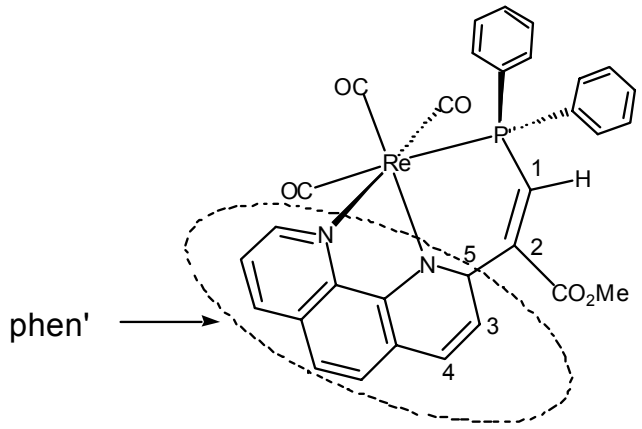
Supplementary Material for Chemical Communications

Supplementary Information

General Procedures for the Experimental Section. All manipulations were carried out under dinitrogen using standard Schlenk techniques. Solvents were distilled from Na (hexanes, diethylether and THF) and CaH_2 (CH_2Cl_2). CD_2Cl_2 and C_6D_6 were dried over 4Å molecular sieves and stored in Young tubes. Elemental analyses were obtained using a Perkin-Elmer 240-B microanalyzer. The IR, ^1H and ^{13}C NMR spectra were recorded on Perkin-Elmer FT 1720-X (over the range 2200-1600 cm^{-1}), and Bruker AC-200 (or AC-300) spectrometers respectively.

Atom-labeling scheme:



X-ray structures. Data in common: Bruker AXS SMART 1000 CCD diffractometer, ϕ and ω scans, $Mo_{K\alpha}$ radiation ($\lambda = 0.71073$ Å),

graphite monochromator, *T* = 295 K. Raw frame data integrated with SAINT[1] program. Structures were solved by direct methods with SHELXTL.[2] Semi-empirical absorption correction with SADABS.[3] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were set in calculated positions and refined as riding atoms, with a common thermal parameter. All calculations were made with SHELXTL

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C31.25 H24.50 Cl0.50 N2 O5 P Re	
Formula weight	742.92	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 25.629(6) Å	α= 90°.
	b = 9.692(2) Å	β= 90.334(4) °.
	c = 24.818(5) Å	γ = 90°.
Volume	6165(2) Å ^{3}	
Z	8	
Density (calculated)	1.601 Mg/m^3	
Absorption coefficient	4.078 mm^{-1}	
F(000)	2916	
Crystal size	0.08 x 0.11 x 0.13 mm^3	
Theta range for data collection	1.59 to 23.34°.	
Index ranges	-25<=h<=28, -10<=k<=8, -27<=l<=24	
Reflections collected	13470	
Independent reflections	4450 [R(int) = 0.0747]	
Completeness to theta = 23.34°	99.4 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.780198	

[1] SAINT+. SAX area detector integration program. Version 6.02. Bruker AXS, Inc. Madison, WI, 1999.

[2] G. M. Sheldrick, SHELXTL, An integrated system for solving, refining, and displaying crystal structures from diffraction data. Version 5.1. Bruker AXS, Inc. Madison, WI, 1998.

[3] G. M. Sheldrick, SADABS, Empirical Absorption Correction Program. University of Göttingen: Göttingen, Germany, 1997.

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4450 / 0 / 371
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0463, wR2 = 0.0857
R indices (all data)	R1 = 0.0876, wR2 = 0.0930
Largest diff. peak and hole	1.135 and -0.754 e. $Å^{-3}$

Table 2. 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 U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	8813(1)	319(1)	7940(1)	35(1)
P(1)	8833(1)	2120(3)	8646(1)	37(1)
N(1)	8525(3)	-803(8)	8620(3)	36(2)
N(2)	7972(3)	384(9)	7828(3)	36(2)
C(1)	8847(4)	-1169(13)	7423(5)	44(3)
O(1)	8906(3)	-2023(10)	7107(4)	74(3)
C(2)	8993(4)	1535(13)	7383(5)	47(3)
O(2)	9103(3)	2327(9)	7038(3)	69(3)
C(3)	9546(4)	4(10)	8073(4)	38(3)
O(3)	9977(3)	-246(9)	8140(3)	58(2)
C(4)	9162(4)	1349(11)	9230(4)	42(3)
C(5)	8868(4)	123(11)	9483(3)	39(3)
C(6)	9162(4)	-292(15)	9989(4)	55(3)
O(6)	9532(4)	-1002(10)	10002(3)	89(3)
C(7)	9271(7)	110(30)	10905(5)	289(19)
O(7)	8971(3)	297(15)	10407(3)	149(6)
C(11)	8813(4)	-1140(11)	9108(4)	41(3)
C(12)	8547(5)	-2321(12)	9417(4)	57(3)
C(13)	8042(5)	-2502(13)	9397(4)	57(3)
C(14)	7726(5)	-1722(13)	9042(5)	56(3)
C(15)	7178(5)	-1792(14)	9006(5)	69(4)
C(16)	6889(5)	-1136(14)	8602(6)	70(4)
C(17)	7139(4)	-367(13)	8190(4)	52(3)
C(18)	6888(4)	297(14)	7758(5)	64(3)
C(19)	7165(5)	972(13)	7379(5)	63(4)
C(20)	7715(4)	1006(12)	7426(4)	51(3)
C(21)	7995(4)	-907(11)	8643(4)	42(3)
C(22)	7694(3)	-296(12)	8216(4)	40(3)
C(31)	9216(4)	3647(11)	8499(4)	34(3)
C(32)	9002(4)	4952(11)	8469(4)	45(3)
C(33)	9286(5)	6090(13)	8316(4)	57(3)
C(34)	9811(5)	5948(16)	8200(5)	69(4)
C(35)	10032(5)	4665(18)	8212(6)	88(4)
C(36)	9734(5)	3539(13)	8360(5)	70(4)
C(41)	8236(4)	2852(11)	8922(5)	45(3)
C(42)	8203(5)	3271(13)	9455(5)	59(4)
C(43)	7751(6)	3852(14)	9648(6)	83(5)
C(44)	7325(6)	4048(15)	9326(7)	88(5)
C(45)	7354(5)	3662(15)	8808(7)	80(4)
C(46)	7815(4)	3078(12)	8592(5)	62(4)
Cl(91)	10343(8)	4630(30)	4958(10)	184(10)
Cl(92)	9380(11)	5530(40)	5393(14)	284(18)
C(90)	10027(13)	6040(40)	5270(30)	170(30)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Re(1)-C(2)	1.876(13)
Re(1)-C(3)	1.929(11)
Re(1)-C(1)	1.932(13)
Re(1)-N(1)	2.142(8)
Re(1)-N(2)	2.173(7)
Re(1)-P(1)	2.475(3)
P(1)-C(31)	1.814(11)
P(1)-C(41)	1.822(11)
P(1)-C(4)	1.831(9)
N(1)-C(21)	1.363(12)
N(1)-C(11)	1.452(11)
N(2)-C(20)	1.336(12)
N(2)-C(22)	1.369(12)
C(1)-O(1)	1.150(12)
C(2)-O(2)	1.186(13)
C(3)-O(3)	1.143(10)
C(4)-C(5)	1.543(13)
C(5)-C(6)	1.515(13)
C(5)-C(11)	1.543(13)
C(6)-O(6)	1.172(12)
C(6)-O(7)	1.285(13)
C(7)-O(7)	1.464(14)
C(11)-C(12)	1.540(14)
C(12)-C(13)	1.307(14)
C(13)-C(14)	1.412(15)
C(14)-C(15)	1.409(15)
C(14)-C(21)	1.446(14)
C(15)-C(16)	1.395(16)
C(16)-C(17)	1.421(15)
C(17)-C(18)	1.403(15)
C(17)-C(22)	1.425(12)
C(18)-C(19)	1.351(15)
C(19)-C(20)	1.415(14)
C(21)-C(22)	1.436(13)
C(31)-C(36)	1.379(14)
C(31)-C(32)	1.381(13)
C(32)-C(33)	1.376(14)
C(33)-C(34)	1.386(16)
C(34)-C(35)	1.367(17)
C(35)-C(36)	1.383(17)
C(41)-C(46)	1.370(14)
C(41)-C(42)	1.387(14)
C(42)-C(43)	1.378(16)
C(43)-C(44)	1.362(18)
C(44)-C(45)	1.343(18)
C(45)-C(46)	1.417(15)
Cl(91)-Cl(92)#1	1.14(4)
Cl(91)-C(90)#1	1.28(5)
Cl(91)-C(90)	1.7700
Cl(91)-Cl(91)#1	1.91(4)
Cl(92)-Cl(91)#1	1.14(4)
Cl(92)-C(90)	1.7612
C(90)-Cl(91)#1	1.28(5)
C(2)-Re(1)-C(3)	89.0(4)
C(2)-Re(1)-C(1)	88.2(5)

C(3)-Re(1)-C(1)	87.0(4)
C(2)-Re(1)-N(1)	170.6(4)
C(3)-Re(1)-N(1)	97.1(3)
C(1)-Re(1)-N(1)	99.3(4)
C(2)-Re(1)-N(2)	97.8(4)
C(3)-Re(1)-N(2)	172.1(4)
C(1)-Re(1)-N(2)	89.2(4)
N(1)-Re(1)-N(2)	76.6(3)
C(2)-Re(1)-P(1)	94.2(4)
C(3)-Re(1)-P(1)	88.5(3)
C(1)-Re(1)-P(1)	174.9(3)
N(1)-Re(1)-P(1)	78.8(2)
N(2)-Re(1)-P(1)	94.9(2)
C(31)-P(1)-C(41)	102.3(5)
C(31)-P(1)-C(4)	104.2(4)
C(41)-P(1)-C(4)	104.2(5)
C(31)-P(1)-Re(1)	116.3(3)
C(41)-P(1)-Re(1)	121.8(4)
C(4)-P(1)-Re(1)	106.3(4)
C(21)-N(1)-C(11)	116.7(8)
C(21)-N(1)-Re(1)	114.8(6)
C(11)-N(1)-Re(1)	126.6(6)
C(20)-N(2)-C(22)	119.1(8)
C(20)-N(2)-Re(1)	126.3(7)
C(22)-N(2)-Re(1)	114.6(6)
O(1)-C(1)-Re(1)	174.7(10)
O(2)-C(2)-Re(1)	178.6(12)
O(3)-C(3)-Re(1)	176.6(9)
C(5)-C(4)-P(1)	114.4(6)
C(6)-C(5)-C(4)	107.5(8)
C(6)-C(5)-C(11)	109.5(9)
C(4)-C(5)-C(11)	114.1(8)
O(6)-C(6)-O(7)	123.5(11)
O(6)-C(6)-C(5)	125.3(11)
O(7)-C(6)-C(5)	111.2(10)
C(6)-O(7)-C(7)	115.1(11)
N(1)-C(11)-C(12)	111.0(8)
N(1)-C(11)-C(5)	111.7(8)
C(12)-C(11)-C(5)	109.2(8)
C(13)-C(12)-C(11)	121.5(11)
C(12)-C(13)-C(14)	121.0(11)
C(15)-C(14)-C(13)	125.7(12)
C(15)-C(14)-C(21)	117.5(12)
C(13)-C(14)-C(21)	116.5(11)
C(16)-C(15)-C(14)	123.3(12)
C(15)-C(16)-C(17)	121.1(11)
C(18)-C(17)-C(16)	125.7(11)
C(18)-C(17)-C(22)	117.8(11)
C(16)-C(17)-C(22)	116.5(11)
C(19)-C(18)-C(17)	120.9(11)
C(18)-C(19)-C(20)	118.8(11)
N(2)-C(20)-C(19)	122.5(11)
N(1)-C(21)-C(22)	118.0(9)
N(1)-C(21)-C(14)	123.3(10)
C(22)-C(21)-C(14)	118.3(10)
N(2)-C(22)-C(17)	121.0(10)
N(2)-C(22)-C(21)	115.9(8)
C(17)-C(22)-C(21)	123.1(10)

C(36)-C(31)-C(32)	116.0(10)
C(36)-C(31)-P(1)	120.8(9)
C(32)-C(31)-P(1)	123.0(8)
C(33)-C(32)-C(31)	122.6(11)
C(32)-C(33)-C(34)	119.6(12)
C(35)-C(34)-C(33)	119.2(12)
C(34)-C(35)-C(36)	119.6(12)
C(31)-C(36)-C(35)	122.8(12)
C(46)-C(41)-C(42)	118.1(10)
C(46)-C(41)-P(1)	119.9(9)
C(42)-C(41)-P(1)	121.9(9)
C(43)-C(42)-C(41)	120.5(12)
C(44)-C(43)-C(42)	121.8(14)
C(45)-C(44)-C(43)	118.3(14)
C(44)-C(45)-C(46)	121.7(13)
C(41)-C(46)-C(45)	119.6(12)
Cl(92)#1-Cl(91)-C(90)#1	94(4)
Cl(92)#1-Cl(91)-C(90)	137(5)
C(90)#1-Cl(91)-C(90)	104(3)
Cl(92)#1-Cl(91)-Cl(91)#1	135(4)
C(90)#1-Cl(91)-Cl(91)#1	64(3)
C(90)-Cl(91)-Cl(91)#1	40.4(16)
Cl(91)#1-Cl(92)-C(90)	46(2)
Cl(91)#1-C(90)-Cl(92)	40.1(17)
Cl(91)#1-C(90)-Cl(91)	76(2)
Cl(92)-C(90)-Cl(91)	106.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	35(1)	36(1)	35(1)	1(1)	1(1)	-1(1)
P(1)	37(2)	35(2)	38(2)	-1(1)	1(1)	2(1)
N(1)	40(5)	30(6)	38(5)	1(4)	-4(4)	-3(4)
N(2)	26(4)	40(6)	42(5)	-12(5)	-3(4)	-5(5)
C(1)	32(6)	55(10)	44(8)	14(6)	2(6)	1(6)
O(1)	89(7)	61(8)	74(7)	-26(5)	10(5)	-16(5)
C(2)	25(6)	68(11)	49(8)	-14(7)	-10(6)	0(6)
O(2)	74(6)	69(7)	64(6)	31(5)	4(5)	-8(5)
C(3)	61(7)	24(9)	29(6)	-9(4)	7(5)	-1(5)
O(3)	28(4)	81(7)	65(5)	-2(5)	-2(4)	11(4)
C(4)	36(6)	43(8)	49(7)	2(6)	-2(5)	0(5)
C(5)	37(6)	45(9)	36(6)	-4(5)	3(5)	5(5)
C(6)	40(7)	81(10)	44(7)	8(7)	-1(6)	4(7)
O(6)	92(7)	105(9)	71(6)	0(5)	-24(5)	42(6)
C(7)	137(16)	690(60)	39(9)	20(20)	-33(10)	180(30)
O(7)	95(8)	318(18)	34(5)	-6(7)	-5(5)	106(10)
C(11)	46(7)	38(8)	38(7)	2(6)	1(5)	0(5)
C(12)	81(10)	35(9)	55(8)	16(6)	2(7)	5(7)
C(13)	64(9)	55(10)	51(8)	23(6)	2(7)	-7(7)
C(14)	55(8)	54(10)	60(8)	-8(7)	22(7)	-17(7)
C(15)	63(10)	81(12)	64(9)	-5(8)	19(8)	-30(8)
C(16)	50(8)	72(11)	89(11)	-21(8)	24(8)	-20(7)

C(17)	39(6)	55(8)	63(7)	-8(7)	-3(6)	-8(7)
C(18)	33(6)	72(10)	87(9)	-23(8)	-11(7)	4(7)
C(19)	50(8)	69(11)	70(9)	5(7)	-14(7)	-1(7)
C(20)	48(8)	55(9)	50(7)	0(6)	-14(6)	-10(6)
C(21)	54(7)	33(8)	37(7)	-14(5)	6(6)	-2(6)
C(22)	28(5)	42(7)	51(6)	-14(6)	5(5)	-6(6)
C(31)	37(6)	28(8)	36(6)	-6(5)	6(5)	5(5)
C(32)	46(7)	31(11)	57(7)	-2(5)	0(5)	1(5)
C(33)	81(10)	33(9)	59(8)	-1(6)	3(7)	-10(7)
C(34)	73(10)	48(11)	86(10)	-8(8)	29(8)	-27(8)
C(35)	69(9)	46(10)	148(13)	2(11)	42(9)	-3(10)
C(36)	50(8)	35(9)	125(12)	0(8)	24(8)	8(7)
C(41)	46(7)	29(8)	61(8)	3(6)	12(6)	4(5)
C(42)	52(8)	66(11)	59(9)	2(7)	21(7)	22(7)
C(43)	109(13)	58(11)	83(11)	13(8)	43(10)	3(9)
C(44)	79(12)	62(12)	123(15)	8(10)	41(11)	14(9)
C(45)	36(8)	82(12)	122(14)	-9(10)	-2(9)	15(7)
C(46)	55(8)	45(9)	85(10)	-14(7)	-11(8)	10(7)

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

	x	y	z	U(eq)
H(4A)	9505	1038	9120	51
H(4B)	9211	2055	9502	51
H(5)	8519	434	9585	47
H(7A)	9177	-754	11068	433
H(7B)	9196	850	11149	433
H(7C)	9637	107	10824	433
H(11)	9163	-1444	9006	49
H(12)	8751	-2920	9623	68
H(13)	7888	-3155	9621	68
H(15)	6999	-2300	9263	83
H(16)	6527	-1204	8602	84
H(18)	6526	272	7732	77
H(19)	6997	1407	7092	76
H(20)	7905	1479	7167	61
H(32)	8652	5067	8554	54
H(33)	9126	6950	8291	69
H(34)	10011	6718	8114	83
H(35)	10381	4549	8122	105
H(36)	9890	2673	8367	84
H(42)	8488	3158	9684	71
H(43)	7736	4119	10008	100
H(44)	7021	4438	9462	106
H(45)	7065	3782	8585	96
H(46)	7830	2849	8228	74
H(90A)	10156	6574	5566	100
H(90B)	10036	6598	4946	100

Table 1. Crystal data and structure refinement for **3**.

Empirical formula	C31 H22 N2 O5 P Re	
Formula weight	719.68	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.844(3) Å	α= 86.592(7)°.
	b = 11.300(4) Å	β= 71.976(6) °.
	c = 13.009(5) Å	γ = 82.823(7) °.
Volume	1365.0(8) $Å^3$	
Z	2	
Density (calculated)	1.751 Mg/m^3	
Absorption coefficient	4.554 mm^{-1}	
F(000)	704	
Crystal size	0.11 x 0.18 x 0.22 mm^3	
Theta range for data collection	1.65 to 23.32°.	
Index ranges	-10<=h<=10, -10<=k<=12, -14<=l<=12	
Reflections collected	6131	
Independent reflections	3917 [R(int) = 0.0212]	
Completeness to theta = 23.32°	99.0 %	
Absorption correction	SADABS	
Max. and min. transmission	1.000000 and 0.690997	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3917 / 0 / 362	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0317, wR2 = 0.0782	
R indices (all data)	R1 = 0.0371, wR2 = 0.0815	
Largest diff. peak and hole	1.484 and -0.899 e. $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{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)	3623(1)	2195(1)	2189(1)	35(1)
P(1)	3877(2)	3183(1)	3752(1)	33(1)
N(1)	5323(5)	3313(4)	1517(4)	34(1)
N(2)	5567(5)	1024(4)	2116(4)	37(1)
C(1)	3559(6)	1547(6)	833(5)	43(2)
O(1)	3475(6)	1157(6)	97(5)	85(2)
C(3)	2034(7)	3348(6)	2146(5)	43(2)
O(3)	1096(6)	4044(5)	2058(4)	67(1)
C(2)	2283(6)	1082(5)	2949(5)	39(1)
O(2)	1523(5)	408(5)	3395(5)	69(1)
C(4)	3940(7)	4769(5)	3428(5)	42(2)
C(5)	4365(6)	5266(5)	2432(5)	39(1)
C(6)	4055(7)	6594(6)	2350(5)	45(2)
O(6)	4213(7)	7297(4)	2933(4)	76(2)
O(7)	3511(6)	6901(4)	1532(4)	59(1)
C(7)	3064(9)	8165(6)	1402(7)	68(2)
C(11)	5082(7)	4613(5)	1370(5)	40(1)
C(12)	6454(8)	5153(6)	753(5)	51(2)
C(13)	7745(8)	4548(6)	525(5)	54(2)
C(14)	7954(7)	3306(6)	830(5)	46(2)
C(15)	6680(7)	2760(6)	1322(5)	40(1)
C(16)	6847(6)	1529(6)	1624(5)	39(1)
C(17)	8206(7)	858(7)	1486(5)	51(2)
C(18)	8225(8)	-310(7)	1848(6)	64(2)
C(19)	6986(8)	-802(6)	2323(6)	57(2)
C(20)	5679(7)	-106(6)	2447(5)	45(2)
C(21)	9290(7)	2610(7)	657(6)	61(2)
C(22)	9439(8)	1436(8)	972(7)	68(2)
C(31)	2474(6)	3237(5)	5070(5)	38(1)
C(32)	2706(7)	3627(6)	5985(5)	50(2)
C(33)	1618(8)	3722(6)	6952(5)	56(2)
C(34)	278(9)	3444(7)	7018(6)	66(2)
C(35)	37(8)	3046(9)	6131(7)	82(3)
C(36)	1130(8)	2949(8)	5144(6)	67(2)
C(41)	5521(6)	2666(5)	4090(4)	37(1)
C(42)	6714(7)	3271(7)	3739(5)	52(2)
C(43)	8015(7)	2786(8)	3914(6)	64(2)
C(44)	8078(8)	1688(8)	4447(6)	64(2)
C(45)	6878(8)	1079(7)	4786(6)	58(2)
C(46)	5613(7)	1564(6)	4614(5)	45(2)

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

Re(1)-C(3)	1.920(7)
Re(1)-C(2)	1.939(6)
Re(1)-C(1)	1.972(6)
Re(1)-N(1)	2.157(4)
Re(1)-N(2)	2.166(5)
Re(1)-P(1)	2.4685(16)
P(1)-C(4)	1.821(6)
P(1)-C(41)	1.824(6)
P(1)-C(31)	1.838(6)
N(1)-C(15)	1.356(8)
N(1)-C(11)	1.469(8)
N(2)-C(20)	1.325(8)
N(2)-C(16)	1.400(7)
C(1)-O(1)	1.107(7)
C(3)-O(3)	1.165(8)
C(2)-O(2)	1.139(7)
C(4)-C(5)	1.344(8)
C(5)-C(6)	1.498(9)
C(5)-C(11)	1.530(9)
C(6)-O(6)	1.186(8)
C(6)-O(7)	1.342(8)
O(7)-C(7)	1.457(8)
C(11)-C(12)	1.522(9)
C(12)-C(13)	1.321(10)
C(13)-C(14)	1.442(10)
C(14)-C(21)	1.407(10)
C(14)-C(15)	1.419(8)
C(15)-C(16)	1.426(9)
C(16)-C(17)	1.418(9)
C(17)-C(18)	1.375(10)
C(17)-C(22)	1.410(10)
C(18)-C(19)	1.356(10)
C(19)-C(20)	1.391(9)
C(21)-C(22)	1.368(11)
C(31)-C(36)	1.375(9)
C(31)-C(32)	1.385(9)
C(32)-C(33)	1.377(9)
C(33)-C(34)	1.370(10)
C(34)-C(35)	1.360(11)
C(35)-C(36)	1.396(10)
C(41)-C(42)	1.373(8)
C(41)-C(46)	1.391(8)
C(42)-C(43)	1.408(10)
C(43)-C(44)	1.389(11)
C(44)-C(45)	1.382(10)
C(45)-C(46)	1.373(9)
C(3)-Re(1)-C(2)	89.6(2)
C(3)-Re(1)-C(1)	88.5(3)
C(2)-Re(1)-C(1)	87.3(3)
C(3)-Re(1)-N(1)	98.0(2)
C(2)-Re(1)-N(1)	170.4(2)
C(1)-Re(1)-N(1)	98.7(2)
C(3)-Re(1)-N(2)	173.7(2)
C(2)-Re(1)-N(2)	96.6(2)
C(1)-Re(1)-N(2)	90.7(2)

N(1)-Re(1)-N(2)	75.94(18)
C(3)-Re(1)-P(1)	90.76(18)
C(2)-Re(1)-P(1)	99.48(18)
C(1)-Re(1)-P(1)	173.19(18)
N(1)-Re(1)-P(1)	74.72(13)
N(2)-Re(1)-P(1)	89.34(13)
C(4)-P(1)-C(41)	106.0(3)
C(4)-P(1)-C(31)	100.6(3)
C(41)-P(1)-C(31)	103.6(3)
C(4)-P(1)-Re(1)	108.42(19)
C(41)-P(1)-Re(1)	114.44(19)
C(31)-P(1)-Re(1)	122.0(2)
C(15)-N(1)-C(11)	120.1(5)
C(15)-N(1)-Re(1)	115.7(4)
C(11)-N(1)-Re(1)	124.0(4)
C(20)-N(2)-C(16)	117.3(5)
C(20)-N(2)-Re(1)	127.8(4)
C(16)-N(2)-Re(1)	114.9(4)
O(1)-C(1)-Re(1)	177.0(6)
O(3)-C(3)-Re(1)	176.2(6)
O(2)-C(2)-Re(1)	178.4(6)
C(5)-C(4)-P(1)	126.2(5)
C(4)-C(5)-C(6)	116.6(6)
C(4)-C(5)-C(11)	126.8(6)
C(6)-C(5)-C(11)	116.6(5)
O(6)-C(6)-O(7)	123.3(6)
O(6)-C(6)-C(5)	126.1(6)
O(7)-C(6)-C(5)	110.5(5)
C(6)-O(7)-C(7)	116.6(5)
N(1)-C(11)-C(12)	112.6(5)
N(1)-C(11)-C(5)	113.3(5)
C(12)-C(11)-C(5)	109.4(5)
C(13)-C(12)-C(11)	123.2(6)
C(12)-C(13)-C(14)	122.0(6)
C(21)-C(14)-C(15)	118.7(6)
C(21)-C(14)-C(13)	125.6(6)
C(15)-C(14)-C(13)	115.6(6)
N(1)-C(15)-C(14)	125.1(6)
N(1)-C(15)-C(16)	117.8(5)
C(14)-C(15)-C(16)	117.1(6)
N(2)-C(16)-C(17)	121.3(6)
N(2)-C(16)-C(15)	115.5(5)
C(17)-C(16)-C(15)	123.2(6)
C(18)-C(17)-C(22)	124.9(7)
C(18)-C(17)-C(16)	117.7(6)
C(22)-C(17)-C(16)	117.4(7)
C(19)-C(18)-C(17)	121.1(7)
C(18)-C(19)-C(20)	119.1(7)
N(2)-C(20)-C(19)	123.5(6)
C(22)-C(21)-C(14)	123.6(6)
C(21)-C(22)-C(17)	119.8(7)
C(36)-C(31)-C(32)	118.7(6)
C(36)-C(31)-P(1)	119.4(5)
C(32)-C(31)-P(1)	121.7(5)
C(33)-C(32)-C(31)	120.9(6)
C(34)-C(33)-C(32)	120.1(7)
C(35)-C(34)-C(33)	119.7(7)
C(34)-C(35)-C(36)	120.7(7)

C(31)-C(36)-C(35)	119.8(7)
C(42)-C(41)-C(46)	119.3(6)
C(42)-C(41)-P(1)	121.8(5)
C(46)-C(41)-P(1)	118.6(4)
C(41)-C(42)-C(43)	120.4(7)
C(44)-C(43)-C(42)	119.2(6)
C(45)-C(44)-C(43)	119.9(7)
C(46)-C(45)-C(44)	120.3(7)
C(45)-C(46)-C(41)	120.8(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	37(1)	38(1)	34(1)	-4(1)	-12(1)	-12(1)
P(1)	36(1)	37(1)	29(1)	-3(1)	-10(1)	-12(1)
N(1)	36(3)	30(3)	35(3)	-1(2)	-7(2)	-12(2)
N(2)	40(3)	40(3)	30(3)	-2(2)	-8(2)	-10(2)
C(1)	37(3)	57(4)	34(3)	-6(3)	-7(3)	-11(3)
O(1)	86(4)	118(5)	61(4)	-33(3)	-29(3)	-22(4)
C(3)	52(4)	41(4)	38(3)	-5(3)	-9(3)	-20(3)
O(3)	57(3)	64(3)	81(4)	3(3)	-27(3)	4(3)
C(2)	37(3)	36(3)	42(3)	-2(3)	-7(3)	-7(3)
O(2)	56(3)	56(3)	88(4)	11(3)	-10(3)	-24(3)
C(4)	52(4)	46(4)	36(3)	-5(3)	-17(3)	-17(3)
C(5)	45(4)	41(3)	37(3)	-1(3)	-16(3)	-15(3)
C(6)	55(4)	42(4)	38(4)	3(3)	-10(3)	-18(3)
O(6)	130(5)	44(3)	68(3)	-6(3)	-46(4)	-23(3)
O(7)	87(4)	42(3)	57(3)	-3(2)	-33(3)	-7(2)
C(7)	93(6)	44(4)	71(5)	4(4)	-28(5)	-12(4)
C(11)	49(4)	41(3)	33(3)	1(3)	-14(3)	-14(3)
C(12)	66(5)	44(4)	43(4)	2(3)	-12(3)	-25(3)
C(13)	52(4)	65(5)	43(4)	-2(3)	-5(3)	-32(4)
C(14)	38(4)	64(4)	37(3)	-4(3)	-8(3)	-15(3)
C(15)	42(4)	48(4)	33(3)	-3(3)	-12(3)	-19(3)
C(16)	36(3)	49(4)	34(3)	-6(3)	-10(3)	-9(3)
C(17)	54(4)	70(5)	30(3)	-6(3)	-14(3)	-9(3)
C(18)	57(5)	61(5)	74(5)	-8(4)	-25(4)	14(4)
C(19)	59(5)	48(4)	62(5)	-3(3)	-18(4)	0(3)
C(20)	49(4)	44(4)	43(4)	-8(3)	-13(3)	-5(3)
C(21)	37(4)	82(6)	58(5)	-13(4)	3(3)	-19(4)
C(22)	38(4)	85(6)	75(5)	-7(5)	-10(4)	-3(4)
C(31)	41(3)	39(3)	32(3)	-1(3)	-6(3)	-9(3)
C(32)	52(4)	61(4)	39(4)	-11(3)	-8(3)	-18(3)
C(33)	67(5)	57(4)	39(4)	-11(3)	-8(3)	-9(4)
C(34)	68(5)	66(5)	47(4)	-10(4)	7(4)	-7(4)
C(35)	44(5)	128(8)	68(5)	-26(5)	3(4)	-26(5)
C(36)	46(4)	111(7)	49(4)	-18(4)	-13(3)	-17(4)
C(41)	38(3)	45(4)	28(3)	-6(3)	-8(3)	-14(3)
C(42)	51(4)	63(5)	48(4)	3(3)	-19(3)	-28(3)
C(43)	41(4)	90(6)	68(5)	7(4)	-20(4)	-31(4)
C(44)	42(4)	88(6)	67(5)	-8(4)	-26(4)	1(4)
C(45)	63(5)	60(5)	60(5)	7(4)	-31(4)	-9(4)
C(46)	39(4)	54(4)	45(4)	3(3)	-14(3)	-14(3)

Supplementary Material for Chemical Communications

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

	x	y	z	U(eq)
H(4)	3651	5284	4007	51
H(7A)	2507	8484	2092	103
H(7B)	2493	8263	917	103
H(7C)	3899	8580	1111	103
H(11)	4425	4767	933	48
H(12)	6379	5948	526	61
H(13)	8543	4933	157	64
H(18)	9102	-771	1766	77
H(19)	7011	-1594	2563	69
H(20)	4838	-451	2781	54
H(21)	10119	2967	309	74
H(22)	10350	1020	847	81
H(32)	3609	3828	5945	60
H(33)	1793	3975	7562	67
H(34)	-464	3528	7666	79
H(35)	-866	2836	6181	99
H(36)	950	2690	4538	81
H(42)	6662	4006	3382	62
H(43)	8822	3196	3676	77
H(44)	8928	1362	4575	77
H(45)	6926	338	5132	70
H(46)	4809	1151	4852	54