Supporting Information for

Formation and Reactivity of $[(tacn)\text{-}N\text{-}CO\text{-}Re^{III}Br(CO)_2]^+$ in Water: a Theoretical and Experimental Study

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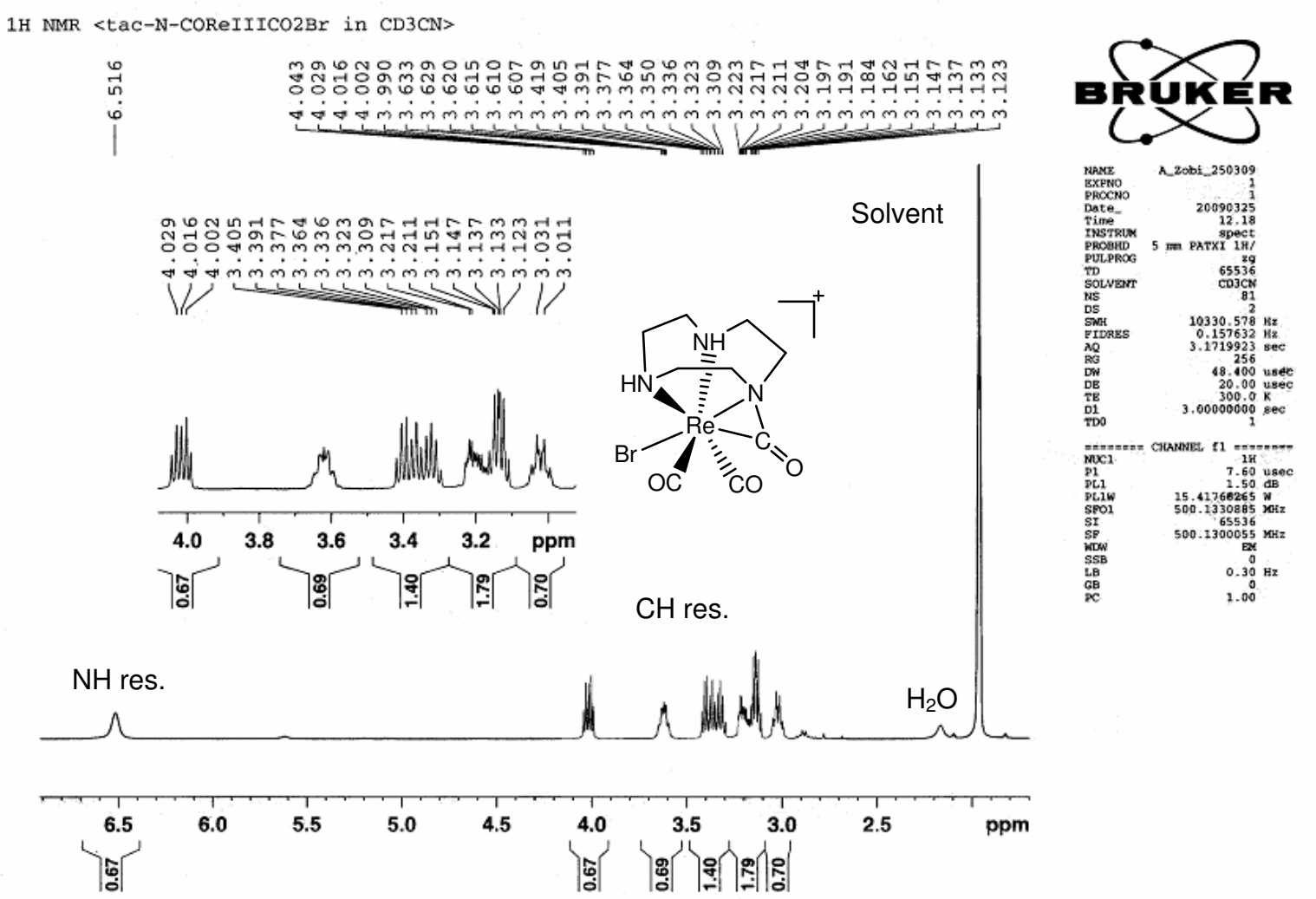

Figure S1. ^{1}H NMR spectrum of **2a** in CD_3CN.

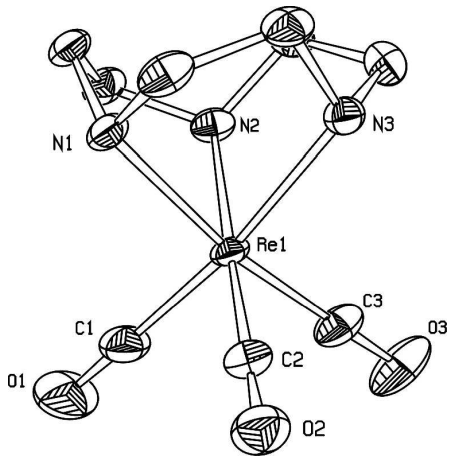

Figure S2. ORTEP presentation of $\mathbf{1}^{+}$ (50% probability of thermal ellipsoids).

Table S1. Crystal data and structure refinement for Structure **1**.

Empirical formula	C9 H15 Br N3 O3 Re	
Formula weight	479.35	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 13.75570(10) Å	α= 90°.
	b = 13.65620(10) Å	β= 90°.
	c = 14.77120(10) Å	γ = 90°.
Volume	2774.78(3) $Å^3$	
Z	8	
Density (calculated)	2.295 Mg/m^3	
Absorption coefficient	11.639 mm^{-1}	
F(000)	1792	
Crystal size	0.44 x 0.42 x 0.17 mm^3	
Crystal description	colorless block	
Theta range for data collection	2.51 to 33.14°.	
Index ranges	-21<=h<=20, -21<=k<=20, -22<=l<=22	
Reflections collected	77765	
Independent reflections	5288 [R(int) = 0.0640]	
Reflections observed	4290	
Criterion for observation	>2sigma(I)	
Completeness to theta = 33.14°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.2437 and 0.0792	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5288 / 0 / 154	
Goodness-of-fit on F^2	1.239	
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0760	
R indices (all data)	R1 = 0.0529, wR2 = 0.0890	
Largest diff. peak and hole	2.964 and -2.195 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Structure **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	6044(1)	1992(1)	3961(1)	20(1)
Br(1)	9115(1)	1560(1)	3491(1)	30(1)
C(1)	4934(4)	1221(4)	4300(5)	38(1)
C(2)	6813(4)	1362(4)	4875(4)	28(1)
C(3)	6400(4)	997(4)	3114(4)	33(1)
C(4)	4986(4)	3972(4)	4289(4)	28(1)
C(5)	4521(4)	3462(4)	3490(4)	29(1)
C(6)	5931(4)	3580(4)	2447(4)	31(1)
C(7)	6989(4)	3287(4)	2572(4)	30(1)
C(8)	7209(4)	3936(4)	4129(4)	29(1)
C(9)	6629(4)	3785(4)	4982(4)	30(1)
N(1)	5691(3)	3301(3)	4766(3)	24(1)
N(2)	5271(3)	2913(3)	2979(3)	25(1)
N(3)	7170(3)	3044(3)	3539(3)	24(1)
O(1)	4267(4)	773(4)	4490(5)	65(2)
O(2)	7285(3)	1008(3)	5428(3)	37(1)
O(3)	6608(4)	405(4)	2589(4)	56(1)

Table **S3**. Bond lengths [Å] and angles [°] for Structure **1**.

Re(1)-C(3)	1.911(5)	C(3)-Re(1)-C(2)	90.1(2)
Re(1)-C(2)	1.919(5)	C(3)-Re(1)-C(1)	89.1(3)
Re(1)-C(1)	1.922(6)	C(2)-Re(1)-C(1)	90.5(3)
Re(1)-N(2)	2.195(4)	C(3)-Re(1)-N(2)	95.7(2)
Re(1)-N(1)	2.201(4)	C(2)-Re(1)-N(2)	171.52(19)
Re(1)-N(3)	2.203(4)	C(1)-Re(1)-N(2)	95.8(2)
C(1)-O(1)	1.137(7)	C(3)-Re(1)-N(1)	171.0(2)
C(2)-O(2)	1.150(7)	C(2)-Re(1)-N(1)	96.07(19)
C(3)-O(3)	1.155(7)	C(1)-Re(1)-N(1)	97.4(2)
C(4)-N(1)	1.508(6)	N(2)-Re(1)-N(1)	77.55(16)
C(4)-C(5)	1.511(8)	C(3)-Re(1)-N(3)	95.7(2)
C(4)-H(4A)	0.9900	C(2)-Re(1)-N(3)	96.0(2)
C(4)-H(4B)	0.9900	C(1)-Re(1)-N(3)	171.9(2)
C(5)-N(2)	1.482(7)	N(2)-Re(1)-N(3)	77.27(16)
C(5)-H(5A)	0.9900	N(1)-Re(1)-N(3)	77.17(16)
C(5)-H(5B)	0.9900	O(1)-C(1)-Re(1)	178.8(7)
C(6)-N(2)	1.506(7)	O(2)-C(2)-Re(1)	178.2(5)
C(6)-C(7)	1.521(8)	O(3)-C(3)-Re(1)	178.8(6)
C(6)-H(6A)	0.9900	N(1)-C(4)-C(5)	110.9(4)
C(6)-H(6B)	0.9900	N(1)-C(4)-H(4A)	109.5
C(7)-N(3)	1.488(7)	C(5)-C(4)-H(4A)	109.5
C(7)-H(7A)	0.9900	N(1)-C(4)-H(4B)	109.5
C(7)-H(7B)	0.9900	C(5)-C(4)-H(4B)	109.5
C(8)-N(3)	1.497(6)	H(4A)-C(4)-H(4B)	108.0
C(8)-C(9)	1.506(8)	N(2)-C(5)-C(4)	109.7(4)
C(8)-H(8A)	0.9900	N(2)-C(5)-H(5A)	109.7
C(8)-H(8B)	0.9900	C(4)-C(5)-H(5A)	109.7
C(9)-N(1)	1.486(7)	N(2)-C(5)-H(5B)	109.7
C(9)-H(9A)	0.9900	C(4)-C(5)-H(5B)	109.7
C(9)-H(9B)	0.9900	H(5A)-C(5)-H(5B)	108.2
N(1)-H(1A)	0.9300	N(2)-C(6)-C(7)	110.8(4)
N(2)-H(2A)	0.9300	N(2)-C(6)-H(6A)	109.5
N(3)-H(3A)	0.9300	C(7)-C(6)-H(6A)	109.5
		N(2)-C(6)-H(6B)	109.5

C(7)-C(6)-H(6B)	109.5	C(8)-N(3)-H(3A)	107.9
H(6A)-C(6)-H(6B)	108.1	Re(1)-N(3)-H(3A)	107.9
N(3)-C(7)-C(6)	109.6(4)		
N(3)-C(7)-H(7A)	109.8		
C(6)-C(7)-H(7A)	109.8		
N(3)-C(7)-H(7B)	109.8		
C(6)-C(7)-H(7B)	109.8		
H(7A)-C(7)-H(7B)	108.2		
N(3)-C(8)-C(9)	110.9(4)		
N(3)-C(8)-H(8A)	109.5		
C(9)-C(8)-H(8A)	109.5		
N(3)-C(8)-H(8B)	109.5		
C(9)-C(8)-H(8B)	109.5		
H(8A)-C(8)-H(8B)	108.0		
N(1)-C(9)-C(8)	109.9(4)		
N(1)-C(9)-H(9A)	109.7		
C(8)-C(9)-H(9A)	109.7		
N(1)-C(9)-H(9B)	109.7		
C(8)-C(9)-H(9B)	109.7		
H(9A)-C(9)-H(9B)	108.2		
C(9)-N(1)-C(4)	112.9(4)		
C(9)-N(1)-Re(1)	106.6(3)		
C(4)-N(1)-Re(1)	112.5(3)		
C(9)-N(1)-H(1A)	108.2		
C(4)-N(1)-H(1A)	108.2		
Re(1)-N(1)-H(1A)	108.2		
C(5)-N(2)-C(6)	112.3(4)		
C(5)-N(2)-Re(1)	106.9(3)		
C(6)-N(2)-Re(1)	113.5(3)		
C(5)-N(2)-H(2A)	108.0		
C(6)-N(2)-H(2A)	108.0		
Re(1)-N(2)-H(2A)	108.0		
C(7)-N(3)-C(8)	112.5(4)		
C(7)-N(3)-Re(1)	107.4(3)		
C(8)-N(3)-Re(1)	113.0(3)		
C(7)-N(3)-H(3A)	107.9		

Table S4. Anisotropic displacement parameters ($Å^2$x 10^3)for Structure **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	20(1)	10(1)	31(1)	-1(1)	0(1)	1(1)
Br(1)	27(1)	30(1)	35(1)	11(1)	2(1)	2(1)
C(1)	31(3)	22(2)	61(4)	7(2)	3(3)	-2(2)
C(2)	33(2)	18(2)	34(3)	1(2)	2(2)	3(2)
C(3)	34(3)	22(2)	44(3)	-10(2)	-7(2)	4(2)
C(4)	26(2)	18(2)	39(3)	-3(2)	3(2)	6(2)
C(5)	21(2)	23(2)	43(3)	1(2)	-4(2)	6(2)
C(6)	38(3)	25(2)	28(2)	2(2)	0(2)	-3(2)
C(7)	30(2)	32(3)	29(2)	2(2)	3(2)	-3(2)
C(8)	28(2)	18(2)	40(3)	-5(2)	-5(2)	-6(2)
C(9)	35(3)	21(2)	33(3)	-8(2)	-9(2)	4(2)
N(1)	29(2)	18(2)	26(2)	0(2)	1(2)	8(2)
N(2)	27(2)	19(2)	29(2)	-1(2)	-7(2)	-1(2)
N(3)	22(2)	19(2)	30(2)	0(2)	0(2)	0(1)
O(1)	43(3)	42(3)	110(5)	19(3)	11(3)	-15(2)
O(2)	44(2)	33(2)	35(2)	6(2)	-2(2)	8(2)
O(3)	60(3)	39(3)	68(3)	-32(2)	-15(3)	19(2)

Table S5. Torsion angles [°] for Structure **1**.

C(3)-Re(1)-C(1)-O(1)	-90(35)
C(2)-Re(1)-C(1)-O(1)	180(100)
N(2)-Re(1)-C(1)-O(1)	5(35)
N(1)-Re(1)-C(1)-O(1)	83(35)
N(3)-Re(1)-C(1)-O(1)	36(36)
C(3)-Re(1)-C(2)-O(2)	130(16)
C(1)-Re(1)-C(2)-O(2)	-141(16)
N(2)-Re(1)-C(2)-O(2)	-3(17)
N(1)-Re(1)-C(2)-O(2)	-44(16)
N(3)-Re(1)-C(2)-O(2)	34(16)
C(2)-Re(1)-C(3)-O(3)	-166(28)
C(1)-Re(1)-C(3)-O(3)	103(28)
N(2)-Re(1)-C(3)-O(3)	7(28)
N(1)-Re(1)-C(3)-O(3)	-33(29)
N(3)-Re(1)-C(3)-O(3)	-70(28)
N(1)-C(4)-C(5)-N(2)	-43.7(6)
N(2)-C(6)-C(7)-N(3)	-42.2(6)
N(3)-C(8)-C(9)-N(1)	-43.3(6)
C(8)-C(9)-N(1)-C(4)	-72.1(5)
C(8)-C(9)-N(1)-Re(1)	51.9(4)
C(5)-C(4)-N(1)-C(9)	134.4(5)
C(5)-C(4)-N(1)-Re(1)	13.6(5)
C(3)-Re(1)-N(1)-C(9)	-71.7(14)
C(2)-Re(1)-N(1)-C(9)	61.0(4)
C(1)-Re(1)-N(1)-C(9)	152.3(4)
N(2)-Re(1)-N(1)-C(9)	-113.3(3)
N(3)-Re(1)-N(1)-C(9)	-33.7(3)
C(3)-Re(1)-N(1)-C(4)	52.6(14)
C(2)-Re(1)-N(1)-C(4)	-174.7(4)
C(1)-Re(1)-N(1)-C(4)	-83.4(4)
N(2)-Re(1)-N(1)-C(4)	11.0(3)
N(3)-Re(1)-N(1)-C(4)	90.6(3)
C(4)-C(5)-N(2)-C(6)	-73.0(5)
C(4)-C(5)-N(2)-Re(1)	52.1(5)

C(7)-C(6)-N(2)-C(5)	134.2(5)
C(7)-C(6)-N(2)-Re(1)	12.9(5)
C(3)-Re(1)-N(2)-C(5)	152.3(3)
C(2)-Re(1)-N(2)-C(5)	-75.5(14)
C(1)-Re(1)-N(2)-C(5)	62.6(4)
N(1)-Re(1)-N(2)-C(5)	-33.7(3)
N(3)-Re(1)-N(2)-C(5)	-113.2(3)
C(3)-Re(1)-N(2)-C(6)	-83.4(4)
C(2)-Re(1)-N(2)-C(6)	48.8(15)
C(1)-Re(1)-N(2)-C(6)	-173.1(4)
N(1)-Re(1)-N(2)-C(6)	90.6(3)
N(3)-Re(1)-N(2)-C(6)	11.2(3)
C(6)-C(7)-N(3)-C(8)	-74.1(5)
C(6)-C(7)-N(3)-Re(1)	50.9(5)
C(9)-C(8)-N(3)-C(7)	134.9(5)
C(9)-C(8)-N(3)-Re(1)	13.0(5)
C(3)-Re(1)-N(3)-C(7)	61.2(4)
C(2)-Re(1)-N(3)-C(7)	151.9(3)
C(1)-Re(1)-N(3)-C(7)	-65.1(18)
N(2)-Re(1)-N(3)-C(7)	-33.3(3)
N(1)-Re(1)-N(3)-C(7)	-113.2(3)
C(3)-Re(1)-N(3)-C(8)	-174.1(4)
C(2)-Re(1)-N(3)-C(8)	-83.4(4)
C(1)-Re(1)-N(3)-C(8)	59.7(18)
N(2)-Re(1)-N(3)-C(8)	91.4(3)
N(1)-Re(1)-N(3)-C(8)	11.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S6. Crystal data and structure refinement for Structure **2a**.

Empirical formula	C9 H14 Br2 Cl2 N3 O3 Re	
Formula weight	629.15	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.0293(2) Å	α= 77.459(2)°.
	b = 14.1786(3) Å	β= 87.532(2)°.
	c = 14.7420(4) Å	γ = 89.378(2)°.
Volume	1636.73(7) $Å^3$	
Z	4	
Density (calculated)	2.553 Mg/m^3	
Absorption coefficient	12.641 mm^{-1}	
F(000)	1168	
Crystal size	0.38 x 0.20 x 0.08 mm^3	
Crystal description	yellow plate	
Theta range for data collection	2.25 to 30.51°.	
Index ranges	-11<=h<=11, -20<=k<=20, -21<=l<=21	
Reflections collected	25692	
Independent reflections	9964 [R(int) = 0.0710]	
Reflections observed	7406	
Criterion for observation	>2sigma(I)	
Completeness to theta = 30.51°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4201 and 0.0857	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9964 / 18 / 361	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0590, wR2 = 0.1514	
R indices (all data)	R1 = 0.0834, wR2 = 0.1607	
Largest diff. peak and hole	4.869 and -3.025 $e.Å^{-3}$	

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Structure **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	9810(1)	8535(1)	8847(1)	20(1)
Re(2)	5573(1)	12077(1)	5807(1)	23(1)
Br(1)	9559(1)	8100(1)	10616(1)	32(1)
Br(2)	5394(2)	13042(1)	4139(1)	43(1)
Br(3)	4769(1)	6075(1)	10855(1)	37(1)
Cl(10)	4792(5)	4613(2)	11870(3)	69(1)
Cl(11)	4717(3)	7759(2)	9860(2)	39(1)
Br(6)	10086(1)	5451(1)	6563(1)	31(1)
Cl(8)	10636(4)	4434(2)	7942(2)	44(1)
Cl(9)	9514(3)	6640(2)	5049(2)	45(1)
C(1)	9959(14)	9434(6)	7604(6)	30(2)
C(2)	11592(13)	9345(6)	9018(6)	27(2)
C(3)	8002(14)	9453(6)	8980(6)	29(2)
C(4)	5628(13)	10889(7)	6806(6)	29(2)
C(5)	7564(14)	11437(8)	5377(7)	35(2)
C(6)	3978(15)	11227(7)	5387(7)	37(2)
C(7)	11780(17)	8147(9)	7205(8)	49(3)
C(8)	12202(16)	7240(9)	7952(7)	42(3)
C(9)	10443(14)	6398(7)	9313(8)	41(3)
C(10)	8847(14)	6448(7)	8873(8)	40(3)
C(11)	7352(15)	7736(9)	7763(8)	44(3)
C(12)	8660(20)	8039(9)	7053(7)	54(4)
C(13)	7297(13)	11970(7)	7578(6)	30(2)
C(14)	7598(13)	13014(7)	7127(7)	30(2)
C(15)	5911(14)	14123(7)	5968(7)	33(2)
C(16)	4251(12)	13896(7)	6434(7)	30(2)
C(17)	2802(12)	12370(6)	7113(6)	29(2)
C(18)	4128(13)	11941(7)	7794(6)	29(2)
N(1)	10115(11)	8476(6)	7428(5)	33(2)
N(2)	11463(11)	7292(6)	8885(5)	29(2)
N(3)	8051(10)	7422(6)	8709(6)	31(2)

N(4)	5641(10)	11672(5)	7285(5)	25(2)
N(5)	7013(9)	13230(5)	6150(5)	24(2)
N(6)	3614(9)	12967(5)	6264(5)	23(2)
O(1)	9980(11)	10203(5)	7113(5)	44(2)
O(2)	12765(10)	9840(5)	9068(6)	43(2)
O(3)	6937(9)	9970(5)	9032(5)	38(2)
O(4)	5523(11)	10038(5)	7094(5)	42(2)
O(5)	8703(10)	11082(6)	5140(5)	44(2)
O(6)	3087(13)	10762(7)	5122(6)	63(3)

Table S8. Bond lengths [Å] and angles [°] for Structure **2a**.

Re(1)-C(2)	1.903(11)	C(9)-N(2)	1.519(14)
Re(1)-C(3)	1.971(9)	C(9)-H(9A)	0.9900
Re(1)-C(1)	1.992(9)	C(9)-H(9B)	0.9900
Re(1)-N(1)	2.115(7)	C(10)-N(3)	1.491(12)
Re(1)-N(3)	2.177(8)	C(10)-H(10A)	0.9900
Re(1)-N(2)	2.188(7)	C(10)-H(10B)	0.9900
Re(1)-Br(1)	2.5459(9)	C(11)-C(12)	1.451(17)
Re(2)-C(6)	1.975(11)	C(11)-N(3)	1.499(13)
Re(2)-C(5)	1.978(11)	C(11)-H(11A)	0.9900
Re(2)-C(4)	1.983(9)	C(11)-H(11B)	0.9900
Re(2)-N(4)	2.133(7)	C(12)-N(1)	1.508(17)
Re(2)-N(5)	2.171(8)	C(12)-H(12A)	0.9900
Re(2)-N(6)	2.180(7)	C(12)-H(12B)	0.9900
Re(2)-Br(2)	2.5507(10)	C(13)-C(14)	1.504(14)
Br(3)-Cl(10)	2.277(3)	C(13)-N(4)	1.507(13)
Br(3)-Cl(11)	2.518(3)	C(13)-H(13A)	0.9900
Br(6)-Cl(8)	2.280(3)	C(13)-H(13B)	0.9900
Br(6)-Cl(9)	2.545(3)	C(14)-N(5)	1.501(11)
C(1)-O(1)	1.170(11)	C(14)-H(14A)	0.9900
C(1)-N(1)	1.439(11)	C(14)-H(14B)	0.9900
C(2)-O(2)	1.195(13)	C(15)-C(16)	1.478(14)
C(3)-O(3)	1.131(11)	C(15)-N(5)	1.519(11)
C(4)-O(4)	1.192(11)	C(15)-H(15A)	0.9900
C(4)-N(4)	1.440(11)	C(15)-H(15B)	0.9900
C(5)-O(5)	1.118(12)	C(16)-N(6)	1.493(12)
C(6)-O(6)	1.115(14)	C(16)-H(16A)	0.9900
C(7)-N(1)	1.459(13)	C(16)-H(16B)	0.9900
C(7)-C(8)	1.546(16)	C(17)-N(6)	1.480(11)
C(7)-H(7A)	0.9900	C(17)-C(18)	1.525(13)
C(7)-H(7B)	0.9900	C(17)-H(17A)	0.9900
C(8)-N(2)	1.490(12)	C(17)-H(17B)	0.9900
C(8)-H(8A)	0.9900	C(18)-N(4)	1.490(12)
C(8)-H(8B)	0.9900	C(18)-H(18A)	0.9900
C(9)-C(10)	1.456(15)	C(18)-H(18B)	0.9900

N(2)-H(2)	0.9300	C(6)-Re(2)-N(6)	93.5(4)
N(3)-H(3)	0.9300	C(5)-Re(2)-N(6)	171.6(4)
N(5)-H(5)	0.9300	C(4)-Re(2)-N(6)	104.9(3)
N(6)-H(6)	0.9300	N(4)-Re(2)-N(6)	77.1(3)
		N(5)-Re(2)-N(6)	78.4(3)
C(2)-Re(1)-C(3)	96.4(4)	C(6)-Re(2)-Br(2)	82.7(3)
C(2)-Re(1)-C(1)	79.4(4)	C(5)-Re(2)-Br(2)	87.3(3)
C(3)-Re(1)-C(1)	78.9(4)	C(4)-Re(2)-Br(2)	155.6(3)
C(2)-Re(1)-N(1)	103.3(4)	N(4)-Re(2)-Br(2)	163.5(2)
C(3)-Re(1)-N(1)	108.7(3)	N(5)-Re(2)-Br(2)	90.07(19)
C(1)-Re(1)-N(1)	40.9(3)	N(6)-Re(2)-Br(2)	90.42(18)
C(2)-Re(1)-N(3)	170.9(3)	Cl(10)-Br(3)-Cl(11)	174.80(13)
C(3)-Re(1)-N(3)	92.2(4)	Cl(8)-Br(6)-Cl(9)	177.74(11)
C(1)-Re(1)-N(3)	105.4(4)	O(1)-C(1)-N(1)	132.7(9)
N(1)-Re(1)-N(3)	76.8(3)	O(1)-C(1)-Re(1)	153.2(8)
C(2)-Re(1)-N(2)	92.6(3)	N(1)-C(1)-Re(1)	74.1(5)
C(3)-Re(1)-N(2)	167.8(4)	O(2)-C(2)-Re(1)	175.3(8)
C(1)-Re(1)-N(2)	111.0(3)	O(3)-C(3)-Re(1)	177.6(9)
N(1)-Re(1)-N(2)	77.1(3)	O(4)-C(4)-N(4)	131.0(8)
N(3)-Re(1)-N(2)	78.6(3)	O(4)-C(4)-Re(2)	153.2(8)
C(2)-Re(1)-Br(1)	85.0(3)	N(4)-C(4)-Re(2)	75.2(5)
C(3)-Re(1)-Br(1)	83.6(2)	O(5)-C(5)-Re(2)	179.1(10)
C(1)-Re(1)-Br(1)	155.0(3)	O(6)-C(6)-Re(2)	177.8(10)
N(1)-Re(1)-Br(1)	164.0(2)	N(1)-C(7)-C(8)	108.3(9)
N(3)-Re(1)-Br(1)	92.9(2)	N(1)-C(7)-H(7A)	110.0
N(2)-Re(1)-Br(1)	88.9(2)	C(8)-C(7)-H(7A)	110.0
C(6)-Re(2)-C(5)	94.3(5)	N(1)-C(7)-H(7B)	110.0
C(6)-Re(2)-C(4)	77.6(4)	C(8)-C(7)-H(7B)	110.0
C(5)-Re(2)-C(4)	80.0(4)	H(7A)-C(7)-H(7B)	108.4
C(6)-Re(2)-N(4)	108.5(4)	N(2)-C(8)-C(7)	111.7(8)
C(5)-Re(2)-N(4)	103.5(3)	N(2)-C(8)-H(8A)	109.3
C(4)-Re(2)-N(4)	40.8(3)	C(7)-C(8)-H(8A)	109.3
C(6)-Re(2)-N(5)	169.2(4)	N(2)-C(8)-H(8B)	109.3
C(5)-Re(2)-N(5)	93.5(4)	C(7)-C(8)-H(8B)	109.3
C(4)-Re(2)-N(5)	111.3(3)	H(8A)-C(8)-H(8B)	107.9
N(4)-Re(2)-N(5)	77.0(3)	C(10)-C(9)-N(2)	109.6(8)

C(10)-C(9)-H(9A)	109.7	C(16)-C(15)-H(15A)	109.7
N(2)-C(9)-H(9A)	109.7	N(5)-C(15)-H(15A)	109.7
C(10)-C(9)-H(9B)	109.7	C(16)-C(15)-H(15B)	109.7
N(2)-C(9)-H(9B)	109.7	N(5)-C(15)-H(15B)	109.7
H(9A)-C(9)-H(9B)	108.2	H(15A)-C(15)-H(15B)	108.2
C(9)-C(10)-N(3)	114.1(9)	C(15)-C(16)-N(6)	110.5(7)
C(9)-C(10)-H(10A)	108.7	C(15)-C(16)-H(16A)	109.5
N(3)-C(10)-H(10A)	108.7	N(6)-C(16)-H(16A)	109.5
C(9)-C(10)-H(10B)	108.7	C(15)-C(16)-H(16B)	109.5
N(3)-C(10)-H(10B)	108.7	N(6)-C(16)-H(16B)	109.5
H(10A)-C(10)-H(10B)	107.6	H(16A)-C(16)-H(16B)	108.1
C(12)-C(11)-N(3)	111.5(10)	N(6)-C(17)-C(18)	109.5(8)
C(12)-C(11)-H(11A)	109.3	N(6)-C(17)-H(17A)	109.8
N(3)-C(11)-H(11A)	109.3	C(18)-C(17)-H(17A)	109.8
C(12)-C(11)-H(11B)	109.3	N(6)-C(17)-H(17B)	109.8
N(3)-C(11)-H(11B)	109.3	C(18)-C(17)-H(17B)	109.8
H(11A)-C(11)-H(11B)	108.0	H(17A)-C(17)-H(17B)	108.2
C(11)-C(12)-N(1)	111.7(8)	N(4)-C(18)-C(17)	110.4(7)
C(11)-C(12)-H(12A)	109.3	N(4)-C(18)-H(18A)	109.6
N(1)-C(12)-H(12A)	109.3	C(17)-C(18)-H(18A)	109.6
C(11)-C(12)-H(12B)	109.3	N(4)-C(18)-H(18B)	109.6
N(1)-C(12)-H(12B)	109.3	C(17)-C(18)-H(18B)	109.6
H(12A)-C(12)-H(12B)	107.9	H(18A)-C(18)-H(18B)	108.1
C(14)-C(13)-N(4)	108.7(7)	C(1)-N(1)-C(7)	117.6(10)
C(14)-C(13)-H(13A)	110.0	C(1)-N(1)-C(12)	119.3(8)
N(4)-C(13)-H(13A)	110.0	C(7)-N(1)-C(12)	117.2(9)
C(14)-C(13)-H(13B)	110.0	C(1)-N(1)-Re(1)	64.9(4)
N(4)-C(13)-H(13B)	110.0	C(7)-N(1)-Re(1)	111.8(7)
H(13A)-C(13)-H(13B)	108.3	C(12)-N(1)-Re(1)	114.3(7)
N(5)-C(14)-C(13)	110.2(7)	C(8)-N(2)-C(9)	111.6(8)
N(5)-C(14)-H(14A)	109.6	C(8)-N(2)-Re(1)	113.1(6)
C(13)-C(14)-H(14A)	109.6	C(9)-N(2)-Re(1)	106.7(6)
N(5)-C(14)-H(14B)	109.6	C(8)-N(2)-H(2)	108.4
C(13)-C(14)-H(14B)	109.6	C(9)-N(2)-H(2)	108.4
H(14A)-C(14)-H(14B)	108.1	Re(1)-N(2)-H(2)	108.4
C(16)-C(15)-N(5)	110.0(8)	C(10)-N(3)-C(11)	113.8(8)

C(10)-N(3)-Re(1)	111.6(6)
C(11)-N(3)-Re(1)	106.4(7)
C(10)-N(3)-H(3)	108.3
C(11)-N(3)-H(3)	108.3
Re(1)-N(3)-H(3)	108.3
C(4)-N(4)-C(18)	121.7(8)
C(4)-N(4)-C(13)	117.8(7)
C(18)-N(4)-C(13)	116.6(7)
C(4)-N(4)-Re(2)	64.0(4)
C(18)-N(4)-Re(2)	114.8(5)
C(13)-N(4)-Re(2)	108.8(6)
C(14)-N(5)-C(15)	111.3(7)
C(14)-N(5)-Re(2)	114.2(6)
C(15)-N(5)-Re(2)	106.2(6)
C(14)-N(5)-H(5)	108.3
C(15)-N(5)-H(5)	108.3
Re(2)-N(5)-H(5)	108.3
C(17)-N(6)-C(16)	111.7(7)
C(17)-N(6)-Re(2)	106.6(5)
C(16)-N(6)-Re(2)	113.0(6)
C(17)-N(6)-H(6)	108.5
C(16)-N(6)-H(6)	108.5
Re(2)-N(6)-H(6)	108.5

Table S9. Anisotropic displacement parameters ($Å^2$x 10^3)for Structure **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	23(1)	20(1)	15(1)	-5(1)	0(1)	2(1)
Re(2)	25(1)	27(1)	16(1)	-4(1)	-1(1)	4(1)
Br(1)	36(1)	42(1)	17(1)	-4(1)	0(1)	3(1)
Br(2)	45(1)	61(1)	19(1)	-1(1)	2(1)	16(1)
Br(3)	33(1)	41(1)	41(1)	-18(1)	-6(1)	1(1)
Cl(10)	76(3)	31(1)	95(3)	0(2)	-27(2)	-9(2)
Cl(11)	32(1)	48(1)	36(1)	-6(1)	-5(1)	-2(1)
Br(6)	27(1)	34(1)	35(1)	-17(1)	1(1)	-2(1)
Cl(8)	59(2)	34(1)	41(1)	-10(1)	-5(1)	1(1)
Cl(9)	24(1)	76(2)	31(1)	-5(1)	2(1)	5(1)
C(1)	46(4)	23(3)	19(3)	1(3)	-3(3)	8(3)
C(2)	45(4)	15(3)	19(3)	1(2)	3(3)	12(3)
C(3)	45(4)	21(3)	18(3)	0(3)	-2(3)	8(3)
C(4)	37(5)	30(4)	19(4)	-1(3)	-8(4)	2(4)
C(5)	41(6)	39(5)	25(4)	-5(4)	-2(4)	2(5)
C(6)	50(7)	27(5)	30(5)	2(4)	-6(5)	-5(4)
C(7)	60(8)	48(6)	34(5)	-4(5)	24(6)	18(6)
C(8)	44(7)	54(7)	30(5)	-15(5)	2(5)	13(5)
C(9)	43(6)	30(5)	52(7)	-11(5)	-16(6)	6(5)
C(10)	34(6)	28(5)	57(7)	-4(5)	10(5)	2(4)
C(11)	41(7)	51(7)	39(6)	-8(5)	-9(5)	-7(5)
C(12)	93(11)	48(7)	23(5)	-9(5)	-13(6)	2(7)
C(13)	36(5)	33(5)	27(4)	-15(4)	-15(4)	9(4)
C(14)	33(5)	27(4)	31(5)	-5(4)	-7(4)	-8(4)
C(15)	40(6)	27(4)	28(5)	0(4)	8(4)	6(4)
C(16)	27(5)	29(4)	33(5)	-7(4)	5(4)	2(4)
C(17)	31(5)	25(4)	30(5)	-2(4)	9(4)	-2(4)
C(18)	37(5)	25(4)	23(4)	-2(3)	5(4)	-7(4)
N(1)	40(5)	40(4)	22(4)	-11(3)	1(4)	17(4)
N(2)	32(4)	33(4)	28(4)	-17(3)	-8(3)	8(3)
N(3)	25(4)	41(4)	29(4)	-13(3)	-9(3)	-4(3)
N(4)	28(4)	28(4)	15(3)	1(3)	3(3)	-4(3)
N(5)	18(4)	32(4)	20(3)	-4(3)	1(3)	4(3)
N(6)	20(4)	26(4)	19(3)	-1(3)	-1(3)	5(3)

O(1)	63(6)	28(4)	34(4)	5(3)	6(4)	11(4)
O(2)	39(5)	37(4)	51(5)	-5(3)	1(4)	-6(3)
O(3)	31(4)	40(4)	43(4)	-10(3)	-6(3)	12(3)
O(4)	65(6)	25(3)	32(4)	-2(3)	-1(4)	2(3)
O(5)	41(5)	48(4)	42(4)	-12(4)	7(4)	19(4)
O(6)	69(7)	75(6)	53(5)	-32(5)	-20(5)	-12(5)

Table S10. Torsion angles [°] for Structure **2a**.

C(2)-Re(1)-C(1)-O(1)	-54(2)
C(3)-Re(1)-C(1)-O(1)	45(2)
N(1)-Re(1)-C(1)-O(1)	-179(2)
N(3)-Re(1)-C(1)-O(1)	134(2)
N(2)-Re(1)-C(1)-O(1)	-143(2)
Br(1)-Re(1)-C(1)-O(1)	-2(3)
C(2)-Re(1)-C(1)-N(1)	124.9(6)
C(3)-Re(1)-C(1)-N(1)	-136.4(7)
N(3)-Re(1)-C(1)-N(1)	-47.2(6)
N(2)-Re(1)-C(1)-N(1)	36.2(7)
Br(1)-Re(1)-C(1)-N(1)	177.1(5)
C(3)-Re(1)-C(2)-O(2)	-130(9)
C(1)-Re(1)-C(2)-O(2)	-52(9)
N(1)-Re(1)-C(2)-O(2)	-19(9)
N(3)-Re(1)-C(2)-O(2)	70(10)
N(2)-Re(1)-C(2)-O(2)	58(9)
Br(1)-Re(1)-C(2)-O(2)	147(9)
C(2)-Re(1)-C(3)-O(3)	139(22)
C(1)-Re(1)-C(3)-O(3)	62(22)
N(1)-Re(1)-C(3)-O(3)	33(22)
N(3)-Re(1)-C(3)-O(3)	-44(22)
N(2)-Re(1)-C(3)-O(3)	-84(22)
Br(1)-Re(1)-C(3)-O(3)	-136(22)
C(6)-Re(2)-C(4)-O(4)	30(2)
C(5)-Re(2)-C(4)-O(4)	-66(2)
N(4)-Re(2)-C(4)-O(4)	169(2)
N(5)-Re(2)-C(4)-O(4)	-156.2(19)
N(6)-Re(2)-C(4)-O(4)	120.6(19)
Br(2)-Re(2)-C(4)-O(4)	-7(3)
C(6)-Re(2)-C(4)-N(4)	-138.8(6)
C(5)-Re(2)-C(4)-N(4)	124.5(6)
N(5)-Re(2)-C(4)-N(4)	34.7(6)
N(6)-Re(2)-C(4)-N(4)	-48.5(6)
Br(2)-Re(2)-C(4)-N(4)	-175.8(5)
C(6)-Re(2)-C(5)-O(5)	-173(100)
C(4)-Re(2)-C(5)-O(5)	-97(66)
N(4)-Re(2)-C(5)-O(5)	-63(66)

N(5)-Re(2)-C(5)-O(5)	14(66)
N(6)-Re(2)-C(5)-O(5)	30(67)
Br(2)-Re(2)-C(5)-O(5)	104(66)
C(5)-Re(2)-C(6)-O(6)	-75(29)
C(4)-Re(2)-C(6)-O(6)	-154(29)
N(4)-Re(2)-C(6)-O(6)	179(100)
N(5)-Re(2)-C(6)-O(6)	60(30)
N(6)-Re(2)-C(6)-O(6)	101(29)
Br(2)-Re(2)-C(6)-O(6)	11(29)
N(1)-C(7)-C(8)-N(2)	-34.2(14)
N(2)-C(9)-C(10)-N(3)	-41.9(12)
N(3)-C(11)-C(12)-N(1)	-31.3(13)
N(4)-C(13)-C(14)-N(5)	-39.1(10)
N(5)-C(15)-C(16)-N(6)	-45.8(11)
N(6)-C(17)-C(18)-N(4)	-37.1(10)
O(1)-C(1)-N(1)-C(7)	76.6(16)
Re(1)-C(1)-N(1)-C(7)	-102.6(8)
O(1)-C(1)-N(1)-C(12)	-75.7(17)
Re(1)-C(1)-N(1)-C(12)	105.0(8)
O(1)-C(1)-N(1)-Re(1)	179.3(15)
C(8)-C(7)-N(1)-C(1)	119.5(10)
C(8)-C(7)-N(1)-C(12)	-87.5(12)
C(8)-C(7)-N(1)-Re(1)	47.3(11)
C(11)-C(12)-N(1)-C(1)	-74.6(12)
C(11)-C(12)-N(1)-C(7)	132.9(10)
C(11)-C(12)-N(1)-Re(1)	-0.8(12)
C(2)-Re(1)-N(1)-C(1)	-56.0(6)
C(3)-Re(1)-N(1)-C(1)	45.5(7)
N(3)-Re(1)-N(1)-C(1)	133.3(6)
N(2)-Re(1)-N(1)-C(1)	-145.6(6)
Br(1)-Re(1)-N(1)-C(1)	-175.6(8)
C(2)-Re(1)-N(1)-C(7)	55.4(8)
C(3)-Re(1)-N(1)-C(7)	156.9(8)
C(1)-Re(1)-N(1)-C(7)	111.4(10)
N(3)-Re(1)-N(1)-C(7)	-115.3(8)
N(2)-Re(1)-N(1)-C(7)	-34.2(7)
Br(1)-Re(1)-N(1)-C(7)	-64.2(14)
C(2)-Re(1)-N(1)-C(12)	-168.4(7)
C(3)-Re(1)-N(1)-C(12)	-66.9(8)

C(1)-Re(1)-N(1)-C(12)	-112.4(9)
N(3)-Re(1)-N(1)-C(12)	20.9(7)
N(2)-Re(1)-N(1)-C(12)	102.0(7)
Br(1)-Re(1)-N(1)-C(12)	72.0(12)
C(7)-C(8)-N(2)-C(9)	127.2(10)
C(7)-C(8)-N(2)-Re(1)	6.8(13)
C(10)-C(9)-N(2)-C(8)	-76.5(11)
C(10)-C(9)-N(2)-Re(1)	47.5(9)
C(2)-Re(1)-N(2)-C(8)	-88.9(8)
C(3)-Re(1)-N(2)-C(8)	134.0(15)
C(1)-Re(1)-N(2)-C(8)	-9.3(9)
N(1)-Re(1)-N(2)-C(8)	14.1(8)
N(3)-Re(1)-N(2)-C(8)	92.9(8)
Br(1)-Re(1)-N(2)-C(8)	-173.9(7)
C(2)-Re(1)-N(2)-C(9)	147.9(6)
C(3)-Re(1)-N(2)-C(9)	10.8(18)
C(1)-Re(1)-N(2)-C(9)	-132.4(6)
N(1)-Re(1)-N(2)-C(9)	-109.0(6)
N(3)-Re(1)-N(2)-C(9)	-30.2(6)
Br(1)-Re(1)-N(2)-C(9)	63.0(6)
C(9)-C(10)-N(3)-C(11)	135.4(10)
C(9)-C(10)-N(3)-Re(1)	14.9(12)
C(12)-C(11)-N(3)-C(10)	-75.8(12)
C(12)-C(11)-N(3)-Re(1)	47.5(10)
C(2)-Re(1)-N(3)-C(10)	-3(2)
C(3)-Re(1)-N(3)-C(10)	-162.6(7)
C(1)-Re(1)-N(3)-C(10)	118.3(7)
N(1)-Re(1)-N(3)-C(10)	88.7(7)
N(2)-Re(1)-N(3)-C(10)	9.4(7)
Br(1)-Re(1)-N(3)-C(10)	-78.9(7)
C(2)-Re(1)-N(3)-C(11)	-127(2)
C(3)-Re(1)-N(3)-C(11)	72.7(7)
C(1)-Re(1)-N(3)-C(11)	-6.4(7)
N(1)-Re(1)-N(3)-C(11)	-36.0(6)
N(2)-Re(1)-N(3)-C(11)	-115.3(7)
Br(1)-Re(1)-N(3)-C(11)	156.4(6)
O(4)-C(4)-N(4)-C(18)	-69.2(15)
Re(2)-C(4)-N(4)-C(18)	104.3(7)
O(4)-C(4)-N(4)-C(13)	87.9(14)

Re(2)-C(4)-N(4)-C(13)	-98.5(7)
O(4)-C(4)-N(4)-Re(2)	-173.5(14)
C(17)-C(18)-N(4)-C(4)	-68.5(10)
C(17)-C(18)-N(4)-C(13)	134.2(8)
C(17)-C(18)-N(4)-Re(2)	5.2(9)
C(14)-C(13)-N(4)-C(4)	120.9(8)
C(14)-C(13)-N(4)-C(18)	-80.8(9)
C(14)-C(13)-N(4)-Re(2)	50.9(8)
C(6)-Re(2)-N(4)-C(4)	42.7(7)
C(5)-Re(2)-N(4)-C(4)	-56.6(7)
N(5)-Re(2)-N(4)-C(4)	-147.1(6)
N(6)-Re(2)-N(4)-C(4)	132.1(6)
Br(2)-Re(2)-N(4)-C(4)	173.9(7)
C(6)-Re(2)-N(4)-C(18)	-72.1(7)
C(5)-Re(2)-N(4)-C(18)	-171.3(6)
C(4)-Re(2)-N(4)-C(18)	-114.8(9)
N(5)-Re(2)-N(4)-C(18)	98.2(6)
N(6)-Re(2)-N(4)-C(18)	17.3(6)
Br(2)-Re(2)-N(4)-C(18)	59.1(11)
C(6)-Re(2)-N(4)-C(13)	155.2(6)
C(5)-Re(2)-N(4)-C(13)	55.9(6)
C(4)-Re(2)-N(4)-C(13)	112.5(8)
N(5)-Re(2)-N(4)-C(13)	-34.6(5)
N(6)-Re(2)-N(4)-C(13)	-115.5(6)
Br(2)-Re(2)-N(4)-C(13)	-73.7(10)
C(13)-C(14)-N(5)-C(15)	130.5(9)
C(13)-C(14)-N(5)-Re(2)	10.2(10)
C(16)-C(15)-N(5)-C(14)	-74.3(10)
C(16)-C(15)-N(5)-Re(2)	50.6(8)
C(6)-Re(2)-N(5)-C(14)	135.1(19)
C(5)-Re(2)-N(5)-C(14)	-89.5(7)
C(4)-Re(2)-N(5)-C(14)	-8.8(7)
N(4)-Re(2)-N(5)-C(14)	13.6(6)
N(6)-Re(2)-N(5)-C(14)	92.9(6)
Br(2)-Re(2)-N(5)-C(14)	-176.7(6)
C(6)-Re(2)-N(5)-C(15)	12(2)
C(5)-Re(2)-N(5)-C(15)	147.5(6)
C(4)-Re(2)-N(5)-C(15)	-131.9(6)
N(4)-Re(2)-N(5)-C(15)	-109.5(6)

N(6)-Re(2)-N(5)-C(15)	-30.2(5)
Br(2)-Re(2)-N(5)-C(15)	60.2(5)
C(18)-C(17)-N(6)-C(16)	-73.2(9)
C(18)-C(17)-N(6)-Re(2)	50.6(8)
C(15)-C(16)-N(6)-C(17)	138.6(8)
C(15)-C(16)-N(6)-Re(2)	18.4(9)
C(6)-Re(2)-N(6)-C(17)	71.5(6)
C(5)-Re(2)-N(6)-C(17)	-132(2)
C(4)-Re(2)-N(6)-C(17)	-6.5(7)
N(4)-Re(2)-N(6)-C(17)	-36.6(6)
N(5)-Re(2)-N(6)-C(17)	-115.8(6)
Br(2)-Re(2)-N(6)-C(17)	154.3(6)
C(6)-Re(2)-N(6)-C(16)	-165.5(6)
C(5)-Re(2)-N(6)-C(16)	-9(2)
C(4)-Re(2)-N(6)-C(16)	116.5(6)
N(4)-Re(2)-N(6)-C(16)	86.4(6)
N(5)-Re(2)-N(6)-C(16)	7.3(6)
Br(2)-Re(2)-N(6)-C(16)	-82.7(6)

Symmetry transformations used to generate equivalent atoms:

Table S11. Crystal data and structure refinement for Structure **3**.

Empirical formula	C8 H15 Br N3 O2 Re	
Formula weight	451.34	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.9948(2) Å	α= 90°.
	b = 8.3696(2) Å	β= 92.410(2)°.
	c = 12.2745(2) Å	γ = 90°.
Volume	1128.53(4) $Å^3$	
Z	4	
Density (calculated)	2.656 Mg/m^3	
Absorption coefficient	14.293 mm^{-1}	
F(000)	840	
Crystal size	0.15 x 0.07 x 0.02 mm^3	
Crystal description	Colorless Plate	
Theta range for data collection	2.95 to 30.51°.	
Index ranges	-15<=h<=15, -11<=k<=11, -17<=l<=17	
Reflections collected	15827	
Independent reflections	3437 [R(int) = 0.0525]	
Reflections observed	2645	
Criterion for observation	>2sigma(I)	
Completeness to theta = 30.51°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7346 and 0.2215	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3437 / 93 / 145	
Goodness-of-fit on F^2	0.979	
Final R indices [I>2sigma(I)]	R1 = 0.0362, wR2 = 0.0700	
R indices (all data)	R1 = 0.0606, wR2 = 0.0747	
Largest diff. peak and hole	2.358 and -1.632 e.$Å^{-3}$	

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Structure **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	7519(1)	852(1)	4231(1)	15(1)
Br(1)	7796(1)	134(1)	6282(1)	29(1)
O(2)	5519(4)	3114(5)	4659(4)	31(1)
C(2)	6215(5)	2362(6)	4498(5)	18(1)
Br(1B)	5860(40)	2760(70)	4590(80)	23(2)
N(3)	8805(4)	-1085(5)	3809(4)	21(1)
O(1)	9309(4)	3620(6)	4417(4)	33(1)
N(2)	7359(4)	836(5)	2470(4)	19(1)
C(1)	8625(6)	2555(7)	4353(4)	22(1)
N(1)	6321(4)	-1262(5)	3906(4)	19(1)
C(6)	9052(6)	-1091(7)	2616(5)	24(1)
C(4)	5556(5)	-814(8)	2918(5)	26(1)
C(7)	6990(6)	-2792(7)	3780(5)	28(1)
C(3)	6366(6)	-261(8)	2027(5)	27(1)
C(5)	8565(6)	404(7)	2053(5)	25(1)
C(8)	8316(6)	-2631(7)	4185(5)	27(1)

Table S13. Bond lengths [Å] and angles [°] for Structure **3**.

Re(1)-C(1)	1.875(6)	C(1)-Re(1)-N(3)	99.0(2)
Re(1)-C(2)	1.949(5)	C(2)-Re(1)-N(3)	171.9(2)
Re(1)-N(2)	2.161(5)	N(2)-Re(1)-N(3)	77.82(18)
Re(1)-N(3)	2.227(5)	C(1)-Re(1)-N(1)	173.0(2)
Re(1)-N(1)	2.232(5)	C(2)-Re(1)-N(1)	96.4(2)
Re(1)-Br(1B)	2.48(2)	N(2)-Re(1)-N(1)	78.10(17)
Re(1)-Br(1)	2.5931(7)	N(3)-Re(1)-N(1)	75.93(18)
O(2)-C(2)	1.017(6)	C(1)-Re(1)-Br(1B)	88.6(15)
N(3)-C(8)	1.483(7)	C(2)-Re(1)-Br(1B)	1(2)
N(3)-C(6)	1.501(8)	N(2)-Re(1)-Br(1B)	99(2)
N(3)-H(3)	0.9300	N(3)-Re(1)-Br(1B)	171.9(16)
O(1)-C(1)	1.166(7)	N(1)-Re(1)-Br(1B)	96.2(15)
N(2)-C(5)	1.486(8)	C(1)-Re(1)-Br(1)	92.85(17)
N(2)-C(3)	1.511(7)	C(2)-Re(1)-Br(1)	92.54(17)
N(2)-H(2)	0.9300	N(2)-Re(1)-Br(1)	166.06(12)
N(1)-C(7)	1.488(8)	N(3)-Re(1)-Br(1)	90.40(12)
N(1)-C(4)	1.494(7)	N(1)-Re(1)-Br(1)	91.93(12)
N(1)-H(1)	0.9300	Br(1B)-Re(1)-Br(1)	92(2)
C(6)-C(5)	1.516(8)	O(2)-C(2)-Re(1)	177.5(5)
C(6)-H(6A)	0.9900	C(8)-N(3)-C(6)	112.6(4)
C(6)-H(6B)	0.9900	C(8)-N(3)-Re(1)	108.7(4)
C(4)-C(3)	1.512(9)	C(6)-N(3)-Re(1)	111.8(3)
C(4)-H(4A)	0.9900	C(8)-N(3)-H(3)	107.9
C(4)-H(4B)	0.9900	C(6)-N(3)-H(3)	107.9
C(7)-C(8)	1.527(9)	Re(1)-N(3)-H(3)	107.9
C(7)-H(7A)	0.9900	C(5)-N(2)-C(3)	111.7(5)
C(7)-H(7B)	0.9900	C(5)-N(2)-Re(1)	108.0(3)
C(3)-H(3A)	0.9900	C(3)-N(2)-Re(1)	113.1(4)
C(3)-H(3B)	0.9900	C(5)-N(2)-H(2)	108.0
C(5)-H(5A)	0.9900	C(3)-N(2)-H(2)	108.0
C(5)-H(5B)	0.9900	Re(1)-N(2)-H(2)	108.0
C(8)-H(8A)	0.9900	O(1)-C(1)-Re(1)	179.3(5)
C(8)-H(8B)	0.9900	C(7)-N(1)-C(4)	113.3(5)
		C(7)-N(1)-Re(1)	114.2(4)
C(1)-Re(1)-C(2)	88.4(3)	C(4)-N(1)-Re(1)	104.7(3)
C(1)-Re(1)-N(2)	96.3(2)	C(7)-N(1)-H(1)	108.1
C(2)-Re(1)-N(2)	98.2(2)	C(4)-N(1)-H(1)	108.1

Re(1)-N(1)-H(1)	108.1
N(3)-C(6)-C(5)	111.5(5)
N(3)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6A)	109.3
N(3)-C(6)-H(6B)	109.3
C(5)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
N(1)-C(4)-C(3)	109.6(5)
N(1)-C(4)-H(4A)	109.7
C(3)-C(4)-H(4A)	109.7
N(1)-C(4)-H(4B)	109.7
C(3)-C(4)-H(4B)	109.7
H(4A)-C(4)-H(4B)	108.2
N(1)-C(7)-C(8)	111.1(5)
N(1)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7A)	109.4
N(1)-C(7)-H(7B)	109.4
C(8)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
N(2)-C(3)-C(4)	111.3(5)
N(2)-C(3)-H(3A)	109.4
C(4)-C(3)-H(3A)	109.4
N(2)-C(3)-H(3B)	109.4
C(4)-C(3)-H(3B)	109.4
H(3A)-C(3)-H(3B)	108.0
N(2)-C(5)-C(6)	110.3(5)
N(2)-C(5)-H(5A)	109.6
C(6)-C(5)-H(5A)	109.6
N(2)-C(5)-H(5B)	109.6
C(6)-C(5)-H(5B)	109.6
H(5A)-C(5)-H(5B)	108.1
N(3)-C(8)-C(7)	109.3(5)
N(3)-C(8)-H(8A)	109.8
C(7)-C(8)-H(8A)	109.8
N(3)-C(8)-H(8B)	109.8
C(7)-C(8)-H(8B)	109.8
H(8A)-C(8)-H(8B)	108.3

Symmetry transformations used to generate equivalent atoms:

Table S14. Anisotropic displacement parameters ($Å^2$x 10^3)for Structure **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	17(1)	12(1)	16(1)	-1(1)	3(1)	-1(1)
Br(1)	38(1)	28(1)	22(1)	3(1)	0(1)	1(1)
O(2)	43(2)	33(2)	17(2)	4(2)	-2(2)	-13(2)
C(2)	29(2)	19(2)	5(2)	1(2)	-5(2)	-16(2)
Br(1B)	32(4)	23(4)	15(4)	-1(4)	2(4)	-8(4)
N(3)	21(2)	19(2)	22(2)	-5(2)	-4(2)	3(2)
O(1)	38(2)	32(2)	29(2)	-6(2)	5(2)	-13(2)
N(2)	23(2)	12(2)	24(2)	0(2)	0(2)	-3(2)
C(1)	31(2)	20(2)	15(2)	-3(2)	6(2)	-4(2)
N(1)	19(2)	17(2)	22(2)	0(2)	5(2)	-4(2)
C(6)	24(3)	21(3)	27(3)	-6(2)	6(2)	-4(2)
C(4)	19(3)	34(3)	27(3)	-7(3)	-3(2)	-9(3)
C(7)	36(4)	20(3)	29(3)	4(3)	7(3)	-7(3)
C(3)	24(3)	33(3)	22(3)	0(3)	-6(3)	-7(3)
C(5)	28(3)	22(3)	24(3)	0(2)	8(3)	-5(2)
C(8)	39(4)	11(3)	31(3)	2(3)	0(3)	10(3)

Table S15. Torsion angles [°] for Structure **3**.

C(1)-Re(1)-C(2)-O(2)	-137(12)
N(2)-Re(1)-C(2)-O(2)	127(12)
N(3)-Re(1)-C(2)-O(2)	67(12)
N(1)-Re(1)-C(2)-O(2)	48(12)
Br(1B)-Re(1)-C(2)-O(2)	-26(100)
Br(1)-Re(1)-C(2)-O(2)	-44(12)
C(1)-Re(1)-N(3)-C(8)	152.7(4)
C(2)-Re(1)-N(3)-C(8)	-51.5(16)
N(2)-Re(1)-N(3)-C(8)	-112.7(4)
N(1)-Re(1)-N(3)-C(8)	-32.1(3)
Br(1B)-Re(1)-N(3)-C(8)	-48(16)
Br(1)-Re(1)-N(3)-C(8)	59.7(3)
C(1)-Re(1)-N(3)-C(6)	-82.4(4)
C(2)-Re(1)-N(3)-C(6)	73.4(16)
N(2)-Re(1)-N(3)-C(6)	12.1(3)
N(1)-Re(1)-N(3)-C(6)	92.7(4)
Br(1B)-Re(1)-N(3)-C(6)	77(16)
Br(1)-Re(1)-N(3)-C(6)	-175.4(3)
C(1)-Re(1)-N(2)-C(5)	64.5(4)
C(2)-Re(1)-N(2)-C(5)	153.9(4)
N(3)-Re(1)-N(2)-C(5)	-33.3(3)
N(1)-Re(1)-N(2)-C(5)	-111.3(4)
Br(1B)-Re(1)-N(2)-C(5)	154.1(16)
Br(1)-Re(1)-N(2)-C(5)	-66.2(7)
C(1)-Re(1)-N(2)-C(3)	-171.3(4)
C(2)-Re(1)-N(2)-C(3)	-82.0(4)
N(3)-Re(1)-N(2)-C(3)	90.8(4)
N(1)-Re(1)-N(2)-C(3)	12.9(4)
Br(1B)-Re(1)-N(2)-C(3)	-81.7(16)
Br(1)-Re(1)-N(2)-C(3)	57.9(7)
C(2)-Re(1)-C(1)-O(1)	-73(47)
N(2)-Re(1)-C(1)-O(1)	25(47)
N(3)-Re(1)-C(1)-O(1)	103(47)
N(1)-Re(1)-C(1)-O(1)	61(48)

Br(1B)-Re(1)-C(1)-O(1)	-74(47)
Br(1)-Re(1)-C(1)-O(1)	-166(47)
C(1)-Re(1)-N(1)-C(7)	52.8(19)
C(2)-Re(1)-N(1)-C(7)	-173.3(4)
N(2)-Re(1)-N(1)-C(7)	89.7(4)
N(3)-Re(1)-N(1)-C(7)	9.4(4)
Br(1B)-Re(1)-N(1)-C(7)	-173(2)
Br(1)-Re(1)-N(1)-C(7)	-80.5(4)
C(1)-Re(1)-N(1)-C(4)	-71.6(18)
C(2)-Re(1)-N(1)-C(4)	62.3(4)
N(2)-Re(1)-N(1)-C(4)	-34.8(4)
N(3)-Re(1)-N(1)-C(4)	-115.0(4)
Br(1B)-Re(1)-N(1)-C(4)	63(2)
Br(1)-Re(1)-N(1)-C(4)	155.0(3)
C(8)-N(3)-C(6)-C(5)	133.9(5)
Re(1)-N(3)-C(6)-C(5)	11.2(6)
C(7)-N(1)-C(4)-C(3)	-73.0(6)
Re(1)-N(1)-C(4)-C(3)	52.1(5)
C(4)-N(1)-C(7)-C(8)	134.2(5)
Re(1)-N(1)-C(7)-C(8)	14.4(6)
C(5)-N(2)-C(3)-C(4)	134.0(5)
Re(1)-N(2)-C(3)-C(4)	11.9(6)
N(1)-C(4)-C(3)-N(2)	-43.5(7)
C(3)-N(2)-C(5)-C(6)	-74.7(6)
Re(1)-N(2)-C(5)-C(6)	50.3(5)
N(3)-C(6)-C(5)-N(2)	-40.3(6)
C(6)-N(3)-C(8)-C(7)	-74.3(6)
Re(1)-N(3)-C(8)-C(7)	50.1(5)
N(1)-C(7)-C(8)-N(3)	-42.5(7)

Symmetry transformations used to generate equivalent atoms:

Table S16. Crystal data and structure refinement for Structure **4**.

Empirical formula	C9 H15 N4 O2 Re	
Formula weight	397.46	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 7.1545(3) Å	α= 90°.
	b = 11.6007(3) Å	β= 108.064(4)°.
	c = 7.3123(2) Å	γ = 90°.
Volume	576.99(4) $Å^3$	
Z	2	
Density (calculated)	2.288 Mg/m^3	
Absorption coefficient	10.522 mm^{-1}	
F(000)	376	
Crystal size	0.11 x 0.07 x 0.035 mm^3	
Crystal description	colorless plate	
Theta range for data collection	2.93 to 26.37°.	
Index ranges	-8<=h<=8, -14<=k<=14, -9<=l<=9	
Reflections collected	6477	
Independent reflections	2349 [R(int) = 0.0385]	
Reflections observed	2063	
Criterion for observation	>2sigma(I)	
Completeness to theta = 26.37°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.692 and 0.442	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2349 / 82 / 146	
Goodness-of-fit on F^2	1.107	
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0540	
R indices (all data)	R1 = 0.0362, wR2 = 0.0586	
Absolute structure parameter	0.49(2)	
Largest diff. peak and hole	1.386 and -0.802 $e.Å^{-3}$	

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Structure **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	12299(15)	13213(9)	6741(14)	20(2)
O(1)	12356(11)	14069(7)	7652(11)	35(2)
C(2)	13776(16)	11127(9)	7258(15)	22(2)
O(2)	15002(12)	10695(6)	8653(10)	34(2)
C(3)	9668(15)	11293(8)	5826(13)	21(2)
N(1)	8355(13)	10853(8)	6087(13)	30(2)
C(4)	9670(16)	10792(9)	1523(16)	29(2)
C(5)	9669(11)	11990(16)	830(10)	29(2)
C(6)	12023(16)	13711(10)	2242(18)	30(2)
C(7)	13852(17)	13086(10)	2244(17)	26(2)
C(8)	15066(15)	11108(8)	3335(15)	24(2)
C(9)	13229(17)	10461(12)	2078(18)	32(2)
N(2)	11546(13)	10541(9)	2890(13)	27(2)
N(3)	10484(14)	12814(8)	2471(13)	23(2)
N(4)	14386(11)	12216(6)	3839(10)	22(2)
Re(1)	12126(1)	11944(1)	5195(1)	14(1)

Table S18. Bond lengths [Å] and angles [°] for Structure **4**.

C(1)-O(1)	1.189(12)	O(1)-C(1)-Re(1)	176.3(9)
C(1)-Re(1)	1.838(11)	O(2)-C(2)-Re(1)	172.8(9)
C(2)-O(2)	1.227(12)	N(1)-C(3)-Re(1)	173.9(9)
C(2)-Re(1)	1.861(11)	N(2)-C(4)-C(5)	109.3(9)
C(3)-N(1)	1.135(12)	N(2)-C(4)-H(4A)	109.8
C(3)-Re(1)	2.093(11)	C(5)-C(4)-H(4A)	109.8
C(4)-N(2)	1.433(11)	N(2)-C(4)-H(4B)	109.8
C(4)-C(5)	1.479(16)	C(5)-C(4)-H(4B)	109.8
C(4)-H(4A)	0.9900	H(4A)-C(4)-H(4B)	108.3
C(4)-H(4B)	0.9900	C(4)-C(5)-N(3)	111.4(8)
C(5)-N(3)	1.504(15)	C(4)-C(5)-H(5A)	109.3
C(5)-H(5A)	0.9900	N(3)-C(5)-H(5A)	109.3
C(5)-H(5B)	0.9900	C(4)-C(5)-H(5B)	109.3
C(6)-C(7)	1.496(13)	N(3)-C(5)-H(5B)	109.3
C(6)-N(3)	1.562(14)	H(5A)-C(5)-H(5B)	108.0
C(6)-H(6A)	0.9900	C(7)-C(6)-N(3)	108.8(9)
C(6)-H(6B)	0.9900	C(7)-C(6)-H(6A)	109.9
C(7)-N(4)	1.500(10)	N(3)-C(6)-H(6A)	109.9
C(7)-H(7A)	0.9900	C(7)-C(6)-H(6B)	109.9
C(7)-H(7B)	0.9900	N(3)-C(6)-H(6B)	109.9
C(8)-N(4)	1.461(10)	H(6A)-C(6)-H(6B)	108.3
C(8)-C(9)	1.545(13)	C(6)-C(7)-N(4)	109.8(9)
C(8)-H(8A)	0.9900	C(6)-C(7)-H(7A)	109.7
C(8)-H(8B)	0.9900	N(4)-C(7)-H(7A)	109.7
C(9)-N(2)	1.502(11)	C(6)-C(7)-H(7B)	109.7
C(9)-H(9A)	0.9900	N(4)-C(7)-H(7B)	109.7
C(9)-H(9B)	0.9900	H(7A)-C(7)-H(7B)	108.2
N(2)-Re(1)	2.285(10)	N(4)-C(8)-C(9)	106.8(9)
N(2)-H(2)	0.9300	N(4)-C(8)-H(8A)	110.4
N(3)-Re(1)	2.217(9)	C(9)-C(8)-H(8A)	110.4
N(3)-H(3)	0.9300	N(4)-C(8)-H(8B)	110.4
N(4)-Re(1)	2.166(8)	C(9)-C(8)-H(8B)	110.4
N(4)-H(4)	0.9300	H(8A)-C(8)-H(8B)	108.6
		N(2)-C(9)-C(8)	111.9(8)

N(2)-C(9)-H(9A)	109.2	C(7)-N(4)-Re(1)	114.1(6)
C(8)-C(9)-H(9A)	109.2	C(8)-N(4)-H(4)	105.7
N(2)-C(9)-H(9B)	109.2	C(7)-N(4)-H(4)	105.7
C(8)-C(9)-H(9B)	109.2	Re(1)-N(4)-H(4)	105.7
H(9A)-C(9)-H(9B)	107.9	C(1)-Re(1)-C(2)	90.2(4)
C(4)-N(2)-C(9)	115.4(9)	C(1)-Re(1)-C(3)	93.1(4)
C(4)-N(2)-Re(1)	106.6(8)	C(2)-Re(1)-C(3)	90.2(4)
C(9)-N(2)-Re(1)	110.6(6)	C(1)-Re(1)-N(4)	104.3(4)
C(4)-N(2)-H(2)	108.0	C(2)-Re(1)-N(4)	94.0(3)
C(9)-N(2)-H(2)	108.0	C(3)-Re(1)-N(4)	162.0(3)
Re(1)-N(2)-H(2)	108.0	C(1)-Re(1)-N(3)	95.9(4)
C(5)-N(3)-C(6)	116.8(8)	C(2)-Re(1)-N(3)	170.5(4)
C(5)-N(3)-Re(1)	113.2(8)	C(3)-Re(1)-N(3)	96.6(4)
C(6)-N(3)-Re(1)	101.8(7)	N(4)-Re(1)-N(3)	77.6(3)
C(5)-N(3)-H(3)	108.2	C(1)-Re(1)-N(2)	170.5(4)
C(6)-N(3)-H(3)	108.2	C(2)-Re(1)-N(2)	99.2(4)
Re(1)-N(3)-H(3)	108.2	C(3)-Re(1)-N(2)	86.2(3)
C(8)-N(4)-C(7)	114.8(8)	N(4)-Re(1)-N(2)	75.9(3)
C(8)-N(4)-Re(1)	110.0(5)	N(3)-Re(1)-N(2)	74.8(4)

Symmetry transformations used to generate equivalent atoms:

Table S19. Anisotropic displacement parameters ($Å^2$x 10^3)for Structure **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	20(6)	16(5)	27(6)	14(5)	12(5)	13(5)
O(1)	39(5)	31(5)	38(4)	-19(4)	17(4)	-9(4)
C(2)	28(6)	14(5)	35(6)	1(5)	24(5)	3(5)
O(2)	41(5)	33(5)	29(4)	11(4)	12(4)	13(4)
C(3)	15(6)	22(6)	21(5)	-8(4)	-1(5)	1(4)
N(1)	23(5)	35(6)	39(5)	2(5)	18(4)	-1(4)
C(4)	24(4)	32(4)	28(5)	-13(4)	3(4)	-5(4)
C(5)	20(4)	43(4)	22(3)	-2(4)	1(3)	-7(5)
C(6)	21(5)	25(5)	40(5)	6(4)	5(4)	-1(3)
C(7)	19(4)	32(5)	27(5)	6(4)	9(4)	-5(4)
C(8)	21(4)	26(5)	27(5)	-2(4)	12(4)	-5(3)
C(9)	27(4)	41(6)	28(5)	-21(4)	9(4)	-1(4)
N(2)	20(4)	23(5)	36(5)	-12(4)	8(3)	-6(4)
N(3)	16(4)	24(4)	31(4)	-1(3)	10(4)	3(3)
N(4)	16(3)	26(5)	20(3)	-2(3)	2(3)	-2(3)
Re(1)	13(1)	16(1)	15(1)	-2(1)	5(1)	-5(1)

Table S20. Torsion angles [°] for Structure **4**.

N(2)-C(4)-C(5)-N(3)	-47.3(11)
N(3)-C(6)-C(7)-N(4)	-45.6(13)
N(4)-C(8)-C(9)-N(2)	-44.6(13)
C(5)-C(4)-N(2)-C(9)	-69.1(13)
C(5)-C(4)-N(2)-Re(1)	54.1(10)
C(8)-C(9)-N(2)-C(4)	135.4(11)
C(8)-C(9)-N(2)-Re(1)	14.2(13)
C(4)-C(5)-N(3)-C(6)	133.6(9)
C(4)-C(5)-N(3)-Re(1)	15.9(9)
C(7)-C(6)-N(3)-C(5)	-67.0(13)
C(7)-C(6)-N(3)-Re(1)	56.8(10)
C(9)-C(8)-N(4)-C(7)	-75.2(10)
C(9)-C(8)-N(4)-Re(1)	55.0(9)
C(6)-C(7)-N(4)-C(8)	138.9(10)
C(6)-C(7)-N(4)-Re(1)	10.7(12)
C(8)-N(4)-Re(1)-C(1)	153.0(7)
C(7)-N(4)-Re(1)-C(1)	-76.3(8)
C(8)-N(4)-Re(1)-C(2)	61.8(7)
C(7)-N(4)-Re(1)-C(2)	-167.6(7)
C(8)-N(4)-Re(1)-C(3)	-41.1(13)
C(7)-N(4)-Re(1)-C(3)	89.5(12)
C(8)-N(4)-Re(1)-N(3)	-113.9(7)
C(7)-N(4)-Re(1)-N(3)	16.7(7)
C(8)-N(4)-Re(1)-N(2)	-36.7(6)
C(7)-N(4)-Re(1)-N(2)	93.9(7)
C(5)-N(3)-Re(1)-C(1)	-168.4(6)
C(6)-N(3)-Re(1)-C(1)	65.4(7)
C(5)-N(3)-Re(1)-C(3)	-74.6(6)
C(6)-N(3)-Re(1)-C(3)	159.3(7)
C(5)-N(3)-Re(1)-N(4)	88.2(6)
C(6)-N(3)-Re(1)-N(4)	-38.0(6)
C(5)-N(3)-Re(1)-N(2)	9.6(6)
C(6)-N(3)-Re(1)-N(2)	-116.6(7)
C(4)-N(2)-Re(1)-C(2)	153.3(7)

C(9)-N(2)-Re(1)-C(2)	-80.5(9)
C(4)-N(2)-Re(1)-C(3)	63.7(7)
C(9)-N(2)-Re(1)-C(3)	-170.1(9)
C(4)-N(2)-Re(1)-N(4)	-114.9(7)
C(9)-N(2)-Re(1)-N(4)	11.3(8)
C(4)-N(2)-Re(1)-N(3)	-34.2(7)
C(9)-N(2)-Re(1)-N(3)	92.0(9)

Symmetry transformations used to generate equivalent atoms:

Table 21. Crystal data and structure refinement for Structure **5**.

Empirical formula	C14 H36 Br2 F12 N6 O6 P2 Re2	
Formula weight	1206.65	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 12.7405(2) Å	α= 90°.
	b = 8.06410(10) Å	β= 92.4263(14)°.
	c = 29.9394(5) Å	γ = 90°.
Volume	3073.24(8) $Å^3$	
Z	4	
Density (calculated)	2.608 Mg/m^3	
Absorption coefficient	10.690 mm^{-1}	
F(000)	2272	
Crystal size	0.521 x 0.061 x 0.040 mm^3	
Crystal description	green needle	
Theta range for data collection	2.53 to 30.51°.	
Index ranges	-18<=h<=17, -11<=k<=11, -42<=l<=39	
Reflections collected	39400	
Independent reflections	9515 [R(int) = 0.0349]	
Reflections observed	8298	
Criterion for observation	>2sigma(I)	
Completeness to theta = 30.51°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.26113	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9515 / 27 / 416	
Goodness-of-fit on F^2	1.250	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0996	
R indices (all data)	R1 = 0.0541, wR2 = 0.1026	
Largest diff. peak and hole	2.449 and -1.992 $e.Å^{-3}$	

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Structure **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	1521(1)	1924(1)	1113(1)	11(1)
Re(2)	-1155(1)	3616(1)	1072(1)	11(1)
C(5)	3868(6)	2300(10)	1383(3)	22(2)
C(4)	3228(6)	2978(11)	1748(3)	21(2)
C(7)	2414(7)	5367(10)	1322(3)	23(2)
C(9)	1858(7)	5460(9)	875(3)	21(2)
C(8)	3038(6)	3599(11)	462(3)	24(2)
C(6)	3445(6)	1884(11)	572(3)	23(2)
C(15)	-2583(6)	2445(11)	305(3)	21(2)
C(14)	-3372(6)	3047(10)	637(3)	20(2)
C(13)	-3250(6)	3522(10)	1462(3)	19(2)
C(11)	-2862(6)	1785(10)	1579(3)	22(2)
C(10)	-1460(6)	41(9)	1250(3)	20(2)
C(12)	-1859(6)	106(9)	767(3)	22(2)
C(2)	1291(6)	327(10)	1565(3)	20(2)
C(3)	-905(6)	5212(11)	1536(3)	22(2)
N(1)	3195(4)	1438(8)	1043(2)	14(1)
N(2)	2235(5)	3730(8)	1550(2)	15(1)
N(3)	1952(5)	3853(7)	629(2)	14(1)
N(4)	-1709(5)	1640(8)	1480(2)	17(1)
N(5)	-1642(5)	1757(7)	555(2)	15(1)
N(6)	-2858(5)	3950(8)	1021(2)	17(1)
F(1)	-5505(4)	-2229(7)	2698(2)	31(1)
F(2)	-5079(5)	-556(7)	2125(2)	37(1)
F(3)	-6678(5)	-312(8)	2437(2)	42(2)
F(4)	-5403(5)	-3280(7)	1999(2)	35(1)
F(5)	-6979(4)	-3050(8)	2303(2)	35(1)
F(6)	-6560(4)	-1330(7)	1736(2)	31(1)
F(7)	-4962(4)	-3914(7)	997(2)	33(1)
F(8)	-3543(4)	-2776(7)	687(2)	34(1)
F(9)	-4556(5)	-1211(8)	1129(2)	44(2)

F(10)	-4557(5)	-730(7)	398(2)	40(2)
F(11)	-6001(4)	-1884(7)	706(2)	37(1)
F(12)	-4991(5)	-3411(8)	262(2)	44(2)
P(1)	-6029(2)	-1795(3)	2217(1)	19(1)
P(2)	-4776(2)	-2316(2)	697(1)	16(1)
Br(1)	1059(1)	-93(1)	492(1)	30(1)
Br(2)	-928(1)	5765(1)	475(1)	26(1)
O(1)	187(4)	2795(6)	1123(2)	12(1)
O(2)	1124(5)	-614(10)	1837(3)	41(2)
O(3)	-765(6)	6157(10)	1812(3)	44(2)
O(4)	-779(5)	2059(8)	2362(2)	26(1)
O(5)	-1144(5)	-1203(8)	2619(2)	28(1)
O(6)	-7042(6)	2772(10)	2915(3)	43(2)

Table S23. Bond lengths [Å] and angles [°] for Structure **5**.

Re(1)-O(1)	1.841(5)	C(15)-C(14)	1.521(11)
Re(1)-C(2)	1.899(8)	C(15)-H(15A)	0.9900
Re(1)-N(2)	2.135(6)	C(15)-H(15B)	0.9900
Re(1)-N(1)	2.187(5)	C(14)-N(6)	1.491(10)
Re(1)-N(3)	2.212(6)	C(14)-H(14A)	0.9900
Re(1)-Br(1)	2.5218(9)	C(14)-H(14B)	0.9900
Re(2)-O(1)	1.835(5)	C(13)-N(6)	1.472(10)
Re(2)-C(3)	1.911(8)	C(13)-C(11)	1.521(11)
Re(2)-N(4)	2.144(6)	C(13)-H(13A)	0.9900
Re(2)-N(6)	2.184(6)	C(13)-H(13B)	0.9900
Re(2)-N(5)	2.225(6)	C(11)-N(4)	1.516(10)
Re(2)-Br(2)	2.5144(9)	C(11)-H(11A)	0.9900
C(5)-N(1)	1.476(10)	C(11)-H(11B)	0.9900
C(5)-C(4)	1.495(12)	C(10)-N(4)	1.502(10)
C(5)-H(5A)	0.9900	C(10)-C(12)	1.512(11)
C(5)-H(5B)	0.9900	C(10)-H(10A)	0.9900
C(4)-N(2)	1.503(9)	C(10)-H(10B)	0.9900
C(4)-H(4A)	0.9900	C(12)-N(5)	1.507(10)
C(4)-H(4B)	0.9900	C(12)-H(12A)	0.9900
C(7)-C(9)	1.488(12)	C(12)-H(12B)	0.9900
C(7)-N(2)	1.509(10)	C(2)-O(2)	1.141(11)
C(7)-H(7A)	0.9900	C(3)-O(3)	1.133(11)
C(7)-H(7B)	0.9900	N(1)-H(1)	0.9300
C(9)-N(3)	1.498(10)	N(2)-H(2)	0.9300
C(9)-H(9A)	0.9900	N(3)-H(3)	0.9300
C(9)-H(9B)	0.9900	N(4)-H(4)	0.9300
C(8)-N(3)	1.505(10)	N(5)-H(5)	0.9300
C(8)-C(6)	1.508(12)	N(6)-H(6)	0.9300
C(8)-H(8A)	0.9900	F(1)-P(1)	1.599(5)
C(8)-H(8B)	0.9900	F(2)-P(1)	1.602(6)
C(6)-N(1)	1.504(10)	F(3)-P(1)	1.611(6)
C(6)-H(6A)	0.9900	F(4)-P(1)	1.593(6)
C(6)-H(6B)	0.9900	F(5)-P(1)	1.607(6)
C(15)-N(5)	1.493(10)	F(6)-P(1)	1.609(5)

F(7)-P(2)	1.594(5)	N(4)-Re(2)-N(5)	78.9(2)
F(8)-P(2)	1.616(5)	N(6)-Re(2)-N(5)	77.8(2)
F(9)-P(2)	1.585(6)	O(1)-Re(2)-Br(2)	99.89(15)
F(10)-P(2)	1.594(6)	C(3)-Re(2)-Br(2)	91.8(3)
F(11)-P(2)	1.601(5)	N(4)-Re(2)-Br(2)	165.26(17)
F(12)-P(2)	1.588(6)	N(6)-Re(2)-Br(2)	90.57(17)
O(4)-H(4D)	0.863(19)	N(5)-Re(2)-Br(2)	90.38(16)
O(4)-H(4E)	0.85(2)	N(1)-C(5)-C(4)	111.0(6)
O(5)-H(5D)	0.858(19)	N(1)-C(5)-H(5A)	109.4
O(5)-H(5E)	0.85(2)	C(4)-C(5)-H(5A)	109.4
O(6)-H(6D)	0.857(19)	N(1)-C(5)-H(5B)	109.4
O(6)-H(6E)	0.859(19)	C(4)-C(5)-H(5B)	109.4
		H(5A)-C(5)-H(5B)	108.0
O(1)-Re(1)-C(2)	94.4(3)	C(5)-C(4)-N(2)	109.6(6)
O(1)-Re(1)-N(2)	95.7(2)	C(5)-C(4)-H(4A)	109.8
C(2)-Re(1)-N(2)	95.8(3)	N(2)-C(4)-H(4A)	109.8
O(1)-Re(1)-N(1)	167.1(2)	C(5)-C(4)-H(4B)	109.8
C(2)-Re(1)-N(1)	97.3(3)	N(2)-C(4)-H(4B)	109.8
N(2)-Re(1)-N(1)	77.8(2)	H(4A)-C(4)-H(4B)	108.2
O(1)-Re(1)-N(3)	89.8(2)	C(9)-C(7)-N(2)	112.0(6)
C(2)-Re(1)-N(3)	173.7(3)	C(9)-C(7)-H(7A)	109.2
N(2)-Re(1)-N(3)	79.1(2)	N(2)-C(7)-H(7A)	109.2
N(1)-Re(1)-N(3)	78.1(2)	C(9)-C(7)-H(7B)	109.2
O(1)-Re(1)-Br(1)	94.07(15)	N(2)-C(7)-H(7B)	109.2
C(2)-Re(1)-Br(1)	92.9(2)	H(7A)-C(7)-H(7B)	107.9
N(2)-Re(1)-Br(1)	166.42(17)	C(7)-C(9)-N(3)	110.7(6)
N(1)-Re(1)-Br(1)	90.71(17)	C(7)-C(9)-H(9A)	109.5
N(3)-Re(1)-Br(1)	91.53(16)	N(3)-C(9)-H(9A)	109.5
O(1)-Re(2)-C(3)	93.3(3)	C(7)-C(9)-H(9B)	109.5
O(1)-Re(2)-N(4)	90.7(2)	N(3)-C(9)-H(9B)	109.5
C(3)-Re(2)-N(4)	97.8(3)	H(9A)-C(9)-H(9B)	108.1
O(1)-Re(2)-N(6)	165.9(2)	N(3)-C(8)-C(6)	111.4(6)
C(3)-Re(2)-N(6)	95.9(3)	N(3)-C(8)-H(8A)	109.3
N(4)-Re(2)-N(6)	77.4(2)	C(6)-C(8)-H(8A)	109.3
O(1)-Re(2)-N(5)	92.6(2)	N(3)-C(8)-H(8B)	109.3
C(3)-Re(2)-N(5)	173.3(3)	C(6)-C(8)-H(8B)	109.3

H(8A)-C(8)-H(8B)	108.0	H(10A)-C(10)-H(10B)	108.2
N(1)-C(6)-C(8)	109.8(7)	N(5)-C(12)-C(10)	111.9(6)
N(1)-C(6)-H(6A)	109.7	N(5)-C(12)-H(12A)	109.2
C(8)-C(6)-H(6A)	109.7	C(10)-C(12)-H(12A)	109.2
N(1)-C(6)-H(6B)	109.7	N(5)-C(12)-H(12B)	109.2
C(8)-C(6)-H(6B)	109.7	C(10)-C(12)-H(12B)	109.2
H(6A)-C(6)-H(6B)	108.2	H(12A)-C(12)-H(12B)	107.9
N(5)-C(15)-C(14)	109.4(6)	O(2)-C(2)-Re(1)	178.0(7)
N(5)-C(15)-H(15A)	109.8	O(3)-C(3)-Re(2)	179.4(8)
C(14)-C(15)-H(15A)	109.8	C(5)-N(1)-C(6)	113.3(6)
N(5)-C(15)-H(15B)	109.8	C(5)-N(1)-Re(1)	113.0(5)
C(14)-C(15)-H(15B)	109.8	C(6)-N(1)-Re(1)	107.0(4)
H(15A)-C(15)-H(15B)	108.2	C(5)-N(1)-H(1)	107.8
N(6)-C(14)-C(15)	112.3(6)	C(6)-N(1)-H(1)	107.8
N(6)-C(14)-H(14A)	109.1	Re(1)-N(1)-H(1)	107.8
C(15)-C(14)-H(14A)	109.1	C(4)-N(2)-C(7)	113.0(6)
N(6)-C(14)-H(14B)	109.1	C(4)-N(2)-Re(1)	107.2(5)
C(15)-C(14)-H(14B)	109.1	C(7)-N(2)-Re(1)	112.8(5)
H(14A)-C(14)-H(14B)	107.9	C(4)-N(2)-H(2)	107.9
N(6)-C(13)-C(11)	107.6(6)	C(7)-N(2)-H(2)	107.9
N(6)-C(13)-H(13A)	110.2	Re(1)-N(2)-H(2)	107.9
C(11)-C(13)-H(13A)	110.2	C(9)-N(3)-C(8)	112.0(6)
N(6)-C(13)-H(13B)	110.2	C(9)-N(3)-Re(1)	105.0(4)
C(11)-C(13)-H(13B)	110.2	C(8)-N(3)-Re(1)	112.2(5)
H(13A)-C(13)-H(13B)	108.5	C(9)-N(3)-H(3)	109.2
N(4)-C(11)-C(13)	109.6(6)	C(8)-N(3)-H(3)	109.2
N(4)-C(11)-H(11A)	109.8	Re(1)-N(3)-H(3)	109.2
C(13)-C(11)-H(11A)	109.8	C(10)-N(4)-C(11)	112.4(6)
N(4)-C(11)-H(11B)	109.8	C(10)-N(4)-Re(2)	107.3(4)
C(13)-C(11)-H(11B)	109.8	C(11)-N(4)-Re(2)	113.5(5)
H(11A)-C(11)-H(11B)	108.2	C(10)-N(4)-H(4)	107.8
N(4)-C(10)-C(12)	109.8(6)	C(11)-N(4)-H(4)	107.8
N(4)-C(10)-H(10A)	109.7	Re(2)-N(4)-H(4)	107.8
C(12)-C(10)-H(10A)	109.7	C(15)-N(5)-C(12)	112.4(6)
N(4)-C(10)-H(10B)	109.7	C(15)-N(5)-Re(2)	107.0(4)
C(12)-C(10)-H(10B)	109.7	C(12)-N(5)-Re(2)	110.6(5)

C(15)-N(5)-H(5)	108.9	F(7)-P(2)-F(8)	89.7(3)
C(12)-N(5)-H(5)	108.9	F(10)-P(2)-F(8)	88.8(3)
Re(2)-N(5)-H(5)	108.9	F(11)-P(2)-F(8)	179.3(3)
C(13)-N(6)-C(14)	115.1(6)	Re(2)-O(1)-Re(1)	174.3(3)
C(13)-N(6)-Re(2)	106.4(4)	H(4D)-O(4)-H(4E)	107(3)
C(14)-N(6)-Re(2)	113.3(4)	H(5D)-O(5)-H(5E)	108(3)
C(13)-N(6)-H(6)	107.2	H(6D)-O(6)-H(6E)	107(3)
C(14)-N(6)-H(6)	107.2		
Re(2)-N(6)-H(6)	107.2		
F(4)-P(1)-F(1)	90.4(3)		
F(4)-P(1)-F(2)	90.2(3)		
F(1)-P(1)-F(2)	90.1(3)		
F(4)-P(1)-F(5)	89.1(3)		
F(1)-P(1)-F(5)	90.4(3)		
F(2)-P(1)-F(5)	179.2(3)		
F(4)-P(1)-F(6)	90.4(3)		
F(1)-P(1)-F(6)	179.1(3)		
F(2)-P(1)-F(6)	89.6(3)		
F(5)-P(1)-F(6)	89.9(3)		
F(4)-P(1)-F(3)	179.1(4)		
F(1)-P(1)-F(3)	89.8(3)		
F(2)-P(1)-F(3)	90.7(4)		
F(5)-P(1)-F(3)	89.9(3)		
F(6)-P(1)-F(3)	89.4(3)		
F(9)-P(2)-F(12)	179.5(4)		
F(9)-P(2)-F(7)	91.2(3)		
F(12)-P(2)-F(7)	89.3(3)		
F(9)-P(2)-F(10)	88.7(4)		
F(12)-P(2)-F(10)	90.7(4)		
F(7)-P(2)-F(10)	178.5(3)		
F(9)-P(2)-F(11)	90.2(3)		
F(12)-P(2)-F(11)	90.0(3)		
F(7)-P(2)-F(11)	89.9(3)		
F(10)-P(2)-F(11)	91.6(3)		
F(9)-P(2)-F(8)	90.4(3)		
F(12)-P(2)-F(8)	89.5(3)		

Table S24. Anisotropic displacement parameters ($Å^2$x 10^3)for Structure **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	7(1)	11(1)	14(1)	1(1)	0(1)	1(1)
Re(2)	8(1)	11(1)	13(1)	-1(1)	-1(1)	1(1)
C(5)	14(3)	20(4)	32(4)	2(3)	-8(3)	-2(3)
C(4)	13(3)	28(4)	21(4)	1(3)	-6(3)	-4(3)
C(7)	26(4)	11(3)	33(4)	1(3)	1(3)	-3(3)
C(9)	25(4)	11(3)	27(4)	2(3)	-4(3)	0(3)
C(8)	16(3)	29(4)	29(4)	11(3)	9(3)	-1(3)
C(6)	16(3)	33(4)	21(4)	6(3)	6(3)	3(3)
C(15)	20(3)	23(4)	20(4)	-3(3)	-4(3)	2(3)
C(14)	13(3)	21(3)	23(4)	-1(3)	-8(3)	4(3)
C(13)	12(3)	25(4)	21(4)	-2(3)	2(3)	2(3)
C(11)	17(3)	24(4)	26(4)	4(3)	5(3)	-4(3)
C(10)	16(3)	14(3)	28(4)	7(3)	-4(3)	5(3)
C(12)	23(4)	13(3)	29(4)	-4(3)	-3(3)	-4(3)
C(2)	10(3)	23(4)	28(4)	0(3)	-5(3)	0(3)
C(3)	13(3)	26(4)	25(4)	-2(3)	0(3)	6(3)
N(1)	7(2)	16(2)	20(2)	2(2)	1(2)	7(2)
N(2)	12(2)	17(2)	17(2)	-3(2)	-1(2)	-1(2)
N(3)	11(2)	13(2)	17(2)	-2(2)	0(2)	0(2)
N(4)	14(3)	19(3)	18(3)	2(2)	1(2)	-1(2)
N(5)	13(3)	13(3)	20(3)	-3(2)	-1(2)	2(2)
N(6)	23(3)	16(3)	11(3)	-3(2)	-4(2)	8(2)
F(1)	35(3)	32(3)	24(3)	2(2)	-8(2)	4(2)
F(2)	41(3)	32(3)	37(3)	2(2)	-5(3)	-17(2)
F(3)	54(4)	42(3)	29(3)	-7(3)	-5(3)	20(3)
F(4)	41(3)	31(3)	34(3)	-5(2)	7(2)	9(2)
F(5)	34(3)	42(3)	29(3)	3(2)	3(2)	-16(3)
F(6)	36(3)	34(3)	21(2)	4(2)	-6(2)	-6(2)
F(7)	26(3)	25(3)	48(3)	16(2)	2(2)	-4(2)
F(8)	16(2)	26(3)	62(4)	9(3)	6(2)	4(2)
F(9)	53(4)	44(3)	33(3)	-18(3)	-1(3)	-15(3)
F(10)	37(3)	31(3)	53(4)	21(3)	6(3)	1(2)
F(11)	16(2)	30(3)	66(4)	-3(3)	4(2)	6(2)
F(12)	49(4)	51(4)	32(3)	-21(3)	2(3)	-6(3)

P(1)	23(1)	18(1)	16(1)	-1(1)	-3(1)	-2(1)
P(2)	14(1)	14(1)	21(1)	-1(1)	1(1)	1(1)
Br(1)	28(1)	29(1)	32(1)	-13(1)	-1(1)	-1(1)
Br(2)	26(1)	25(1)	28(1)	8(1)	0(1)	0(1)
O(1)	16(2)	12(2)	8(2)	1(2)	0(2)	1(2)
O(2)	23(3)	46(4)	52(4)	29(4)	2(3)	4(3)
O(3)	40(4)	42(4)	49(4)	-21(4)	-15(3)	6(3)
O(4)	23(3)	33(3)	22(3)	-2(3)	0(2)	-4(3)
O(5)	32(3)	26(3)	28(3)	3(3)	6(3)	2(3)
O(6)	30(3)	51(5)	48(5)	-19(4)	3(3)	-2(3)

Table S25. Torsion angles [°] for Structure **5**.

N(1)-C(5)-C(4)-N(2)	-41.7(9)
N(2)-C(7)-C(9)-N(3)	-41.5(9)
N(3)-C(8)-C(6)-N(1)	-43.4(9)
N(5)-C(15)-C(14)-N(6)	42.0(9)
N(6)-C(13)-C(11)-N(4)	45.7(8)
N(4)-C(10)-C(12)-N(5)	42.3(9)
O(1)-Re(1)-C(2)-O(2)	-2(23)
N(2)-Re(1)-C(2)-O(2)	94(23)
N(1)-Re(1)-C(2)-O(2)	172(100)
N(3)-Re(1)-C(2)-O(2)	129(22)
Br(1)-Re(1)-C(2)-O(2)	-96(23)
O(1)-Re(2)-C(3)-O(3)	-148(100)
N(4)-Re(2)-C(3)-O(3)	-57(89)
N(6)-Re(2)-C(3)-O(3)	21(89)
N(5)-Re(2)-C(3)-O(3)	3(90)
Br(2)-Re(2)-C(3)-O(3)	112(88)
C(4)-C(5)-N(1)-C(6)	134.5(7)
C(4)-C(5)-N(1)-Re(1)	12.6(8)
C(8)-C(6)-N(1)-C(5)	-74.5(8)
C(8)-C(6)-N(1)-Re(1)	50.7(7)
O(1)-Re(1)-N(1)-C(5)	72.7(12)
C(2)-Re(1)-N(1)-C(5)	-82.5(6)
N(2)-Re(1)-N(1)-C(5)	11.8(5)
N(3)-Re(1)-N(1)-C(5)	93.1(5)
Br(1)-Re(1)-N(1)-C(5)	-175.5(5)
O(1)-Re(1)-N(1)-C(6)	-52.7(12)
C(2)-Re(1)-N(1)-C(6)	152.2(5)
N(2)-Re(1)-N(1)-C(6)	-113.5(5)
N(3)-Re(1)-N(1)-C(6)	-32.2(5)
Br(1)-Re(1)-N(1)-C(6)	59.2(5)
C(5)-C(4)-N(2)-C(7)	-73.9(8)
C(5)-C(4)-N(2)-Re(1)	51.1(7)
C(9)-C(7)-N(2)-C(4)	133.7(7)
C(9)-C(7)-N(2)-Re(1)	11.9(8)
O(1)-Re(1)-N(2)-C(4)	158.0(5)
C(2)-Re(1)-N(2)-C(4)	63.0(5)
N(1)-Re(1)-N(2)-C(4)	-33.3(5)

N(3)-Re(1)-N(2)-C(4)	-113.3(5)
Br(1)-Re(1)-N(2)-C(4)	-66.2(9)
O(1)-Re(1)-N(2)-C(7)	-76.9(5)
C(2)-Re(1)-N(2)-C(7)	-172.0(5)
N(1)-Re(1)-N(2)-C(7)	91.8(5)
N(3)-Re(1)-N(2)-C(7)	11.8(5)
Br(1)-Re(1)-N(2)-C(7)	58.8(10)
C(7)-C(9)-N(3)-C(8)	-73.1(8)
C(7)-C(9)-N(3)-Re(1)	48.9(7)
C(6)-C(8)-N(3)-C(9)	132.5(7)
C(6)-C(8)-N(3)-Re(1)	14.7(8)
O(1)-Re(1)-N(3)-C(9)	63.6(5)
C(2)-Re(1)-N(3)-C(9)	-68(3)
N(2)-Re(1)-N(3)-C(9)	-32.3(4)
N(1)-Re(1)-N(3)-C(9)	-112.0(5)
Br(1)-Re(1)-N(3)-C(9)	157.6(4)
O(1)-Re(1)-N(3)-C(8)	-174.5(5)
C(2)-Re(1)-N(3)-C(8)	54(3)
N(2)-Re(1)-N(3)-C(8)	89.6(5)
N(1)-Re(1)-N(3)-C(8)	9.9(5)
Br(1)-Re(1)-N(3)-C(8)	-80.5(5)
C(12)-C(10)-N(4)-C(11)	74.3(8)
C(12)-C(10)-N(4)-Re(2)	-51.1(7)
C(13)-C(11)-N(4)-C(10)	-136.4(7)
C(13)-C(11)-N(4)-Re(2)	-14.5(8)
O(1)-Re(2)-N(4)-C(10)	-59.1(5)
C(3)-Re(2)-N(4)-C(10)	-152.5(5)
N(6)-Re(2)-N(4)-C(10)	113.2(5)
N(5)-Re(2)-N(4)-C(10)	33.4(4)
Br(2)-Re(2)-N(4)-C(10)	77.2(8)
O(1)-Re(2)-N(4)-C(11)	176.1(5)
C(3)-Re(2)-N(4)-C(11)	82.8(5)
N(6)-Re(2)-N(4)-C(11)	-11.5(5)
N(5)-Re(2)-N(4)-C(11)	-91.4(5)
Br(2)-Re(2)-N(4)-C(11)	-47.5(10)
C(14)-C(15)-N(5)-C(12)	72.8(8)
C(14)-C(15)-N(5)-Re(2)	-48.8(7)
C(10)-C(12)-N(5)-C(15)	-132.4(7)
C(10)-C(12)-N(5)-Re(2)	-13.0(8)

O(1)-Re(2)-N(5)-C(15)	-158.5(5)
C(3)-Re(2)-N(5)-C(15)	51(3)
N(4)-Re(2)-N(5)-C(15)	111.3(5)
N(6)-Re(2)-N(5)-C(15)	31.9(5)
Br(2)-Re(2)-N(5)-C(15)	-58.6(5)
O(1)-Re(2)-N(5)-C(12)	78.8(5)
C(3)-Re(2)-N(5)-C(12)	-72(3)
N(4)-Re(2)-N(5)-C(12)	-11.4(5)
N(6)-Re(2)-N(5)-C(12)	-90.8(5)
Br(2)-Re(2)-N(5)-C(12)	178.7(5)
C(11)-C(13)-N(6)-C(14)	71.6(7)
C(11)-C(13)-N(6)-Re(2)	-54.8(6)
C(15)-C(14)-N(6)-C(13)	-136.5(7)
C(15)-C(14)-N(6)-Re(2)	-13.7(8)
O(1)-Re(2)-N(6)-C(13)	69.5(10)
C(3)-Re(2)-N(6)-C(13)	-60.5(5)
N(4)-Re(2)-N(6)-C(13)	36.2(5)
N(5)-Re(2)-N(6)-C(13)	117.4(5)
Br(2)-Re(2)-N(6)-C(13)	-152.4(5)
O(1)-Re(2)-N(6)-C(14)	-57.9(11)
C(3)-Re(2)-N(6)-C(14)	172.1(5)
N(4)-Re(2)-N(6)-C(14)	-91.2(5)
N(5)-Re(2)-N(6)-C(14)	-10.1(5)
Br(2)-Re(2)-N(6)-C(14)	80.2(5)
C(3)-Re(2)-O(1)-Re(1)	-150(3)
N(4)-Re(2)-O(1)-Re(1)	113(3)
N(6)-Re(2)-O(1)-Re(1)	80(3)
N(5)-Re(2)-O(1)-Re(1)	34(3)
Br(2)-Re(2)-O(1)-Re(1)	-57(3)
C(2)-Re(1)-O(1)-Re(2)	-123(3)
N(2)-Re(1)-O(1)-Re(2)	140(3)
N(1)-Re(1)-O(1)-Re(2)	81(3)
N(3)-Re(1)-O(1)-Re(2)	61(3)
Br(1)-Re(1)-O(1)-Re(2)	-30(3)

Symmetry transformations used to generate equivalent atoms: