Electronic Supplementary Material (ESI) for Dalton Transactions.

Rhenium and Technetium Bi and Tricarbonyl Complexes in a New Strategy for Biomolecule Incorporation using Click Chemistry

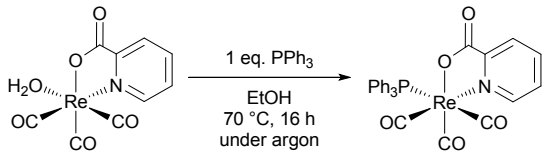
Thomas R. Hayes, Benjamin B. Kasten, Charles L. Barnes, Paul D. Benny

Supporting Information

Experimental

All reagents and organic solvents of reagent grade or better were used as purchased from Aldrich, Acros, or Fluka without further purification. Rhenium starting material *fac*-[$Re^{I}(OH_2)_3(CO)_3$](SO_3CF_3) was prepared by literature methods from $Re_2(CO)_{10}$ purchased from Strem.[1] ^{99m}Tc was obtained in the form of Na[$^{99m}TcO_4$]$^-$ from Cardinal Health (Spokane, WA) and the *fac*-[$^{99m}Tc^{I}(OH_2)_3(CO)_3$]$^+$ complex was prepared using a commercially available Isolink® kit from Covidien. Radiochemical percent yields were determined from the radio-HPLC chromatograms by dividing the radioactive area of the peak of interest by the total radioactive area of all species present in the chromatogram. The preparation of compounds **1** and **4** was performed as previously reported.[2, 3] ^1H and ^{13}C NMR spectra were recorded on a Varian 300 MHz instrument at 25 ºC in CD_3OD or $CDCl_3$. Elemental analyses were performed by Intertek Pharmaceutical Services (Whitehouse, NJ). FT-IR spectra were obtained on a Thermo Nicolet 6700 FT-IR with an ATR cell and analyzed with OMNIC 7.1 software. Mass spectra were obtained on a Thermo-Finnigan LCQ Advantage ESI-MS.

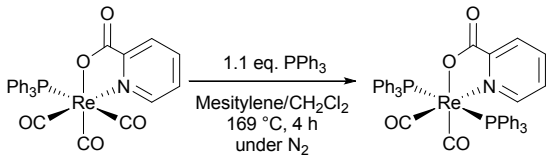
Separation and identification of compounds were conducted on a Perkin Elmer Series 200 High Performance Liquid Chromatography (HPLC) system equipped with a UV/VIS Series 200 detector and a Radiomatic 610TR detector. Utilizing a Varian Pursuit XRs 5µm particle and 250 x 4.6 mm C-18 column, the compounds were separated with a reverse phase gradient system beginning with 70% 0.1% trifluoroacetic acid (TFA) and 30% methanol eluent gradually shifting to 100% methanol. HPLC analysis was performed using 0-3.0 min (70% TFA, 30% MeOH), 3.0-9.0 min (50% TFA, 50% MeOH), 9.0-18.5 min (50% to 100% MeOH linear gradient), 18.5-28.0 min (100% MeOH) at a flow rate of 1.0 mL/min.



1 **2**

***fac*-[$Re^{I}(CO)_3$(pic)(PPh_3)], 2.**

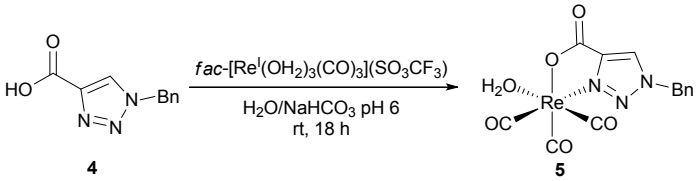
Triphenylphosphine (6.4 mg, 2.44x10^{-5} mol) and **1** (10 mg, 2.44x10^{-5} mol) were added to a 5 mL sealable vial followed by the addition of absolute EtOH (2 mL). The vial was sealed, sparged with argon and heated at 70 °C overnight. The solvent was removed in vaccuo to yield a yellow residue that was purified by silica column chromatography with 1.5% methanol in dichloromethane. The product eluted as a faint yellow solution (R_f 0.2) that was dried by rotary evaporation to yield 8.4 mg (53%) of **2** as a tannish-yellow solid. X-ray quality crystals were obtained by slow evaporation from a dichloromethane/MeOH (2:1) solution containing **2**. ^1H NMR [300 MHz δ (ppm), $CDCl_3$] 7.24-7.40 (m, 16H), 7.56 (d, 1H), 7.62 (dt, 1H), 8.50 (d, 1H). ^{13}C NMR [75 MHz, δ (ppm), $CDCl_3$] 171.2, 151.7, 150.7, 138.6, 133.8, 130.7, 129.5, 128.9, 127.5. ^{31}P NMR [121.5 MHz δ (ppm), $CDCl_3$] 20.38. MS (+ESI): 656.0 m/z; 656.1 m/z calcd for $[M + H]^+$. IR (neat powder, cm^{-1}): 2015.0, 1902.8, 1665.5, 1329.4, 759.7, 695.5, 520.0.



2 **3**

***cis-trans*-[Re^{I}(CO)$_2$(pic)(PPh$_3$)$_2$], 3.**

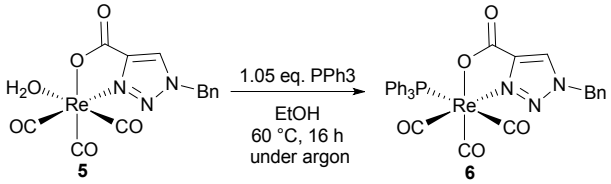
2 (30 mg, 4.6x10^{-5} mol) dissolved in CH_2Cl_2 (300 µL) and triphenylphosphine (13.2 mg, 5.0x10^{-5} mol) were combined in 2 mL mesitylene sparged with N_2. The reaction was refluxed at 169 °C with stirring for 4 h under N_2, during which a tannish-yellow precipitate formed. After cooling the reaction mixture, the precipitate was collected by filtration and rinsed with ice-cold EtOH to yield 37.4 mg (92%) of pure **3**. X-ray quality crystals were obtained by slow diffusion of hexanes into a chloroform solution containing **3**. ^{1}H NMR [300 MHz δ (ppm), $CDCl_3$] 6.71 (ddd, 1H), 7.10 (ddd, 1H), 7.19-7.34 (m, 19H), 7.37-7.45 (m, 12H), 7.91 (ddd, 1H). ^{13}C NMR [75 MHz δ (ppm), $CDCl_3$] 170.8, 150.6, 135.9, 133.8 (t, J_{CP} = 5.7 Hz), 132.3 (t, J_{CP} = 22.4 Hz), 129.7, 128.4 (t, J_{CP} = 4.7 Hz), 126.6 (d, J_{CP} = 7.0 Hz). ^{31}P NMR [121.5 MHz δ (ppm), $CDCl_3$] 24.99. MS (+ESI): 890.0 m/z; 890.2 m/z calcd for [M]$^+$. IR (neat powder, cm^{-1}): 1926.4, 1832.7, 1649.7, 1431.4, 1330.5, 1086.9, 690.4, 499.7.



4 **5**

***fac*-[Re^{I}(OH$_2$)(CO)$_3$(4)], 5.**

4 (41 mg, 0.20 mmol) was dissolved in deionized water (5 ml) and adjusted to pH 6 with sodium bicarbonate. A 0.1 M solution of *fac*-[Re^{I}(OH$_2$)$_3$(CO)$_3$](SO$_3$CF$_3$) (2 ml, 0.20 mmol) was added and the solution was stirred at room temperature for 18 h. The resulting precipitate was then collected by filtration, washed with H_2O and dried in vacuo to yield **5** (48.2 mg, 49% yield) as a white powder. X-ray quality crystals were obtained by slow evaporation from a solution of **5** dissolved in acetone and water. Anal. calcd for $C_{13}H_{10}N_3O_6Re$: C, 31.84%; H, 2.06%; N, 8.57%. Found: C, 31.91%; H, 1.69%; N, 8.02%. ^{1}H NMR [300 MHz δ (ppm), CD_3OD] 8.56 (s, 1H), 8.49 (s, 1H), 7.43-7.45 (m, 5H), 5.75 (d, 2H, J=4.4 Hz). ^{13}C NMR [75 MHz δ (ppm), CD_3OD] 197.5, 196.2, 193.8, 169.8, 144.0, 135.2, 130.4, 130.3, 129.7, 128.2, 56.7. MS (+ESI): 513.6 m/z; 514.0 m/z calcd for [M + Na]$^+$. IR (neat powder, cm^{-1}): 2031.4, 1896.8, 1881.8, 1573.4, 1313.4, 1080.0, 723.7.

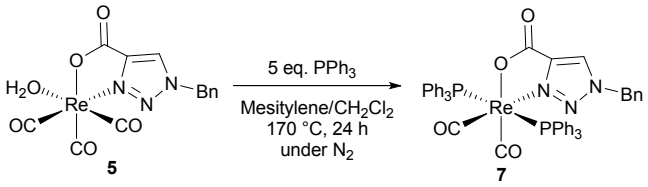


5 **6**

***fac*-[Re^{I}(CO)$_3$(4)(PPh$_3$)], 6.**

5 (100 mg, 0.204 mmol) was dissolved in 10 mL absolute EtOH sparged with argon. Triphenylphosphine (56.2 mg, 0.214 mmol) was then added and the reaction was stirred at 60 °C in a sealed vial for 16 h. After 16 h, the solution was concentrated to dryness and 3 mL of MeOH was added. The mixture was then cooled to 0 °C, filtered and washed with cold MeOH to give 136.2 mg (91%) of **6** as a white solid. X-ray quality crystals were obtained by slow evaporation from a chloroform/EtOH solution containing **6**. Anal. calcd for $C_{31}H_{23}N_3O_5PRe$: C, 50.68%; H, 3.16%; N, 5.72%. Found: C, 50.77%; H, 2.34%; N,

5.47%. ^{1}H NMR [300 MHz, δ (ppm), $CDCl_3$] 7.61 (s, 1H), 7.44-7.30 (m, 14H), 7.22-7.16 (m, 6H), 5.42 (ABq, 2H, J_{AB} = 14.2 Hz). ^{13}C NMR [75 MHz δ (ppm), $CDCl_3$] 166.2, 143.0, 134.1, 134.0, 132.6, 130.8, 130.0, 129.7, 129.5, 128.7, 125.5, 56.0. ^{31}P NMR [121.5 MHz δ (ppm), $CDCl_3$] 19.76. MS (+ESI): 758.0 m/z; 758.1 m/z calcd for $[M + Na]^+$. IR (neat powder, cm^{-1}): 3064.6, 2028.1, 1926.5, 1894.6, 1651.9, 1558.5, 1434.4, 1278.7, 1098.0, 695.0.



***cis-trans*-[$Re^{I}(CO)_2(PPh_3)_2$(4)], 7.**

Triphenylphosphine (66.8 mg, 0.255 mmol) was dissolved in 2 mL of mesitylene sparged with N_2 with stirring. **5** (25 mg, 0.051 mmol) dissolved in 1 mL CH_2Cl_2 was then added and the reaction was refluxed at 170 °C under N_2 for 24 h. The reaction mixture was then cooled, filtered and the precipitate was washed with ice cold EtOH and dried in vacuo to give **7** (34.1 mg, 69.0 % yield) as a white solid. X-ray quality crystals were obtained by slow diffusion of hexanes into a chloroform solution containing **7**. Anal. calcd for $C_{48}H_{38}N_3O_4P_2Re$: C, 59.50%; H, 3.95%; N, 4.34%. Found: C, 59.85%; H, 3.36%; N, 4.08%. ^{1}H NMR [300 MHz, δ (ppm), $CDCl_3$] 7.21-7.48 (m, 15H), 7.28-7.19 (m, 20H), 6.64 (s, 1H), 5.06 (s, 1H). ^{13}C NMR [75 MHz, δ (ppm), $CDCl_3$] 165.7, 142.9, 134.1 (t, J_{CP} = 5.7 Hz), 133.0 (t, J_{CP} = 22.3 Hz), 132.3, 130.1, 129.7 (t, J_{CP} = 4.7 Hz), 128.3 (d, J_{CP} = 4.7 Hz), 123.7, 55.6. ^{31}P NMR [121.5 MHz δ (ppm), $CDCl_3$] 23.96. MS (+ESI): 970.2 m/z; 970.2 m/z calcd for $[M + H]^+$. IR (neat powder, cm^{-1}): 3060.9, 2029.4, 1945.3, 1898.9, 1866.9, 1644.6, 1557.9, 1433.2, 1278.7, 1095.7, 692.0.

X-ray Crystallography Procedures

Complexes 2, 3, 5, 6 and 7

For all structures intensity data were obtained on a Bruker SMART CCD Area Detector system using the ω scan technique with Mo Kα radiation from a graphite monochromator. For **2**, **3** and **5** data were collected at -100 °C; for **6** and **7** data were collected at -173 °C. Intensities were corrected for Lorentz and polarization effects. Equivalent reflections were merged, and absorption corrections were made using the multi-scan method.[4] Space group, lattice parameters and other relevant information are given in supporting information tables S3 through S34. The structures were solved by direct methods with full-matrix least-squares refinement, using the SHELX package[5-7] with the aid of the program X-SEED.[8] All non-hydrogen atoms were refined with anisotropic thermal parameters. The hydrogen atoms were placed at calculated positions and included in the refinement using a riding model, with fixed isotropic *U*. For **3**, the final difference map showed some residual density in the vicinity of solvent chloroform, while the final map for **7** contained peaks as high as 0.7 $e^{-}/Å^{-3}$ perhaps due to unresolved twinning in the data. Final difference maps for **2**, **5**, and **6** contained no features of chemical significance.

^{99m}Tc synthesis

***fac*-[^{99m}Tc^{I}(OH$_2$)(CO)$_3$(pic)], 1a**

A 10^{-2} M solution of picolinic acid in EtOH (100 μL) was added to 10 mM $NaHCO_3$ (800 μL) in a sealable vial and sparged with N_2 for 5 min. A solution of *fac*-[^{99m}Tc^{I}(OH$_2$)$_3$(CO)$_3$]$^+$ (100 μL, 549 μCi) prepared from a Isolink® kit from Covidien was then injected and the solution was heated to 90 °C for 30 min. The solution was then cooled and analyzed by radio-HPLC to give **2a** in >98% yield. Peak purified samples for log *P* analysis were obtained by RP-HPLC.

***fac*-[^{99m}Tc^{I}(CO)$_3$(pic)(PPh$_3$)], 2a**

EtOH (800 μL) was added to a 10^{-2} M solution of triphenylphosphine in EtOH (100 μL) in a sealable vial. The reaction solution was then sparged with N_2 for 5 min. A solution of **1a** (100 μL, 46 μCi) was then added and the reaction was heated to 60 °C for 1 h. The solution was then cooled and analyzed by radio-HPLC to give **2a** in 93% yield. Peak purified solutions for stability and log *P* analysis were obtained by RP-HPLC.

***cis-trans*-[^{99m}Tc^{I}(CO)$_2$(pic)(PPh$_3$)$_2$], 3a**

EtOH (800 μL) was added to a 10^{-2} M solution of triphenylphosphine in EtOH (100 μL) in a sealable vial. The reaction solution was then sparged with N_2 for 5 min. A solution of **1a** (100 μL, 55 μCi) was then added and the reaction was heated to 90 °C for 1 h. The solution was then cooled and analyzed by radio-HPLC to give **3a** in >99% yield. Peak purified solutions for stability and log *P* analysis were obtained by RP-HPLC.

***fac*-[^{99m}Tc^{I}(OH$_2$)(CO)$_3$(4)], 5a.**

A $5x10^{-2}$ solution of **4** in EtOH was added to 10 mM $NaHCO_3$ (800 μL) in a sealable vial. The vial was sparged with N_2 for 5 min and a solution of *fac*-[^{99m}Tc^{I}(OH$_2$)$_3$(CO)$_3$]$^+$ (100 μL, 663 μCi) was added and the reaction solution was heated at 50 °C for 1 h. The solution was then cooled and analyzed by radio-HPLC to give **5a** in 98% yield. Peak purified samples for log *P* analysis were obtained by RP-HPLC.

***fac*-[^{99m}Tc^{I}(CO)$_3$(4)(PPh$_3$)], 6a**

EtOH (800 μL) was added to a 10^{-2} M solution of triphenylphosphine in EtOH (100 μL) in a sealable vial. The reaction solution was then sparged with N_2 for 5 min. A solution of **5a** (100 μL, 46 μCi) was then added and the reaction was heated to 60 °C for 1 h. The solution was then cooled and analyzed by radio-HPLC to give **2a** in 81% yield. Peak purified solutions for stability and log *P* analysis were obtained by RP-HPLC.

***cis-trans*-[^{99m}Tc^{I}(CO)$_2$(4)(PPh$_3$)$_2$], 7a**

EtOH (800 μL) was added to a 10^{-2} M solution of triphenylphosphine in EtOH (100 μL) in a sealable vial. The reaction solution was then sparged with N_2 for 5 min. A solution of **5a** (100 μL, 56 μCi) was then added and the reaction was heated to 90 °C for 1 h. The solution was then cooled and analyzed by radio-HPLC to give **3a** in >99% yield. Peak purified solutions for stability and log *P* analysis were obtained by RP-HPLC.

Log *P* Determination

Equal volumes of 10 mM pH 7.4 phosphate buffered saline (PBS) and 1-octanol (500 μL each) were vortexed (30 sec) in centrifuge tubes and allowed to stand (2 h) at room temperature. RP-HPLC purified solutions of the complexes were dried under a stream of N_2 and re-dissolved in either 10 mM pH 7.4 PBS (**1a** and **5a**) or 1-octanol (**2a**, **3a**, **6a**, **7a**). Aliquots of solutions containing the reconstituted complexes (0.1 μCi in 3-8 μL) were added to triplicate sets of tubes after an equal volume of the corresponding aqueous or organic phase was removed. The tubes were vortexed (1 min) and centrifuged (2,000 × g, 5 min). Aliquots (50 μL) from each layer were removed and counted with a γ-counter to determine the ratio of radioactivity present in the octanol layer compared to the aqueous layer.

Stability Studies of ^{99m}Tc complexes

Purified solutions of **2a**, **3a**, **6a**, or **7a** (500 μL, approximately 5 μCi) were mixed 1:1 with either 2 mM histidine or 2 mM cysteine in 10 mM pH 7.4 phosphate buffer to give a final concentration of 1 mM amino acid in N_2 sparged sealable vials. The solutions were then placed in a 37 °C water bath and samples were taken at 4 and 18 h.

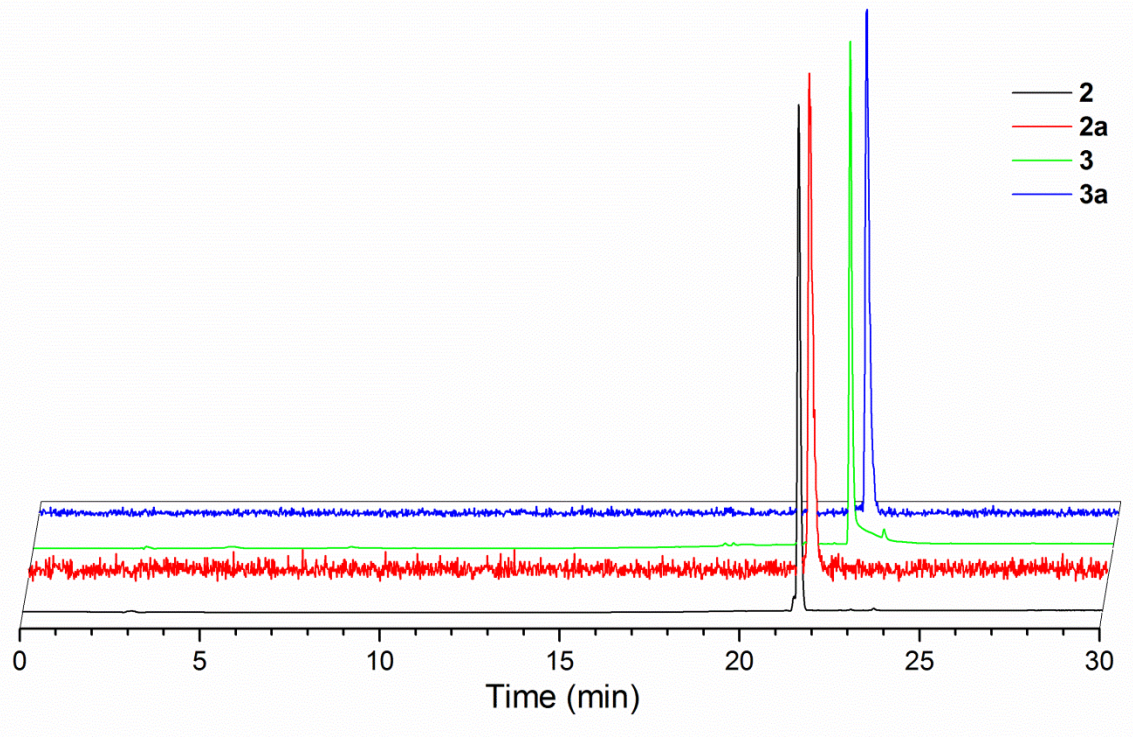


Figure S1. Normalized and offset UV and radio- HPLC chromatograms of complexes **2** (t_R = 21.6 min), **2a** (t_R = 21.7 min), **3** (t_R = 22.7 min) and **3a** (t_R = 23.0 min).

Table S1. Log *P* analysis of ^{99m}Tc complexes between ocatanol and pH 7.4 PBS.

Complex	Log *P*
1a	0.82 ± 0.06
2a	1.06 ± 0.09
3a	1.23 ± 0.03
5a	1.06 ± 0.01
6a	1.13 ± 0.11
7a	1.44 ± 0.06

Table S2. Stability of ^{99m}Tc complexes to amino acid challenges. 1 mM cysteine or histidine, 10 mM pH 7.4 phosphate buffer, 37 °C.

Complex	Amino Acid	4 h	18 h
2a	Cysteine	99%	99%
	Hisidine	99%	99%
3a	Cysteine	99%	99%
	Histidine	99%	99%
6a	Cysteine	99%	5%
	Histidine	99%	95%
7a	Cysteine	99%	99%
	Histidine	99%	99%

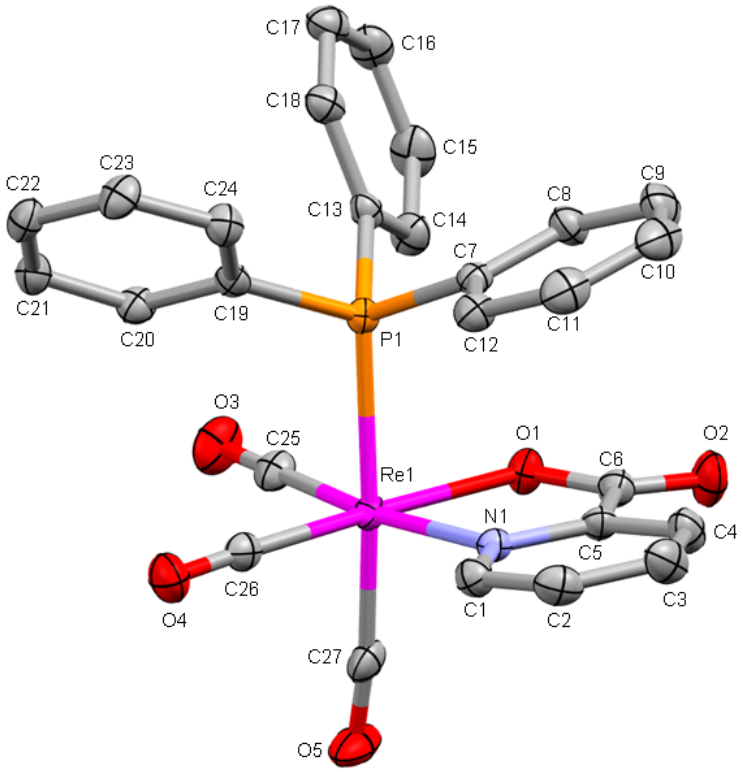


Table S3. Crystal data and structure refinement for **2**.

Empirical formula	$C_{27}H_{19}NO_5PRe$	
Formula weight	654.60	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 9.9334(15) Å	α = 90°
	b = 29.643(4) Å	β = 110.9850(10)°
	c = 8.6911(13) Å	γ = 90°
Volume	2389.4(6) Å^3	
Z, Calculated density	4, 1.820 Mg/m^3	
Absorption coefficient	5.192 mm^{-1}	
F(000)	1272	
Crystal size	0.40 x 0.10 x 0.10 mm	
Theta range for data collection	2.20 to 27.49°	
Limiting indices	-12<=h<=12, -38<=k<=38, -11<=l<=11	
Reflections collected / unique	27882 / 5484 [R_{int}=0.0377]	
Completeness to theta = 27.49	99.8%	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.62 and 0.38	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5484 / 0 / 316	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2σ(I)]	R_1 = 0.0199, wR_2=0.0414	
R indices (all data)	R_1 = 0.0242, wR_2=0.0429	
Largest diff. peak and hole	0.653 and -0.568 e.Å^{-3}	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Re(1)	5741(1)	806(1)	7084(1)	17(1)
P(1)	4047(1)	1245(1)	8045(1)	16(1)
O(1)	6636(2)	1443(1)	6783(2)	23(1)
O(2)	8428(2)	1935(1)	7895(3)	35(1)
O(3)	3329(2)	751(1)	3686(2)	38(1)
O(4)	4786(2)	-97(1)	8080(3)	33(1)
O(5)	7473(2)	248(1)	5430(3)	43(1)
N(1)	7451(2)	940(1)	9466(2)	17(1)
C(1)	7786(3)	683(1)	10837(3)	23(1)
C(2)	8792(3)	822(1)	12318(3)	27(1)
C(3)	9497(3)	1228(1)	12415(4)	32(1)
C(4)	9181(3)	1485(1)	11008(3)	28(1)
C(5)	8157(3)	1332(1)	9556(3)	20(1)
C(6)	7740(3)	1601(1)	7973(3)	23(1)
C(7)	4933(3)	1569(1)	9909(3)	18(1)
C(8)	5233(3)	2026(1)	9783(3)	25(1)
C(9)	6043(3)	2270(1)	11173(4)	35(1)
C(10)	6552(3)	2059(1)	12697(4)	35(1)
C(11)	6257(3)	1607(1)	12840(3)	31(1)
C(12)	5472(3)	1360(1)	11450(3)	24(1)
C(13)	2902(3)	1654(1)	6580(3)	19(1)
C(14)	3291(3)	1829(1)	5306(3)	26(1)
C(15)	2401(3)	2143(1)	4216(4)	32(1)
C(16)	1126(3)	2281(1)	4380(4)	30(1)
C(17)	739(3)	2107(1)	5641(3)	27(1)
C(18)	1610(3)	1798(1)	6732(3)	23(1)
C(19)	2675(3)	895(1)	8387(3)	19(1)
C(20)	1889(3)	613(1)	7097(3)	22(1)
C(21)	752(3)	360(1)	7193(3)	25(1)
C(22)	410(3)	374(1)	8601(3)	25(1)
C(23)	1193(3)	643(1)	9903(3)	26(1)
C(24)	2313(3)	912(1)	9796(3)	24(1)
C(25)	4237(3)	772(1)	4965(3)	24(1)
C(26)	5115(3)	244(1)	7675(3)	22(1)
C(27)	6913(3)	462(1)	6120(3)	26(1)

Table S5. Bond lengths [Å] and angles [°] for **2**.

Re(1)-C(26)	1.912(3)	C(9)-C(10)	1.385(4)
Re(1)-C(25)	1.914(3)	C(9)-H(9)	0.95
Re(1)-C(27)	1.947(3)	C(10)-C(11)	1.388(4)
Re(1)-O(1)	2.1439(18)	C(10)-H(10)	0.95
Re(1)-N(1)	2.193(2)	C(11)-C(12)	1.387(4)
Re(1)-P(1)	2.4975(7)	C(11)-H(11)	0.95
P(1)-C(7)	1.816(3)	C(12)-H(12)	0.95
P(1)-C(19)	1.820(3)	C(13)-C(14)	1.396(4)
P(1)-C(13)	1.829(3)	C(13)-C(18)	1.402(4)
O(1)-C(6)	1.295(3)	C(14)-C(15)	1.395(4)
O(2)-C(6)	1.219(3)	C(14)-H(14)	0.95
O(3)-C(25)	1.155(3)	C(15)-C(16)	1.386(4)
O(4)-C(26)	1.154(3)	C(15)-H(15)	0.95
O(5)-C(27)	1.145(3)	C(16)-C(17)	1.385(4)
N(1)-C(5)	1.346(3)	C(16)-H(16)	0.95
N(1)-C(1)	1.351(3)	C(17)-C(18)	1.379(4)
C(1)-C(2)	1.380(4)	C(17)-H(17)	0.95
C(1)-H(1)	0.95	C(18)-H(18)	0.95
C(2)-C(3)	1.380(4)	C(19)-C(20)	1.394(4)
C(2)-H(2)	0.95	C(19)-C(24)	1.394(4)
C(3)-C(4)	1.377(4)	C(20)-C(21)	1.382(4)
C(3)-H(3)	0.95	C(20)-H(20)	0.95
C(4)-C(5)	1.384(4)	C(21)-C(22)	1.383(4)
C(4)-H(4)	0.95	C(21)-H(21)	0.95
C(5)-C(6)	1.513(4)	C(22)-C(23)	1.375(4)
C(7)-C(12)	1.397(4)	C(22)-H(22)	0.95
C(7)-C(8)	1.401(4)	C(23)-C(24)	1.398(4)
C(8)-C(9)	1.390(4)	C(23)-H(23)	0.95
C(8)-H(8)	0.95	C(24)-H(24)	0.95

C(26)-Re(1)-C(25)	89.76(11)	C(25)-Re(1)-P(1)	87.83(8)
C(26)-Re(1)-C(27)	87.84(11)	C(27)-Re(1)-P(1)	174.35(8)
C(25)-Re(1)-C(27)	86.53(11)	O(1)-Re(1)-P(1)	86.52(5)
C(26)-Re(1)-O(1)	171.84(9)	N(1)-Re(1)-P(1)	88.65(6)
C(25)-Re(1)-O(1)	98.28(10)	C(7)-P(1)-C(19)	107.89(12)
C(27)-Re(1)-O(1)	94.03(10)	C(7)-P(1)-C(13)	104.65(12)
C(26)-Re(1)-N(1)	96.92(9)	C(19)-P(1)-C(13)	100.15(12)
C(25)-Re(1)-N(1)	172.57(10)	C(7)-P(1)-Re(1)	113.89(8)
C(27)-Re(1)-N(1)	96.92(10)	C(19)-P(1)-Re(1)	113.00(9)
O(1)-Re(1)-N(1)	74.98(7)	C(13)-P(1)-Re(1)	116.00(9)
C(26)-Re(1)-P(1)	92.40(8)	C(6)-O(1)-Re(1)	119.33(16)

C(5)-N(1)-C(1)	118.5(2)
C(5)-N(1)-Re(1)	114.99(16)
C(1)-N(1)-Re(1)	126.43(18)
N(1)-C(1)-C(2)	121.5(3)
N(1)-C(1)-H(1)	119.3
C(2)-C(1)-H(1)	119.3
C(1)-C(2)-C(3)	120.0(3)
C(1)-C(2)-H(2)	120
C(3)-C(2)-H(2)	120
C(4)-C(3)-C(2)	118.6(3)
C(4)-C(3)-H(3)	120.7
C(2)-C(3)-H(3)	120.7
C(3)-C(4)-C(5)	119.2(3)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N(1)-C(5)-C(4)	122.3(2)
N(1)-C(5)-C(6)	115.8(2)
C(4)-C(5)-C(6)	121.9(2)
O(2)-C(6)-O(1)	125.4(3)
O(2)-C(6)-C(5)	120.1(2)
O(1)-C(6)-C(5)	114.4(2)
C(12)-C(7)-C(8)	119.0(2)
C(12)-C(7)-P(1)	121.2(2)
C(8)-C(7)-P(1)	119.34(19)
C(9)-C(8)-C(7)	120.5(3)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	119.8(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(11)	120.3(3)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(12)-C(11)-C(10)	120.1(3)
C(12)-C(11)-H(11)	119.9
C(10)-C(11)-H(11)	119.9
C(11)-C(12)-C(7)	120.3(3)
C(11)-C(12)-H(12)	119.9
C(7)-C(12)-H(12)	119.9
C(14)-C(13)-C(18)	119.0(2)
C(14)-C(13)-P(1)	121.2(2)
C(18)-C(13)-P(1)	119.8(2)
C(15)-C(14)-C(13)	119.9(3)
C(15)-C(14)-H(14)	120.1
C(13)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	120.5(3)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	119.6(3)
C(17)-C(16)-H(16)	120.2
C(15)-C(16)-H(16)	120.2
C(18)-C(17)-C(16)	120.6(3)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(17)-C(18)-C(13)	120.5(3)
C(17)-C(18)-H(18)	119.8
C(13)-C(18)-H(18)	119.8
C(20)-C(19)-C(24)	118.8(2)
C(20)-C(19)-P(1)	116.58(19)
C(24)-C(19)-P(1)	124.6(2)
C(21)-C(20)-C(19)	120.7(2)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(20)-C(21)-C(22)	120.2(3)
C(20)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(23)-C(22)-C(21)	119.9(3)
C(23)-C(22)-H(22)	120
C(21)-C(22)-H(22)	120
C(22)-C(23)-C(24)	120.3(3)
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-H(23)	119.9
C(19)-C(24)-C(23)	120.0(3)
C(19)-C(24)-H(24)	120
C(23)-C(24)-H(24)	120
O(3)-C(25)-Re(1)	180.0(3)
O(4)-C(26)-Re(1)	177.4(2)
O(5)-C(27)-Re(1)	173.0(2)

Table S6. Anisotropic displacement parameters ($Å^2$ x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Re(1)	16(1)	20(1)	14(1)	-1(1)	5(1)	-2(1)
P(1)	17(1)	18(1)	14(1)	1(1)	5(1)	-1(1)
O(1)	22(1)	26(1)	19(1)	5(1)	4(1)	-5(1)
O(2)	30(1)	28(1)	42(1)	10(1)	5(1)	-10(1)
O(3)	32(1)	57(2)	18(1)	-3(1)	0(1)	-4(1)
O(4)	38(1)	24(1)	37(1)	1(1)	13(1)	-5(1)
O(5)	25(1)	62(2)	41(1)	-26(1)	12(1)	1(1)
N(1)	17(1)	19(1)	15(1)	0(1)	5(1)	2(1)
C(1)	24(1)	21(1)	22(1)	1(1)	8(1)	0(1)
C(2)	31(2)	30(2)	19(1)	3(1)	6(1)	8(1)
C(3)	29(2)	32(2)	23(2)	-6(1)	-4(1)	4(1)
C(4)	27(2)	23(2)	26(2)	-2(1)	1(1)	-2(1)
C(5)	18(1)	19(1)	22(1)	3(1)	5(1)	3(1)
C(6)	21(1)	23(1)	24(1)	1(1)	8(1)	-1(1)
C(7)	17(1)	21(1)	16(1)	-3(1)	6(1)	1(1)
C(8)	28(2)	20(1)	24(1)	-2(1)	6(1)	0(1)
C(9)	35(2)	26(2)	37(2)	-11(1)	5(1)	-3(1)
C(10)	27(2)	46(2)	26(2)	-18(1)	4(1)	2(1)
C(11)	30(2)	44(2)	18(1)	-3(1)	7(1)	3(1)
C(12)	24(1)	28(2)	20(1)	-1(1)	8(1)	0(1)
C(13)	21(1)	16(1)	17(1)	-1(1)	2(1)	-1(1)
C(14)	26(2)	24(2)	28(2)	7(1)	9(1)	0(1)
C(15)	36(2)	30(2)	26(2)	12(1)	6(1)	-3(1)
C(16)	30(2)	25(2)	27(2)	5(1)	1(1)	2(1)
C(17)	26(2)	26(2)	25(1)	-5(1)	4(1)	6(1)
C(18)	26(1)	23(1)	18(1)	-1(1)	5(1)	2(1)
C(19)	19(1)	16(1)	20(1)	4(1)	6(1)	2(1)
C(20)	23(1)	26(1)	20(1)	-2(1)	9(1)	0(1)
C(21)	22(1)	25(2)	25(1)	-3(1)	5(1)	-3(1)
C(22)	20(1)	27(2)	26(1)	4(1)	6(1)	-4(1)
C(23)	25(2)	35(2)	22(1)	2(1)	13(1)	-3(1)
C(24)	25(1)	26(2)	20(1)	-1(1)	8(1)	-2(1)
C(25)	23(1)	31(2)	20(1)	-1(1)	11(1)	-2(1)
C(26)	20(1)	26(2)	17(1)	-4(1)	3(1)	1(1)
C(27)	16(1)	36(2)	24(1)	-4(1)	5(1)	-4(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **2**.

	x	y	z	U(eq)
H(1)	7319	401	10780	27
H(2)	8998	639	13270	33
H(3)	10186	1329	13430	38
H(4)	9659	1764	11035	33
H(8)	4881	2171	8739	30
H(9)	6247	2579	11079	42
H(10)	7106	2225	13648	42
H(11)	6593	1465	13890	37
H(12)	5300	1048	11548	28
H(14)	4160	1734	5182	31
H(15)	2670	2263	3354	38
H(16)	523	2495	3633	36
H(17)	-135	2201	5755	33
H(18)	1334	1681	7592	27
H(20)	2137	594	6140	27
H(21)	204	177	6289	30
H(22)	-366	198	8668	30
H(23)	972	646	10880	31
H(24)	2828	1105	10683	28

Table S8. Torsion angles [°] for **2**.

C(26)-Re(1)-P(1)-C(7)	109.44(12)	Re(1)-O(1)-C(6)-O(2)	172.6(2)
C(25)-Re(1)-P(1)-C(7)	-160.90(12)	Re(1)-O(1)-C(6)-C(5)	-7.4(3)
C(27)-Re(1)-P(1)-C(7)	-158.3(9)	N(1)-C(5)-C(6)-O(2)	-172.2(3)
O(1)-Re(1)-P(1)-C(7)	-62.47(11)	C(4)-C(5)-C(6)-O(2)	8.9(4)
N(1)-Re(1)-P(1)-C(7)	12.56(11)	N(1)-C(5)-C(6)-O(1)	7.8(3)
C(26)-Re(1)-P(1)-C(19)	-14.14(12)	C(4)-C(5)-C(6)-O(1)	-171.1(2)
C(25)-Re(1)-P(1)-C(19)	75.53(12)	C(19)-P(1)-C(7)-C(12)	50.6(2)
C(27)-Re(1)-P(1)-C(19)	78.2(9)	C(13)-P(1)-C(7)-C(12)	156.6(2)
O(1)-Re(1)-P(1)-C(19)	173.96(10)	Re(1)-P(1)-C(7)-C(12)	-75.7(2)
N(1)-Re(1)-P(1)-C(19)	-111.01(11)	C(19)-P(1)-C(7)-C(8)	-137.0(2)
C(26)-Re(1)-P(1)-C(13)	-128.98(12)	C(13)-P(1)-C(7)-C(8)	-31.0(2)
C(25)-Re(1)-P(1)-C(13)	-39.32(12)	Re(1)-P(1)-C(7)-C(8)	96.7(2)
C(27)-Re(1)-P(1)-C(13)	-36.7(9)	C(12)-C(7)-C(8)-C(9)	-0.6(4)
O(1)-Re(1)-P(1)-C(13)	59.11(10)	P(1)-C(7)-C(8)-C(9)	-173.2(2)
N(1)-Re(1)-P(1)-C(13)	134.14(11)	C(7)-C(8)-C(9)-C(10)	-0.3(4)
C(26)-Re(1)-O(1)-C(6)	11.0(7)	C(8)-C(9)-C(10)-C(11)	0.0(5)
C(25)-Re(1)-O(1)-C(6)	-179.1(2)	C(9)-C(10)-C(11)-C(12)	1.2(5)
C(27)-Re(1)-O(1)-C(6)	-92.1(2)	C(10)-C(11)-C(12)-C(7)	-2.1(4)
N(1)-Re(1)-O(1)-C(6)	4.02(18)	C(8)-C(7)-C(12)-C(11)	1.9(4)
P(1)-Re(1)-O(1)-C(6)	93.56(19)	P(1)-C(7)-C(12)-C(11)	174.2(2)
C(26)-Re(1)-N(1)-C(5)	-178.41(19)	C(7)-P(1)-C(13)-C(14)	103.8(2)
C(25)-Re(1)-N(1)-C(5)	-24.4(8)	C(19)-P(1)-C(13)-C(14)	-144.5(2)
C(27)-Re(1)-N(1)-C(5)	92.94(19)	Re(1)-P(1)-C(13)-C(14)	-22.6(2)
O(1)-Re(1)-N(1)-C(5)	0.61(17)	C(7)-P(1)-C(13)-C(18)	-76.0(2)
P(1)-Re(1)-N(1)-C(5)	-86.15(17)	C(19)-P(1)-C(13)-C(18)	35.6(2)
C(26)-Re(1)-N(1)-C(1)	-2.6(2)	Re(1)-P(1)-C(13)-C(18)	157.57(18)
C(25)-Re(1)-N(1)-C(1)	151.4(7)	C(18)-C(13)-C(14)-C(15)	0.4(4)
C(27)-Re(1)-N(1)-C(1)	-91.2(2)	P(1)-C(13)-C(14)-C(15)	-179.5(2)
O(1)-Re(1)-N(1)-C(1)	176.4(2)	C(13)-C(14)-C(15)-C(16)	-0.4(4)
P(1)-Re(1)-N(1)-C(1)	89.7(2)	C(14)-C(15)-C(16)-C(17)	0.2(4)
C(5)-N(1)-C(1)-C(2)	2.1(4)	C(15)-C(16)-C(17)-C(18)	0.1(4)
Re(1)-N(1)-C(1)-C(2)	-173.5(2)	C(16)-C(17)-C(18)-C(13)	-0.1(4)
N(1)-C(1)-C(2)-C(3)	-1.0(4)	C(14)-C(13)-C(18)-C(17)	-0.1(4)
C(1)-C(2)-C(3)-C(4)	-0.5(4)	P(1)-C(13)-C(18)-C(17)	179.7(2)
C(2)-C(3)-C(4)-C(5)	0.9(4)	C(7)-P(1)-C(19)-C(20)	-178.8(2)
C(1)-N(1)-C(5)-C(4)	-1.7(4)	C(13)-P(1)-C(19)-C(20)	72.1(2)
Re(1)-N(1)-C(5)-C(4)	174.4(2)	Re(1)-P(1)-C(19)-C(20)	-51.9(2)
C(1)-N(1)-C(5)-C(6)	179.4(2)	C(7)-P(1)-C(19)-C(24)	5.1(3)
Re(1)-N(1)-C(5)-C(6)	-4.4(3)	C(13)-P(1)-C(19)-C(24)	-104.1(2)
C(3)-C(4)-C(5)-N(1)	0.2(4)	Re(1)-P(1)-C(19)-C(24)	131.9(2)
C(3)-C(4)-C(5)-C(6)	179.0(3)	C(24)-C(19)-C(20)-C(21)	1.4(4)

P(1)-C(19)-C(20)-C(21)	-175.0(2)	P(1)-Re(1)-C(25)-O(3)	-62(100)
C(19)-C(20)-C(21)-C(22)	-2.1(4)	C(25)-Re(1)-C(26)-O(4)	164(5)
C(20)-C(21)-C(22)-C(23)	0.6(4)	C(27)-Re(1)-C(26)-O(4)	77(5)
C(21)-C(22)-C(23)-C(24)	1.6(4)	O(1)-Re(1)-C(26)-O(4)	-26(6)
C(20)-C(19)-C(24)-C(23)	0.8(4)	N(1)-Re(1)-C(26)-O(4)	-20(5)
P(1)-C(19)-C(24)-C(23)	176.9(2)	P(1)-Re(1)-C(26)-O(4)	-108(5)
C(22)-C(23)-C(24)-C(19)	-2.3(4)	C(26)-Re(1)-C(27)-O(5)	71(2)
C(26)-Re(1)-C(25)-O(3)	30(100)	C(25)-Re(1)-C(27)-O(5)	-19(2)
C(27)-Re(1)-C(25)-O(3)	118(100)	O(1)-Re(1)-C(27)-O(5)	-117(2)
O(1)-Re(1)-C(25)-O(3)	-148(100)	N(1)-Re(1)-C(27)-O(5)	167(2)
N(1)-Re(1)-C(25)-O(3)	-124(100)	P(1)-Re(1)-C(27)-O(5)	-22(3)

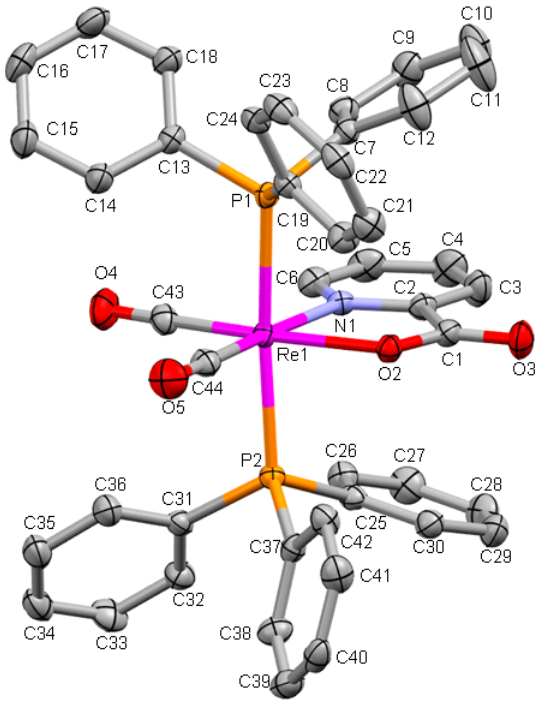


Table S9. Crystal data and structure refinement for **3**.

Empirical formula	$C_{46}H_{36}Cl_6NO_4P_2Re$
Formula weight	1127.60
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, *P*-1
Unit cell dimensions	a = 10.8612(3) Å, α = 77.9590(10)°
	b = 14.6446(5) Å, β = 82.0390(10)°
	c = 15.5216(5) Å, γ = 72.2150(10)°
Volume	2291.70(12) $Å^3$
Z, Calculated density	2, 1.634 Mg/m^3
Absorption coefficient	3.115 mm^{-1}
F(000)	1116
Crystal size	0.50 x 0.30 x 0.25 mm
Theta range for data collection	1.82 to 27.61°
Limiting indices	-14<=h<=14, -19<=k<=19, -20<=l<=20
Reflections collected / unique	21139 / 10429 [R(int) = 0.0210]
Completeness to theta = 27.61	98.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.51 and 0.40
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10429 / 0 / 541
Goodness-of-fit on F^2	1.042
Final R indices [I>2σ(I)]	R_1 = 0.0230, wR_2 = 0.0555
R indices (all data)	R_1 = 0.0259, wR_2 = 0.0569
Largest diff. peak and hole	0.820 and -1.267 e.$Å^{-3}$

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	2726(1)	3538(1)	6486(1)	17(1)
Cl(1)	4479(2)	808(1)	10962(1)	94(1)
Cl(2)	3420(1)	2877(1)	10412(1)	57(1)
Cl(3)	5772(1)	1845(1)	9505(1)	72(1)
Cl(4)	1011(2)	152(1)	10851(1)	101(1)
Cl(5)	-1302(1)	1703(1)	10454(1)	58(1)
Cl(6)	547(1)	1934(1)	11496(1)	56(1)
P(1)	3751(1)	2082(1)	5860(1)	18(1)
P(2)	1821(1)	4912(1)	7237(1)	18(1)
O(2)	2977(2)	2654(1)	7793(1)	21(1)
O(3)	2098(2)	1791(2)	8931(1)	33(1)
O(4)	1840(2)	4737(2)	4713(1)	38(1)
O(5)	5313(2)	4032(2)	6059(1)	40(1)
N(1)	948(2)	3107(2)	6875(1)	19(1)
C(1)	2069(3)	2293(2)	8185(2)	23(1)
C(2)	897(3)	2533(2)	7679(2)	22(1)
C(3)	-180(3)	2213(2)	8005(2)	34(1)
C(4)	-1248(3)	2504(2)	7515(2)	38(1)
C(5)	-1201(3)	3096(2)	6705(2)	32(1)
C(6)	-93(3)	3375(2)	6399(2)	26(1)
C(7)	2963(2)	1108(2)	6206(2)	21(1)
C(8)	1720(3)	1254(2)	5946(2)	25(1)
C(9)	1051(3)	572(2)	6272(2)	34(1)
C(10)	1599(3)	-269(2)	6848(2)	42(1)
C(11)	2823(4)	-427(3)	7099(3)	53(1)
C(12)	3501(3)	262(2)	6786(2)	40(1)
C(13)	3929(2)	2278(2)	4654(2)	21(1)
C(14)	4411(3)	3048(2)	4213(2)	28(1)
C(15)	4554(3)	3244(2)	3296(2)	35(1)
C(16)	4204(3)	2689(2)	2815(2)	38(1)
C(17)	3730(3)	1925(2)	3237(2)	37(1)
C(18)	3608(3)	1709(2)	4156(2)	28(1)
C(19)	5397(2)	1441(2)	6168(2)	20(1)
C(20)	5690(3)	1405(2)	7026(2)	27(1)
C(21)	6877(3)	827(2)	7321(2)	30(1)
C(22)	7792(3)	295(2)	6766(2)	29(1)
C(23)	7527(3)	345(2)	5907(2)	28(1)
C(24)	6335(2)	910(2)	5608(2)	23(1)

C(25)	402(2)	4814(2)	7987(2)	21(1)
C(26)	-804(3)	5001(2)	7659(2)	25(1)
C(27)	-1849(3)	4832(2)	8220(2)	33(1)
C(28)	-1702(3)	4460(2)	9105(2)	35(1)
C(29)	-513(3)	4252(2)	9438(2)	31(1)
C(30)	536(3)	4432(2)	8886(2)	25(1)
C(31)	1341(2)	6120(2)	6548(2)	21(1)
C(32)	206(3)	6837(2)	6713(2)	27(1)
C(33)	-16(3)	7770(2)	6224(2)	33(1)
C(34)	895(3)	8000(2)	5573(2)	33(1)
C(35)	2027(3)	7287(2)	5392(2)	33(1)
C(36)	2243(3)	6352(2)	5868(2)	27(1)
C(37)	2915(2)	5112(2)	7938(2)	21(1)
C(38)	2675(3)	6018(2)	8185(2)	28(1)
C(39)	3535(3)	6179(2)	8676(2)	30(1)
C(40)	4642(3)	5447(2)	8924(2)	29(1)
C(41)	4873(3)	4542(2)	8699(2)	31(1)
C(42)	4015(3)	4373(2)	8205(2)	26(1)
C(43)	2206(3)	4286(2)	5385(2)	24(1)
C(44)	4327(2)	3846(2)	6230(2)	23(1)
C(45)	4262(4)	1769(3)	10058(2)	46(1)
C(46)	348(3)	1404(2)	10627(2)	39(1)

Table S11. Bond lengths [Å] and angles [°] for **3**.

Re(1)-C(43)	1.884(3)	C(11)-C(12)	1.394(4)
Re(1)-C(44)	1.897(3)	C(11)-H(11)	0.95
Re(1)-O(2)	2.1701(16)	C(12)-H(12)	0.95
Re(1)-N(1)	2.181(2)	C(13)-C(18)	1.390(4)
Re(1)-P(2)	2.4130(6)	C(13)-C(14)	1.398(3)
Re(1)-P(1)	2.4182(6)	C(14)-C(15)	1.388(4)
Cl(1)-C(45)	1.752(4)	C(14)-H(14)	0.95
Cl(2)-C(45)	1.759(4)	C(15)-C(16)	1.374(4)
Cl(3)-C(45)	1.767(4)	C(15)-H(15)	0.95
Cl(4)-C(46)	1.731(3)	C(16)-C(17)	1.377(4)
Cl(5)-C(46)	1.756(3)	C(16)-H(16)	0.95
Cl(6)-C(46)	1.756(3)	C(17)-C(18)	1.391(4)
P(1)-C(19)	1.825(3)	C(17)-H(17)	0.95
P(1)-C(13)	1.826(2)	C(18)-H(18)	0.95
P(1)-C(7)	1.831(2)	C(19)-C(24)	1.397(3)
P(2)-C(25)	1.822(2)	C(19)-C(20)	1.399(4)
P(2)-C(31)	1.829(2)	C(20)-C(21)	1.387(4)
P(2)-C(37)	1.840(3)	C(20)-H(20)	0.95
O(2)-C(1)	1.281(3)	C(21)-C(22)	1.381(4)
O(3)-C(1)	1.234(3)	C(21)-H(21)	0.95
O(4)-C(43)	1.161(3)	C(22)-C(23)	1.384(4)
O(5)-C(44)	1.167(3)	C(22)-H(22)	0.95
N(1)-C(6)	1.348(3)	C(23)-C(24)	1.389(4)
N(1)-C(2)	1.356(3)	C(23)-H(23)	0.95
C(1)-C(2)	1.500(4)	C(24)-H(24)	0.95
C(2)-C(3)	1.384(4)	C(25)-C(26)	1.399(4)
C(3)-C(4)	1.383(4)	C(25)-C(30)	1.400(3)
C(3)-H(3)	0.95	C(26)-C(27)	1.384(4)
C(4)-C(5)	1.374(4)	C(26)-H(26)	0.95
C(4)-H(4)	0.95	C(27)-C(28)	1.380(4)
C(5)-C(6)	1.379(4)	C(27)-H(27)	0.95
C(5)-H(5)	0.95	C(28)-C(29)	1.381(4)
C(6)-H(6)	0.95	C(28)-H(28)	0.95
C(7)-C(12)	1.388(4)	C(29)-C(30)	1.387(4)
C(7)-C(8)	1.404(4)	C(29)-H(29)	0.95
C(8)-C(9)	1.383(4)	C(30)-H(30)	0.95
C(8)-H(8)	0.95	C(31)-C(32)	1.386(4)
C(9)-C(10)	1.383(4)	C(31)-C(36)	1.399(3)
C(9)-H(9)	0.95	C(32)-C(33)	1.384(4)
C(10)-C(11)	1.375(5)	C(32)-H(32)	0.95
C(10)-H(10)	0.95	C(33)-C(34)	1.378(4)

C(33)-H(33)	0.95
C(34)-C(35)	1.386(4)
C(34)-H(34)	0.95
C(35)-C(36)	1.380(4)
C(35)-H(35)	0.95
C(36)-H(36)	0.95
C(37)-C(42)	1.390(4)
C(37)-C(38)	1.397(4)
C(38)-C(39)	1.384(4)
C(38)-H(38)	0.95
C(39)-C(40)	1.382(4)
C(39)-H(39)	0.95
C(40)-C(41)	1.380(4)
C(40)-H(40)	0.95
C(41)-C(42)	1.391(4)
C(41)-H(41)	0.95
C(42)-H(42)	0.95
C(45)-H(45)	1
C(46)-H(46)	1

C(43)-Re(1)-C(44)	88.96(11)
C(43)-Re(1)-O(2)	169.83(9)
C(44)-Re(1)-O(2)	101.16(9)
C(43)-Re(1)-N(1)	95.56(9)
C(44)-Re(1)-N(1)	175.46(9)
O(2)-Re(1)-N(1)	74.33(7)
C(43)-Re(1)-P(2)	92.73(8)
C(44)-Re(1)-P(2)	90.69(8)
O(2)-Re(1)-P(2)	86.16(5)
N(1)-Re(1)-P(2)	89.55(5)
C(43)-Re(1)-P(1)	92.67(8)
C(44)-Re(1)-P(1)	87.88(8)
O(2)-Re(1)-P(1)	88.79(5)
N(1)-Re(1)-P(1)	91.46(6)
P(2)-Re(1)-P(1)	174.39(2)
C(19)-P(1)-C(13)	103.43(11)
C(19)-P(1)-C(7)	101.05(11)
C(13)-P(1)-C(7)	105.87(11)
C(19)-P(1)-Re(1)	114.81(8)
C(13)-P(1)-Re(1)	114.84(8)
C(7)-P(1)-Re(1)	115.23(8)
C(25)-P(2)-C(31)	105.64(11)
C(25)-P(2)-C(37)	103.75(11)
C(31)-P(2)-C(37)	100.03(11)
C(25)-P(2)-Re(1)	113.15(8)
C(31)-P(2)-Re(1)	117.23(8)
C(37)-P(2)-Re(1)	115.35(9)
C(1)-O(2)-Re(1)	119.15(16)
C(6)-N(1)-C(2)	118.2(2)
C(6)-N(1)-Re(1)	125.94(16)
C(2)-N(1)-Re(1)	115.86(16)
O(3)-C(1)-O(2)	124.7(2)
O(3)-C(1)-C(2)	119.9(2)
O(2)-C(1)-C(2)	115.4(2)
N(1)-C(2)-C(3)	121.6(2)
N(1)-C(2)-C(1)	115.3(2)
C(3)-C(2)-C(1)	123.1(2)
C(4)-C(3)-C(2)	119.6(3)
C(4)-C(3)-H(3)	120.2
C(2)-C(3)-H(3)	120.2
C(5)-C(4)-C(3)	118.8(3)
C(5)-C(4)-H(4)	120.6
C(3)-C(4)-H(4)	120.6
C(4)-C(5)-C(6)	119.4(3)
C(4)-C(5)-H(5)	120.3
C(6)-C(5)-H(5)	120.3
N(1)-C(6)-C(5)	122.4(2)
N(1)-C(6)-H(6)	118.8
C(5)-C(6)-H(6)	118.8
C(12)-C(7)-C(8)	118.3(2)
C(12)-C(7)-P(1)	122.1(2)
C(8)-C(7)-P(1)	119.29(19)
C(9)-C(8)-C(7)	120.3(3)
C(9)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
C(10)-C(9)-C(8)	120.8(3)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	119.5(3)
C(11)-C(10)-H(10)	120.3
C(9)-C(10)-H(10)	120.3
C(10)-C(11)-C(12)	120.4(3)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(7)-C(12)-C(11)	120.7(3)
C(7)-C(12)-H(12)	119.7

C(11)-C(12)-H(12)	119.7
C(18)-C(13)-C(14)	118.7(2)
C(18)-C(13)-P(1)	123.71(19)
C(14)-C(13)-P(1)	117.60(19)
C(15)-C(14)-C(13)	120.5(3)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(16)-C(15)-C(14)	120.0(3)
C(16)-C(15)-H(15)	120
C(14)-C(15)-H(15)	120
C(15)-C(16)-C(17)	120.3(3)
C(15)-C(16)-H(16)	119.9
C(17)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	120.2(3)
C(16)-C(17)-H(17)	119.9
C(18)-C(17)-H(17)	119.9
C(13)-C(18)-C(17)	120.3(3)
C(13)-C(18)-H(18)	119.8
C(17)-C(18)-H(18)	119.8
C(24)-C(19)-C(20)	118.8(2)
C(24)-C(19)-P(1)	122.29(19)
C(20)-C(19)-P(1)	118.60(19)
C(21)-C(20)-C(19)	120.3(3)
C(21)-C(20)-H(20)	119.8
C(19)-C(20)-H(20)	119.8
C(22)-C(21)-C(20)	120.4(3)
C(22)-C(21)-H(21)	119.8
C(20)-C(21)-H(21)	119.8
C(21)-C(22)-C(23)	119.8(3)
C(21)-C(22)-H(22)	120.1
C(23)-C(22)-H(22)	120.1
C(22)-C(23)-C(24)	120.4(3)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(19)	120.2(2)
C(23)-C(24)-H(24)	119.9
C(19)-C(24)-H(24)	119.9
C(26)-C(25)-C(30)	118.8(2)
C(26)-C(25)-P(2)	120.49(18)
C(30)-C(25)-P(2)	120.2(2)
C(27)-C(26)-C(25)	120.3(2)
C(27)-C(26)-H(26)	119.8
C(25)-C(26)-H(26)	119.8
C(28)-C(27)-C(26)	120.2(3)
C(28)-C(27)-H(27)	119.9
C(26)-C(27)-H(27)	119.9
C(27)-C(28)-C(29)	120.4(3)
C(27)-C(28)-H(28)	119.8
C(29)-C(28)-H(28)	119.8
C(28)-C(29)-C(30)	120.0(3)
C(28)-C(29)-H(29)	120
C(30)-C(29)-H(29)	120
C(29)-C(30)-C(25)	120.3(3)
C(29)-C(30)-H(30)	119.8
C(25)-C(30)-H(30)	119.8
C(32)-C(31)-C(36)	118.7(2)
C(32)-C(31)-P(2)	124.03(19)
C(36)-C(31)-P(2)	116.9(2)
C(33)-C(32)-C(31)	120.5(2)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
C(34)-C(33)-C(32)	120.4(3)
C(34)-C(33)-H(33)	119.8
C(32)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	119.8(2)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(36)-C(35)-C(34)	120.0(3)
C(36)-C(35)-H(35)	120
C(34)-C(35)-H(35)	120
C(35)-C(36)-C(31)	120.5(3)
C(35)-C(36)-H(36)	119.8
C(31)-C(36)-H(36)	119.8
C(42)-C(37)-C(38)	119.0(2)
C(42)-C(37)-P(2)	120.5(2)
C(38)-C(37)-P(2)	120.5(2)
C(39)-C(38)-C(37)	120.3(3)
C(39)-C(38)-H(38)	119.9
C(37)-C(38)-H(38)	119.9
C(40)-C(39)-C(38)	120.4(3)
C(40)-C(39)-H(39)	119.8
C(38)-C(39)-H(39)	119.8
C(41)-C(40)-C(39)	119.8(3)
C(41)-C(40)-H(40)	120.1
C(39)-C(40)-H(40)	120.1
C(40)-C(41)-C(42)	120.2(3)

C(40)-C(41)-H(41)	119.9	Cl(1)-C(45)-H(45)	108.7
C(42)-C(41)-H(41)	119.9	Cl(2)-C(45)-H(45)	108.7
C(37)-C(42)-C(41)	120.3(3)	Cl(3)-C(45)-H(45)	108.7
C(37)-C(42)-H(42)	119.8	Cl(4)-C(46)-Cl(6)	110.48(18)
C(41)-C(42)-H(42)	119.8	Cl(4)-C(46)-Cl(5)	110.5(2)
O(4)-C(43)-Re(1)	177.2(2)	Cl(6)-C(46)-Cl(5)	110.29(17)
O(5)-C(44)-Re(1)	179.0(2)	Cl(4)-C(46)-H(46)	108.5
Cl(1)-C(45)-Cl(2)	110.20(19)	Cl(6)-C(46)-H(46)	108.5
Cl(1)-C(45)-Cl(3)	110.7(2)	Cl(5)-C(46)-H(46)	108.5
Cl(2)-C(45)-Cl(3)	109.79(19)		

Table S12. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Re(1)	16(1)	16(1)	16(1)	-2(1)	-1(1)	-3(1)
Cl(1)	164(2)	61(1)	57(1)	12(1)	-21(1)	-41(1)
Cl(2)	63(1)	63(1)	47(1)	-10(1)	-8(1)	-21(1)
Cl(3)	47(1)	68(1)	97(1)	-13(1)	-1(1)	-13(1)
Cl(4)	131(1)	44(1)	127(1)	-35(1)	-94(1)	27(1)
Cl(5)	41(1)	72(1)	56(1)	-24(1)	-3(1)	2(1)
Cl(6)	72(1)	51(1)	50(1)	-17(1)	-7(1)	-18(1)
P(1)	17(1)	18(1)	17(1)	-2(1)	-2(1)	-5(1)
P(2)	17(1)	18(1)	19(1)	-3(1)	-1(1)	-4(1)
O(2)	22(1)	23(1)	19(1)	-3(1)	-3(1)	-7(1)
O(3)	41(1)	39(1)	20(1)	6(1)	-7(1)	-19(1)
O(4)	43(1)	35(1)	26(1)	6(1)	-9(1)	-2(1)
O(5)	26(1)	48(1)	48(1)	-11(1)	5(1)	-18(1)
N(1)	20(1)	20(1)	19(1)	-5(1)	-2(1)	-6(1)
C(1)	26(1)	23(1)	19(1)	-5(1)	-2(1)	-7(1)
C(2)	25(1)	25(1)	20(1)	-5(1)	-3(1)	-10(1)
C(3)	40(2)	44(2)	25(1)	-3(1)	2(1)	-26(2)
C(4)	31(2)	54(2)	38(2)	-12(1)	4(1)	-28(2)
C(5)	24(1)	44(2)	34(1)	-12(1)	-6(1)	-14(1)
C(6)	23(1)	27(1)	25(1)	-6(1)	-4(1)	-3(1)
C(7)	21(1)	22(1)	21(1)	-4(1)	1(1)	-6(1)
C(8)	24(1)	27(1)	24(1)	-5(1)	-4(1)	-8(1)
C(9)	30(2)	46(2)	31(1)	-6(1)	-1(1)	-20(1)
C(10)	41(2)	40(2)	48(2)	3(1)	2(1)	-25(2)
C(11)	44(2)	38(2)	70(2)	25(2)	-15(2)	-19(2)
C(12)	27(2)	36(2)	53(2)	13(1)	-11(1)	-13(1)
C(13)	18(1)	24(1)	18(1)	-4(1)	-1(1)	-4(1)
C(14)	32(2)	31(1)	22(1)	-5(1)	1(1)	-14(1)
C(15)	41(2)	39(2)	23(1)	1(1)	3(1)	-17(1)
C(16)	43(2)	50(2)	17(1)	-5(1)	1(1)	-12(2)
C(17)	45(2)	48(2)	25(1)	-15(1)	-1(1)	-19(2)
C(18)	33(2)	32(1)	23(1)	-8(1)	0(1)	-13(1)
C(19)	17(1)	18(1)	24(1)	-2(1)	-3(1)	-5(1)
C(20)	23(1)	27(1)	27(1)	-5(1)	-4(1)	-2(1)
C(21)	27(1)	29(1)	32(1)	-2(1)	-12(1)	-5(1)
C(22)	20(1)	22(1)	41(2)	3(1)	-8(1)	-5(1)
C(23)	20(1)	21(1)	41(2)	-5(1)	2(1)	-4(1)

C(24)	23(1)	20(1)	27(1)	-4(1)	-1(1)	-8(1)
C(25)	21(1)	19(1)	22(1)	-6(1)	0(1)	-5(1)
C(26)	22(1)	25(1)	27(1)	-3(1)	-1(1)	-6(1)
C(27)	20(1)	37(2)	40(2)	-7(1)	-1(1)	-7(1)
C(28)	29(2)	42(2)	36(2)	-10(1)	11(1)	-15(1)
C(29)	38(2)	36(2)	22(1)	-6(1)	4(1)	-16(1)
C(30)	26(1)	26(1)	24(1)	-6(1)	-1(1)	-8(1)
C(31)	24(1)	17(1)	21(1)	-3(1)	-5(1)	-6(1)
C(32)	27(1)	23(1)	27(1)	-5(1)	-2(1)	-4(1)
C(33)	33(2)	21(1)	41(2)	-3(1)	-10(1)	2(1)
C(34)	46(2)	22(1)	32(1)	3(1)	-13(1)	-12(1)
C(35)	41(2)	29(2)	29(1)	1(1)	-3(1)	-17(1)
C(36)	28(1)	27(1)	26(1)	-4(1)	-1(1)	-10(1)
C(37)	19(1)	26(1)	18(1)	-3(1)	-1(1)	-8(1)
C(38)	23(1)	30(1)	30(1)	-11(1)	-2(1)	-4(1)
C(39)	33(2)	35(2)	29(1)	-14(1)	2(1)	-13(1)
C(40)	31(2)	41(2)	19(1)	-4(1)	-2(1)	-21(1)
C(41)	27(1)	35(2)	32(1)	1(1)	-10(1)	-12(1)
C(42)	25(1)	24(1)	29(1)	-1(1)	-6(1)	-8(1)
C(43)	23(1)	22(1)	25(1)	-2(1)	-1(1)	-4(1)
C(44)	22(1)	22(1)	25(1)	-5(1)	0(1)	-5(1)
C(45)	53(2)	57(2)	38(2)	-2(2)	-16(2)	-27(2)
C(46)	40(2)	45(2)	27(1)	-6(1)	0(1)	-4(2)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(3)	-186	1795	8563	41
H(4)	-1999	2299	7733	45
H(5)	-1925	3311	6358	39
H(6)	-62	3771	5832	31
H(8)	1336	1824	5544	29
H(9)	205	683	6098	40
H(10)	1133	-734	7069	51
H(11)	3210	-1008	7487	64
H(12)	4340	150	6972	48
H(14)	4642	3440	4543	33
H(15)	4895	3763	3002	42
H(16)	4288	2832	2187	45
H(17)	3487	1545	2901	44
H(18)	3303	1171	4444	34
H(20)	5073	1779	7409	32
H(21)	7061	796	7909	36
H(22)	8601	-103	6972	34
H(23)	8164	-9	5521	34
H(24)	6156	935	5020	28
H(26)	-906	5245	7048	30
H(27)	-2669	4973	7995	39
H(28)	-2423	4346	9486	42
H(29)	-414	3985	10046	38
H(30)	1351	4296	9118	30
H(32)	-424	6688	7164	32
H(33)	-802	8254	6338	40
H(34)	749	8645	5250	40
H(35)	2653	7442	4940	39
H(36)	3010	5862	5732	32
H(38)	1918	6526	8017	33
H(39)	3364	6797	8844	36
H(40)	5241	5566	9247	34
H(41)	5621	4032	8883	37
H(42)	4182	3750	8050	31
H(45)	3737	1647	9636	56
H(46)	814	1669	10076	47

Table S14. Torsion angles [°] for **3**.

C(43)-Re(1)-P(1)-C(19)	130.98(11)	C(44)-Re(1)-N(1)-C(2)	6.2(12)
C(44)-Re(1)-P(1)-C(19)	42.13(11)	O(2)-Re(1)-N(1)-C(2)	-0.66(17)
O(2)-Re(1)-P(1)-C(19)	-59.09(9)	P(2)-Re(1)-N(1)-C(2)	-86.80(17)
N(1)-Re(1)-P(1)-C(19)	-133.38(10)	P(1)-Re(1)-N(1)-C(2)	87.68(17)
P(2)-Re(1)-P(1)-C(19)	-33.1(2)	Re(1)-O(2)-C(1)-O(3)	-179.0(2)
C(43)-Re(1)-P(1)-C(13)	11.25(12)	Re(1)-O(2)-C(1)-C(2)	-0.2(3)
C(44)-Re(1)-P(1)-C(13)	-77.61(12)	C(6)-N(1)-C(2)-C(3)	1.0(4)
O(2)-Re(1)-P(1)-C(13)	-178.83(10)	Re(1)-N(1)-C(2)-C(3)	179.7(2)
N(1)-Re(1)-P(1)-C(13)	106.88(10)	C(6)-N(1)-C(2)-C(1)	-177.9(2)
P(2)-Re(1)-P(1)-C(13)	-152.9(2)	Re(1)-N(1)-C(2)-C(1)	0.8(3)
C(43)-Re(1)-P(1)-C(7)	-112.20(12)	O(3)-C(1)-C(2)-N(1)	178.5(2)
C(44)-Re(1)-P(1)-C(7)	158.95(12)	O(2)-C(1)-C(2)-N(1)	-0.4(3)
O(2)-Re(1)-P(1)-C(7)	57.73(10)	O(3)-C(1)-C(2)-C(3)	-0.4(4)
N(1)-Re(1)-P(1)-C(7)	-16.56(11)	O(2)-C(1)-C(2)-C(3)	-179.3(3)
P(2)-Re(1)-P(1)-C(7)	83.7(2)	N(1)-C(2)-C(3)-C(4)	-1.9(4)
C(43)-Re(1)-P(2)-C(25)	110.68(12)	C(1)-C(2)-C(3)-C(4)	177.0(3)
C(44)-Re(1)-P(2)-C(25)	-160.33(12)	C(2)-C(3)-C(4)-C(5)	1.0(5)
O(2)-Re(1)-P(2)-C(25)	-59.19(10)	C(3)-C(4)-C(5)-C(6)	0.6(5)
N(1)-Re(1)-P(2)-C(25)	15.14(11)	C(2)-N(1)-C(6)-C(5)	0.7(4)
P(1)-Re(1)-P(2)-C(25)	-85.2(2)	Re(1)-N(1)-C(6)-C(5)	-177.8(2)
C(43)-Re(1)-P(2)-C(31)	-12.66(12)	C(4)-C(5)-C(6)-N(1)	-1.5(4)
C(44)-Re(1)-P(2)-C(31)	76.33(12)	C(19)-P(1)-C(7)-C(12)	17.0(3)
O(2)-Re(1)-P(2)-C(31)	177.47(10)	C(13)-P(1)-C(7)-C(12)	124.6(2)
N(1)-Re(1)-P(2)-C(31)	-108.20(11)	Re(1)-P(1)-C(7)-C(12)	-107.3(2)
P(1)-Re(1)-P(2)-C(31)	151.4(2)	C(19)-P(1)-C(7)-C(8)	-169.1(2)
C(43)-Re(1)-P(2)-C(37)	-130.07(11)	C(13)-P(1)-C(7)-C(8)	-61.5(2)
C(44)-Re(1)-P(2)-C(37)	-41.09(11)	Re(1)-P(1)-C(7)-C(8)	66.5(2)
O(2)-Re(1)-P(2)-C(37)	60.06(9)	C(12)-C(7)-C(8)-C(9)	0.7(4)
N(1)-Re(1)-P(2)-C(37)	134.38(10)	P(1)-C(7)-C(8)-C(9)	-173.4(2)
P(1)-Re(1)-P(2)-C(37)	34.0(2)	C(7)-C(8)-C(9)-C(10)	-0.9(4)
C(43)-Re(1)-O(2)-C(1)	7.0(6)	C(8)-C(9)-C(10)-C(11)	0.0(5)
C(44)-Re(1)-O(2)-C(1)	-179.01(18)	C(9)-C(10)-C(11)-C(12)	1.0(6)
N(1)-Re(1)-O(2)-C(1)	0.44(17)	C(8)-C(7)-C(12)-C(11)	0.3(5)
P(2)-Re(1)-O(2)-C(1)	91.05(17)	P(1)-C(7)-C(12)-C(11)	174.2(3)
P(1)-Re(1)-O(2)-C(1)	-91.41(17)	C(10)-C(11)-C(12)-C(7)	-1.2(6)
C(43)-Re(1)-N(1)-C(6)	-0.9(2)	C(19)-P(1)-C(13)-C(18)	100.9(2)
C(44)-Re(1)-N(1)-C(6)	-175.2(11)	C(7)-P(1)-C(13)-C(18)	-5.0(3)
O(2)-Re(1)-N(1)-C(6)	177.9(2)	Re(1)-P(1)-C(13)-C(18)	-133.3(2)
P(2)-Re(1)-N(1)-C(6)	91.8(2)	C(19)-P(1)-C(13)-C(14)	-79.4(2)
P(1)-Re(1)-N(1)-C(6)	-93.7(2)	C(7)-P(1)-C(13)-C(14)	174.7(2)
C(43)-Re(1)-N(1)-C(2)	-179.50(18)	Re(1)-P(1)-C(13)-C(14)	46.4(2)

C(18)-C(13)-C(14)-C(15)	0.5(4)	C(37)-P(2)-C(31)-C(32)	-96.9(2)
P(1)-C(13)-C(14)-C(15)	-179.2(2)	Re(1)-P(2)-C(31)-C(32)	137.7(2)
C(13)-C(14)-C(15)-C(16)	1.0(5)	C(25)-P(2)-C(31)-C(36)	-175.7(2)
C(14)-C(15)-C(16)-C(17)	-1.1(5)	C(37)-P(2)-C(31)-C(36)	76.8(2)
C(15)-C(16)-C(17)-C(18)	-0.2(5)	Re(1)-P(2)-C(31)-C(36)	-48.6(2)
C(14)-C(13)-C(18)-C(17)	-1.9(4)	C(36)-C(31)-C(32)-C(33)	-1.3(4)
P(1)-C(13)-C(18)-C(17)	177.8(2)	P(2)-C(31)-C(32)-C(33)	172.3(2)
C(16)-C(17)-C(18)-C(13)	1.7(5)	C(31)-C(32)-C(33)-C(34)	-0.7(4)
C(13)-P(1)-C(19)-C(24)	-23.3(2)	C(32)-C(33)-C(34)-C(35)	1.6(5)
C(7)-P(1)-C(19)-C(24)	86.1(2)	C(33)-C(34)-C(35)-C(36)	-0.6(4)
Re(1)-P(1)-C(19)-C(24)	-149.21(17)	C(34)-C(35)-C(36)-C(31)	-1.5(4)
C(13)-P(1)-C(19)-C(20)	162.9(2)	C(32)-C(31)-C(36)-C(35)	2.4(4)
C(7)-P(1)-C(19)-C(20)	-87.6(2)	P(2)-C(31)-C(36)-C(35)	-171.7(2)
Re(1)-P(1)-C(19)-C(20)	37.0(2)	C(25)-P(2)-C(37)-C(42)	106.8(2)
C(24)-C(19)-C(20)-C(21)	-2.0(4)	C(31)-P(2)-C(37)-C(42)	-144.2(2)
P(1)-C(19)-C(20)-C(21)	171.9(2)	Re(1)-P(2)-C(37)-C(42)	-17.5(2)
C(19)-C(20)-C(21)-C(22)	1.3(4)	C(25)-P(2)-C(37)-C(38)	-75.3(2)
C(20)-C(21)-C(22)-C(23)	0.4(4)	C(31)-P(2)-C(37)-C(38)	33.7(2)
C(21)-C(22)-C(23)-C(24)	-1.4(4)	Re(1)-P(2)-C(37)-C(38)	160.40(17)
C(22)-C(23)-C(24)-C(19)	0.7(4)	C(42)-C(37)-C(38)-C(39)	1.2(4)
C(20)-C(19)-C(24)-C(23)	1.0(4)	P(2)-C(37)-C(38)-C(39)	-176.8(2)
P(1)-C(19)-C(24)-C(23)	-172.70(19)	C(37)-C(38)-C(39)-C(40)	0.2(4)
C(31)-P(2)-C(25)-C(26)	52.6(2)	C(38)-C(39)-C(40)-C(41)	-1.6(4)
C(37)-P(2)-C(25)-C(26)	157.3(2)	C(39)-C(40)-C(41)-C(42)	1.7(4)
Re(1)-P(2)-C(25)-C(26)	-76.9(2)	C(38)-C(37)-C(42)-C(41)	-1.1(4)
C(31)-P(2)-C(25)-C(30)	-135.6(2)	P(2)-C(37)-C(42)-C(41)	176.9(2)
C(37)-P(2)-C(25)-C(30)	-30.9(2)	C(40)-C(41)-C(42)-C(37)	-0.3(4)
Re(1)-P(2)-C(25)-C(30)	94.9(2)	C(44)-Re(1)-C(43)-O(4)	178(100)
C(30)-C(25)-C(26)-C(27)	1.6(4)	O(2)-Re(1)-C(43)-O(4)	-8(5)
P(2)-C(25)-C(26)-C(27)	173.5(2)	N(1)-Re(1)-C(43)-O(4)	-1(5)
C(25)-C(26)-C(27)-C(28)	-1.3(4)	P(2)-Re(1)-C(43)-O(4)	-91(5)
C(26)-C(27)-C(28)-C(29)	0.0(5)	P(1)-Re(1)-C(43)-O(4)	90(5)
C(27)-C(28)-C(29)-C(30)	1.1(5)	C(43)-Re(1)-C(44)-O(5)	-48(14)
C(28)-C(29)-C(30)-C(25)	-0.8(4)	O(2)-Re(1)-C(44)-O(5)	133(14)
C(26)-C(25)-C(30)-C(29)	-0.5(4)	N(1)-Re(1)-C(44)-O(5)	127(14)
P(2)-C(25)-C(30)-C(29)	-172.5(2)	P(2)-Re(1)-C(44)-O(5)	-141(14)
C(25)-P(2)-C(31)-C(32)	10.6(3)	P(1)-Re(1)-C(44)-O(5)	45(14)

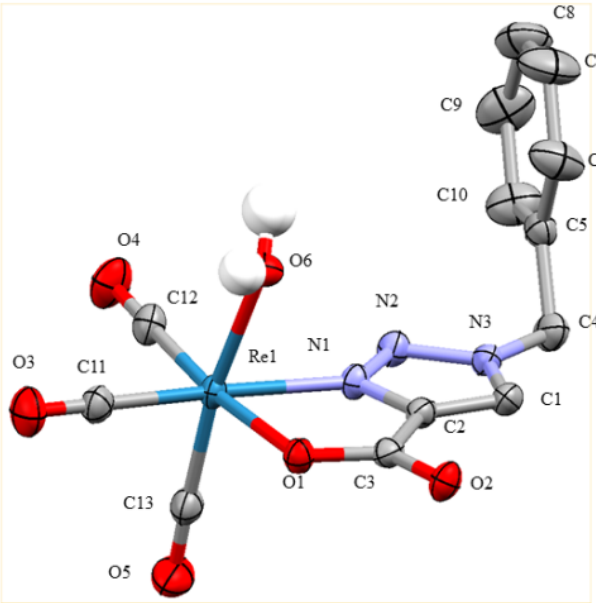


Table S15. Crystal data and structure refinement for **5**.

Empirical formula	$C_{16}H_{16}N_3O_7Re$	
Formula weight	548.52	
Temperature	173(2) K	
Wavelength	0.71073 A	
Crystal system, space group	Triclinic, *P*-1	
Unit cell dimensions	a = 8.6015(9) Å	α = 88.9500(10)°
	b = 10.2481(11) Å	β = 74.7110(10)°
	c = 11.3012(12) Å	γ = 86.0810(10)°
Volume	958.69(18) $Å^3$	
Z, Calculated density	2, 1.900 Mg/m^3	
Absorption coefficient	6.380 mm^{-1}	
F(000)	528	
Crystal size	0.35 x 0.25 x 0.15 mm	
Theta range for data collection	1.87 to 27.56°	
Limiting indices	-11<=h<=11, -13<=k<=13, -14<=l<=14	
Reflections collected / unique	11290 / 4355 [R(int) = 0.0216]	
Completeness to theta = 27.56	98.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.45 and 0.29	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4355 / 0 / 248	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2σ(I)]	R_1 = 0.0166, wR_2 = 0.0398	
R indices (all data)	R_1 = 0.0181, wR_2 = 0.0404	
Largest diff. peak and hole	0.534 and -0.553 e. $Å^{-3}$	

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	842(1)	704(1)	2089(1)	20(1)
O(1)	1242(2)	-483(2)	3595(2)	24(1)
O(2)	2658(2)	-761(2)	4988(2)	28(1)
O(3)	-2315(2)	-499(2)	2045(2)	41(1)
O(4)	391(3)	2665(2)	117(2)	42(1)
O(5)	2725(3)	-1213(2)	103(2)	47(1)
O(6)	-239(2)	1967(2)	3653(2)	29(1)
O(7)	-1063(3)	4520(2)	3864(2)	57(1)
N(1)	2980(2)	1396(2)	2446(2)	22(1)
N(2)	3981(3)	2294(2)	1953(2)	25(1)
N(3)	5046(2)	2282(2)	2638(2)	24(1)
C(1)	4732(3)	1397(2)	3553(2)	25(1)
C(2)	3386(3)	829(2)	3425(2)	22(1)
C(3)	2367(3)	-211(2)	4072(2)	22(1)
C(4)	6374(3)	3163(3)	2307(3)	33(1)
C(5)	5767(3)	4577(3)	2304(3)	27(1)
C(6)	4789(4)	5160(3)	3360(3)	46(1)
C(7)	4261(5)	6475(3)	3353(3)	58(1)
C(8)	4687(5)	7193(3)	2300(4)	53(1)
C(9)	5626(4)	6626(3)	1243(3)	53(1)
C(10)	6159(4)	5304(3)	1254(3)	45(1)
C(11)	-1133(3)	-50(3)	2056(2)	28(1)
C(12)	560(3)	1916(3)	859(3)	29(1)
C(13)	1996(3)	-480(3)	843(3)	30(1)
C(14)	-1250(6)	6808(3)	3748(5)	79(1)
C(15)	-532(4)	5488(3)	3317(3)	44(1)
C(16)	793(5)	5373(4)	2169(4)	73(1)

Table S17. Bond lengths [Å] and angles [°] for **5**.

Re(1)-C(13)	1.898(3)	C(4)-C(5)	1.507(4)
Re(1)-C(12)	1.899(3)	C(4)-H(4A)	0.9900
Re(1)-C(11)	1.923(3)	C(4)-H(4B)	0.9900
Re(1)-N(1)	2.152(2)	C(5)-C(10)	1.366(4)
Re(1)-O(1)	2.1612(17)	C(5)-C(6)	1.385(4)
Re(1)-O(6)	2.1719(18)	C(6)-C(7)	1.393(4)
O(1)-C(3)	1.274(3)	C(6)-H(6)	0.9500
O(2)-C(3)	1.244(3)	C(7)-C(8)	1.366(5)
O(3)-C(11)	1.147(3)	C(7)-H(7)	0.9500
O(4)-C(12)	1.157(3)	C(8)-C(9)	1.367(5)
O(5)-C(13)	1.157(3)	C(8)-H(8)	0.9500
O(6)-H(2O)	0.8588	C(9)-C(10)	1.402(5)
O(6)-H(1O)	0.8985	C(9)-H(9)	0.9500
O(7)-C(15)	1.210(4)	C(10)-H(10)	0.9500
N(1)-N(2)	1.316(3)	C(14)-C(15)	1.483(5)
N(1)-C(2)	1.355(3)	C(14)-H(14A)	0.9800
N(2)-N(3)	1.345(3)	C(14)-H(14B)	0.9800
N(3)-C(1)	1.348(3)	C(14)-H(14C)	0.9800
N(3)-C(4)	1.471(3)	C(15)-C(16)	1.484(5)
C(1)-C(2)	1.372(3)	C(16)-H(16A)	0.9800
C(1)-H(1)	0.9500	C(16)-H(16B)	0.9800
C(2)-C(3)	1.483(3)	C(16)-H(16C)	0.9800

C(13)-Re(1)-C(12)	89.38(12)	N(2)-N(3)-C(4)	119.0(2)
C(13)-Re(1)-C(11)	89.48(11)	C(1)-N(3)-C(4)	128.7(2)
C(12)-Re(1)-C(11)	89.76(11)	N(3)-C(1)-C(2)	104.4(2)
C(13)-Re(1)-N(1)	94.38(10)	N(3)-C(1)-H(1)	127.8
C(12)-Re(1)-N(1)	99.73(9)	C(2)-C(1)-H(1)	127.8
C(11)-Re(1)-N(1)	169.77(9)	N(1)-C(2)-C(1)	107.4(2)
C(13)-Re(1)-O(1)	95.29(9)	N(1)-C(2)-C(3)	117.0(2)
C(12)-Re(1)-O(1)	173.25(9)	C(1)-C(2)-C(3)	135.6(2)
C(11)-Re(1)-O(1)	95.15(9)	O(2)-C(3)-O(1)	125.0(2)
N(1)-Re(1)-O(1)	75.09(7)	O(2)-C(3)-C(2)	120.4(2)
C(13)-Re(1)-O(6)	172.08(9)	O(1)-C(3)-C(2)	114.5(2)
C(12)-Re(1)-O(6)	96.82(10)	N(3)-C(4)-C(5)	112.1(2)
C(11)-Re(1)-O(6)	95.44(9)	N(3)-C(4)-H(4A)	109.2
N(1)-Re(1)-O(6)	79.76(7)	C(5)-C(4)-H(4A)	109.2
O(1)-Re(1)-O(6)	78.13(7)	N(3)-C(4)-H(4B)	109.2
C(3)-O(1)-Re(1)	118.59(15)	C(5)-C(4)-H(4B)	109.2
Re(1)-O(6)-H(2O)	110.5	H(4A)-C(4)-H(4B)	107.9
Re(1)-O(6)-H(1O)	129.2	C(10)-C(5)-C(6)	118.8(3)
H(2O)-O(6)-H(1O)	110.8	C(10)-C(5)-C(4)	120.5(3)
N(2)-N(1)-C(2)	110.9(2)	C(6)-C(5)-C(4)	120.7(3)
N(2)-N(1)-Re(1)	134.59(16)	C(5)-C(6)-C(7)	120.2(3)
C(2)-N(1)-Re(1)	114.41(16)	C(5)-C(6)-H(6)	119.9
N(1)-N(2)-N(3)	105.0(2)	C(7)-C(6)-H(6)	119.9
N(2)-N(3)-C(1)	112.3(2)	C(8)-C(7)-C(6)	120.2(3)

C(8)-C(7)-H(7)	119.9	C(15)-C(14)-H(14B)	109.5
C(6)-C(7)-H(7)	119.9	H(14A)-C(14)-H(14B)	109.5
C(7)-C(8)-C(9)	120.4(3)	C(15)-C(14)-H(14C)	109.5
C(7)-C(8)-H(8)	119.8	H(14A)-C(14)-H(14C)	109.5
C(9)-C(8)-H(8)	119.8	H(14B)-C(14)-H(14C)	109.5
C(8)-C(9)-C(10)	119.3(3)	O(7)-C(15)-C(14)	120.5(4)
C(8)-C(9)-H(9)	120.4	O(7)-C(15)-C(16)	120.6(3)
C(10)-C(9)-H(9)	120.4	C(14)-C(15)-C(16)	118.8(3)
C(5)-C(10)-C(9)	121.1(3)	C(15)-C(16)-H(16A)	109.5
C(5)-C(10)-H(10)	119.4	C(15)-C(16)-H(16B)	109.5
C(9)-C(10)-H(10)	119.4	H(16A)-C(16)-H(16B)	109.5
O(3)-C(11)-Re(1)	179.5(3)	C(15)-C(16)-H(16C)	109.5
O(4)-C(12)-Re(1)	179.3(3)	H(16A)-C(16)-H(16C)	109.5
O(5)-C(13)-Re(1)	178.2(2)	H(16B)-C(16)-H(16C)	109.5
C(15)-C(14)-H(14A)	109.5		

Table S18. Anisotropic displacement parameters ($Å^2$ x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Re(1)	20(1)	24(1)	20(1)	2(1)	-8(1)	-2(1)
O(1)	26(1)	24(1)	25(1)	4(1)	-11(1)	-4(1)
O(2)	27(1)	33(1)	25(1)	8(1)	-12(1)	-1(1)
O(3)	32(1)	48(1)	48(1)	3(1)	-16(1)	-14(1)
O(4)	44(1)	48(1)	38(1)	20(1)	-18(1)	-4(1)
O(5)	47(1)	55(1)	38(1)	-16(1)	-16(1)	15(1)
O(6)	32(1)	25(1)	26(1)	0(1)	-1(1)	-1(1)
O(7)	70(2)	26(1)	63(2)	3(1)	2(1)	-6(1)
N(1)	23(1)	25(1)	21(1)	4(1)	-8(1)	-3(1)
N(2)	23(1)	27(1)	27(1)	3(1)	-9(1)	-3(1)
N(3)	21(1)	22(1)	33(1)	0(1)	-11(1)	-1(1)
C(1)	26(1)	23(1)	29(1)	0(1)	-13(1)	2(1)
C(2)	24(1)	22(1)	22(1)	-1(1)	-8(1)	3(1)
C(3)	23(1)	22(1)	22(1)	-1(1)	-6(1)	3(1)
C(4)	22(1)	29(1)	48(2)	0(1)	-10(1)	-4(1)
C(5)	26(1)	27(1)	32(1)	0(1)	-11(1)	-5(1)
C(6)	74(2)	31(2)	28(2)	0(1)	-7(2)	-2(2)
C(7)	85(3)	37(2)	44(2)	-12(2)	-5(2)	8(2)
C(8)	63(2)	26(2)	69(3)	5(2)	-16(2)	1(2)
C(9)	57(2)	46(2)	49(2)	23(2)	-4(2)	-5(2)
C(10)	42(2)	44(2)	37(2)	6(1)	7(1)	2(1)
C(11)	29(1)	30(1)	26(1)	2(1)	-12(1)	-1(1)
C(12)	24(1)	37(1)	27(1)	2(1)	-9(1)	-3(1)
C(13)	28(1)	36(1)	29(2)	0(1)	-13(1)	1(1)
C(14)	90(3)	26(2)	125(4)	1(2)	-35(3)	-7(2)
C(15)	52(2)	33(2)	53(2)	7(1)	-24(2)	-9(1)
C(16)	81(3)	70(3)	66(3)	21(2)	-13(2)	-19(2)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(1)	5311	1209	4152	30
H(4A)	7071	2926	1482	39
H(4B)	7041	3045	2899	39
H(6)	4479	4663	4092	55
H(7)	3601	6874	4083	70
H(8)	4329	8091	2303	64
H(9)	5915	7124	509	63
H(10)	6805	4906	519	54
H(14A)	-1956	6745	4581	119
H(14B)	-1883	7166	3198	119
H(14C)	-387	7384	3749	119
H(16A)	1316	4488	2105	110
H(16B)	1588	6010	2181	110
H(16C)	348	5545	1463	110
H(2O)	-1036	1610	4143	49(10)
H(1O)	-394	2843	3681	64(12)

Table S20. Torsion angles [°] for **5**.

C(13)-Re(1)-O(1)-C(3)	98.93(19)	N(1)-C(2)-C(3)-O(1)	2.3(3)
C(12)-Re(1)-O(1)-C(3)	-34.6(8)	C(1)-C(2)-C(3)-O(1)	-176.7(3)
C(11)-Re(1)-O(1)-C(3)	-171.12(18)	N(2)-N(3)-C(4)-C(5)	58.3(3)
N(1)-Re(1)-O(1)-C(3)	5.79(17)	C(1)-N(3)-C(4)-C(5)	-123.4(3)
O(6)-Re(1)-O(1)-C(3)	-76.62(17)	N(3)-C(4)-C(5)-C(10)	-119.2(3)
C(13)-Re(1)-N(1)-N(2)	84.4(2)	N(3)-C(4)-C(5)-C(6)	60.3(4)
C(12)-Re(1)-N(1)-N(2)	-5.7(3)	C(10)-C(5)-C(6)-C(7)	-1.8(5)
C(11)-Re(1)-N(1)-N(2)	-163.6(5)	C(4)-C(5)-C(6)-C(7)	178.7(3)
O(1)-Re(1)-N(1)-N(2)	178.8(2)	C(5)-C(6)-C(7)-C(8)	0.8(6)
O(6)-Re(1)-N(1)-N(2)	-100.9(2)	C(6)-C(7)-C(8)-C(9)	0.4(6)
C(13)-Re(1)-N(1)-C(2)	-98.43(18)	C(7)-C(8)-C(9)-C(10)	-0.6(6)
C(12)-Re(1)-N(1)-C(2)	171.46(18)	C(6)-C(5)-C(10)-C(9)	1.7(5)
C(11)-Re(1)-N(1)-C(2)	13.5(6)	C(4)-C(5)-C(10)-C(9)	-178.9(3)
O(1)-Re(1)-N(1)-C(2)	-4.11(16)	C(8)-C(9)-C(10)-C(5)	-0.5(6)
O(6)-Re(1)-N(1)-C(2)	76.21(17)	C(13)-Re(1)-C(11)-O(3)	144(30)
C(2)-N(1)-N(2)-N(3)	0.3(3)	C(12)-Re(1)-C(11)-O(3)	-127(30)
Re(1)-N(1)-N(2)-N(3)	177.54(17)	N(1)-Re(1)-C(11)-O(3)	31(30)
N(1)-N(2)-N(3)-C(1)	-0.1(3)	O(1)-Re(1)-C(11)-O(3)	48(30)
N(1)-N(2)-N(3)-C(4)	178.4(2)	O(6)-Re(1)-C(11)-O(3)	-30(30)
N(2)-N(3)-C(1)-C(2)	-0.1(3)	C(13)-Re(1)-C(12)-O(4)	-141(20)
C(4)-N(3)-C(1)-C(2)	-178.5(2)	C(11)-Re(1)-C(12)-O(4)	129(20)
N(2)-N(1)-C(2)-C(1)	-0.4(3)	N(1)-Re(1)-C(12)-O(4)	-47(20)
Re(1)-N(1)-C(2)-C(1)	-178.21(16)	O(1)-Re(1)-C(12)-O(4)	-8(20)
N(2)-N(1)-C(2)-C(3)	-179.6(2)	O(6)-Re(1)-C(12)-O(4)	34(20)
Re(1)-N(1)-C(2)-C(3)	2.6(3)	C(12)-Re(1)-C(13)-O(5)	147(9)
N(3)-C(1)-C(2)-N(1)	0.3(3)	C(11)-Re(1)-C(13)-O(5)	-124(9)
N(3)-C(1)-C(2)-C(3)	179.3(3)	N(1)-Re(1)-C(13)-O(5)	47(9)
Re(1)-O(1)-C(3)-O(2)	175.21(18)	O(1)-Re(1)-C(13)-O(5)	-28(9)
Re(1)-O(1)-C(3)-C(2)	-6.1(3)	O(6)-Re(1)-C(13)-O(5)	5(9)
N(1)-C(2)-C(3)-O(2)	-179.0(2)		
C(1)-C(2)-C(3)-O(2)	2.1(4)		

Table S21. Hydrogen bonds for **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(6)-H(2O)...O(2)#1	0.86	1.75	2.610(3)	173.6
O(6)-H(1O)...O(7)	0.90	1.77	2.662(3)	169.8

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1

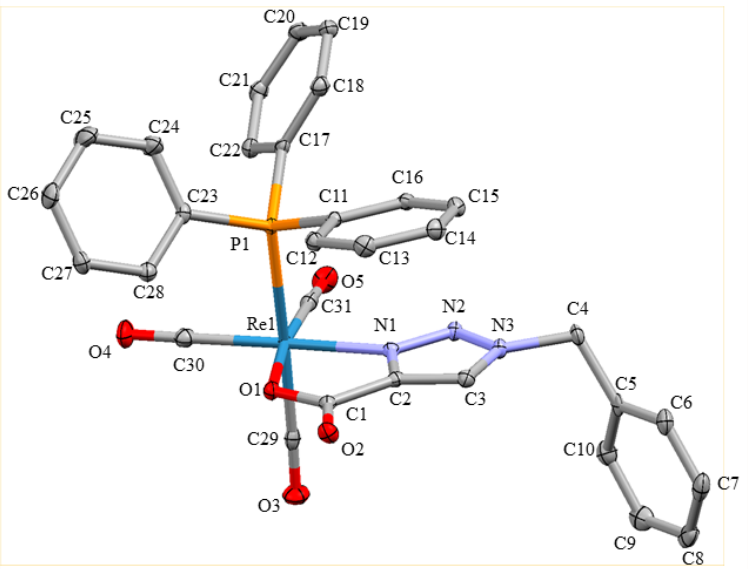


Table S22. Crystal data and structure refinement for **6**.

Empirical formula	$C_{33}H_{29}N_3O_6PRe$	
Formula weight	780.76	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Triclinic, P-1	
Unit cell dimensions	a = 10.1876(14) Å	α= 86.0620(10)°
	b = 10.5072(14) Å	β= 70.4170(10)°
	c = 15.090(2) Å	γ = 86.9510(10)°
Volume	1517.5(4) Å^3	
Z	2	
Density (calculated)	1.709 Mg/m^3	
Absorption coefficient	4.107 mm^{-1}	
F(000)	772	
Crystal size	0.500 x 0.500 x 0.200 mm^3	
Theta range for data collection	1.434 to 26.367°	
Index ranges	-12<=h<=12, -13<=k<=13, -18<=l<=18	
Reflections collected	16777	
Independent reflections	6183 [R(int) = 0.0175]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.49 and 0.33	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6183 / 0 / 402	
Goodness-of-fit on F^2	1.079	
Final R indices [I>2σ(I)]	R_1 = 0.0141, wR_2 = 0.0338	
R indices (all data)	R_1 = 0.0145, wR_2 = 0.0339	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.875 and -0.635 e.Å^{-3}	

Table S23. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	4464(1)	4209(1)	2878(1)	9(1)
P(1)	3976(1)	2560(1)	1911(1)	9(1)
O(1)	6130(1)	2874(1)	2984(1)	12(1)
N(1)	3522(2)	2983(1)	4112(1)	10(1)
C(1)	5867(2)	2045(2)	3684(1)	11(1)
O(2)	6724(1)	1280(1)	3853(1)	15(1)
N(2)	2252(2)	2897(2)	4719(1)	12(1)
C(2)	4391(2)	2072(2)	4317(1)	10(1)
O(3)	5342(2)	6087(1)	4059(1)	21(1)
N(3)	2331(2)	1910(2)	5318(1)	11(1)
C(3)	3622(2)	1373(2)	5102(1)	12(1)
O(4)	6107(2)	5669(2)	1036(1)	24(1)
C(4)	1072(2)	1552(2)	6111(1)	15(1)
O(5)	1890(2)	5934(1)	3004(1)	21(1)
C(5)	1264(2)	1769(2)	7039(1)	14(1)
C(6)	1328(2)	745(2)	7658(1)	17(1)
C(7)	1542(2)	952(2)	8501(1)	21(1)
C(8)	1729(2)	2176(2)	8714(2)	23(1)
C(9)	1655(2)	3201(2)	8101(2)	22(1)
C(10)	1414(2)	3006(2)	7271(2)	18(1)
C(11)	3739(2)	995(2)	2542(1)	10(1)
C(12)	4879(2)	145(2)	2419(1)	13(1)
C(13)	4761(2)	-969(2)	2994(1)	15(1)
C(14)	3508(2)	-1238(2)	3695(1)	15(1)
C(15)	2362(2)	-400(2)	3817(1)	14(1)
C(16)	2469(2)	712(2)	3248(1)	12(1)
C(17)	2455(2)	2911(2)	1543(1)	11(1)
C(18)	1494(2)	2000(2)	1555(1)	14(1)
C(19)	332(2)	2363(2)	1301(1)	16(1)
C(20)	128(2)	3622(2)	1021(1)	16(1)
C(21)	1102(2)	4520(2)	972(1)	16(1)
C(22)	2260(2)	4170(2)	1233(1)	13(1)
C(23)	5392(2)	2290(2)	805(1)	11(1)
C(24)	5120(2)	1991(2)	-1(2)	20(1)
C(25)	6209(2)	1786(2)	-833(2)	25(1)
C(26)	7581(2)	1863(2)	-864(1)	20(1)
C(27)	7857(2)	2145(2)	-63(1)	16(1)
C(28)	6777(2)	2372(2)	767(1)	14(1)
C(29)	5000(2)	5391(2)	3629(1)	14(1)
C(30)	5498(2)	5125(2)	1728(1)	15(1)
C(31)	2860(2)	5281(2)	2942(1)	14(1)
O(1S)	9300(2)	1886(1)	3904(1)	22(1)
C(1S)	8592(3)	3957(2)	4565(2)	32(1)
C(2S)	9504(2)	3229(2)	3754(2)	19(1)

Table S24. Bond lengths [Å] and angles [°] for **6**.

Re(1)-C(31)	1.913(2)	C(12)-H(12)	0.9500
Re(1)-C(30)	1.924(2)	C(13)-C(14)	1.386(3)
Re(1)-C(29)	1.951(2)	C(13)-H(13)	0.9500
Re(1)-N(1)	2.1570(15)	C(14)-C(15)	1.392(3)
Re(1)-O(1)	2.1843(13)	C(14)-H(14)	0.9500
Re(1)-P(1)	2.5098(5)	C(15)-C(16)	1.389(3)
P(1)-C(17)	1.8247(19)	C(15)-H(15)	0.9500
P(1)-C(11)	1.8279(19)	C(16)-H(16)	0.9500
P(1)-C(23)	1.8316(19)	C(17)-C(22)	1.399(3)
O(1)-C(1)	1.287(2)	C(17)-C(18)	1.400(3)
N(1)-N(2)	1.314(2)	C(18)-C(19)	1.390(3)
N(1)-C(2)	1.360(2)	C(18)-H(18)	0.9500
C(1)-O(2)	1.233(2)	C(19)-C(20)	1.387(3)
C(1)-C(2)	1.486(3)	C(19)-H(19)	0.9500
N(2)-N(3)	1.345(2)	C(20)-C(21)	1.386(3)
C(2)-C(3)	1.369(3)	C(20)-H(20)	0.9500
O(3)-C(29)	1.149(2)	C(21)-C(22)	1.389(3)
N(3)-C(3)	1.346(2)	C(21)-H(21)	0.9500
N(3)-C(4)	1.476(2)	C(22)-H(22)	0.9500
C(3)-H(3)	0.9500	C(23)-C(24)	1.393(3)
O(4)-C(30)	1.150(2)	C(23)-C(28)	1.400(3)
C(4)-C(5)	1.511(3)	C(24)-C(25)	1.390(3)
C(4)-H(4A)	0.9900	C(24)-H(24)	0.9500
C(4)-H(4B)	0.9900	C(25)-C(26)	1.390(3)
O(5)-C(31)	1.154(2)	C(25)-H(25)	0.9500
C(5)-C(6)	1.390(3)	C(26)-C(27)	1.384(3)
C(5)-C(10)	1.397(3)	C(26)-H(26)	0.9500
C(6)-C(7)	1.393(3)	C(27)-C(28)	1.388(3)
C(6)-H(6)	0.9500	C(27)-H(27)	0.9500
C(7)-C(8)	1.385(3)	C(28)-H(28)	0.9500
C(7)-H(7)	0.9500	O(1S)-C(2S)	1.429(2)
C(8)-C(9)	1.387(3)	O(1S)-H(1OS)	0.74(3)
C(8)-H(8)	0.9500	C(1S)-C(2S)	1.495(3)
C(9)-C(10)	1.385(3)	C(1S)-H(1S1)	0.9800
C(9)-H(9)	0.9500	C(1S)-H(1S2)	0.9800
C(10)-H(10)	0.9500	C(1S)-H(1S3)	0.9800
C(11)-C(12)	1.396(3)	C(2S)-H(2S1)	0.9900
C(11)-C(16)	1.404(3)	C(2S)-H(2S2)	0.9900
C(12)-C(13)	1.393(3)		

C(31)-Re(1)-C(30)	89.51(8)	N(1)-Re(1)-O(1)	74.68(5)
C(31)-Re(1)-C(29)	89.44(8)	C(31)-Re(1)-P(1)	96.01(6)
C(30)-Re(1)-C(29)	91.34(8)	C(30)-Re(1)-P(1)	88.82(6)
C(31)-Re(1)-N(1)	97.85(7)	C(29)-Re(1)-P(1)	174.56(6)
C(30)-Re(1)-N(1)	172.28(7)	N(1)-Re(1)-P(1)	88.10(4)
C(29)-Re(1)-N(1)	91.07(7)	O(1)-Re(1)-P(1)	84.80(4)
C(31)-Re(1)-O(1)	172.47(6)	C(17)-P(1)-C(11)	107.32(8)
C(30)-Re(1)-O(1)	97.99(7)	C(17)-P(1)-C(23)	103.76(9)
C(29)-Re(1)-O(1)	89.79(7)	C(11)-P(1)-C(23)	104.28(8)

C(17)-P(1)-Re(1)	115.22(6)	C(14)-C(13)-H(13)	120.0
C(11)-P(1)-Re(1)	111.16(6)	C(12)-C(13)-H(13)	120.0
C(23)-P(1)-Re(1)	114.19(6)	C(13)-C(14)-C(15)	119.88(18)
C(1)-O(1)-Re(1)	118.77(11)	C(13)-C(14)-H(14)	120.1
N(2)-N(1)-C(2)	110.91(15)	C(15)-C(14)-H(14)	120.1
N(2)-N(1)-Re(1)	133.83(12)	C(16)-C(15)-C(14)	120.50(18)
C(2)-N(1)-Re(1)	115.24(12)	C(16)-C(15)-H(15)	119.8
O(2)-C(1)-O(1)	125.42(17)	C(14)-C(15)-H(15)	119.8
O(2)-C(1)-C(2)	120.40(17)	C(15)-C(16)-C(11)	119.88(17)
O(1)-C(1)-C(2)	114.18(16)	C(15)-C(16)-H(16)	120.1
N(1)-N(2)-N(3)	104.77(14)	C(11)-C(16)-H(16)	120.1
N(1)-C(2)-C(3)	107.40(16)	C(22)-C(17)-C(18)	119.12(17)
N(1)-C(2)-C(1)	117.06(16)	C(22)-C(17)-P(1)	117.04(14)
C(3)-C(2)-C(1)	135.54(17)	C(18)-C(17)-P(1)	123.83(14)
N(2)-N(3)-C(3)	112.68(15)	C(19)-C(18)-C(17)	119.98(18)
N(2)-N(3)-C(4)	119.31(15)	C(19)-C(18)-H(18)	120.0
C(3)-N(3)-C(4)	128.00(16)	C(17)-C(18)-H(18)	120.0
N(3)-C(3)-C(2)	104.23(16)	C(20)-C(19)-C(18)	120.34(18)
N(3)-C(3)-H(3)	127.9	C(20)-C(19)-H(19)	119.8
C(2)-C(3)-H(3)	127.9	C(18)-C(19)-H(19)	119.8
N(3)-C(4)-C(5)	110.45(15)	C(21)-C(20)-C(19)	120.03(18)
N(3)-C(4)-H(4A)	109.6	C(21)-C(20)-H(20)	120.0
C(5)-C(4)-H(4A)	109.6	C(19)-C(20)-H(20)	120.0
N(3)-C(4)-H(4B)	109.6	C(20)-C(21)-C(22)	120.06(18)
C(5)-C(4)-H(4B)	109.6	C(20)-C(21)-H(21)	120.0
H(4A)-C(4)-H(4B)	108.1	C(22)-C(21)-H(21)	120.0
C(6)-C(5)-C(10)	119.40(19)	C(21)-C(22)-C(17)	120.38(18)
C(6)-C(5)-C(4)	120.57(18)	C(21)-C(22)-H(22)	119.8
C(10)-C(5)-C(4)	120.01(18)	C(17)-C(22)-H(22)	119.8
C(5)-C(6)-C(7)	120.12(19)	C(24)-C(23)-C(28)	119.10(18)
C(5)-C(6)-H(6)	119.9	C(24)-C(23)-P(1)	121.31(15)
C(7)-C(6)-H(6)	119.9	C(28)-C(23)-P(1)	119.58(14)
C(8)-C(7)-C(6)	120.2(2)	C(25)-C(24)-C(23)	120.50(19)
C(8)-C(7)-H(7)	119.9	C(25)-C(24)-H(24)	119.7
C(6)-C(7)-H(7)	119.9	C(23)-C(24)-H(24)	119.7
C(7)-C(8)-C(9)	119.8(2)	C(26)-C(25)-C(24)	120.0(2)
C(7)-C(8)-H(8)	120.1	C(26)-C(25)-H(25)	120.0
C(9)-C(8)-H(8)	120.1	C(24)-C(25)-H(25)	120.0
C(10)-C(9)-C(8)	120.4(2)	C(27)-C(26)-C(25)	119.70(19)
C(10)-C(9)-H(9)	119.8	C(27)-C(26)-H(26)	120.2
C(8)-C(9)-H(9)	119.8	C(25)-C(26)-H(26)	120.2
C(9)-C(10)-C(5)	120.1(2)	C(26)-C(27)-C(28)	120.64(19)
C(9)-C(10)-H(10)	120.0	C(26)-C(27)-H(27)	119.7
C(5)-C(10)-H(10)	120.0	C(28)-C(27)-H(27)	119.7
C(12)-C(11)-C(16)	119.23(17)	C(27)-C(28)-C(23)	119.99(18)
C(12)-C(11)-P(1)	119.88(14)	C(27)-C(28)-H(28)	120.0
C(16)-C(11)-P(1)	120.27(14)	C(23)-C(28)-H(28)	120.0
C(13)-C(12)-C(11)	120.46(17)	O(3)-C(29)-Re(1)	178.63(18)
C(13)-C(12)-H(12)	119.8	O(4)-C(30)-Re(1)	179.29(18)
C(11)-C(12)-H(12)	119.8	O(5)-C(31)-Re(1)	178.24(17)
C(14)-C(13)-C(12)	120.05(18)	C(2S)-O(1S)-H(1OS)	107(2)

C(2S)-C(1S)-H(1S1)	109.5	O(1S)-C(2S)-C(1S)	112.27(18)
C(2S)-C(1S)-H(1S2)	109.5	O(1S)-C(2S)-H(2S1)	109.2
H(1S1)-C(1S)-H(1S2)	109.5	C(1S)-C(2S)-H(2S1)	109.2
C(2S)-C(1S)-H(1S3)	109.5	O(1S)-C(2S)-H(2S2)	109.2
H(1S1)-C(1S)-H(1S3)	109.5	C(1S)-C(2S)-H(2S2)	109.2
H(1S2)-C(1S)-H(1S3)	109.5	H(2S1)-C(2S)-H(2S2)	107.9

Table S25. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	9(1)	8(1)	8(1)	1(1)	-2(1)	-1(1)
P(1)	8(1)	10(1)	8(1)	0(1)	-2(1)	0(1)
O(1)	10(1)	13(1)	10(1)	1(1)	-2(1)	0(1)
N(1)	11(1)	10(1)	10(1)	-1(1)	-3(1)	-1(1)
C(1)	12(1)	12(1)	10(1)	-2(1)	-3(1)	-3(1)
O(2)	12(1)	14(1)	18(1)	2(1)	-6(1)	1(1)
N(2)	12(1)	12(1)	9(1)	0(1)	-1(1)	-1(1)
C(2)	13(1)	9(1)	10(1)	-1(1)	-6(1)	0(1)
O(3)	27(1)	17(1)	22(1)	-5(1)	-11(1)	-3(1)
N(3)	11(1)	11(1)	10(1)	1(1)	-1(1)	-2(1)
C(3)	12(1)	12(1)	11(1)	-1(1)	-4(1)	-1(1)
O(4)	27(1)	24(1)	16(1)	7(1)	-2(1)	-9(1)
C(4)	10(1)	18(1)	13(1)	2(1)	1(1)	-4(1)
O(5)	21(1)	21(1)	20(1)	-2(1)	-7(1)	9(1)
C(5)	7(1)	18(1)	11(1)	0(1)	3(1)	0(1)
C(6)	15(1)	17(1)	14(1)	1(1)	2(1)	-1(1)
C(7)	16(1)	28(1)	13(1)	5(1)	1(1)	4(1)
C(8)	14(1)	39(1)	12(1)	-7(1)	-1(1)	4(1)
C(9)	17(1)	24(1)	25(1)	-10(1)	-3(1)	3(1)
C(10)	16(1)	17(1)	20(1)	-1(1)	-3(1)	1(1)
C(11)	12(1)	10(1)	10(1)	0(1)	-5(1)	-2(1)
C(12)	11(1)	14(1)	13(1)	-1(1)	-2(1)	-1(1)
C(13)	15(1)	12(1)	18(1)	-1(1)	-6(1)	2(1)
C(14)	19(1)	12(1)	16(1)	4(1)	-7(1)	-3(1)
C(15)	13(1)	17(1)	13(1)	1(1)	-2(1)	-5(1)
C(16)	10(1)	14(1)	12(1)	-3(1)	-4(1)	0(1)
C(17)	9(1)	16(1)	7(1)	-1(1)	-1(1)	1(1)
C(18)	16(1)	13(1)	13(1)	2(1)	-6(1)	-1(1)
C(19)	15(1)	21(1)	13(1)	2(1)	-6(1)	-5(1)
C(20)	13(1)	23(1)	14(1)	0(1)	-6(1)	2(1)
C(21)	18(1)	16(1)	13(1)	1(1)	-6(1)	2(1)
C(22)	14(1)	15(1)	11(1)	0(1)	-3(1)	-2(1)
C(23)	12(1)	9(1)	10(1)	1(1)	-1(1)	0(1)
C(24)	14(1)	29(1)	17(1)	-4(1)	-6(1)	0(1)
C(25)	23(1)	40(1)	14(1)	-10(1)	-6(1)	0(1)
C(26)	17(1)	25(1)	12(1)	-4(1)	2(1)	1(1)
C(27)	10(1)	18(1)	16(1)	0(1)	-1(1)	-1(1)
C(28)	14(1)	15(1)	13(1)	-1(1)	-3(1)	-2(1)
C(29)	15(1)	13(1)	12(1)	4(1)	-1(1)	1(1)
C(30)	17(1)	14(1)	15(1)	-1(1)	-7(1)	-1(1)
C(31)	19(1)	13(1)	9(1)	0(1)	-4(1)	-2(1)
O(1S)	12(1)	16(1)	38(1)	-2(1)	-7(1)	0(1)
C(1S)	45(2)	21(1)	22(1)	-2(1)	-1(1)	3(1)
C(2S)	18(1)	18(1)	20(1)	1(1)	-4(1)	-1(1)

Table S26. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(3)	3930	671	5421	14
H(4A)	888	642	6087	18
H(4B)	259	2069	6056	18
H(6)	1224	-99	7507	20
H(7)	1561	252	8930	25
H(8)	1907	2313	9278	27
H(9)	1770	4042	8251	27
H(10)	1351	3713	6858	22
H(12)	5741	327	1941	15
H(13)	5540	-1544	2905	18
H(14)	3430	-1992	4092	19
H(15)	1502	-591	4294	17
H(16)	1684	1280	3335	14
H(18)	1637	1135	1737	17
H(19)	-326	1746	1319	19
H(20)	-680	3869	862	19
H(21)	976	5376	761	19
H(22)	2924	4788	1200	16
H(24)	4184	1926	19	24
H(25)	6014	1594	-1382	30
H(26)	8326	1724	-1433	24
H(27)	8796	2183	-81	19
H(28)	6977	2584	1309	17
H(1OS)	8610(30)	1770(20)	3879(19)	25(7)
H(1S1)	7617	3906	4603	48
H(1S2)	8857	4852	4472	48
H(1S3)	8706	3589	5150	48
H(2S1)	9303	3536	3176	23
H(2S2)	10492	3397	3655	23

Table S27. Torsion angles [°] for **6**.

Re(1)-O(1)-C(1)-O(2)	-176.35(14)	C(16)-C(11)-C(12)-C(13)	-0.3(3)
Re(1)-O(1)-C(1)-C(2)	3.2(2)	P(1)-C(11)-C(12)-C(13)	170.59(15)
C(2)-N(1)-N(2)-N(3)	0.07(19)	C(11)-C(12)-C(13)-C(14)	-0.2(3)
Re(1)-N(1)-N(2)-N(3)	178.41(12)	C(12)-C(13)-C(14)-C(15)	0.7(3)
N(2)-N(1)-C(2)-C(3)	-0.2(2)	C(13)-C(14)-C(15)-C(16)	-0.7(3)
Re(1)-N(1)-C(2)-C(3)	-178.85(12)	C(14)-C(15)-C(16)-C(11)	0.1(3)
N(2)-N(1)-C(2)-C(1)	179.62(15)	C(12)-C(11)-C(16)-C(15)	0.4(3)
Re(1)-N(1)-C(2)-C(1)	0.9(2)	P(1)-C(11)-C(16)-C(15)	-170.50(14)
O(2)-C(1)-C(2)-N(1)	176.84(16)	C(11)-P(1)-C(17)-C(22)	166.27(14)
O(1)-C(1)-C(2)-N(1)	-2.7(2)	C(23)-P(1)-C(17)-C(22)	-83.70(16)
O(2)-C(1)-C(2)-C(3)	-3.5(3)	Re(1)-P(1)-C(17)-C(22)	41.88(16)
O(1)-C(1)-C(2)-C(3)	177.0(2)	C(11)-P(1)-C(17)-C(18)	-13.82(18)
N(1)-N(2)-N(3)-C(3)	0.1(2)	C(23)-P(1)-C(17)-C(18)	96.20(17)
N(1)-N(2)-N(3)-C(4)	179.21(15)	Re(1)-P(1)-C(17)-C(18)	-138.22(14)
N(2)-N(3)-C(3)-C(2)	-0.2(2)	C(22)-C(17)-C(18)-C(19)	-2.8(3)
C(4)-N(3)-C(3)-C(2)	-179.22(17)	P(1)-C(17)-C(18)-C(19)	177.25(15)
N(1)-C(2)-C(3)-N(3)	0.2(2)	C(17)-C(18)-C(19)-C(20)	1.0(3)
C(1)-C(2)-C(3)-N(3)	-179.5(2)	C(18)-C(19)-C(20)-C(21)	1.5(3)
N(2)-N(3)-C(4)-C(5)	-114.85(18)	C(19)-C(20)-C(21)-C(22)	-2.1(3)
C(3)-N(3)-C(4)-C(5)	64.1(2)	C(20)-C(21)-C(22)-C(17)	0.2(3)
N(3)-C(4)-C(5)-C(6)	-113.47(19)	C(18)-C(17)-C(22)-C(21)	2.3(3)
N(3)-C(4)-C(5)-C(10)	64.9(2)	P(1)-C(17)-C(22)-C(21)	-177.79(15)
C(10)-C(5)-C(6)-C(7)	-0.1(3)	C(17)-P(1)-C(23)-C(24)	-19.73(18)
C(4)-C(5)-C(6)-C(7)	178.24(18)	C(11)-P(1)-C(23)-C(24)	92.52(17)
C(5)-C(6)-C(7)-C(8)	-1.7(3)	Re(1)-P(1)-C(23)-C(24)	-145.96(15)
C(6)-C(7)-C(8)-C(9)	2.2(3)	C(17)-P(1)-C(23)-C(28)	160.85(15)
C(7)-C(8)-C(9)-C(10)	-0.9(3)	C(11)-P(1)-C(23)-C(28)	-86.90(16)
C(8)-C(9)-C(10)-C(5)	-0.9(3)	Re(1)-P(1)-C(23)-C(28)	34.62(17)
C(6)-C(5)-C(10)-C(9)	1.4(3)	C(28)-C(23)-C(24)-C(25)	-0.5(3)
C(4)-C(5)-C(10)-C(9)	-176.98(18)	P(1)-C(23)-C(24)-C(25)	-179.88(17)
C(17)-P(1)-C(11)-C(12)	141.15(15)	C(23)-C(24)-C(25)-C(26)	0.8(3)
C(23)-P(1)-C(11)-C(12)	31.48(17)	C(24)-C(25)-C(26)-C(27)	0.0(3)
Re(1)-P(1)-C(11)-C(12)	-92.03(15)	C(25)-C(26)-C(27)-C(28)	-1.1(3)
C(17)-P(1)-C(11)-C(16)	-48.02(17)	C(26)-C(27)-C(28)-C(23)	1.4(3)
C(23)-P(1)-C(11)-C(16)	-157.69(15)	C(24)-C(23)-C(28)-C(27)	-0.7(3)
Re(1)-P(1)-C(11)-C(16)	78.81(15)	P(1)-C(23)-C(28)-C(27)	178.78(15)

Table S28. Hydrogen bonds for **6**. [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1S)-H(1OS)...O(2)	0.74(3)	2.03(3)	2.761(2)	175(3)

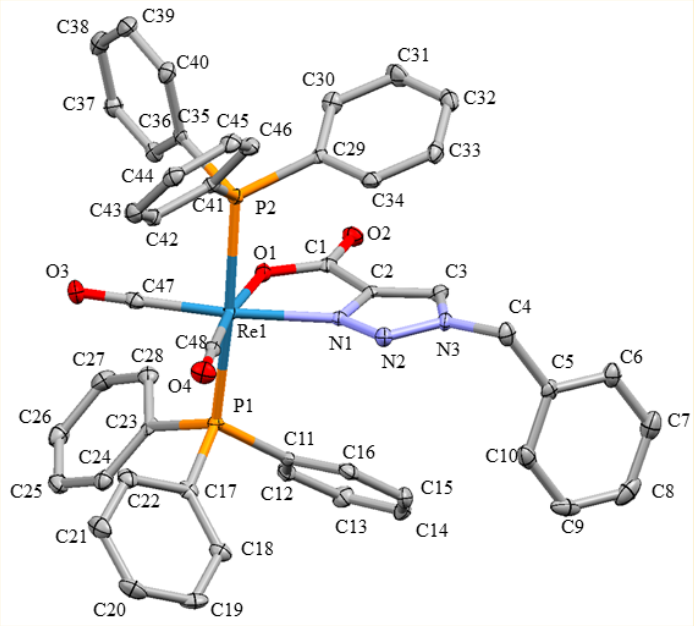


Table S29. Crystal data and structure refinement for **7**.

Empirical formula	$C_{49}H_{39}Cl_3N_3O_4P_2Re$	
Formula weight	1088.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, $P2_1/c$	
Unit cell dimensions	a = 17.1322(6) Å	α = 90°
	b = 12.2900(4) Å	β = 100.7630(10)°
	c = 21.1693(8) Å	γ = 90°
Volume	4378.9(3) Å^3	
Z	4	
Density (calculated)	1.651 Mg/m^3	
Absorption coefficient	3.081 mm^{-1}	
F(000)	2168	
Crystal size	0.200 x 0.200 x 0.150 mm^3	
Theta range for data collection	1.210 to 26.371°	
Index ranges	-21<=h<=21, -15<=k<=14, -25<=l<=26	
Reflections collected	31375	
Independent reflections	8949 [R(int) = 0.0473]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.66 and 0.60	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8949 / 0 / 559	
Goodness-of-fit on F^2	1.032	
Final R indices [I>2σ(I)]	R_1 = 0.0299, wR_2 = 0.0537	
R indices (all data)	R_1 = 0.0426, wR_2 = 0.0587	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.753 and -0.622 e.Å^{-3}	

Table S30. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	2205(1)	5448(1)	3486(1)	10(1)
P(1)	2127(1)	7355(1)	3197(1)	11(1)
O(1)	2682(1)	5909(2)	4486(1)	13(1)
N(1)	3490(2)	5378(2)	3589(1)	10(1)
C(1)	3441(2)	5843(3)	4696(2)	14(1)
P(2)	2210(1)	3592(1)	3884(1)	11(1)
O(2)	3777(1)	5971(2)	5261(1)	16(1)
N(2)	3975(2)	5090(2)	3200(1)	14(1)
C(2)	3904(2)	5574(2)	4193(2)	11(1)
O(3)	425(1)	5521(2)	3519(1)	22(1)
N(3)	4713(2)	5102(2)	3572(1)	14(1)
C(3)	4696(2)	5393(3)	4183(2)	14(1)
O(4)	1793(1)	4792(2)	2072(1)	19(1)
C(4)	5400(2)	4785(3)	3287(2)	17(1)
C(5)	5945(2)	5732(3)	3236(2)	14(1)
C(6)	6692(2)	5779(3)	3623(2)	18(1)
C(7)	7191(2)	6652(3)	3585(2)	25(1)
C(8)	6941(2)	7507(3)	3176(2)	26(1)
C(9)	6194(2)	7478(3)	2791(2)	25(1)
C(10)	5699(2)	6587(3)	2809(2)	21(1)
C(11)	3030(2)	8182(3)	3419(2)	12(1)
C(12)	3078(2)	9053(3)	3856(2)	16(1)
C(13)	3775(2)	9637(3)	4026(2)	18(1)
C(14)	4437(2)	9392(3)	3771(2)	19(1)
C(15)	4400(2)	8525(3)	3342(2)	18(1)
C(16)	3708(2)	7913(3)	3172(2)	16(1)
C(17)	1769(2)	7625(3)	2341(2)	13(1)
C(18)	2160(2)	8258(3)	1952(2)	16(1)
C(19)	1821(2)	8453(3)	1309(2)	21(1)
C(20)	1076(2)	8036(3)	1054(2)	22(1)
C(21)	680(2)	7398(3)	1433(2)	21(1)
C(22)	1029(2)	7182(3)	2068(2)	17(1)
C(23)	1414(2)	8135(3)	3568(2)	12(1)
C(24)	901(2)	8899(3)	3228(2)	16(1)
C(25)	424(2)	9537(3)	3540(2)	20(1)
C(26)	462(2)	9445(3)	4189(2)	21(1)
C(27)	963(2)	8676(3)	4537(2)	20(1)
C(28)	1433(2)	8016(3)	4228(2)	16(1)
C(29)	3178(2)	3041(3)	4271(2)	11(1)
C(30)	3360(2)	2834(3)	4928(2)	16(1)
C(31)	4115(2)	2457(3)	5207(2)	23(1)
C(32)	4689(2)	2297(3)	4836(2)	20(1)
C(33)	4507(2)	2498(3)	4182(2)	18(1)
C(34)	3761(2)	2872(3)	3902(2)	16(1)
C(35)	1597(2)	3372(3)	4495(2)	12(1)
C(36)	1349(2)	4241(3)	4835(2)	15(1)

C(37)	890(2)	4057(3)	5296(2)	17(1)
C(38)	685(2)	3008(3)	5441(2)	19(1)
C(39)	942(2)	2136(3)	5117(2)	21(1)
C(40)	1387(2)	2311(3)	4646(2)	16(1)
C(41)	1840(2)	2572(3)	3268(2)	12(1)
C(42)	1141(2)	2798(3)	2829(2)	14(1)
C(43)	864(2)	2078(3)	2330(2)	17(1)
C(44)	1273(2)	1124(3)	2266(2)	17(1)
C(45)	1950(2)	884(3)	2708(2)	17(1)
C(46)	2230(2)	1592(3)	3211(2)	16(1)
C(47)	1106(2)	5502(3)	3508(2)	15(1)
C(48)	1944(2)	5032(3)	2618(2)	14(1)
Cl(1S)	2737(1)	10289(1)	5534(1)	45(1)
C(1S)	2872(2)	9142(3)	6042(2)	21(1)
Cl(2S)	3535(1)	9452(1)	6764(1)	28(1)
Cl(3S)	3216(1)	8022(1)	5660(1)	26(1)

Table S31. Bond lengths [Å] and angles [°] for **7**.

Re(1)-C(48)	1.879(4)	C(17)-C(22)	1.402(4)
Re(1)-C(47)	1.892(4)	C(18)-C(19)	1.397(5)
Re(1)-N(1)	2.173(3)	C(18)-H(18)	0.9500
Re(1)-O(1)	2.198(2)	C(19)-C(20)	1.388(5)
Re(1)-P(1)	2.4196(9)	C(19)-H(19)	0.9500
Re(1)-P(2)	2.4318(9)	C(20)-C(21)	1.386(5)
P(1)-C(17)	1.832(4)	C(20)-H(20)	0.9500
P(1)-C(11)	1.838(3)	C(21)-C(22)	1.390(5)
P(1)-C(23)	1.839(4)	C(21)-H(21)	0.9500
O(1)-C(1)	1.295(4)	C(22)-H(22)	0.9500
N(1)-N(2)	1.323(4)	C(23)-C(24)	1.393(4)
N(1)-C(2)	1.361(4)	C(23)-C(28)	1.400(5)
C(1)-O(2)	1.237(4)	C(24)-C(25)	1.386(5)
C(1)-C(2)	1.480(5)	C(24)-H(24)	0.9500
P(2)-C(35)	1.832(4)	C(25)-C(26)	1.367(5)
P(2)-C(41)	1.833(3)	C(25)-H(25)	0.9500
P(2)-C(29)	1.836(3)	C(26)-C(27)	1.391(5)
N(2)-N(3)	1.358(3)	C(26)-H(26)	0.9500
C(2)-C(3)	1.379(5)	C(27)-C(28)	1.390(5)
O(3)-C(47)	1.172(4)	C(27)-H(27)	0.9500
N(3)-C(3)	1.347(4)	C(28)-H(28)	0.9500
N(3)-C(4)	1.472(4)	C(29)-C(30)	1.391(5)
C(3)-H(3)	0.9500	C(29)-C(34)	1.394(5)
O(4)-C(48)	1.173(4)	C(30)-C(31)	1.397(5)
C(4)-C(5)	1.509(5)	C(30)-H(30)	0.9500
C(4)-H(4A)	0.9900	C(31)-C(32)	1.383(5)
C(4)-H(4B)	0.9900	C(31)-H(31)	0.9500
C(5)-C(6)	1.386(4)	C(32)-C(33)	1.382(5)
C(5)-C(10)	1.398(5)	C(32)-H(32)	0.9500
C(6)-C(7)	1.383(5)	C(33)-C(34)	1.385(4)
C(6)-H(6)	0.9500	C(33)-H(33)	0.9500
C(7)-C(8)	1.379(5)	C(34)-H(34)	0.9500
C(7)-H(7)	0.9500	C(35)-C(36)	1.399(5)
C(8)-C(9)	1.383(5)	C(35)-C(40)	1.405(4)
C(8)-H(8)	0.9500	C(36)-C(37)	1.383(5)
C(9)-C(10)	1.390(5)	C(36)-H(36)	0.9500
C(9)-H(9)	0.9500	C(37)-C(38)	1.386(5)
C(10)-H(10)	0.9500	C(37)-H(37)	0.9500
C(11)-C(16)	1.400(5)	C(38)-C(39)	1.387(5)
C(11)-C(12)	1.407(5)	C(38)-H(38)	0.9500
C(12)-C(13)	1.382(5)	C(39)-C(40)	1.381(5)
C(12)-H(12)	0.9500	C(39)-H(39)	0.9500
C(13)-C(14)	1.378(5)	C(40)-H(40)	0.9500
C(13)-H(13)	0.9500	C(41)-C(46)	1.395(5)
C(14)-C(15)	1.395(5)	C(41)-C(42)	1.399(4)
C(14)-H(14)	0.9500	C(42)-C(43)	1.391(5)
C(15)-C(16)	1.393(5)	C(42)-H(42)	0.9500
C(15)-H(15)	0.9500	C(43)-C(44)	1.387(5)
C(16)-H(16)	0.9500	C(43)-H(43)	0.9500
C(17)-C(18)	1.392(5)	C(44)-C(45)	1.380(5)

C(44)-H(44)	0.9500	Cl(1S)-C(1S)	1.763(4)
C(45)-C(46)	1.389(5)	C(1S)-Cl(3S)	1.754(4)
C(45)-H(45)	0.9500	C(1S)-Cl(2S)	1.767(3)
C(46)-H(46)	0.9500	C(1S)-H(1S)	1.0000

C(48)-Re(1)-C(47)	88.73(15)	N(3)-C(4)-H(4A)	109.2
C(48)-Re(1)-N(1)	98.01(13)	C(5)-C(4)-H(4A)	109.2
C(47)-Re(1)-N(1)	172.90(13)	N(3)-C(4)-H(4B)	109.2
C(48)-Re(1)-O(1)	172.06(12)	C(5)-C(4)-H(4B)	109.2
C(47)-Re(1)-O(1)	99.20(12)	H(4A)-C(4)-H(4B)	107.9
N(1)-Re(1)-O(1)	74.05(9)	C(6)-C(5)-C(10)	118.9(3)
C(48)-Re(1)-P(1)	91.44(10)	C(6)-C(5)-C(4)	120.4(3)
C(47)-Re(1)-P(1)	87.96(10)	C(10)-C(5)-C(4)	120.7(3)
N(1)-Re(1)-P(1)	94.10(7)	C(7)-C(6)-C(5)	120.7(3)
O(1)-Re(1)-P(1)	89.25(6)	C(7)-C(6)-H(6)	119.6
C(48)-Re(1)-P(2)	93.90(10)	C(5)-C(6)-H(6)	119.6
C(47)-Re(1)-P(2)	87.88(10)	C(8)-C(7)-C(6)	120.3(4)
N(1)-Re(1)-P(2)	89.40(7)	C(8)-C(7)-H(7)	119.8
O(1)-Re(1)-P(2)	86.05(6)	C(6)-C(7)-H(7)	119.8
P(1)-Re(1)-P(2)	173.15(3)	C(7)-C(8)-C(9)	119.7(4)
C(17)-P(1)-C(11)	105.23(16)	C(7)-C(8)-H(8)	120.2
C(17)-P(1)-C(23)	101.66(15)	C(9)-C(8)-H(8)	120.2
C(11)-P(1)-C(23)	101.38(15)	C(8)-C(9)-C(10)	120.3(4)
C(17)-P(1)-Re(1)	114.70(11)	C(8)-C(9)-H(9)	119.8
C(11)-P(1)-Re(1)	117.84(11)	C(10)-C(9)-H(9)	119.8
C(23)-P(1)-Re(1)	113.98(11)	C(9)-C(10)-C(5)	120.0(3)
C(1)-O(1)-Re(1)	118.9(2)	C(9)-C(10)-H(10)	120.0
N(2)-N(1)-C(2)	110.7(3)	C(5)-C(10)-H(10)	120.0
N(2)-N(1)-Re(1)	133.7(2)	C(16)-C(11)-C(12)	118.4(3)
C(2)-N(1)-Re(1)	115.3(2)	C(16)-C(11)-P(1)	119.4(3)
O(2)-C(1)-O(1)	125.5(3)	C(12)-C(11)-P(1)	122.1(3)
O(2)-C(1)-C(2)	120.6(3)	C(13)-C(12)-C(11)	120.5(3)
O(1)-C(1)-C(2)	113.9(3)	C(13)-C(12)-H(12)	119.8
C(35)-P(2)-C(41)	103.47(15)	C(11)-C(12)-H(12)	119.8
C(35)-P(2)-C(29)	102.65(15)	C(14)-C(13)-C(12)	121.3(3)
C(41)-P(2)-C(29)	103.22(15)	C(14)-C(13)-H(13)	119.4
C(35)-P(2)-Re(1)	114.71(11)	C(12)-C(13)-H(13)	119.4
C(41)-P(2)-Re(1)	114.62(11)	C(13)-C(14)-C(15)	118.8(3)
C(29)-P(2)-Re(1)	116.44(11)	C(13)-C(14)-H(14)	120.6
N(1)-N(2)-N(3)	105.1(3)	C(15)-C(14)-H(14)	120.6
N(1)-C(2)-C(3)	107.4(3)	C(16)-C(15)-C(14)	120.9(3)
N(1)-C(2)-C(1)	117.4(3)	C(16)-C(15)-H(15)	119.5
C(3)-C(2)-C(1)	135.1(3)	C(14)-C(15)-H(15)	119.5
C(3)-N(3)-N(2)	112.0(3)	C(15)-C(16)-C(11)	120.1(3)
C(3)-N(3)-C(4)	128.8(3)	C(15)-C(16)-H(16)	120.0
N(2)-N(3)-C(4)	119.2(3)	C(11)-C(16)-H(16)	120.0
N(3)-C(3)-C(2)	104.8(3)	C(18)-C(17)-C(22)	118.1(3)
N(3)-C(3)-H(3)	127.6	C(18)-C(17)-P(1)	125.3(3)
C(2)-C(3)-H(3)	127.6	C(22)-C(17)-P(1)	116.6(3)
N(3)-C(4)-C(5)	112.2(3)	C(17)-C(18)-C(19)	121.0(3)

C(17)-C(18)-H(18)	119.5	C(33)-C(34)-C(29)	120.7(3)
C(19)-C(18)-H(18)	119.5	C(33)-C(34)-H(34)	119.7
C(20)-C(19)-C(18)	120.0(4)	C(29)-C(34)-H(34)	119.7
C(20)-C(19)-H(19)	120.0	C(36)-C(35)-C(40)	118.5(3)
C(18)-C(19)-H(19)	120.0	C(36)-C(35)-P(2)	121.3(3)
C(21)-C(20)-C(19)	119.9(3)	C(40)-C(35)-P(2)	120.2(3)
C(21)-C(20)-H(20)	120.1	C(37)-C(36)-C(35)	120.4(3)
C(19)-C(20)-H(20)	120.1	C(37)-C(36)-H(36)	119.8
C(20)-C(21)-C(22)	120.0(3)	C(35)-C(36)-H(36)	119.8
C(20)-C(21)-H(21)	120.0	C(36)-C(37)-C(38)	120.6(3)
C(22)-C(21)-H(21)	120.0	C(36)-C(37)-H(37)	119.7
C(21)-C(22)-C(17)	121.1(3)	C(38)-C(37)-H(37)	119.7
C(21)-C(22)-H(22)	119.5	C(37)-C(38)-C(39)	119.6(4)
C(17)-C(22)-H(22)	119.5	C(37)-C(38)-H(38)	120.2
C(24)-C(23)-C(28)	118.8(3)	C(39)-C(38)-H(38)	120.2
C(24)-C(23)-P(1)	122.4(3)	C(40)-C(39)-C(38)	120.4(3)
C(28)-C(23)-P(1)	118.6(3)	C(40)-C(39)-H(39)	119.8
C(25)-C(24)-C(23)	120.4(3)	C(38)-C(39)-H(39)	119.8
C(25)-C(24)-H(24)	119.8	C(39)-C(40)-C(35)	120.6(3)
C(23)-C(24)-H(24)	119.8	C(39)-C(40)-H(40)	119.7
C(26)-C(25)-C(24)	120.7(3)	C(35)-C(40)-H(40)	119.7
C(26)-C(25)-H(25)	119.6	C(46)-C(41)-C(42)	118.5(3)
C(24)-C(25)-H(25)	119.6	C(46)-C(41)-P(2)	123.0(3)
C(25)-C(26)-C(27)	119.7(4)	C(42)-C(41)-P(2)	118.4(3)
C(25)-C(26)-H(26)	120.1	C(43)-C(42)-C(41)	120.5(3)
C(27)-C(26)-H(26)	120.1	C(43)-C(42)-H(42)	119.7
C(28)-C(27)-C(26)	120.2(4)	C(41)-C(42)-H(42)	119.7
C(28)-C(27)-H(27)	119.9	C(44)-C(43)-C(42)	120.3(3)
C(26)-C(27)-H(27)	119.9	C(44)-C(43)-H(43)	119.8
C(27)-C(28)-C(23)	120.1(3)	C(42)-C(43)-H(43)	119.8
C(27)-C(28)-H(28)	120.0	C(45)-C(44)-C(43)	119.4(3)
C(23)-C(28)-H(28)	120.0	C(45)-C(44)-H(44)	120.3
C(30)-C(29)-C(34)	118.9(3)	C(43)-C(44)-H(44)	120.3
C(30)-C(29)-P(2)	122.0(3)	C(44)-C(45)-C(46)	120.8(3)
C(34)-C(29)-P(2)	119.1(3)	C(44)-C(45)-H(45)	119.6
C(29)-C(30)-C(31)	120.1(4)	C(46)-C(45)-H(45)	119.6
C(29)-C(30)-H(30)	120.0	C(45)-C(46)-C(41)	120.4(3)
C(31)-C(30)-H(30)	120.0	C(45)-C(46)-H(46)	119.8
C(32)-C(31)-C(30)	120.5(3)	C(41)-C(46)-H(46)	119.8
C(32)-C(31)-H(31)	119.8	O(3)-C(47)-Re(1)	179.1(3)
C(30)-C(31)-H(31)	119.8	O(4)-C(48)-Re(1)	178.4(3)
C(33)-C(32)-C(31)	119.5(3)	Cl(3S)-C(1S)-Cl(1S)	111.3(2)
C(33)-C(32)-H(32)	120.3	Cl(3S)-C(1S)-Cl(2S)	110.58(19)
C(31)-C(32)-H(32)	120.3	Cl(1S)-C(1S)-Cl(2S)	110.2(2)
C(32)-C(33)-C(34)	120.4(4)	Cl(3S)-C(1S)-H(1S)	108.2
C(32)-C(33)-H(33)	119.8	Cl(1S)-C(1S)-H(1S)	108.2
C(34)-C(33)-H(33)	119.8	Cl(2S)-C(1S)-H(1S)	108.2

Table S32. Anisotropic displacement parameters ($Å^2$ x 10^3) for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	9(1)	9(1)	11(1)	1(1)	1(1)	0(1)
P(1)	11(1)	10(1)	11(1)	1(1)	2(1)	0(1)
O(1)	10(1)	14(1)	15(1)	-1(1)	2(1)	-1(1)
N(1)	11(1)	9(1)	12(2)	1(1)	2(1)	0(1)
C(1)	14(2)	7(2)	22(2)	3(2)	4(2)	-1(1)
P(2)	10(1)	10(1)	12(1)	1(1)	2(1)	0(1)
O(2)	18(1)	18(1)	12(1)	1(1)	-2(1)	-1(1)
N(2)	11(2)	15(2)	16(2)	1(1)	2(1)	0(1)
C(2)	11(2)	7(2)	15(2)	3(1)	2(1)	-2(1)
O(3)	11(1)	26(2)	30(2)	6(1)	2(1)	3(1)
N(3)	9(2)	14(2)	20(2)	1(1)	3(1)	0(1)
C(3)	15(2)	14(2)	13(2)	1(2)	4(1)	-2(2)
O(4)	25(2)	20(1)	12(1)	-3(1)	1(1)	0(1)
C(4)	14(2)	20(2)	17(2)	-4(2)	6(2)	4(2)
C(5)	14(2)	17(2)	14(2)	-2(2)	7(2)	2(2)
C(6)	15(2)	23(2)	18(2)	-3(2)	5(2)	1(2)
C(7)	17(2)	34(2)	24(2)	-6(2)	6(2)	-4(2)
C(8)	28(2)	25(2)	33(3)	-9(2)	21(2)	-8(2)
C(9)	41(3)	16(2)	23(2)	6(2)	20(2)	11(2)
C(10)	16(2)	30(2)	17(2)	2(2)	5(2)	8(2)
C(11)	14(2)	10(2)	12(2)	4(2)	0(2)	-1(1)
C(12)	13(2)	12(2)	21(2)	1(2)	2(2)	1(2)
C(13)	19(2)	15(2)	21(2)	-3(2)	2(2)	-4(2)
C(14)	13(2)	19(2)	22(2)	5(2)	-1(2)	-6(2)
C(15)	11(2)	20(2)	24(2)	5(2)	5(2)	3(2)
C(16)	18(2)	12(2)	18(2)	4(2)	2(2)	5(2)
C(17)	17(2)	6(2)	15(2)	-4(1)	3(2)	3(1)
C(18)	20(2)	12(2)	15(2)	-1(2)	2(2)	2(2)
C(19)	34(2)	10(2)	20(2)	3(2)	8(2)	-1(2)
C(20)	33(2)	19(2)	13(2)	1(2)	-2(2)	6(2)
C(21)	22(2)	16(2)	21(2)	0(2)	-7(2)	-3(2)
C(22)	18(2)	10(2)	23(2)	1(2)	1(2)	2(2)
C(23)	11(2)	7(2)	18(2)	-2(2)	2(2)	-5(1)
C(24)	15(2)	13(2)	21(2)	-2(2)	5(2)	-1(2)
C(25)	16(2)	14(2)	27(2)	3(2)	2(2)	2(2)
C(26)	21(2)	16(2)	30(2)	-3(2)	13(2)	0(2)
C(27)	24(2)	19(2)	20(2)	0(2)	9(2)	-5(2)
C(28)	16(2)	11(2)	23(2)	-1(2)	3(2)	-1(2)
C(29)	10(2)	7(2)	16(2)	-1(1)	1(2)	-3(1)
C(30)	17(2)	17(2)	16(2)	-5(2)	3(2)	-2(2)
C(31)	21(2)	24(2)	19(2)	2(2)	-6(2)	-1(2)
C(32)	14(2)	14(2)	29(2)	1(2)	-3(2)	0(2)
C(33)	12(2)	13(2)	30(2)	-2(2)	8(2)	2(2)
C(34)	18(2)	11(2)	19(2)	3(2)	2(2)	-2(2)
C(35)	9(2)	15(2)	12(2)	0(2)	-2(1)	1(1)
C(36)	14(2)	14(2)	16(2)	0(2)	2(2)	1(2)
C(37)	16(2)	18(2)	18(2)	-2(2)	4(2)	2(2)

C(38)	15(2)	28(2)	13(2)	-2(2)	2(2)	-6(2)
C(39)	17(2)	19(2)	26(2)	5(2)	2(2)	-5(2)
C(40)	14(2)	16(2)	19(2)	-2(2)	4(2)	-3(2)
C(41)	13(2)	12(2)	12(2)	-1(2)	3(2)	-2(1)
C(42)	13(2)	12(2)	17(2)	1(2)	2(2)	1(1)
C(43)	16(2)	19(2)	16(2)	2(2)	-1(2)	-2(2)
C(44)	19(2)	15(2)	16(2)	-2(2)	3(2)	-5(2)
C(45)	19(2)	11(2)	23(2)	-1(2)	5(2)	-2(2)
C(46)	17(2)	12(2)	18(2)	0(2)	-1(2)	-4(2)
C(47)	19(2)	10(2)	14(2)	0(2)	0(2)	1(2)
C(48)	10(2)	9(2)	24(2)	3(2)	4(2)	2(1)
Cl(1S)	79(1)	26(1)	25(1)	4(1)	-3(1)	9(1)
C(1S)	24(2)	21(2)	15(2)	-6(2)	0(2)	5(2)
Cl(2S)	30(1)	29(1)	21(1)	-5(1)	-4(1)	3(1)
Cl(3S)	28(1)	24(1)	26(1)	-8(1)	7(1)	3(1)

Table S33. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **7**.

	x	y	z	U(eq)
H(3)	5133	5459	4530	17
H(4A)	5208	4480	2853	20
H(4B)	5702	4208	3554	20
H(6)	6862	5206	3918	22
H(7)	7708	6661	3842	30
H(8)	7280	8114	3158	32
H(9)	6018	8071	2512	30
H(10)	5195	6559	2532	25
H(12)	2628	9241	4036	19
H(13)	3798	10219	4325	22
H(14)	4910	9807	3885	22
H(15)	4853	8348	3163	22
H(16)	3697	7312	2888	20
H(18)	2664	8562	2126	19
H(19)	2101	8871	1046	25
H(20)	838	8187	621	27
H(21)	171	7109	1259	26
H(22)	761	6727	2321	21
H(24)	877	8984	2778	20
H(25)	67	10044	3301	23
H(26)	147	9904	4402	26
H(27)	984	8603	4986	24
H(28)	1768	7483	4466	20
H(30)	2971	2948	5187	20
H(31)	4236	2311	5655	27
H(32)	5204	2049	5028	24
H(33)	4897	2380	3924	21
H(34)	3644	3016	3453	19
H(36)	1497	4963	4749	18
H(37)	713	4656	5516	21
H(38)	371	2886	5759	23
H(39)	811	1414	5220	25
H(40)	1552	1709	4422	19
H(42)	855	3447	2872	17
H(43)	391	2242	2033	21
H(44)	1089	640	1920	20
H(45)	2228	226	2668	21
H(46)	2690	1407	3517	19
H(1S)	2346	8946	6152	25

Table S34. Torsion angles [°] for **7**.

Re(1)-O(1)-C(1)-O(2)	-172.4(3)	Re(1)-P(1)-C(17)-C(22)	55.9(3)
Re(1)-O(1)-C(1)-C(2)	6.7(4)	C(22)-C(17)-C(18)-C(19)	0.5(5)
C(2)-N(1)-N(2)-N(3)	0.3(3)	P(1)-C(17)-C(18)-C(19)	-177.3(3)
Re(1)-N(1)-N(2)-N(3)	-173.0(2)	C(17)-C(18)-C(19)-C(20)	1.6(5)
N(2)-N(1)-C(2)-C(3)	-0.3(4)	C(18)-C(19)-C(20)-C(21)	-2.0(5)
Re(1)-N(1)-C(2)-C(3)	174.3(2)	C(19)-C(20)-C(21)-C(22)	0.3(6)
N(2)-N(1)-C(2)-C(1)	-176.5(3)	C(20)-C(21)-C(22)-C(17)	1.8(5)
Re(1)-N(1)-C(2)-C(1)	-1.9(4)	C(18)-C(17)-C(22)-C(21)	-2.2(5)
O(2)-C(1)-C(2)-N(1)	176.0(3)	P(1)-C(17)-C(22)-C(21)	175.8(3)
O(1)-C(1)-C(2)-N(1)	-3.1(4)	C(17)-P(1)-C(23)-C(24)	-13.3(3)
O(2)-C(1)-C(2)-C(3)	1.2(6)	C(11)-P(1)-C(23)-C(24)	95.1(3)
O(1)-C(1)-C(2)-C(3)	-177.9(3)	Re(1)-P(1)-C(23)-C(24)	-137.2(2)
N(1)-N(2)-N(3)-C(3)	-0.1(4)	C(17)-P(1)-C(23)-C(28)	171.9(3)
N(1)-N(2)-N(3)-C(4)	178.3(3)	C(11)-P(1)-C(23)-C(28)	-79.7(3)
N(2)-N(3)-C(3)-C(2)	-0.1(4)	Re(1)-P(1)-C(23)-C(28)	47.9(3)
C(4)-N(3)-C(3)-C(2)	-178.3(3)	C(28)-C(23)-C(24)-C(25)	0.7(5)
N(1)-C(2)-C(3)-N(3)	0.2(4)	P(1)-C(23)-C(24)-C(25)	-174.2(3)
C(1)-C(2)-C(3)-N(3)	175.4(3)	C(23)-C(24)-C(25)-C(26)	1.5(5)
C(3)-N(3)-C(4)-C(5)	-69.9(4)	C(24)-C(25)-C(26)-C(27)	-2.3(5)
N(2)-N(3)-C(4)-C(5)	112.0(3)	C(25)-C(26)-C(27)-C(28)	1.0(5)
N(3)-C(4)-C(5)-C(6)	110.2(4)	C(26)-C(27)-C(28)-C(23)	1.1(5)
N(3)-C(4)-C(5)-C(10)	-68.3(4)	C(24)-C(23)-C(28)-C(27)	-1.9(5)
C(10)-C(5)-C(6)-C(7)	-0.6(5)	P(1)-C(23)-C(28)-C(27)	173.1(3)
C(4)-C(5)-C(6)-C(7)	-179.1(3)	C(35)-P(2)-C(29)-C(30)	-15.5(3)
C(5)-C(6)-C(7)-C(8)	2.2(6)	C(41)-P(2)-C(29)-C(30)	-122.8(3)
C(6)-C(7)-C(8)-C(9)	-1.5(6)	Re(1)-P(2)-C(29)-C(30)	110.7(3)
C(7)-C(8)-C(9)-C(10)	-0.8(6)	C(35)-P(2)-C(29)-C(34)	167.6(3)
C(8)-C(9)-C(10)-C(5)	2.4(6)	C(41)-P(2)-C(29)-C(34)	60.2(3)
C(6)-C(5)-C(10)-C(9)	-1.7(5)	Re(1)-P(2)-C(29)-C(34)	-66.3(3)
C(4)-C(5)-C(10)-C(9)	176.8(3)	C(34)-C(29)-C(30)-C(31)	-0.4(5)
C(17)-P(1)-C(11)-C(16)	-68.5(3)	P(2)-C(29)-C(30)-C(31)	-177.3(3)
C(23)-P(1)-C(11)-C(16)	-174.1(3)	C(29)-C(30)-C(31)-C(32)	0.6(5)
Re(1)-P(1)-C(11)-C(16)	60.8(3)	C(30)-C(31)-C(32)-C(33)	-0.8(5)
C(17)-P(1)-C(11)-C(12)	114.7(3)	C(31)-C(32)-C(33)-C(34)	0.9(5)
C(23)-P(1)-C(11)-C(12)	9.1(3)	C(32)-C(33)-C(34)-C(29)	-0.7(5)
Re(1)-P(1)-C(11)-C(12)	-116.0(3)	C(30)-C(29)-C(34)-C(33)	0.4(5)
C(16)-C(11)-C(12)-C(13)	1.2(5)	P(2)-C(29)-C(34)-C(33)	177.5(3)
P(1)-C(11)-C(12)-C(13)	178.1(3)	C(41)-P(2)-C(35)-C(36)	-143.7(3)
C(11)-C(12)-C(13)-C(14)	0.5(5)	C(29)-P(2)-C(35)-C(36)	109.2(3)
C(12)-C(13)-C(14)-C(15)	-1.1(5)	Re(1)-P(2)-C(35)-C(36)	-18.1(3)
C(13)-C(14)-C(15)-C(16)	0.0(5)	C(41)-P(2)-C(35)-C(40)	38.4(3)
C(14)-C(15)-C(16)-C(11)	1.7(5)	C(29)-P(2)-C(35)-C(40)	-68.8(3)
C(12)-C(11)-C(16)-C(15)	-2.3(5)	Re(1)-P(2)-C(35)-C(40)	164.0(2)
P(1)-C(11)-C(16)-C(15)	-179.2(3)	C(40)-C(35)-C(36)-C(37)	-1.7(5)
C(11)-P(1)-C(17)-C(18)	4.8(3)	P(2)-C(35)-C(36)-C(37)	-179.7(2)
C(23)-P(1)-C(17)-C(18)	110.2(3)	C(35)-C(36)-C(37)-C(38)	1.7(5)
Re(1)-P(1)-C(17)-C(18)	-126.3(3)	C(36)-C(37)-C(38)-C(39)	-0.2(5)
C(11)-P(1)-C(17)-C(22)	-173.0(3)	C(37)-C(38)-C(39)-C(40)	-1.1(5)
C(23)-P(1)-C(17)-C(22)	-67.6(3)	C(38)-C(39)-C(40)-C(35)	1.1(5)

C(36)-C(35)-C(40)-C(39)	0.3(5)	C(46)-C(41)-C(42)-C(43)	-2.7(5)
P(2)-C(35)-C(40)-C(39)	178.4(3)	P(2)-C(41)-C(42)-C(43)	176.1(3)
C(35)-P(2)-C(41)-C(46)	-100.9(3)	C(41)-C(42)-C(43)-C(44)	0.5(5)
C(29)-P(2)-C(41)-C(46)	5.8(3)	C(42)-C(43)-C(44)-C(45)	1.3(5)
Re(1)-P(2)-C(41)-C(46)	133.5(3)	C(43)-C(44)-C(45)-C(46)	-0.8(5)
C(35)-P(2)-C(41)-C(42)	80.3(3)	C(44)-C(45)-C(46)-C(41)	-1.5(6)
C(29)-P(2)-C(41)-C(42)	-173.0(3)	C(42)-C(41)-C(46)-C(45)	3.2(5)
Re(1)-P(2)-C(41)-C(42)	-45.3(3)	P(2)-C(41)-C(46)-C(45)	-175.6(3)

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