89852500
C	-3.22737900	-0.02691600	1.71541400
C	-0.13386900	-2.68442000	-1.43582400
H	0.43670300	-3.25928200	-2.17772200
C	-3.20361500	-1.13417800	-0.93424200
C	2.54276600	0.01719700	2.83003100
H	1.62384900	-0.54998100	2.75353900
C	3.09732900	-1.75181500	-1.83282400
H	2.51713600	-1.15945000	-2.53061100
C	-3.17731900	1.73828300	-0.52375500
C	2.58234300	2.84801500	-0.81120800
H	1.76769700	2.97797800	-0.10448400
C	4.14969000	3.73645600	-2.42922200
H	4.55051100	4.57948300	-2.98691200
C	-2.56705000	2.93515900	-0.11259800
H	-1.64621200	2.87614900	0.46789200
C	4.67641000	2.45906800	-2.61607800
H	5.49193900	2.30116900	-3.31771500
C	3.66047200	-2.95969400	-2.24213400
H	3.54231300	-3.28263500	-3.27336300
C	4.31427400	1.30654900	1.79559800
H	4.77731600	1.73441000	0.91241000
C	3.10460800	3.92747400	-1.51935200
H	2.68842900	4.92015300	-1.36777900

C	4.49118200	-3.33518900	-0.00868800
H	5.02450300	-3.95172500	0.71032900
C	-2.51735400	-0.54505100	2.80735100
H	-1.46630000	-0.78274300	2.70956200
C	-3.13000300	-1.04991800	-2.33515100
H	-2.66964800	-0.18142700	-2.79206400
C	4.35467400	-3.75886600	-1.33062000
H	4.78190000	-4.70682100	-1.64841100
C	-3.17024400	-0.75223400	4.02628600
H	-2.60848000	-1.15443300	4.86521600
C	4.90481700	1.50657100	3.04414400
H	5.82073900	2.08764100	3.12048900
C	4.31911600	0.96084700	4.18849900
H	4.77667400	1.11712200	5.16283300
C	4.16269100	1.37374600	-1.89841100
H	4.58796400	0.38679000	-2.04535200
C	3.14414200	0.21613700	4.07533700
H	2.67918700	-0.20754100	4.96172200
C	-4.34625600	1.79347300	-1.29475500
H	-4.82780600	0.87701200	-1.62050500
C	-3.76392200	-2.27712900	-0.34817000
H	-3.81315700	-2.35990400	0.73268300
C	-3.12492700	4.16165000	-0.47255200
H	-2.64296500	5.08242500	-0.15326800
C	-4.58878900	0.28441500	1.86725800
H	-5.14750900	0.69481900	1.03179500
C	-4.52247500	-0.44194100	4.17153500
H	-5.02220700	-0.60127700	5.12435900
C	-4.28756300	4.21278800	-1.24685800
H	-4.71563500	5.17157500	-1.52994700
C	-4.18409900	-3.22098800	-2.53669200
H	-4.56055100	-4.03004900	-3.15781000
C	-5.23309400	0.07881900	3.08659900
H	-6.28681700	0.32682400	3.18943000
C	-4.25249600	-3.31476300	-1.14564300

H	-4.68095700	-4.19688100	-0.67701000
C	-3.62408100	-2.08509300	-3.12787600
H	-3.55471600	-2.01086000	-4.20995900
C	-4.89590200	3.02608200	-1.65779200
H	-5.80001200	3.05537100	-2.26138700
O	-0.04693400	0.91916500	1.95412100
O	0.11259100	1.96310800	1.00395600
H	-0.05616000	1.33095700	-3.90821000
C	0.80111800	-4.15096400	0.40666300
H	0.99074100	-4.99227600	-0.25551800
H	1.06161400	-4.25391500	1.45599900
H	-1.18986100	-2.97682900	-1.55572200

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