Supporting Information (28 pages) For

Seven Coordinate $[\text{Re}^{\text{V}}\text{ON}_4\text{X}_2]^+$ Complexes (X = O and Cl)

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Supporting Information

The ^1H - ^1H COSY spectrum of $[\text{ReO}(\text{L1})]\text{PF}_6$ in acetone- d_6 .

Table Crystal data, data collection, and solution and refinement for

Crystal Data

Empirical formula

 $C_{16}H_{26}Cl_3N_4O_3Re$ $[ReO(H_2Pmu)Cl_2]$ $\cdot 2CH_3OH$

Crystal color, Habit

light brown plate

Crystal size

0.19 x 0.14 x 0.09 mm

Crystal system

Monoclinic

Space group

 $P2_1/n$ $a = 7.3495(4) \text{ \AA} \quad \alpha = 90^\circ$ $b = 13.7679(8) \text{ \AA} \quad \beta = 90.227(1)^\circ$ $c = 20.492(2) \text{ \AA} \quad \gamma = 90^\circ$

Volume

 $2073.5(2) \text{ \AA}^3$

Z

4

Formula weight

614.96

Density (calculated)

 1.970 Mg/m^3

Absorption coefficient

 6.272 mm^{-1}

F(000)

1200

Data Collection

Diffractometer

Bruker SMART Platform CCD

Wavelength

 $0.71073 \text{ \AA}$

Temperature

 $173(2) \text{ K}$ θ range for data collection $1.78 \text{ to } 27.49^\circ$

Index ranges

 $-9 \leq h \leq 9, -17 \leq k \leq 17, -26 \leq l \leq 26$

Reflections collected

20365

Independent reflections

4736 ($R_{\text{int}} = 0.0422$)Completeness to $\theta = 27.49^\circ$

99.5 %

Solution and Refinement

System used

SHELXTL-V5.4

Solution

Direct methods

Refinement method

Full-matrix least-squares on F^2

Weighting scheme

 $w = [\sigma^2(F_o^2) + (AP)^2 + (BP)]^{-1}$, where $P = (F_o^2 + 2F_c^2)/3$, $A = 0.0272$, and $B = 0$

Absorption correction

Semi-empirical from equivalents,

SADABS, R. Blessing (1995)

Max. and min. transmission

1.000000 and 0.724814

Data / restraints / parameters

4736 / 0 / 248

R indices ($I > 2\sigma(I)$) = 3876) $R1 = 0.0253, wR2 = 0.0549$

R indices (all data)

 $R1 = 0.0342, wR2 = 0.0571$ Goodness-of-fit on F^2

0.988

Largest diff. peak and hole

1.405 and $-0.557 \text{ e\AA}^{-3}$

Table . Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Re(1)	8522.7(2)	3064.9(1)	5820.57(7)	17.71(5)	1
Cl(1)	11121(1)	3820.1(7)	6273.4(5)	26.1(2)	1
Cl(2)	5833(1)	2149.1(7)	5704.4(5)	29.1(2)	1
O(1)	8801(4)	3411(2)	5040(1)	24(1)	1
N(1)	9208(4)	1888(2)	6587(2)	23(1)	1
N(2)	7307(4)	3477(2)	6808(2)	23(1)	1
N(3)	10159(4)	1840(2)	5398(2)	23(1)	1
N(4)	7088(4)	4512(2)	5795(2)	19(1)	1
C(1)	8944(6)	2176(3)	7277(2)	27(1)	1
C(2)	7169(6)	2695(3)	7302(2)	26(1)	1
C(3)	10984(6)	1434(3)	6486(2)	29(1)	1
C(4)	11195(5)	1262(3)	5780(2)	23(1)	1
C(5)	12352(5)	555(3)	5522(2)	30(1)	1
C(6)	12445(5)	447(3)	4860(2)	33(1)	1
C(7)	11355(6)	1018(3)	4467(2)	33(1)	1
C(8)	10233(6)	1695(3)	4752(2)	31(1)	1
C(9)	5588(5)	3999(3)	6753(2)	25(1)	1
C(10)	5834(5)	4750(3)	6246(2)	21(1)	1
C(11)	4919(5)	5632(3)	6235(2)	24(1)	1
C(12)	5285(5)	6295(3)	5751(2)	28(1)	1
C(13)	6560(5)	6058(3)	5287(2)	27(1)	1
C(14)	7419(5)	5170(3)	5320(2)	22(1)	1
Cl(3)	16706(2)	9987.8(8)	7000.5(5)	33.6(2)	1
O(2)	11245(4)	6172(2)	7196(1)	37(1)	1
C(15)	10338(6)	6326(3)	6592(2)	38(1)	1
O(3)	13843(5)	8486(3)	6443(2)	56(1)	1
C(16)	12455(6)	8686(4)	6898(2)	43(1)	1

Table Bond lengths [Å] and angles [°] for

Re(1)-O(1)	1.682(3)	Re(1)-N(3)	2.247(3)
Re(1)-N(4)	2.254(3)	Re(1)-N(2)	2.286(3)
Re(1)-N(1)	2.310(3)	Re(1)-Cl(2)	2.3557(10)
Re(1)-Cl(1)	2.3609(10)	N(1)-C(3)	1.463(5)
N(1)-C(1)	1.481(5)	N(2)-C(9)	1.458(5)
N(2)-C(2)	1.482(5)	N(3)-C(8)	1.340(5)
N(3)-C(4)	1.350(5)	N(4)-C(10)	1.347(5)
N(4)-C(14)	1.354(5)	C(1)-C(2)	1.489(6)
C(3)-C(4)	1.475(6)	C(4)-C(5)	1.398(5)
C(5)-C(6)	1.367(6)	C(6)-C(7)	1.378(6)
C(7)-C(8)	1.376(6)	C(9)-C(10)	1.478(5)
C(10)-C(11)	1.388(5)	C(11)-C(12)	1.375(6)
C(12)-C(13)	1.377(6)	C(13)-C(14)	1.378(5)
O(2)-C(15)	1.419(5)	O(3)-C(16)	1.412(6)
O(1)-Re(1)-N(3)	77.23(12)	O(1)-Re(1)-N(4)	77.65(12)
N(3)-Re(1)-N(4)	154.86(12)	O(1)-Re(1)-N(2)	145.11(12)
N(3)-Re(1)-N(2)	137.66(12)	N(4)-Re(1)-N(2)	67.46(11)
O(1)-Re(1)-N(1)	144.90(12)	N(3)-Re(1)-N(1)	67.70(12)
N(4)-Re(1)-N(1)	137.37(11)	N(2)-Re(1)-N(1)	69.96(11)
O(1)-Re(1)-Cl(2)	99.26(10)	N(3)-Re(1)-Cl(2)	90.54(8)
N(4)-Re(1)-Cl(2)	94.49(8)	N(2)-Re(1)-Cl(2)	83.76(9)
N(1)-Re(1)-Cl(2)	82.76(9)	O(1)-Re(1)-Cl(1)	98.48(10)
N(3)-Re(1)-Cl(1)	92.81(8)	N(4)-Re(1)-Cl(1)	89.85(8)
N(2)-Re(1)-Cl(1)	82.03(9)	N(1)-Re(1)-Cl(1)	82.41(9)
Cl(2)-Re(1)-Cl(1)	162.25(4)	C(3)-N(1)-C(1)	111.7(3)
C(3)-N(1)-Re(1)	113.3(2)	C(1)-N(1)-Re(1)	115.6(2)
C(9)-N(2)-C(2)	110.4(3)	C(9)-N(2)-Re(1)	113.3(2)
C(2)-N(2)-Re(1)	117.0(2)	C(8)-N(3)-C(4)	117.4(3)
C(8)-N(3)-Re(1)	121.1(3)	C(4)-N(3)-Re(1)	121.3(3)
C(10)-N(4)-C(14)	117.1(3)	C(10)-N(4)-Re(1)	121.4(2)
C(14)-N(4)-Re(1)	121.5(2)	N(1)-C(1)-C(2)	106.3(3)
N(2)-C(2)-C(1)	105.2(3)	N(1)-C(3)-C(4)	107.8(3)
N(3)-C(4)-C(5)	122.2(4)	N(3)-C(4)-C(3)	114.4(3)
C(5)-C(4)-C(3)	123.4(4)	C(6)-C(5)-C(4)	119.0(4)
C(5)-C(6)-C(7)	119.1(4)	C(8)-C(7)-C(6)	119.2(4)
N(3)-C(8)-C(7)	123.1(4)	N(2)-C(9)-C(10)	106.9(3)
N(4)-C(10)-C(11)	122.4(4)	N(4)-C(10)-C(9)	113.4(3)
C(11)-C(10)-C(9)	124.3(4)	C(12)-C(11)-C(10)	119.7(4)
C(11)-C(12)-C(13)	118.5(4)	C(12)-C(13)-C(14)	119.3(4)
N(4)-C(14)-C(13)	123.1(4)		

Symmetry transformations used to generate equivalent atoms:

Table . Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for
 anisotropic displacement factor exponent takes the form: $-2\pi^2 [$
 $(ha)^2 U_{11} + \dots + 2hka b U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	19.2(1)	15.7(1)	18.2(1)	0.3(1)	-0.2(1)	-0.2(1)
Cl(1)	21.5(5)	26.5(5)	30.1(6)	-1.4(4)	-1.5(4)	-5.5(4)
Cl(2)	25.3(5)	23.5(5)	38.3(6)	1.3(4)	-6.7(4)	-4.5(4)
O(1)	29(2)	21(1)	23(2)	-1(1)	3(1)	4(1)
N(1)	27(2)	19(2)	22(2)	2(1)	-3(1)	1(2)
N(2)	25(2)	20(2)	23(2)	2(1)	4(1)	0(1)
N(3)	24(2)	20(2)	25(2)	-4(1)	0(1)	0(1)
N(4)	16(2)	19(2)	22(2)	-1(1)	-2(1)	-2(1)
C(1)	39(2)	24(2)	19(2)	7(2)	-4(2)	-1(2)
C(2)	35(2)	24(2)	20(2)	5(2)	3(2)	-4(2)
C(3)	30(2)	23(2)	34(3)	2(2)	-4(2)	6(2)
C(4)	18(2)	18(2)	34(2)	3(2)	-2(2)	-5(2)
C(5)	23(2)	22(2)	47(3)	3(2)	-1(2)	3(2)
C(6)	20(2)	27(2)	51(3)	-6(2)	4(2)	2(2)
C(7)	40(3)	30(2)	30(2)	-9(2)	6(2)	3(2)
C(8)	34(2)	30(2)	29(2)	-3(2)	-4(2)	4(2)
C(9)	21(2)	32(2)	21(2)	2(2)	1(2)	2(2)
C(10)	17(2)	26(2)	22(2)	-4(2)	-2(2)	-3(2)
C(11)	20(2)	29(2)	24(2)	-6(2)	0(2)	6(2)
C(12)	29(2)	22(2)	33(2)	-3(2)	-8(2)	8(2)
C(13)	29(2)	21(2)	30(2)	2(2)	-3(2)	-1(2)
C(14)	20(2)	19(2)	26(2)	1(2)	1(2)	-1(2)
Cl(3)	44.7(6)	24.1(5)	32.0(6)	1.3(4)	7.0(5)	-1.9(5)
O(2)	40(2)	40(2)	30(2)	4(2)	-1(1)	-3(2)
C(15)	46(3)	34(3)	34(3)	-2(2)	-2(2)	8(2)
O(3)	57(2)	58(3)	51(2)	-11(2)	7(2)	-4(2)
C(16)	38(3)	42(3)	49(3)	4(2)	-3(2)	0(2)

Table Torsion angles [°] for

O(1)-Re(1)-N(1)-C(3)	31.7(4)	N(3)-Re(1)-N(1)-C(3)	34.0(3)
N(4)-Re(1)-N(1)-C(3)	-143.7(2)	N(2)-Re(1)-N(1)-C(3)	-146.5(3)
Cl(2)-Re(1)-N(1)-C(3)	127.6(3)	Cl(1)-Re(1)-N(1)-C(3)	-62.2(3)
O(1)-Re(1)-N(1)-C(1)	162.5(3)	N(3)-Re(1)-N(1)-C(1)	164.8(3)
N(4)-Re(1)-N(1)-C(1)	-12.9(3)	N(2)-Re(1)-N(1)-C(1)	-15.7(3)
Cl(2)-Re(1)-N(1)-C(1)	-101.7(3)	Cl(1)-Re(1)-N(1)-C(1)	68.5(3)
O(1)-Re(1)-N(2)-C(9)	35.2(4)	N(3)-Re(1)-N(2)-C(9)	-146.0(2)
N(4)-Re(1)-N(2)-C(9)	35.4(2)	N(1)-Re(1)-N(2)-C(9)	-146.6(3)
Cl(2)-Re(1)-N(2)-C(9)	-62.1(3)	Cl(1)-Re(1)-N(2)-C(9)	128.6(3)
O(1)-Re(1)-N(2)-C(2)	165.4(3)	N(3)-Re(1)-N(2)-C(2)	-15.8(4)
N(4)-Re(1)-N(2)-C(2)	165.7(3)	N(1)-Re(1)-N(2)-C(2)	-16.4(3)
Cl(2)-Re(1)-N(2)-C(2)	68.2(3)	Cl(1)-Re(1)-N(2)-C(2)	-101.2(3)
O(1)-Re(1)-N(3)-C(8)	-19.3(3)	N(4)-Re(1)-N(3)-C(8)	-21.7(5)
N(2)-Re(1)-N(3)-C(8)	161.4(3)	N(1)-Re(1)-N(3)-C(8)	162.1(3)
Cl(2)-Re(1)-N(3)-C(8)	80.1(3)	Cl(1)-Re(1)-N(3)-C(8)	-117.3(3)
O(1)-Re(1)-N(3)-C(4)	156.4(3)	N(4)-Re(1)-N(3)-C(4)	154.0(3)
N(2)-Re(1)-N(3)-C(4)	-22.9(4)	N(1)-Re(1)-N(3)-C(4)	-22.2(3)
Cl(2)-Re(1)-N(3)-C(4)	-104.2(3)	Cl(1)-Re(1)-N(3)-C(4)	58.4(3)
O(1)-Re(1)-N(4)-C(10)	159.2(3)	N(3)-Re(1)-N(4)-C(10)	161.6(3)
N(2)-Re(1)-N(4)-C(10)	-20.7(3)	N(1)-Re(1)-N(4)-C(10)	-23.5(3)
Cl(2)-Re(1)-N(4)-C(10)	60.7(3)	Cl(1)-Re(1)-N(4)-C(10)	-102.1(3)
O(1)-Re(1)-N(4)-C(14)	-19.4(3)	N(3)-Re(1)-N(4)-C(14)	-17.0(4)
N(2)-Re(1)-N(4)-C(14)	160.7(3)	N(1)-Re(1)-N(4)-C(14)	157.9(3)
Cl(2)-Re(1)-N(4)-C(14)	-117.9(3)	Cl(1)-Re(1)-N(4)-C(14)	79.3(3)
C(3)-N(1)-C(1)-C(2)	175.6(3)	Re(1)-N(1)-C(1)-C(2)	44.0(4)
C(9)-N(2)-C(2)-C(1)	176.0(3)	Re(1)-N(2)-C(2)-C(1)	44.4(4)
N(1)-C(1)-C(2)-N(2)	-54.2(4)	C(1)-N(1)-C(3)-C(4)	-174.5(3)
Re(1)-N(1)-C(3)-C(4)	-41.8(4)	C(8)-N(3)-C(4)-C(5)	1.9(5)
Re(1)-N(3)-C(4)-C(5)	-173.9(3)	C(8)-N(3)-C(4)-C(3)	-177.4(4)
Re(1)-N(3)-C(4)-C(3)	6.7(4)	N(1)-C(3)-C(4)-N(3)	23.1(5)
N(1)-C(3)-C(4)-C(5)	-156.2(4)	N(3)-C(4)-C(5)-C(6)	0.3(6)
C(3)-C(4)-C(5)-C(6)	179.6(4)	C(4)-C(5)-C(6)-C(7)	-2.0(6)
C(5)-C(6)-C(7)-C(8)	1.5(6)	C(4)-N(3)-C(8)-C(7)	-2.5(6)
Re(1)-N(3)-C(8)-C(7)	173.3(3)	C(6)-C(7)-C(8)-N(3)	0.9(7)
C(2)-N(2)-C(9)-C(10)	-179.2(3)	Re(1)-N(2)-C(9)-C(10)	-45.7(4)
C(14)-N(4)-C(10)-C(11)	-0.6(5)	Re(1)-N(4)-C(10)-C(11)	-179.2(3)
C(14)-N(4)-C(10)-C(9)	-178.8(3)	Re(1)-N(4)-C(10)-C(9)	2.6(4)
N(2)-C(9)-C(10)-N(4)	27.6(4)	N(2)-C(9)-C(10)-C(11)	-150.6(4)
N(4)-C(10)-C(11)-C(12)	0.1(6)	C(9)-C(10)-C(11)-C(12)	178.1(4)
C(10)-C(11)-C(12)-C(13)	0.1(6)	C(11)-C(12)-C(13)-C(14)	0.2(6)
C(10)-N(4)-C(14)-C(13)	0.9(5)	Re(1)-N(4)-C(14)-C(13)	179.6(3)
C(12)-C(13)-C(14)-N(4)	-0.7(6)		

Symmetry transformations used to generate equivalent atoms:

Table Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for

	x	y	z	U(eq)	SOF
H(1N)	8366	1396	6514	27	1
H(2N)	8118	3923	6985	27	1
H(1A)	9943	2608	7423	33	1
H(1B)	8922	1596	7562	33	1
H(2A)	6154	2249	7196	31	1
H(2B)	6965	2972	7742	31	1
H(3A)	11054	811	6727	35	1
H(3B)	11965	1865	6647	35	1
H(5)	13062	155	5802	36	1
H(6)	13250	-14	4672	39	1
H(7)	11378	944	4007	40	1
H(8)	9475	2077	4477	37	1
H(9A)	5273	4304	7175	30	1
H(9B)	4596	3549	6627	30	1
H(11)	4043	5777	6560	29	1
H(12)	4673	6902	5737	34	1
H(13)	6843	6502	4947	32	1
H(14)	8285	5012	4993	26	1
H(2O)	10572	5848	7445	55	1
H(15A)	9022	6265	6655	57	1
H(15B)	10746	5841	6275	57	1
H(15C)	10620	6978	6430	57	1
H(3O)	14657	8912	6472	83	1
H(16A)	12891	9169	7214	64	1
H(16B)	12128	8087	7128	64	1
H(16C)	11385	8941	6669	64	1

Table Hydrogen bonds for [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1N)...Cl(3)#1	0.93	2.50	3.310(3)	145.8
N(2)-H(2N)...Cl(3)#2	0.93	2.55	3.287(4)	136.9
O(2)-H(2O)...Cl(3)#2	0.84	2.35	3.178(3)	169.9
O(3)-H(3O)...Cl(3)	0.84	2.37	3.161(4)	156.9

Symmetry transformations used to generate equivalent atoms:

#1 $x-1, y-1, z$ #2 $-x+5/2, y-1/2, -z+3/2$

Table Crystal data, data collection, and solution and refinement for

Crystal Data	
Empirical formula	$C_{38}H_{48}N_8O_{20}Re_4$
Crystal Habit, color	Needle, Light green
Crystal size	0.32 x 0.04 x 0.02 mm
Crystal system	Orthorhombic
Space group	$Pca2_1$
	$a = 23.0314(11) \text{ \AA} \quad \alpha = 90^\circ$
	$b = 8.7674(4) \text{ \AA} \quad \beta = 90^\circ$
	$c = 23.1256(11) \text{ \AA} \quad \gamma = 90^\circ$
Volume	$4669.6(4) \text{ \AA}^3$
Z	4
Formula weight	1681.64
Density (calculated)	2.392 Mg/m^3
Absorption coefficient	10.423 mm^{-1}
F(000)	3168
Data Collection	
Diffractometer	Siemens SMART Platform CCD
Wavelength	$0.71073 \text{ \AA}$
Temperature	$173(2) \text{ K}$
θ range for data collection	1.76 to 25.05°
Index ranges	$0 \leq h \leq 27, 0 \leq k \leq 10, -27 \leq l \leq 27$
Reflections collected	26470
Independent reflections	8232 ($R_{\text{int}} = 0.0393$)
Completeness to $\theta = 25.05^\circ$	99.9 %
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2) + (AP)^2 + (BP)]^{-1}$, where $P = (F_o^2 + 2F_c^2)/3$, $A = 0.034$, and $B = 0.14$
Absorption correction	Analytical
Max. and min. transmission	0.814 and 0.416
Absolute structure parameter	0.270(9)
Data / restraints / parameters	8232 / 837 / 667
R indices ($I > 2\sigma(I)$) = 7279)	$R1 = 0.0304, wR2 = 0.0654$
R indices (all data)	$R1 = 0.0383, wR2 = 0.0679$
Goodness-of-fit on F^2	1.052
Largest diff. peak and hole	2.522 and $-1.017 \text{ e\AA}^{-3}$

Table Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for . U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Re(1)	7826.4(2)	557.2(4)	698.0(2)	15.74(8)	1
O(5)	8306(2)	565(5)	1250(2)	19(1)	1
O(1)	8156(2)	2131(5)	155(2)	22(1)	1
C(4)	8391(3)	1764(7)	-349(3)	24(2)	1
O(2)	8705(3)	2592(7)	-623(2)	32(2)	1
C(3)	8224(3)	166(7)	-550(3)	22(2)	1
N(1)	7680(2)	-291(5)	-241(2)	20(1)	1
O(3)	7254(2)	-1034(5)	967(2)	24(1)	1
C(12)	6716(3)	-685(7)	1124(4)	24(2)	1
O(4)	6410(2)	-1525(6)	1403(3)	32(2)	1
C(11)	6531(3)	908(7)	931(3)	22(2)	1
N(2)	6904(2)	1346(5)	427(2)	20(1)	1
N(3)	8275(2)	-1659(5)	537(2)	19(1)	1
C(10)	8703(3)	-2147(7)	886(3)	23(2)	1
C(9)	8937(3)	-3583(7)	844(3)	26(2)	1
C(8)	8731(3)	-4586(7)	428(3)	26(2)	1
C(7)	8290(3)	-4084(7)	73(3)	25(2)	1
C(6)	8079(3)	-2608(6)	128(3)	21(1)	1
C(5)	7620(3)	-1962(6)	-255(3)	21(2)	1
N(4)	7590(2)	2771(5)	1108(2)	20(1)	1
C(18)	7881(3)	3291(7)	1571(3)	20(2)	1
C(17)	7809(4)	4740(7)	1781(3)	21(2)	1
C(16)	7433(3)	5736(7)	1503(3)	22(2)	1
C(15)	7123(4)	5185(7)	1037(3)	25(2)	1
C(14)	7206(3)	3698(6)	851(3)	22(1)	1
C(13)	6890(3)	3015(6)	352(3)	22(2)	1
C(1)	7177(3)	453(8)	-524(2)	22(2)	1
C(2)	6691(2)	559(8)	-100(2)	21(2)	1
Re(2)	9905.4(2)	4505.5(4)	2687.8(2)	15.8(1)	1
O(10)	9437(2)	4509(5)	2127(2)	23(1)	1
O(6)	9559(2)	2926(5)	3216(2)	21(1)	1
C(22)	9312(3)	3295(7)	3715(3)	23(2)	1
O(7)	8991(3)	2447(6)	3973(3)	33(2)	1
C(21)	9482(3)	4878(7)	3928(3)	21(2)	1
N(5)	10031(2)	5342(5)	3631(2)	18(1)	1
O(8)	10486(2)	6097(5)	2434(2)	20(1)	1
C(30)	11021(2)	5726(7)	2274(3)	21(2)	1
O(9)	11330(2)	6542(6)	1988(3)	32(2)	1
C(29)	11210(3)	4157(7)	2489(3)	19(2)	1
N(6)	10820(2)	3710(5)	2980(2)	17(1)	1
N(7)	9452(2)	6718(5)	2845(2)	19(1)	1
C(28)	9030(3)	7202(7)	2488(3)	23(2)	1
C(27)	8788(3)	8629(7)	2530(3)	26(2)	1
C(26)	8979(3)	9621(7)	2957(3)	26(2)	1
C(25)	9408(3)	9113(7)	3326(3)	24(2)	1
C(24)	9633(3)	7656(6)	3262(3)	21(1)	1
C(23)	10088(3)	7015(6)	3652(3)	20(2)	1
N(8)	10146(2)	2289(5)	2283(2)	20(1)	1
C(36)	9850(3)	1762(7)	1824(3)	22(2)	1
C(35)	9903(4)	290(7)	1630(3)	23(2)	1
C(34)	10292(4)	-686(7)	1902(3)	23(2)	1
C(33)	10601(3)	-127(7)	2367(3)	22(2)	1
C(32)	10523(3)	1362(6)	2549(3)	19(1)	1
C(31)	10837(3)	2038(5)	3050(3)	18(2)	1

C(19)	10529(3)	4606(8)	3928(2)	21(2)	1
C(20)	11024(2)	4469(7)	3516(2)	18(2)	1
Re(3)	9919(1)	-229(1)	-40(1)	24.0(1)	1
O(11)	10445(2)	1092(6)	-185(3)	35(2)	1
O(12)	9644(3)	-929(7)	-674(2)	43(2)	1
O(13)	10218(3)	-1678(6)	358(3)	42(2)	1
O(14)	9370(2)	604(7)	342(2)	38(2)	1
O(19)	10860(7)	4039(18)	293(5)	150(7)	1
C(37)	10459(7)	4300(17)	753(6)	68(4)	1
Re(4)	7801(3)	5110(8)	3557(3)	33(1)	0.50
O(15)	7378(7)	3520(15)	3647(8)	96(7)	0.50
O(16)	7370(9)	6588(14)	3336(10)	48(3)	0.50
O(17)	8125(7)	5540(20)	4200(5)	104(8)	0.50
O(18)	8319(7)	4760(30)	3044(7)	46(3)	0.50
Re(4')	7722(3)	4979(7)	3462(2)	24(1)	0.50
O(15')	7245(6)	3655(15)	3197(6)	57(5)	0.50
O(16')	7454(10)	6763(11)	3321(9)	48(3)	0.50
O(17')	7788(7)	4730(20)	4193(3)	58(5)	0.50
O(18')	8384(5)	4770(30)	3139(7)	46(3)	0.50
O(20)	6873(4)	785(11)	3048(3)	71(3)	1
C(38)	7246(7)	370(18)	2614(7)	86(5)	1

Table Bond lengths [Å] and angles [°] for

Re(1)-O(5)	1.689(4)	Re(1)-O(1)	2.014(3)
Re(1)-O(3)	2.017(4)	Re(1)-N(4)	2.228(4)
Re(1)-N(3)	2.232(4)	Re(1)-N(2)	2.320(4)
Re(1)-N(1)	2.320(4)	O(1)-C(4)	1.325(5)
C(4)-O(2)	1.205(5)	C(4)-C(3)	1.525(6)
C(3)-N(1)	1.496(6)	N(1)-C(5)	1.472(5)
N(1)-C(1)	1.483(5)	O(3)-C(12)	1.328(5)
C(12)-O(4)	1.205(5)	C(12)-C(11)	1.527(6)
C(11)-N(2)	1.498(5)	N(2)-C(13)	1.474(5)
N(2)-C(2)	1.484(5)	N(3)-C(6)	1.338(5)
N(3)-C(10)	1.344(6)	C(10)-C(9)	1.373(6)
C(9)-C(8)	1.387(6)	C(8)-C(7)	1.379(6)
C(7)-C(6)	1.388(6)	C(6)-C(5)	1.491(6)
N(4)-C(14)	1.339(5)	N(4)-C(18)	1.343(6)
C(18)-C(17)	1.371(6)	C(17)-C(16)	1.388(6)
C(16)-C(15)	1.379(6)	C(15)-C(14)	1.386(6)
C(14)-C(13)	1.491(6)	C(1)-C(2)	1.491(8)
Re(2)-O(10)	1.687(4)	Re(2)-O(6)	2.012(3)
Re(2)-O(8)	2.020(4)	Re(2)-N(8)	2.227(4)
Re(2)-N(7)	2.232(4)	Re(2)-N(5)	2.319(4)
Re(2)-N(6)	2.320(4)	O(6)-C(22)	1.327(5)
C(22)-O(7)	1.206(5)	C(22)-C(21)	1.524(6)
C(21)-N(5)	1.497(6)	N(5)-C(23)	1.474(5)
N(5)-C(19)	1.484(5)	O(8)-C(30)	1.327(5)
C(30)-O(9)	1.206(5)	C(30)-C(29)	1.526(6)
C(29)-N(6)	1.499(5)	N(6)-C(31)	1.475(5)
N(6)-C(20)	1.484(5)	N(7)-C(24)	1.335(5)
N(7)-C(28)	1.345(6)	C(28)-C(27)	1.372(6)
C(27)-C(26)	1.388(6)	C(26)-C(25)	1.380(6)
C(25)-C(24)	1.386(6)	C(24)-C(23)	1.493(6)
N(8)-C(32)	1.338(6)	N(8)-C(36)	1.344(6)
C(36)-C(35)	1.372(6)	C(35)-C(34)	1.389(6)
C(34)-C(33)	1.379(6)	C(33)-C(32)	1.383(6)
C(32)-C(31)	1.490(6)	C(19)-C(20)	1.490(8)
Re(3)-O(14)	1.708(4)	Re(3)-O(11)	1.708(4)
Re(3)-O(12)	1.711(4)	Re(3)-O(13)	1.713(4)
O(19)-C(37)	1.426(17)	Re(4)-O(18)	1.708(4)
Re(4)-O(17)	1.708(4)	Re(4)-O(16)	1.711(4)
Re(4)-O(15)	1.714(4)	Re(4')-O(18')	1.707(4)
Re(4')-O(17')	1.710(4)	Re(4')-O(15')	1.712(4)
Re(4')-O(16')	1.712(4)	O(20)-C(38)	1.370(16)

O(5)-Re(1)-O(1)	102.8(2)	O(5)-Re(1)-O(3)	101.3(2)
O(1)-Re(1)-O(3)	155.9(2)	O(5)-Re(1)-N(4)	80.49(17)
O(1)-Re(1)-N(4)	76.13(18)	O(3)-Re(1)-N(4)	108.15(19)
O(5)-Re(1)-N(3)	80.05(17)	O(1)-Re(1)-N(3)	108.49(18)
O(3)-Re(1)-N(3)	75.66(18)	N(4)-Re(1)-N(3)	160.53(19)
O(5)-Re(1)-N(2)	143.32(19)	O(1)-Re(1)-N(2)	88.44(17)
O(3)-Re(1)-N(2)	72.06(16)	N(4)-Re(1)-N(2)	68.35(15)
N(3)-Re(1)-N(2)	129.68(16)	O(5)-Re(1)-N(1)	143.52(18)
O(1)-Re(1)-N(1)	72.00(15)	O(3)-Re(1)-N(1)	88.44(17)
N(4)-Re(1)-N(1)	129.94(16)	N(3)-Re(1)-N(1)	68.38(15)
N(2)-Re(1)-N(1)	73.15(18)	C(4)-O(1)-Re(1)	122.4(3)
O(2)-C(4)-O(1)	124.1(5)	O(2)-C(4)-C(3)	123.0(5)
O(1)-C(4)-C(3)	112.9(4)	N(1)-C(3)-C(4)	108.2(4)
C(5)-N(1)-C(1)	110.8(4)	C(5)-N(1)-C(3)	109.6(4)
C(1)-N(1)-C(3)	109.0(4)	C(5)-N(1)-Re(1)	110.7(3)
C(1)-N(1)-Re(1)	112.7(3)	C(3)-N(1)-Re(1)	103.9(3)
C(12)-O(3)-Re(1)	122.3(4)	O(4)-C(12)-O(3)	123.4(5)

O(4)-C(12)-C(11)	123.6(5)	O(3)-C(12)-C(11)	113.0(4)
N(2)-C(11)-C(12)	107.6(4)	C(13)-N(2)-C(2)	111.0(4)
C(13)-N(2)-C(11)	109.5(4)	C(2)-N(2)-C(11)	109.2(4)
C(13)-N(2)-Re(1)	110.4(3)	C(2)-N(2)-Re(1)	112.7(3)
C(11)-N(2)-Re(1)	103.8(3)	C(6)-N(3)-C(10)	118.3(4)
C(6)-N(3)-Re(1)	120.2(3)	C(10)-N(3)-Re(1)	121.1(3)
N(3)-C(10)-C(9)	122.5(5)	C(10)-C(9)-C(8)	119.7(5)
C(7)-C(8)-C(9)	117.6(5)	C(8)-C(7)-C(6)	120.0(5)
N(3)-C(6)-C(7)	121.8(5)	N(3)-C(6)-C(5)	115.0(4)
C(7)-C(6)-C(5)	123.2(5)	N(1)-C(5)-C(6)	107.3(4)
C(14)-N(4)-C(18)	118.5(4)	C(14)-N(4)-Re(1)	120.1(3)
C(18)-N(4)-Re(1)	120.8(4)	N(4)-C(18)-C(17)	122.5(5)
C(18)-C(17)-C(16)	119.6(5)	C(15)-C(16)-C(17)	117.7(5)
C(16)-C(15)-C(14)	120.1(5)	N(4)-C(14)-C(15)	121.6(5)
N(4)-C(14)-C(13)	114.9(4)	C(15)-C(14)-C(13)	123.5(5)
N(2)-C(13)-C(14)	107.2(4)	N(1)-C(1)-C(2)	108.9(4)
N(2)-C(2)-C(1)	108.7(4)	O(10)-Re(2)-O(6)	102.4(2)
O(10)-Re(2)-O(8)	101.43(19)	O(6)-Re(2)-O(8)	156.1(2)
O(10)-Re(2)-N(8)	80.67(17)	O(6)-Re(2)-N(8)	75.73(18)
O(8)-Re(2)-N(8)	108.38(18)	O(10)-Re(2)-N(7)	79.89(17)
O(6)-Re(2)-N(7)	108.29(18)	O(8)-Re(2)-N(7)	75.93(17)
N(8)-Re(2)-N(7)	160.55(19)	O(10)-Re(2)-N(5)	143.36(18)
O(6)-Re(2)-N(5)	72.28(15)	O(8)-Re(2)-N(5)	88.42(17)
N(8)-Re(2)-N(5)	129.79(16)	N(7)-Re(2)-N(5)	68.33(15)
O(10)-Re(2)-N(6)	143.62(18)	O(6)-Re(2)-N(6)	88.61(17)
O(8)-Re(2)-N(6)	72.01(15)	N(8)-Re(2)-N(6)	68.51(15)
N(7)-Re(2)-N(6)	129.69(16)	N(5)-Re(2)-N(6)	73.00(17)
C(22)-O(6)-Re(2)	122.1(3)	O(7)-C(22)-O(6)	122.9(5)
O(7)-C(22)-C(21)	123.9(5)	O(6)-C(22)-C(21)	113.2(4)
N(5)-C(21)-C(22)	108.4(4)	C(23)-N(5)-C(19)	110.4(4)
C(23)-N(5)-C(21)	109.3(4)	C(19)-N(5)-C(21)	108.8(4)
C(23)-N(5)-Re(2)	110.9(3)	C(19)-N(5)-Re(2)	113.2(3)
C(21)-N(5)-Re(2)	103.9(3)	C(30)-O(8)-Re(2)	121.8(4)
O(9)-C(30)-O(8)	123.7(5)	O(9)-C(30)-C(29)	123.1(5)
O(8)-C(30)-C(29)	113.2(4)	N(6)-C(29)-C(30)	108.2(4)
C(31)-N(6)-C(20)	110.2(4)	C(31)-N(6)-C(29)	109.1(4)
C(20)-N(6)-C(29)	109.1(4)	C(31)-N(6)-Re(2)	110.8(3)
C(20)-N(6)-Re(2)	113.3(3)	C(29)-N(6)-Re(2)	104.1(3)
C(24)-N(7)-C(28)	118.3(4)	C(24)-N(7)-Re(2)	120.5(3)
C(28)-N(7)-Re(2)	120.9(3)	N(7)-C(28)-C(27)	122.5(5)
C(28)-C(27)-C(26)	119.6(5)	C(25)-C(26)-C(27)	117.7(5)
C(26)-C(25)-C(24)	119.9(5)	N(7)-C(24)-C(25)	122.0(5)
N(7)-C(24)-C(23)	115.1(4)	C(25)-C(24)-C(23)	123.0(5)
N(5)-C(23)-C(24)	107.0(4)	C(32)-N(8)-C(36)	118.9(4)
C(32)-N(8)-Re(2)	119.9(3)	C(36)-N(8)-Re(2)	120.3(4)
N(8)-C(36)-C(35)	122.4(5)	C(36)-C(35)-C(34)	119.3(5)
C(33)-C(34)-C(35)	117.8(5)	C(34)-C(33)-C(32)	120.3(5)
N(8)-C(32)-C(33)	121.2(5)	N(8)-C(32)-C(31)	115.5(4)
C(33)-C(32)-C(31)	123.3(5)	N(6)-C(31)-C(32)	107.2(4)
N(5)-C(19)-C(20)	109.3(4)	N(6)-C(20)-C(19)	109.1(4)
O(14)-Re(3)-O(11)	109.7(3)	O(14)-Re(3)-O(12)	108.8(3)
O(11)-Re(3)-O(12)	109.8(3)	O(14)-Re(3)-O(13)	109.6(3)
O(11)-Re(3)-O(13)	108.9(3)	O(12)-Re(3)-O(13)	110.1(3)
O(18)-Re(4)-O(17)	109.8(4)	O(18)-Re(4)-O(16)	109.5(4)
O(17)-Re(4)-O(16)	110.1(4)	O(18)-Re(4)-O(15)	109.6(4)
O(17)-Re(4)-O(15)	108.9(5)	O(16)-Re(4)-O(15)	108.8(4)
O(18')-Re(4')-O(17')	109.9(4)	O(18')-Re(4')-O(15')	110.1(4)
O(17')-Re(4')-O(15')	109.0(5)	O(18')-Re(4')-O(16')	109.6(4)
O(17')-Re(4')-O(16')	109.6(4)	O(15')-Re(4')-O(16')	108.7(4)

Symmetry transformations used to generate equivalent atoms:

Table Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for
 anisotropic displacement factor exponent takes the form: $-2\pi^2 [(h a)^2 U_{11} + \dots + 2 h k a b U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	17(1)	14(1)	16(1)	1(1)	-1(1)	0(1)
O(5)	25(3)	15(3)	19(3)	-6(3)	-6(3)	7(3)
O(1)	28(3)	22(3)	16(3)	0(2)	2(2)	0(3)
C(4)	27(3)	25(3)	20(3)	1(3)	3(3)	-1(3)
O(2)	37(4)	33(4)	25(3)	9(3)	7(3)	-8(3)
C(3)	27(3)	24(3)	16(3)	1(3)	2(3)	-1(3)
N(1)	22(3)	18(3)	18(3)	0(2)	-1(2)	-2(2)
O(3)	24(2)	23(2)	26(2)	-4(2)	-2(2)	5(2)
C(12)	24(3)	22(3)	27(3)	-2(3)	4(3)	2(3)
O(4)	38(4)	25(3)	34(4)	7(3)	17(3)	-3(3)
C(11)	20(3)	23(3)	24(3)	-1(3)	2(3)	2(3)
N(2)	18(3)	19(3)	23(3)	4(2)	0(2)	3(2)
N(3)	17(3)	18(3)	24(3)	1(3)	2(3)	-4(3)
C(10)	18(3)	22(3)	30(3)	-1(3)	1(3)	-2(3)
C(9)	22(3)	23(3)	32(4)	4(3)	2(3)	1(3)
C(8)	26(4)	19(3)	32(3)	1(3)	5(3)	-1(3)
C(7)	26(3)	19(3)	30(3)	-3(3)	5(3)	-6(3)
C(6)	19(3)	19(3)	24(3)	0(3)	4(3)	-6(3)
C(5)	21(3)	20(3)	21(3)	-4(3)	1(3)	-3(3)
N(4)	21(3)	15(3)	23(3)	3(3)	4(3)	-2(3)
C(18)	22(3)	16(3)	20(3)	2(3)	3(3)	-2(3)
C(17)	22(4)	17(3)	26(3)	-1(3)	6(3)	-7(3)
C(16)	23(4)	12(3)	29(3)	-4(3)	13(3)	1(3)
C(15)	27(4)	16(3)	31(3)	1(3)	10(3)	3(3)
C(14)	22(3)	17(3)	28(3)	2(3)	6(3)	1(3)
C(13)	21(3)	16(3)	27(3)	1(3)	1(3)	5(3)
C(1)	27(3)	21(3)	19(3)	0(3)	-5(3)	2(3)
C(2)	24(3)	18(3)	21(3)	1(3)	-8(3)	2(3)
Re(2)	17(1)	14(1)	16(1)	0(1)	-1(1)	0(1)
O(10)	20(3)	16(3)	31(3)	3(3)	-1(3)	2(3)
O(6)	19(3)	25(3)	20(3)	-3(2)	5(3)	-4(3)
C(22)	21(3)	24(3)	23(3)	-3(3)	4(3)	-1(3)
O(7)	35(4)	26(4)	39(4)	1(3)	21(3)	-9(3)
C(21)	20(3)	24(3)	18(3)	-6(3)	1(3)	1(3)
N(5)	19(3)	19(3)	16(3)	-7(2)	-5(2)	2(2)
O(8)	21(3)	17(3)	21(3)	1(2)	3(2)	1(3)
C(30)	21(3)	23(3)	20(3)	-3(3)	5(3)	-2(3)
O(9)	27(4)	29(4)	38(4)	12(3)	14(3)	0(3)
C(29)	20(3)	21(3)	16(3)	-2(3)	1(3)	-1(3)
N(6)	16(3)	20(3)	15(3)	0(2)	-4(2)	0(2)
N(7)	14(3)	19(3)	23(3)	0(3)	1(3)	-1(2)
C(28)	21(3)	22(3)	27(3)	2(3)	-1(3)	2(3)
C(27)	24(3)	26(3)	28(4)	1(3)	0(3)	4(3)
C(26)	26(4)	23(3)	30(4)	0(3)	2(3)	4(3)
C(25)	21(3)	23(3)	27(3)	-4(3)	0(3)	2(3)
C(24)	19(3)	21(3)	24(3)	-3(3)	-1(3)	-1(3)
C(23)	23(3)	18(3)	18(3)	-7(3)	-5(3)	-1(3)
N(8)	24(3)	18(3)	16(3)	-5(3)	2(3)	-2(3)
C(36)	27(4)	23(3)	18(3)	-4(3)	2(3)	-1(3)
C(35)	29(4)	23(3)	18(3)	-1(3)	6(3)	0(3)
C(34)	30(4)	19(3)	19(3)	-2(3)	8(3)	1(3)
C(33)	26(4)	23(3)	18(3)	-1(3)	6(3)	2(3)
C(32)	22(3)	19(3)	16(3)	0(2)	3(3)	-1(3)
C(31)	19(3)	18(3)	16(3)	0(3)	-3(3)	2(3)

C(19)	22(3)	24(3)	17(3)	0(3)	-6(3)	0(3)
C(20)	16(3)	22(3)	17(3)	2(3)	-7(3)	-3(3)
Re(3)	22(1)	29(1)	21(1)	1(1)	-3(1)	1(1)
O(11)	26(4)	37(4)	43(4)	3(3)	-2(3)	-1(3)
O(12)	35(4)	54(5)	41(4)	-15(3)	-17(3)	7(3)
O(13)	38(5)	37(4)	51(4)	14(3)	-13(4)	3(3)
O(14)	30(4)	50(5)	34(4)	5(3)	1(3)	8(3)
O(19)	184(15)	196(15)	69(8)	25(8)	-22(9)	-140(13)
C(37)	69(10)	87(11)	48(9)	0(8)	-1(8)	-18(9)
Re(4)	36(2)	37(2)	25(2)	-6(1)	4(1)	4(1)
O(15)	44(13)	57(8)	190(20)	58(14)	35(12)	-3(6)
O(16)	36(7)	45(4)	65(6)	27(4)	-6(5)	2(4)
O(17)	120(20)	140(20)	54(8)	-62(11)	-48(9)	101(12)
O(18)	28(4)	84(6)	27(5)	16(5)	0(4)	5(4)
Re(4')	32(1)	20(1)	19(2)	-1(1)	2(1)	-4(1)
O(15')	40(8)	57(8)	75(11)	-19(10)	0(9)	-19(8)
O(16')	36(7)	45(4)	65(6)	27(4)	-6(5)	2(4)
O(17')	75(15)	84(14)	14(4)	4(6)	3(5)	52(10)
O(18')	28(4)	84(6)	27(5)	16(5)	0(4)	5(4)
O(20)	79(7)	96(8)	39(5)	15(5)	-13(5)	-42(6)
C(38)	77(12)	109(13)	72(10)	21(10)	36(10)	-7(9)

Table Torsion angles [°] for

[ReO₆]/[ReO₄]-CH₃OH

O(5)-Re(1)-O(1)-C(4)	110.0(6)	O(3)-Re(1)-O(1)-C(4)	-69.8(7)
N(4)-Re(1)-O(1)-C(4)	-173.3(6)	N(3)-Re(1)-O(1)-C(4)	26.4(6)
N(2)-Re(1)-O(1)-C(4)	-105.2(6)	N(1)-Re(1)-O(1)-C(4)	-32.5(6)
Re(1)-O(1)-C(4)-O(2)	-162.4(7)	Re(1)-O(1)-C(4)-C(3)	17.3(9)
O(2)-C(4)-C(3)-N(1)	-159.3(8)	O(1)-C(4)-C(3)-N(1)	21.0(9)
C(4)-C(3)-N(1)-C(5)	-159.8(5)	C(4)-C(3)-N(1)-C(1)	78.9(7)
C(4)-C(3)-N(1)-Re(1)	-41.5(6)	O(5)-Re(1)-N(1)-C(5)	68.8(5)
O(1)-Re(1)-N(1)-C(5)	156.0(4)	O(3)-Re(1)-N(1)-C(5)	-38.3(4)
N(4)-Re(1)-N(1)-C(5)	-150.9(4)	N(3)-Re(1)-N(1)-C(5)	36.9(4)
N(2)-Re(1)-N(1)-C(5)	-110.0(4)	O(5)-Re(1)-N(1)-C(1)	-166.6(4)
O(1)-Re(1)-N(1)-C(1)	-79.3(4)	O(3)-Re(1)-N(1)-C(1)	86.3(4)
N(4)-Re(1)-N(1)-C(1)	-26.3(5)	N(3)-Re(1)-N(1)-C(1)	161.5(4)
N(2)-Re(1)-N(1)-C(1)	14.6(3)	O(5)-Re(1)-N(1)-C(3)	-48.8(5)
O(1)-Re(1)-N(1)-C(3)	38.5(3)	O(3)-Re(1)-N(1)-C(3)	-155.9(3)
N(4)-Re(1)-N(1)-C(3)	91.5(4)	N(3)-Re(1)-N(1)-C(3)	-80.7(4)
N(2)-Re(1)-N(1)-C(3)	132.4(4)	O(5)-Re(1)-O(3)-C(12)	111.1(6)
O(1)-Re(1)-O(3)-C(12)	-69.1(7)	N(4)-Re(1)-O(3)-C(12)	27.5(6)
N(3)-Re(1)-O(3)-C(12)	-172.4(6)	N(2)-Re(1)-O(3)-C(12)	-31.5(6)
N(1)-Re(1)-O(3)-C(12)	-104.3(6)	Re(1)-O(3)-C(12)-O(4)	-163.0(7)
Re(1)-O(3)-C(12)-C(11)	15.3(10)	O(4)-C(12)-C(11)-N(2)	-158.7(8)
O(3)-C(12)-C(11)-N(2)	23.0(9)	C(12)-C(11)-N(2)-C(13)	-160.7(5)
C(12)-C(11)-N(2)-C(2)	77.6(6)	C(12)-C(11)-N(2)-Re(1)	-42.8(6)
O(5)-Re(1)-N(2)-C(13)	71.3(5)	O(1)-Re(1)-N(2)-C(13)	-38.3(3)
O(3)-Re(1)-N(2)-C(13)	156.2(4)	N(4)-Re(1)-N(2)-C(13)	37.4(3)
N(3)-Re(1)-N(2)-C(13)	-151.2(3)	N(1)-Re(1)-N(2)-C(13)	-109.9(4)
O(5)-Re(1)-N(2)-C(2)	-164.0(4)	O(1)-Re(1)-N(2)-C(2)	86.4(4)
O(3)-Re(1)-N(2)-C(2)	-79.1(4)	N(4)-Re(1)-N(2)-C(2)	162.1(4)
N(3)-Re(1)-N(2)-C(2)	-26.5(4)	N(1)-Re(1)-N(2)-C(2)	14.8(3)
O(5)-Re(1)-N(2)-C(11)	-46.0(5)	O(1)-Re(1)-N(2)-C(11)	-155.5(3)
O(3)-Re(1)-N(2)-C(11)	38.9(3)	N(4)-Re(1)-N(2)-C(11)	-79.8(4)
N(3)-Re(1)-N(2)-C(11)	91.6(4)	N(1)-Re(1)-N(2)-C(11)	132.8(4)
O(5)-Re(1)-N(3)-C(6)	173.0(6)	O(1)-Re(1)-N(3)-C(6)	-86.8(6)
O(3)-Re(1)-N(3)-C(6)	68.4(6)	N(4)-Re(1)-N(3)-C(6)	172.4(6)
N(2)-Re(1)-N(3)-C(6)	17.1(6)	N(1)-Re(1)-N(3)-C(6)	-25.6(5)
O(5)-Re(1)-N(3)-C(10)	0.5(6)	O(1)-Re(1)-N(3)-C(10)	100.8(6)
O(3)-Re(1)-N(3)-C(10)	-104.0(6)	N(4)-Re(1)-N(3)-C(10)	0.0(9)
N(2)-Re(1)-N(3)-C(10)	-155.3(5)	N(1)-Re(1)-N(3)-C(10)	161.9(6)
C(6)-N(3)-C(10)-C(9)	-1.1(12)	Re(1)-N(3)-C(10)-C(9)	171.5(7)
N(3)-C(10)-C(9)-C(8)	0.1(14)	C(10)-C(9)-C(8)-C(7)	-0.5(13)
C(9)-C(8)-C(7)-C(6)	1.9(13)	C(10)-N(3)-C(6)-C(7)	2.5(12)
Re(1)-N(3)-C(6)-C(7)	-170.1(6)	C(10)-N(3)-C(6)-C(5)	-177.9(7)
Re(1)-N(3)-C(6)-C(5)	9.4(9)	C(8)-C(7)-C(6)-N(3)	-3.0(13)
C(8)-C(7)-C(6)-C(5)	177.5(8)	C(1)-N(1)-C(5)-C(6)	-169.8(5)
C(3)-N(1)-C(5)-C(6)	69.9(7)	Re(1)-N(1)-C(5)-C(6)	-44.1(6)
N(3)-C(6)-C(5)-N(1)	23.7(9)	C(7)-C(6)-C(5)-N(1)	-156.7(8)
O(5)-Re(1)-N(4)-C(14)	173.3(6)	O(1)-Re(1)-N(4)-C(14)	67.4(6)
O(3)-Re(1)-N(4)-C(14)	-87.8(6)	N(3)-Re(1)-N(4)-C(14)	173.8(6)
N(2)-Re(1)-N(4)-C(14)	-26.5(5)	N(1)-Re(1)-N(4)-C(14)	15.9(6)
O(5)-Re(1)-N(4)-C(18)	2.1(6)	O(1)-Re(1)-N(4)-C(18)	-103.7(6)
O(3)-Re(1)-N(4)-C(18)	101.0(6)	N(3)-Re(1)-N(4)-C(18)	2.6(9)
N(2)-Re(1)-N(4)-C(18)	162.4(6)	N(1)-Re(1)-N(4)-C(18)	-155.3(5)
C(14)-N(4)-C(18)-C(17)	-1.4(12)	Re(1)-N(4)-C(18)-C(17)	170.0(7)
N(4)-C(18)-C(17)-C(16)	-1.6(14)	C(18)-C(17)-C(16)-C(15)	3.2(13)
C(17)-C(16)-C(15)-C(14)	-1.8(13)	C(18)-N(4)-C(14)-C(15)	2.8(12)
Re(1)-N(4)-C(14)-C(15)	-168.6(6)	C(18)-N(4)-C(14)-C(13)	-178.3(7)
Re(1)-N(4)-C(14)-C(13)	10.3(9)	C(16)-C(15)-C(14)-N(4)	-1.2(13)
C(16)-C(15)-C(14)-C(13)	-180.0(8)	C(2)-N(2)-C(13)-C(14)	-170.0(5)
C(11)-N(2)-C(13)-C(14)	69.3(6)	Re(1)-N(2)-C(13)-C(14)	-44.4(6)
N(4)-C(14)-C(13)-N(2)	23.4(9)	C(15)-C(14)-C(13)-N(2)	-157.7(8)

C(5)-N(1)-C(1)-C(2)	82.9(6)	C(3)-N(1)-C(1)-C(2)	-156.4(5)
Re(1)-N(1)-C(1)-C(2)	-41.7(6)	C(13)-N(2)-C(2)-C(1)	82.6(6)
C(11)-N(2)-C(2)-C(1)	-156.6(5)	Re(1)-N(2)-C(2)-C(1)	-41.8(6)
N(1)-C(1)-C(2)-N(2)	54.5(7)	O(10)-Re(2)-O(6)-C(22)	-109.8(6)
O(8)-Re(2)-O(6)-C(22)	70.1(7)	N(8)-Re(2)-O(6)-C(22)	173.3(6)
N(7)-Re(2)-O(6)-C(22)	-26.5(6)	N(5)-Re(2)-O(6)-C(22)	32.6(6)
N(6)-Re(2)-O(6)-C(22)	105.2(6)	Re(2)-O(6)-C(22)-O(7)	162.6(7)
Re(2)-O(6)-C(22)-C(21)	-18.0(9)	O(7)-C(22)-C(21)-N(5)	159.4(8)
O(6)-C(22)-C(21)-N(5)	-19.9(9)	C(22)-C(21)-N(5)-C(23)	159.0(5)
C(22)-C(21)-N(5)-C(19)	-80.4(6)	C(22)-C(21)-N(5)-Re(2)	40.5(6)
O(10)-Re(2)-N(5)-C(23)	-68.3(5)	O(6)-Re(2)-N(5)-C(23)	-155.4(4)
O(8)-Re(2)-N(5)-C(23)	38.8(4)	N(8)-Re(2)-N(5)-C(23)	151.6(4)
N(7)-Re(2)-N(5)-C(23)	-36.6(3)	N(6)-Re(2)-N(5)-C(23)	110.5(4)
O(10)-Re(2)-N(5)-C(19)	166.9(4)	O(6)-Re(2)-N(5)-C(19)	79.8(4)
O(8)-Re(2)-N(5)-C(19)	-85.9(4)	N(8)-Re(2)-N(5)-C(19)	26.9(5)
N(7)-Re(2)-N(5)-C(19)	-161.4(4)	N(6)-Re(2)-N(5)-C(19)	-14.2(3)
O(10)-Re(2)-N(5)-C(21)	49.1(5)	O(6)-Re(2)-N(5)-C(21)	-38.0(3)
O(8)-Re(2)-N(5)-C(21)	156.2(3)	N(8)-Re(2)-N(5)-C(21)	-91.0(4)
N(7)-Re(2)-N(5)-C(21)	80.7(4)	N(6)-Re(2)-N(5)-C(21)	-132.1(4)
O(10)-Re(2)-O(8)-C(30)	-109.4(6)	O(6)-Re(2)-O(8)-C(30)	70.8(7)
N(8)-Re(2)-O(8)-C(30)	-25.5(6)	N(7)-Re(2)-O(8)-C(30)	174.3(6)
N(5)-Re(2)-O(8)-C(30)	106.2(5)	N(6)-Re(2)-O(8)-C(30)	33.6(5)
Re(2)-O(8)-C(30)-O(9)	160.6(7)	Re(2)-O(8)-C(30)-C(29)	-19.3(9)
O(9)-C(30)-C(29)-N(6)	161.0(8)	O(8)-C(30)-C(29)-N(6)	-19.0(9)
C(30)-C(29)-N(6)-C(31)	158.9(5)	C(30)-C(29)-N(6)-C(20)	-80.7(6)
C(30)-C(29)-N(6)-Re(2)	40.5(6)	O(10)-Re(2)-N(6)-C(31)	-70.8(5)
O(6)-Re(2)-N(6)-C(31)	38.5(3)	O(8)-Re(2)-N(6)-C(31)	-155.7(4)
N(8)-Re(2)-N(6)-C(31)	-36.7(3)	N(7)-Re(2)-N(6)-C(31)	151.3(3)
N(5)-Re(2)-N(6)-C(31)	110.4(4)	O(10)-Re(2)-N(6)-C(20)	164.7(4)
O(6)-Re(2)-N(6)-C(20)	-86.0(4)	O(8)-Re(2)-N(6)-C(20)	79.8(4)
N(8)-Re(2)-N(6)-C(20)	-161.2(4)	N(7)-Re(2)-N(6)-C(20)	26.8(4)
N(5)-Re(2)-N(6)-C(20)	-14.1(3)	O(10)-Re(2)-N(6)-C(29)	46.3(5)
O(6)-Re(2)-N(6)-C(29)	155.6(3)	O(8)-Re(2)-N(6)-C(29)	-38.5(3)
N(8)-Re(2)-N(6)-C(29)	80.4(3)	N(7)-Re(2)-N(6)-C(29)	-91.5(4)
N(5)-Re(2)-N(6)-C(29)	-132.5(4)	O(10)-Re(2)-N(7)-C(24)	-173.6(6)
O(6)-Re(2)-N(7)-C(24)	86.5(6)	O(8)-Re(2)-N(7)-C(24)	-69.0(6)
N(8)-Re(2)-N(7)-C(24)	-174.5(6)	N(5)-Re(2)-N(7)-C(24)	24.9(6)
N(6)-Re(2)-N(7)-C(24)	-17.5(7)	O(10)-Re(2)-N(7)-C(28)	-0.2(6)
O(6)-Re(2)-N(7)-C(28)	-100.1(6)	O(8)-Re(2)-N(7)-C(28)	104.4(6)
N(8)-Re(2)-N(7)-C(28)	-1.1(10)	N(5)-Re(2)-N(7)-C(28)	-161.6(6)
N(6)-Re(2)-N(7)-C(28)	156.0(5)	C(24)-N(7)-C(28)-C(27)	1.3(12)
Re(2)-N(7)-C(28)-C(27)	-172.2(7)	N(7)-C(28)-C(27)-C(26)	-0.5(14)
C(28)-C(27)-C(26)-C(25)	-0.2(14)	C(27)-C(26)-C(25)-C(24)	0.0(14)
C(28)-N(7)-C(24)-C(25)	-1.5(12)	Re(2)-N(7)-C(24)-C(25)	172.1(7)
C(28)-N(7)-C(24)-C(23)	178.0(7)	Re(2)-N(7)-C(24)-C(23)	-8.4(9)
C(26)-C(25)-C(24)-N(7)	0.9(14)	C(26)-C(25)-C(24)-C(23)	-178.6(8)
C(19)-N(5)-C(23)-C(24)	170.5(5)	C(21)-N(5)-C(23)-C(24)	-69.9(7)
Re(2)-N(5)-C(23)-C(24)	44.2(6)	N(7)-C(24)-C(23)-N(5)	-24.3(9)
C(25)-C(24)-C(23)-N(5)	155.2(8)	O(10)-Re(2)-N(8)-C(32)	-173.3(6)
O(6)-Re(2)-N(8)-C(32)	-67.9(6)	O(8)-Re(2)-N(8)-C(32)	87.6(6)
N(7)-Re(2)-N(8)-C(32)	-172.5(6)	N(5)-Re(2)-N(8)-C(32)	-16.2(6)
N(6)-Re(2)-N(8)-C(32)	26.3(5)	O(10)-Re(2)-N(8)-C(36)	-4.1(6)
O(6)-Re(2)-N(8)-C(36)	101.4(6)	O(8)-Re(2)-N(8)-C(36)	-103.1(6)
N(7)-Re(2)-N(8)-C(36)	-3.2(10)	N(5)-Re(2)-N(8)-C(36)	153.1(5)
N(6)-Re(2)-N(8)-C(36)	-164.4(6)	C(32)-N(8)-C(36)-C(35)	2.4(13)
Re(2)-N(8)-C(36)-C(35)	-167.0(7)	N(8)-C(36)-C(35)-C(34)	-2.2(14)
C(36)-C(35)-C(34)-C(33)	1.2(13)	C(35)-C(34)-C(33)-C(32)	-0.3(13)
C(36)-N(8)-C(32)-C(33)	-1.5(12)	Re(2)-N(8)-C(32)-C(33)	168.0(6)
C(36)-N(8)-C(32)-C(31)	179.6(7)	Re(2)-N(8)-C(32)-C(31)	-11.0(9)
C(34)-C(33)-C(32)-N(8)	0.5(13)	C(34)-C(33)-C(32)-C(31)	179.3(8)
C(20)-N(6)-C(31)-C(32)	169.2(5)	C(29)-N(6)-C(31)-C(32)	-71.0(6)
Re(2)-N(6)-C(31)-C(32)	43.0(6)	N(8)-C(32)-C(31)-N(6)	-22.1(9)
C(33)-C(32)-C(31)-N(6)	159.0(7)	C(23)-N(5)-C(19)-C(20)	-84.6(6)

C(21)-N(5)-C(19)-C(20)	155.4(5)	Re(2)-N(5)-C(19)-C(20)	40.4(6)
C(31)-N(6)-C(20)-C(19)	-84.6(6)	C(29)-N(6)-C(20)-C(19)	155.6(5)
Re(2)-N(6)-C(20)-C(19)	40.2(6)	N(5)-C(19)-C(20)-N(6)	-52.4(7)

Symmetry transformations used to generate equivalent atoms:

Table Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Re}(\text{C}(\text{bped}))][\text{ReO}_4] \cdot \text{CH}_3\text{OH}$

	x	y	z	U(eq)	SOF
H(3A)	8158	162	-973	27	1
H(3B)	8540	-562	-461	27	1
H(11B)	6117	906	816	27	1
H(11C)	6582	1646	1251	27	1
H(10B)	8849	-1473	1173	28	1
H(9A)	9239	-3888	1099	31	1
H(8A)	8888	-5582	389	31	1
H(7A)	8130	-4749	-210	30	1
H(5B)	7668	-2345	-655	25	1
H(5C)	7231	-2266	-114	25	1
H(18B)	8148	2629	1759	23	1
H(17B)	8015	5060	2116	26	1
H(16B)	7390	6761	1629	26	1
H(15B)	6854	5826	843	30	1
H(13B)	6483	3382	343	26	1
H(13C)	7080	3305	-16	26	1
H(1A)	7053	-151	-865	27	1
H(1B)	7287	1486	-658	27	1
H(2A)	6364	1136	-271	25	1
H(2B)	6552	-476	0	25	1
H(21A)	9169	5616	3840	25	1
H(21B)	9541	4861	4352	25	1
H(29A)	11179	3401	2172	23	1
H(29B)	11618	4191	2621	23	1
H(28A)	8893	6531	2196	28	1
H(27A)	8493	8936	2268	31	1
H(26A)	8819	10616	2995	31	1
H(25A)	9550	9761	3624	29	1
H(23A)	10479	7328	3519	24	1
H(23B)	10031	7387	4052	24	1
H(36A)	9593	2433	1627	27	1
H(35A)	9677	-59	1313	28	1
H(34A)	10343	-1706	1773	28	1
H(33A)	10869	-768	2563	27	1
H(31A)	10647	1738	3417	22	1
H(31B)	11244	1675	3059	22	1
H(19A)	10414	3582	4067	25	1
H(19B)	10646	5225	4266	25	1
H(20A)	11178	5494	3424	22	1
H(20B)	11340	3864	3695	22	1
H(19E)	10772	3227	122	225	1
H(37A)	10400	5399	801	102	1
H(37B)	10615	3870	1112	102	1
H(37C)	10088	3809	662	102	1
H(20E)	6946	1683	3152	106	1
H(38A)	7206	-724	2537	129	1
H(38B)	7646	591	2731	129	1
H(38C)	7153	946	2263	129	1

Table Hydrogen bonds for [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(19)-H(19E)...O(11)	0.84	2.14	2.969(14)	169.5
O(20)-H(20E)...O(15')	0.84	1.86	2.680(13)	163.6

Symmetry transformations used to generate equivalent atoms:

Table Crystal data, data collection, and solution and refinement for

Crystal Data

Empirical formula	$C_{28}H_{28}F_6N_4O_3PRe$
Crystal Habit, color	plate, violet
Crystal size	0.76 x 0.6 x 0.2 mm
Crystal system	Monoclinic
Space group	P2/c
	$a = 11.9219(4) \text{ \AA}$ $\alpha = 90.000(1)^\circ$
	$b = 10.1817(4) \text{ \AA}$ $\beta = 111.001(1)^\circ$
	$c = 12.7269(4) \text{ \AA}$ $\gamma = 90.000(1)^\circ$
Volume	$1442.24(9) \text{ \AA}^3$
Z	2
Formula weight	799.71
Density (calculated)	1.842 Mg/m^3
Absorption coefficient	4.345 mm^{-1}
F(000)	784

[R₂C(bbpen)]PF₆

Data Collection

Diffractionmeter	Siemens SMART Platform CCD
Wavelength	0.71073 \AA
Temperature	173(2) K
θ range for data collection	1.83 to 25.04°
Index ranges	$-13 \leq h \leq 14$, $-12 \leq k \leq 12$, $-15 \leq l \leq 15$
Reflections collected	10422
Independent reflections	2558 ($R_{\text{int}} = 0.0217$)

Solution and Refinement

System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2) + (AP)^2 + (BP)]^{-1}$, where $P = (F_o^2 + 2F_c^2)/3$, $A = 0.0332$, and $B = 1.0179$
Absorption correction	SADABS, Sheldrick, 1986
Max. and min. transmission	1.000000 and 0.632904
Data / restraints / parameters	2558 / 12 / 233
R indices ($I > 2\sigma(I)$) = 2329)	$R1 = 0.0186$, $wR2 = 0.0505$
R indices (all data)	$R1 = 0.0209$, $wR2 = 0.0514$
Goodness-of-fit on F^2	1.059
Largest diff. peak and hole	1.027 and $-1.020 \text{ e\AA}^{-3}$

Table Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Re (1)	5000	7442 (1)	2500	15 (1)	1
O (1)	5426 (2)	7043 (2)	4137 (2)	21 (1)	1
O (2)	5000	9102 (3)	2500	22 (1)	1
N (2)	3048 (2)	7964 (2)	2085 (2)	19 (1)	1
N (1)	3777 (2)	5575 (2)	2356 (2)	19 (1)	1
P (1)	0	3144 (4)	2500	35 (1)	0.611 (7)
F (1)	1143 (7)	3173 (10)	2136 (9)	87 (4)	0.611 (7)
F (2)	-523 (4)	2018 (5)	1612 (3)	71 (2)	0.611 (7)
F (3)	-585 (6)	4231 (5)	1587 (4)	178 (5)	0.611 (7)
P (1D)	0	3490 (7)	2500	35 (1)	0.389 (7)
F (1D)	842 (16)	3415 (24)	1789 (17)	94 (6)	0.389 (7)
F (4D)	0	1950 (9)	2500	100 (5)	0.389 (7)
F (5D)	-1142 (6)	3460 (9)	1389 (5)	72 (3)	0.389 (7)
F (6D)	0	5020 (8)	2500	94 (4)	0.389 (7)
C (1)	2172 (3)	7104 (3)	1537 (2)	23 (1)	1
C (2)	968 (4)	7435 (3)	1189 (4)	34 (1)	1
C (3)	654 (3)	8674 (4)	1435 (3)	39 (1)	1
C (4)	1540 (3)	9537 (3)	2029 (3)	34 (1)	1
C (5)	2724 (3)	9151 (3)	2343 (3)	24 (1)	1
C (6)	2641 (3)	5799 (3)	1377 (2)	23 (1)	1
C (7)	3479 (3)	5317 (3)	3405 (2)	23 (1)	1
C (8)	3465 (3)	6500 (3)	4109 (2)	20 (1)	1
C (9)	4502 (3)	7271 (3)	4503 (3)	20 (1)	1
C (10)	4576 (3)	8308 (3)	5247 (2)	25 (1)	1
C (11)	3599 (3)	8582 (3)	5559 (3)	30 (1)	1
C (12)	2560 (3)	7845 (3)	5152 (3)	29 (1)	1
C (13)	2495 (3)	6799 (3)	4424 (2)	24 (1)	1
C (14)	4350 (3)	4358 (3)	2126 (2)	22 (1)	1

Table Bond lengths [Å] and angles [°] for

[ReO(bbbp)]PF₆

Re(1)-O(2)	1.689(3)	Re(1)-O(1)#1	2.002(2)
Re(1)-O(1)	2.002(2)	Re(1)-N(2)	2.257(2)
Re(1)-N(2)#1	2.257(2)	Re(1)-N(1)#1	2.363(2)
Re(1)-N(1)	2.363(2)	O(1)-C(9)	1.361(4)
N(2)-C(5)	1.345(4)	N(2)-C(1)	1.350(4)
N(1)-C(6)	1.494(4)	N(1)-C(14)	1.494(3)
N(1)-C(7)	1.521(4)	P(1)-F(2)	1.574(4)
P(1)-F(2)#2	1.574(4)	P(1)-F(3)#2	1.575(4)
P(1)-F(3)	1.575(4)	P(1)-F(1)	1.588(4)
P(1)-F(1)#2	1.588(4)	P(1D)-F(6D)	1.558(6)
P(1D)-F(4D)	1.569(6)	P(1D)-F(5D)#2	1.573(5)
P(1D)-F(5D)	1.573(5)	P(1D)-F(1D)	1.576(5)
P(1D)-F(1D)#2	1.576(5)	C(1)-C(2)	1.384(5)
C(1)-C(6)	1.484(4)	C(2)-C(3)	1.383(5)
C(2)-H(2)	0.90(4)	C(3)-C(4)	1.374(5)
C(3)-H(3)	0.95	C(4)-C(5)	1.379(4)
C(4)-H(4)	0.95	C(5)-H(5)	0.95
C(6)-H(6B)	0.99	C(6)-H(6A)	0.99
C(7)-C(8)	1.505(4)	C(7)-H(7A)	0.99
C(7)-H(7B)	0.99	C(8)-C(13)	1.387(4)
C(8)-C(9)	1.397(4)	C(9)-C(10)	1.399(4)
C(10)-C(11)	1.388(5)	C(10)-H(10)	0.95
C(11)-C(12)	1.380(5)	C(11)-H(11)	0.95
C(12)-C(13)	1.396(5)	C(12)-H(12)	0.95
C(13)-H(13)	0.95	C(14)-C(14)#1	1.500(6)
C(14)-H(14B)	0.99	C(14)-H(14A)	0.99
O(2)-Re(1)-O(1)#1	101.73(6)	O(2)-Re(1)-O(1)	101.73(6)
O(1)#1-Re(1)-O(1)	156.54(12)	O(2)-Re(1)-N(2)	76.40(6)
O(1)#1-Re(1)-N(2)	87.04(8)	O(1)-Re(1)-N(2)	98.47(8)
O(2)-Re(1)-N(2)#1	76.40(6)	O(1)#1-Re(1)-N(2)#1	98.47(8)
O(1)-Re(1)-N(2)#1	87.04(8)	N(2)-Re(1)-N(2)#1	152.80(12)
O(2)-Re(1)-N(1)#1	143.59(6)	O(1)#1-Re(1)-N(1)#1	80.57(8)
O(1)-Re(1)-N(1)#1	80.60(8)	N(2)-Re(1)-N(1)#1	139.73(9)
N(2)#1-Re(1)-N(1)#1	67.38(8)	O(2)-Re(1)-N(1)	143.58(6)
O(1)#1-Re(1)-N(1)	80.60(8)	O(1)-Re(1)-N(1)	80.57(8)
N(2)-Re(1)-N(1)	67.38(8)	N(2)#1-Re(1)-N(1)	139.73(9)
N(1)#1-Re(1)-N(1)	72.83(11)	C(9)-O(1)-Re(1)	112.8(2)
C(5)-N(2)-C(1)	118.2(3)	C(5)-N(2)-Re(1)	121.1(2)
C(1)-N(2)-Re(1)	120.7(2)	C(6)-N(1)-C(14)	107.7(2)
C(6)-N(1)-C(7)	109.4(2)	C(14)-N(1)-C(7)	107.2(2)
C(6)-N(1)-Re(1)	106.9(2)	C(14)-N(1)-Re(1)	111.7(2)
C(7)-N(1)-Re(1)	113.7(2)	F(2)-P(1)-F(2)#2	86.5(4)
F(2)-P(1)-F(3)#2	177.1(4)	F(2)#2-P(1)-F(3)#2	91.5(3)
F(2)-P(1)-F(3)	91.5(3)	F(2)#2-P(1)-F(3)	177.1(3)
F(3)#2-P(1)-F(3)	90.7(5)	F(2)-P(1)-F(1)	88.0(4)
F(2)#2-P(1)-F(1)	93.6(5)	F(3)#2-P(1)-F(1)	90.1(4)
F(3)-P(1)-F(1)	88.4(4)	F(2)-P(1)-F(1)#2	93.6(5)
F(2)#2-P(1)-F(1)#2	88.0(4)	F(3)#2-P(1)-F(1)#2	88.4(4)
F(3)-P(1)-F(1)#2	90.1(4)	F(1)-P(1)-F(1)#2	177.8(8)
F(6D)-P(1D)-F(4D)	180.000(2)	F(6D)-P(1D)-F(5D)#2	91.1(4)
F(4D)-P(1D)-F(5D)#2	88.9(4)	F(6D)-P(1D)-F(5D)	91.1(4)
F(4D)-P(1D)-F(5D)	88.9(4)	F(5D)#2-P(1D)-F(5D)	177.7(9)
F(6D)-P(1D)-F(1D)	92.8(9)	F(4D)-P(1D)-F(1D)	87.2(9)
F(5D)#2-P(1D)-F(1D)	89.5(9)	F(5D)-P(1D)-F(1D)	90.4(9)
F(6D)-P(1D)-F(1D)#2	92.8(9)	F(4D)-P(1D)-F(1D)#2	87.2(9)
F(5D)#2-P(1D)-F(1D)#2	90.4(9)	F(5D)-P(1D)-F(1D)#2	89.5(9)
F(1D)-P(1D)-F(1D)#2	174(2)	N(2)-C(1)-C(2)	122.0(3)
N(2)-C(1)-C(6)	113.0(3)	C(2)-C(1)-C(6)	125.0(3)

C(3)-C(2)-C(1)	118.9(3)	C(3)-C(2)-H(2)	121(3)
C(1)-C(2)-H(2)	120(3)	C(4)-C(3)-C(2)	119.4(3)
C(4)-C(3)-H(3)	120.3(2)	C(2)-C(3)-H(3)	120.3(2)
C(3)-C(4)-C(5)	118.9(3)	C(3)-C(4)-H(4)	120.6(2)
C(5)-C(4)-H(4)	120.6(2)	N(2)-C(5)-C(4)	122.6(3)
N(2)-C(5)-H(5)	118.7(2)	C(4)-C(5)-H(5)	118.7(2)
C(1)-C(6)-N(1)	107.2(2)	C(1)-C(6)-H(6B)	110.3(2)
N(1)-C(6)-H(6B)	110.3(2)	C(1)-C(6)-H(6A)	110.3(2)
N(1)-C(6)-H(6A)	110.27(14)	H(6B)-C(6)-H(6A)	108.5
C(8)-C(7)-N(1)	116.1(2)	C(8)-C(7)-H(7A)	108.3(2)
N(1)-C(7)-H(7A)	108.26(14)	C(8)-C(7)-H(7B)	108.3(2)
N(1)-C(7)-H(7B)	108.26(14)	H(7A)-C(7)-H(7B)	107.4
C(13)-C(8)-C(9)	119.7(3)	C(13)-C(8)-C(7)	122.4(3)
C(9)-C(8)-C(7)	117.8(3)	O(1)-C(9)-C(8)	120.1(3)
O(1)-C(9)-C(10)	119.8(3)	C(8)-C(9)-C(10)	120.0(3)
C(11)-C(10)-C(9)	119.3(3)	C(11)-C(10)-H(10)	120.4(2)
C(9)-C(10)-H(10)	120.4(2)	C(12)-C(11)-C(10)	121.1(3)
C(12)-C(11)-H(11)	119.5(2)	C(10)-C(11)-H(11)	119.5(2)
C(11)-C(12)-C(13)	119.5(3)	C(11)-C(12)-H(12)	120.2(2)
C(13)-C(12)-H(12)	120.2(2)	C(8)-C(13)-C(12)	120.4(3)
C(8)-C(13)-H(13)	119.8(2)	C(12)-C(13)-H(13)	119.8(2)
N(1)-C(14)-C(14)#1	108.4(2)	N(1)-C(14)-H(14B)	110.0(2)
C(14)#1-C(14)-H(14B)	110.0(2)	N(1)-C(14)-H(14A)	110.00(14)
C(14)#1-C(14)-H(14A)	110.00(12)	H(14B)-C(14)-H(14A)	108.4

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x,y,-z+1/2

Table Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for
 anisotropic displacement factor exponent takes the form: $-2\pi^2 [$
 $(ha)^2 U_{11} + \dots + 2hka b U_{12}]$

	U11	U22	U33	U23	U13	U12
Re(1)	17(1)	14(1)	16(1)	0	7(1)	0
O(1)	21(1)	22(1)	19(1)	0(1)	8(1)	-1(1)
O(2)	22(2)	17(1)	29(2)	0	12(1)	0
N(2)	18(1)	20(1)	18(1)	2(1)	7(1)	1(1)
N(1)	22(1)	18(1)	18(1)	-2(1)	7(1)	-2(1)
P(1)	43(1)	3(2)	69(1)	0	32(1)	0
F(1)	81(6)	59(4)	158(10)	-34(6)	87(7)	-29(4)
F(2)	69(3)	83(3)	66(3)	-25(3)	31(3)	-26(3)
F(3)	246(10)	106(6)	270(10)	152(7)	199(9)	128(7)
P(1D)	43(1)	3(2)	69(1)	0	32(1)	0
F(1D)	71(7)	135(15)	100(9)	-16(8)	59(7)	-39(8)
C(1)	22(2)	29(1)	19(2)	0(1)	8(1)	-2(1)
C(2)	21(2)	44(2)	34(2)	-5(1)	6(2)	-2(1)
C(3)	24(2)	51(2)	44(2)	-1(2)	12(2)	11(2)
C(4)	34(2)	34(2)	39(2)	4(1)	21(2)	10(1)
C(5)	28(2)	21(1)	25(2)	2(1)	13(1)	3(1)
C(6)	22(2)	26(1)	21(2)	-4(1)	5(1)	-5(1)
C(7)	31(2)	21(1)	22(2)	-1(1)	14(1)	-5(1)
C(8)	25(2)	19(1)	17(1)	2(1)	9(1)	0(1)
C(9)	27(2)	18(1)	17(2)	4(1)	10(1)	2(1)
C(10)	33(2)	20(1)	22(2)	-3(1)	10(1)	-5(1)
C(11)	43(2)	23(1)	28(2)	-3(1)	17(2)	3(1)
C(12)	34(2)	30(1)	29(2)	4(1)	18(2)	9(2)
C(13)	25(2)	27(1)	21(2)	4(1)	9(1)	1(1)
C(14)	28(2)	15(1)	24(2)	-3(1)	10(1)	-3(1)

Table Torsion angles [°] for

[ReO(bbpen)]PF₆

O(2)-Re(1)-O(1)-C(9)	74.0(2)	O(1)#1-Re(1)-O(1)-C(9)	-106.0(2)
N(2)-Re(1)-O(1)-C(9)	-3.8(2)	N(2)#1-Re(1)-O(1)-C(9)	149.4(2)
N(1)#1-Re(1)-O(1)-C(9)	-143.0(2)	N(1)-Re(1)-O(1)-C(9)	-69.0(2)
O(2)-Re(1)-N(2)-C(5)	-21.0(2)	O(1)#1-Re(1)-N(2)-C(5)	-123.8(2)
O(1)-Re(1)-N(2)-C(5)	79.1(2)	N(2)#1-Re(1)-N(2)-C(5)	-21.0(2)
N(1)#1-Re(1)-N(2)-C(5)	164.5(2)	N(1)-Re(1)-N(2)-C(5)	155.1(2)
O(2)-Re(1)-N(2)-C(1)	156.9(2)	O(1)#1-Re(1)-N(2)-C(1)	54.1(2)
O(1)-Re(1)-N(2)-C(1)	-103.0(2)	N(2)#1-Re(1)-N(2)-C(1)	156.9(2)
N(1)#1-Re(1)-N(2)-C(1)	-17.6(3)	N(1)-Re(1)-N(2)-C(1)	-27.0(2)
O(2)-Re(1)-N(1)-C(6)	47.0(2)	O(1)#1-Re(1)-N(1)-C(6)	-50.0(2)
O(1)-Re(1)-N(1)-C(6)	144.0(2)	N(2)-Re(1)-N(1)-C(6)	40.7(2)
N(2)#1-Re(1)-N(1)-C(6)	-142.1(2)	N(1)#1-Re(1)-N(1)-C(6)	-133.0(2)
O(2)-Re(1)-N(1)-C(14)	164.65(13)	O(1)#1-Re(1)-N(1)-C(14)	67.6(2)
O(1)-Re(1)-N(1)-C(14)	-98.3(2)	N(2)-Re(1)-N(1)-C(14)	158.3(2)
N(2)#1-Re(1)-N(1)-C(14)	-24.4(2)	N(1)#1-Re(1)-N(1)-C(14)	-15.35(13)
O(2)-Re(1)-N(1)-C(7)	-73.8(2)	O(1)#1-Re(1)-N(1)-C(7)	-170.9(2)
O(1)-Re(1)-N(1)-C(7)	23.2(2)	N(2)-Re(1)-N(1)-C(7)	-80.2(2)
N(2)#1-Re(1)-N(1)-C(7)	97.1(2)	N(1)#1-Re(1)-N(1)-C(7)	106.2(2)
C(5)-N(2)-C(1)-C(2)	3.4(4)	Re(1)-N(2)-C(1)-C(2)	-174.6(3)
C(5)-N(2)-C(1)-C(6)	-175.7(2)	Re(1)-N(2)-C(1)-C(6)	6.4(3)
N(2)-C(1)-C(2)-C(3)	-1.6(5)	C(6)-C(1)-C(2)-C(3)	177.3(3)
C(1)-C(2)-C(3)-C(4)	-0.9(6)	C(2)-C(3)-C(4)-C(5)	1.4(5)
C(1)-N(2)-C(5)-C(4)	-2.8(4)	Re(1)-N(2)-C(5)-C(4)	175.1(2)
C(3)-C(4)-C(5)-N(2)	0.4(5)	N(2)-C(1)-C(6)-N(1)	31.4(3)
C(2)-C(1)-C(6)-N(1)	-147.6(3)	C(14)-N(1)-C(6)-C(1)	-172.1(2)
C(7)-N(1)-C(6)-C(1)	71.7(3)	Re(1)-N(1)-C(6)-C(1)	-51.8(2)
C(6)-N(1)-C(7)-C(8)	-91.9(3)	C(14)-N(1)-C(7)-C(8)	151.5(2)
Re(1)-N(1)-C(7)-C(8)	27.5(3)	N(1)-C(7)-C(8)-C(13)	127.4(3)
N(1)-C(7)-C(8)-C(9)	-56.2(4)	Re(1)-O(1)-C(9)-C(8)	66.7(3)
Re(1)-O(1)-C(9)-C(10)	-111.2(3)	C(13)-C(8)-C(9)-O(1)	-175.4(3)
C(7)-C(8)-C(9)-O(1)	8.2(4)	C(13)-C(8)-C(9)-C(10)	2.4(4)
C(7)-C(8)-C(9)-C(10)	-174.0(3)	O(1)-C(9)-C(10)-C(11)	176.0(3)
C(8)-C(9)-C(10)-C(11)	-1.9(4)	C(9)-C(10)-C(11)-C(12)	0.3(5)
C(10)-C(11)-C(12)-C(13)	0.6(5)	C(9)-C(8)-C(13)-C(12)	-1.5(4)
C(7)-C(8)-C(13)-C(12)	174.8(3)	C(11)-C(12)-C(13)-C(8)	0.0(5)
C(6)-N(1)-C(14)-C(14)#1	161.1(3)	C(7)-N(1)-C(14)-C(14)#1	-81.3(3)
Re(1)-N(1)-C(14)-C(14)#1	43.9(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2 #2 -x,y,-z+1/2

Table Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Ru}(\text{ocbbpen})]\text{PF}_6$

	x	y	z	U(eq)	SOF
H(2)	411(38)	6867(42)	775(35)	44(11)	1
H(3)	-167(3)	8926(4)	1195(3)	42(10)	1
H(4)	1341(3)	10385(3)	2220(3)	33(9)	1
H(5)	3335(3)	9748(3)	2758(3)	22(8)	1
H(6B)	2802(3)	5783(3)	665(2)	24(8)	1
H(6A)	2048(3)	5105(3)	1343(2)	27(8)	1
H(7A)	2680(3)	4893(3)	3171(2)	16(7)	1
H(7B)	4072(3)	4682(3)	3884(2)	19(7)	1
H(10)	5288(3)	8818(3)	5535(2)	19(8)	1
H(11)	3645(3)	9289(3)	6060(3)	45(11)	1
H(12)	1894(3)	8049(3)	5367(3)	25(8)	1
H(13)	1782(3)	6289(3)	4143(2)	29(9)	1
H(14B)	4277(3)	4337(3)	1327(2)	21(8)	1
H(14A)	3944(3)	3572(3)	2279(2)	23(8)	1