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Table S1. Crystallographic data and Structure Refinement for [ReO(RP294)].

Identification code	[ReO(RP294)]
Empirical formula	$C_{12}\ H_{20}\ N_5\ O_6\ Re\ S$
Formula weight	548.59 g/mole
Temperature	300(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a= 6.954(1) Å
	b = 8.0472(1) Å
	c = 32.9183(4) Å
Volume, Z	1842.01(3) Å^3 , 4
Density (calculated)	1.978 g/cm^3
Absorption coefficient	6.748 mm^{-1}
F(000)	1064
Crystal size	0.4 x 0.2 x 0.2 mm
Theta range for data collection	2.47 to 26.38°
Limiting indices	-8<=h<=8, -9<=k<=9, -40<=l<=40
Reflections collected	10447
Independent reflections	3698 [R(int) = 0.0273]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3698 / 0 / 235
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0838
R indices (all data)	R1 = 0.0335, wR2 = 0.0843
Absolute structure parameter	0.03(2)
Largest diff. peak and hole	1.562 and -2.317 e. Å^{-3}

Table S2. Bond lengths [Å] and angles [°] for [ReO(RP294)].

Re(1)-O(1)	1.682(5)	N(4)-C(5)	1.453(9)
Re(1)-N(7)	1.954(6)	C(8)-N(7)	1.490(8)
Re(1)-N(4)	1.980(5)	C(8)-C(17)	1.521(10)
Re(1)-N(1)	2.165(6)	C(8)-C(9)	1.530(11)
Re(1)-S(1)	2.281(2)	C(19)-C(20)	1.504(11)
S(1)-C(9)	1.827(9)	O(17)-C(17)	1.214(10)
N(1)-C(2)	1.483(9)	C(14)-O(15)	1.401(9)
N(1)-C(11)	1.493(10)	C(14)-C(5)	1.525(10)
N(1)-C(12)	1.514(10)	C(6)-N(7)	1.365(9)
O(13)-C(3)	1.197(10)	C(6)-C(5)	1.509(9)
N(18)-C(17)	1.340(10)	C(2)-C(3)	1.516(11)
N(18)-C(19)	1.449(9)	C(20)-O(20)	1.229(10)
O(16)-C(6)	1.236(9)	C(20)-N(20)	1.328(11)
N(4)-C(3)	1.380(9)		
O(1)-Re(1)-N(7)	113.0(3)	N(7)-C(6)-C(5)	113.9(6)
O(1)-Re(1)-N(4)	111.2(2)	N(1)-C(2)-C(3)	110.0(6)
N(7)-Re(1)-N(4)	78.1(2)	O(20)-C(20)-N(20)	123.0(8)
O(1)-Re(1)-N(1)	109.8(3)	O(20)-C(20)-C(19)	123.6(8)
N(7)-Re(1)-N(1)	135.9(2)	N(20)-C(20)-C(19)	113.4(7)
N(4)-Re(1)-N(1)	77.4(2)	O(17)-C(17)-N(18)	122.5(7)
O(1)-Re(1)-S(1)	108.7(2)	O(17)-C(17)-C(8)	123.0(7)
N(7)-Re(1)-S(1)	83.5(2)	N(18)-C(17)-C(8)	114.5(6)
N(4)-Re(1)-S(1)	140.0(2)	C(6)-N(7)-C(8)	114.8(6)
N(1)-Re(1)-S(1)	92.5(2)	C(6)-N(7)-Re(1)	120.2(5)
C(9)-S(1)-Re(1)	96.8(3)	C(8)-N(7)-Re(1)	124.0(4)
C(2)-N(1)-C(11)	109.6(7)	N(4)-C(5)-C(6)	106.2(5)
C(2)-N(1)-C(12)	110.3(6)	N(4)-C(5)-C(14)	114.7(6)
C(11)-N(1)-C(12)	108.8(7)	C(6)-C(5)-C(14)	109.8(6)
C(2)-N(1)-Re(1)	105.3(4)	O(13)-C(3)-N(4)	125.4(8)
C(11)-N(1)-Re(1)	113.5(5)	O(13)-C(3)-C(2)	123.2(7)
C(12)-N(1)-Re(1)	109.3(5)	N(4)-C(3)-C(2)	111.3(6)
C(17)-N(18)-C(19)	120.0(7)	C(8)-C(9)-S(1)	110.5(5)
C(3)-N(4)-C(5)	121.0(6)	C(17)-C(8)-C(9)	112.5(6)
C(3)-N(4)-Re(1)	119.6(5)	N(18)-C(19)-C(20)	114.0(7)
C(5)-N(4)-Re(1)	119.4(4)	O(15)-C(14)-C(5)	112.6(6)
N(7)-C(8)-C(17)	110.4(6)	O(16)-C(6)-N(7)	124.2(7)
N(7)-C(8)-C(9)	108.6(6)	O(16)-C(6)-C(5)	121.9(7)

Table S3. Anisotropic Thermal Parameters ($Å^2 \times 10^3$) for [ReO(RP294)].

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Re(1)	20(1)	21(1)	18(1)	3(1)	0(1)	3(1)
S(1)	32(1)	35(1)	23(1)	-1(1)	-10(1)	-4(1)
N(1)	25(3)	21(3)	28(3)	-5(2)	-2(2)	-2(3)
O(13)	31(4)	41(3)	51(3)	16(3)	-18(3)	5(3)
N(18)	36(3)	23(3)	10(3)	0(2)	4(2)	4(3)
O(16)	29(3)	31(3)	27(3)	10(2)	5(2)	1(2)
N(4)	19(3)	23(3)	19(3)	4(3)	-5(2)	1(2)
O(1)	23(3)	37(3)	18(3)	-2(2)	6(2)	6(2)
C(8)	33(4)	23(4)	15(3)	4(3)	1(3)	7(3)
C(19)	39(4)	30(4)	17(3)	5(3)	7(3)	-5(4)
O(17)	47(3)	27(3)	30(3)	-1(2)	7(3)	17(3)
C(14)	27(4)	27(4)	25(4)	-1(3)	-1(3)	-5(3)
C(6)	21(3)	17(3)	21(3)	-1(3)	8(3)	2(3)
C(2)	40(4)	20(4)	22(4)	11(3)	-4(3)	7(3)
C(20)	32(4)	25(4)	26(4)	2(3)	-2(3)	6(3)
C(17)	25(3)	24(4)	25(4)	0(3)	-2(3)	0(3)
N(7)	19(3)	26(3)	9(3)	5(2)	-1(2)	0(2)
C(5)	16(3)	24(3)	14(3)	4(3)	0(2)	3(3)
C(3)	28(4)	26(4)	23(4)	2(3)	-4(3)	5(3)
O(20)	27(3)	40(4)	51(4)	-13(3)	-2(3)	-5(3)
O(15)	50(4)	26(3)	34(3)	-1(3)	12(3)	6(3)
N(20)	33(3)	37(4)	48(5)	-25(4)	7(3)	1(3)
C(9)	28(4)	44(5)	18(4)	9(3)	-10(3)	0(4)
C(12)	50(5)	36(5)	39(5)	-24(4)	-2(4)	11(4)
C(11)	42(5)	39(5)	58(7)	2(5)	-5(5)	-17(4)
O(21)	32(3)	38(4)	79(5)	9(4)	8(3)	-3(3)

Table S4. Hydrogen Atom Coordinates (x 10^4) and Isotropic Thermal Parameters ($Å^2$ x 10^3) for [ReO(RP294)].

	x	y	z	B_{eq}
H(18A)	3947(9)	5145(8)	2283(2)	27
H(8A)	4526(10)	5222(10)	1598(2)	28
H(19A)	1682(12)	5170(10)	2754(2)	35
H(19B)	478(12)	6347(10)	2474(2)	35
H(14A)	-528(10)	5575(10)	506(2)	32
H(14B)	107(10)	6922(10)	189(2)	32
H(2A)	4113(12)	11205(10)	142(2)	33
H(2B)	2795(12)	12500(10)	366(2)	33
H(5A)	-212(9)	7997(9)	863(2)	22
H(15A)	2991(10)	5902(7)	240(2)	55
H(20A)	790(11)	9000(10)	3234(2)	47
H(20B)	-447(11)	7755(10)	3025(2)	47
H(9A)	7416(12)	6380(11)	1532(2)	36
H(9B)	6805(12)	7147(11)	1951(2)	36
H(12A)	4495(14)	12073(12)	1341(3)	63
H(12B)	2478(14)	11568(12)	1167(3)	63
H(12C)	3397(14)	13277(12)	1047(3)	63
H(11A)	7287(14)	12155(13)	896(3)	69
H(11B)	6201(14)	13351(13)	599(3)	69
H(11C)	7102(14)	11695(13)	435(3)	69