 # Supplementary Material (ESI) for Dalton Transactions

Rigidity-modulated conformation control: A strategy for incorporating flexible building motifs into metallacycles

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Contents

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Experimental Section

All starting materials and products were found to be stable toward moisture and air. Commercial grade reagents, $Re_2(CO)_{10}$, 6,11-dihydroxy-5,12-naphthacenedione (H_2-dhnq), and solvents were used as received. The ligands 2,2'-bisbenzimidazolyl (H_2-Bim) and α,α'-bis(benzimidazol-1-yl)-*o*-xylene (XyBim) were synthesized by published methods.[S1,S2] H_2-Bim was obtained from the reaction of hexachloroacetone with 1,2-phenylenediamine in ethyleneglycol. The ligand XyBim was synthesized from the reaction of benzimidazole with α,α'-dibromo-*p*-xylene. Elemental analyses were performed on a Perkin-Elmer 2400 CHN elemental analyzer. Infrared spectra were recorded on a Perkin-Elmer FT-IR Spectrometer PARAGON 1000. ^{1}H NMR spectra were recorded on a Bruker AMX-400 FT-NMR spectrometer. FAB-MS data were obtained using a JEOL JMS-700 double focusing mass spectrometer.

References

S1. M. C. Rezende, E. L. Dall'Oglio, *Tetrahedron Lett.,* 1996, **37**, 5265–5268.

S2. Z. Shi, R. P. Thummel, *J. Org. Chem*., 1995, **60**, 5935–5945.

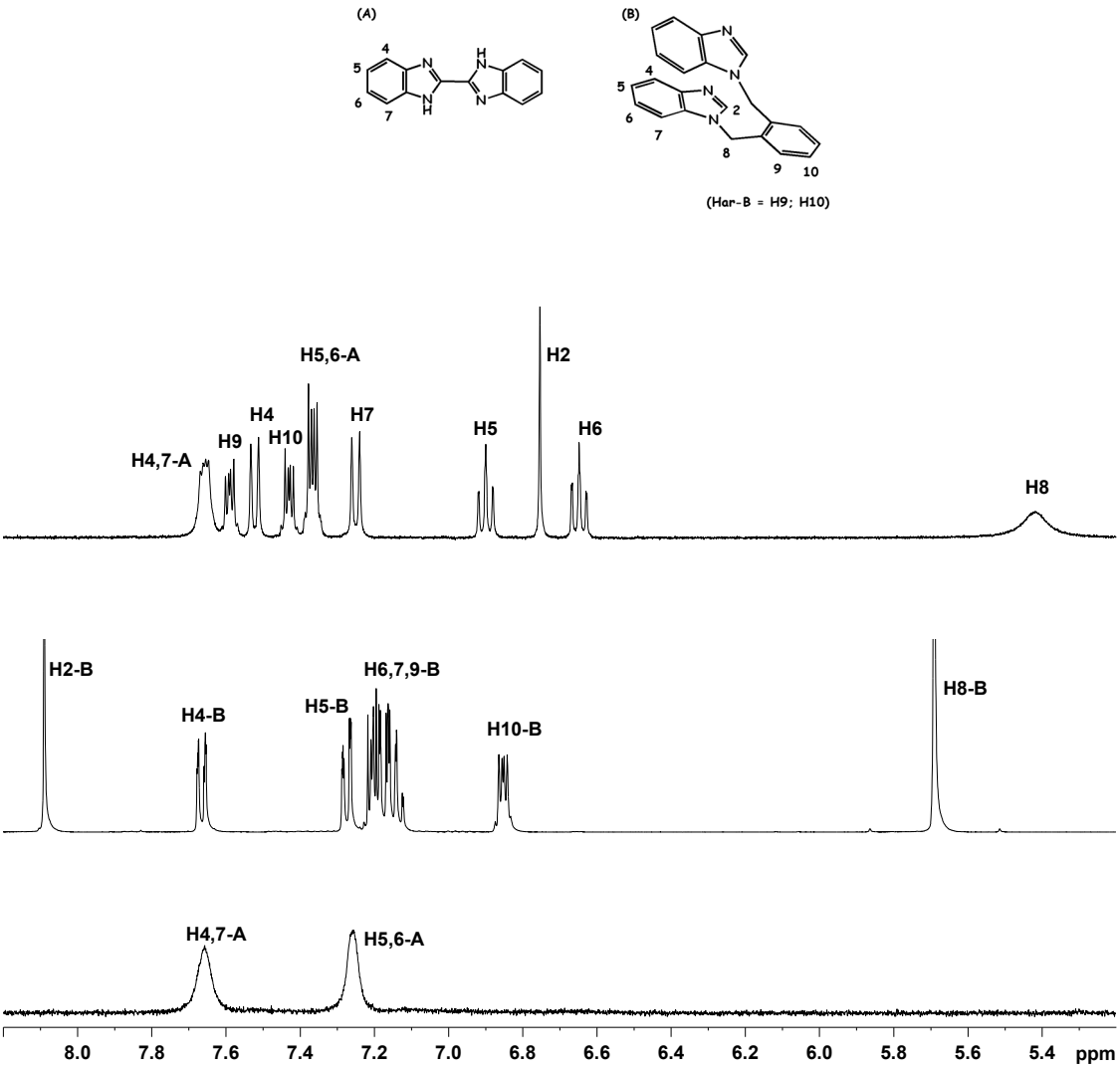

Figure S1. Partial ^{1}H NMR spectra of H_2-Bim, XyBim and **1** (from bottom to top).

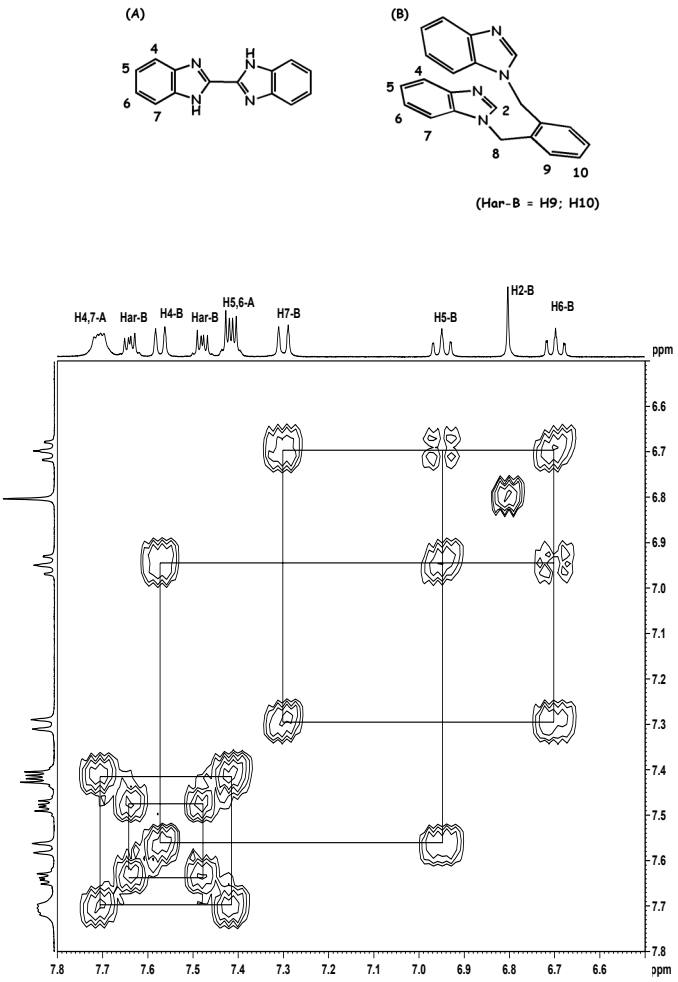

Figure S2. Partial ^{1}H-^{1}H COSY spectrum of **1**.

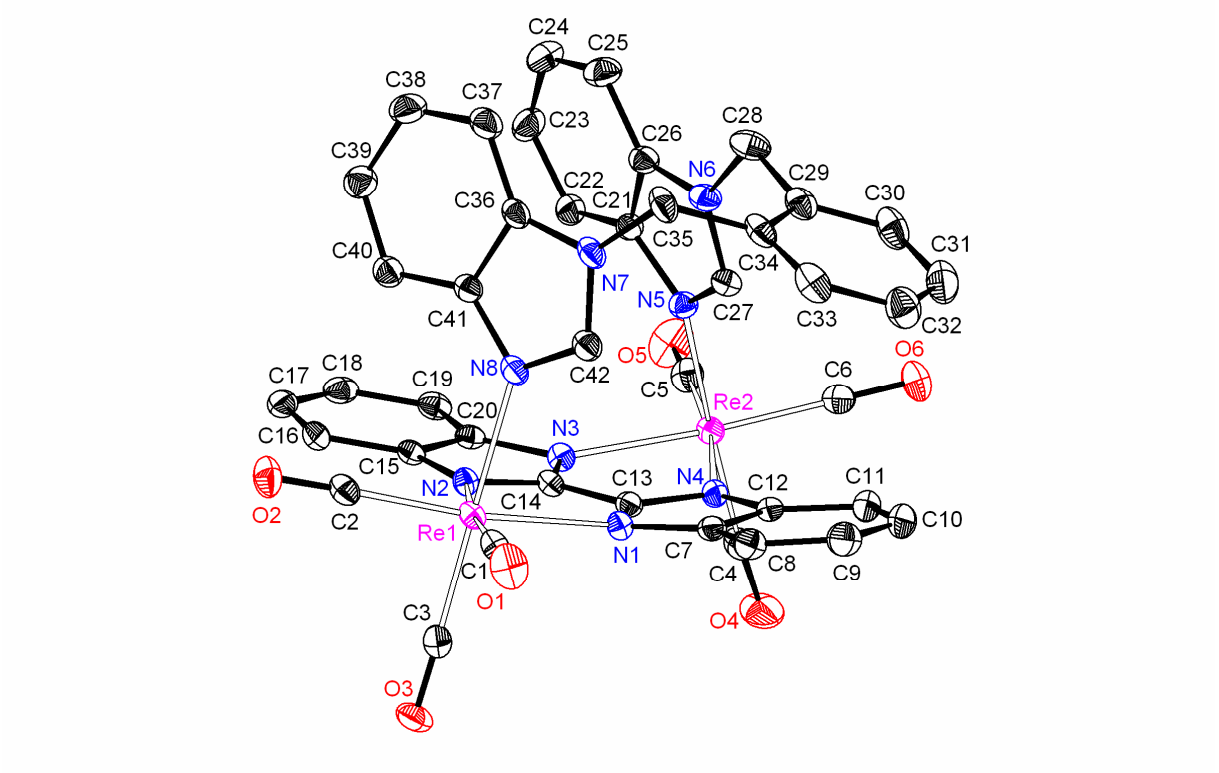

Figure S3. Labeled ORTEP diagram of **1**. Hydrogen atoms were omitted for clarity. Thermal ellipsoids are shown at 30% probability.

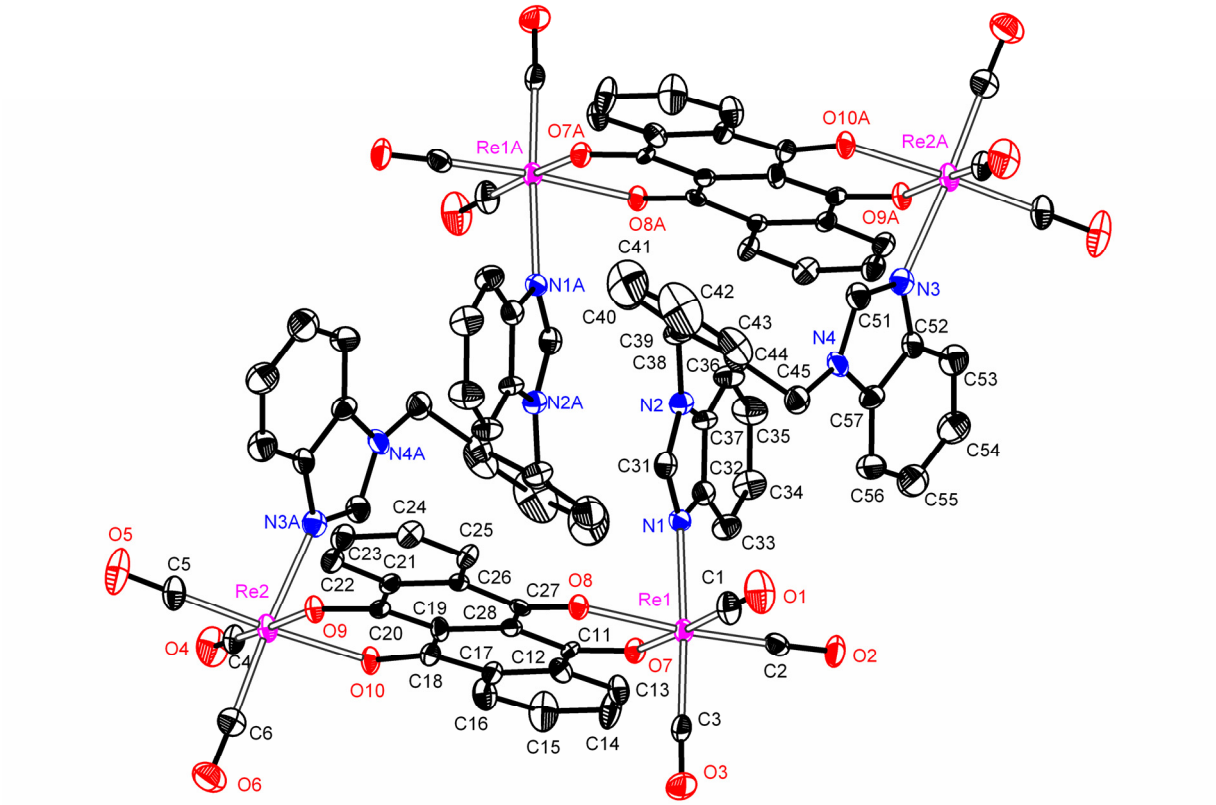

Figure S4. Labeled ORTEP diagram of **2**. Atomic labeling with "A" represents equivalent atoms generated from symmetry code (-x+1, -y+1, -z+1). Solvent molecule and hydrogen atoms were omitted for clarity. Thermal ellipsoids are shown at 30% probability.

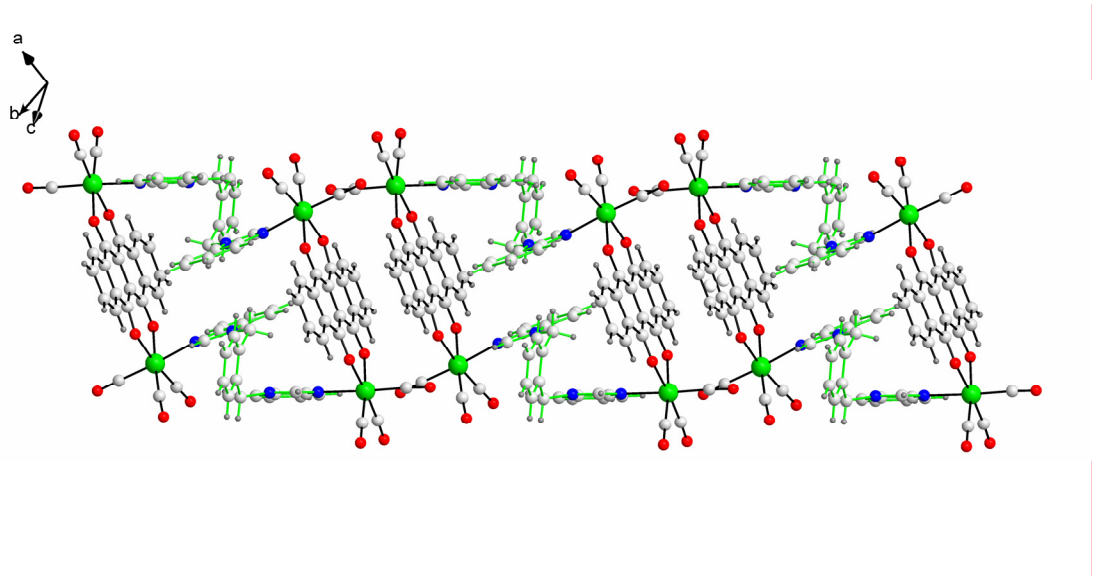

Figure S5. One-dimensional supramolecular chain generated by inter molecular π···π interactions in compound **2**.

 # Supplementary Material (ESI) for Dalton Transactions

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

Identification code	3609	
Empirical formula	$C_{42}H_{26}N_8O_6Re_2$	
Formula weight	1111.11	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 18.82300(10) Å	α = 90°
	b = 10.48100(10) Å	β = 114.59°
	c = 21.4330(2) Å	γ = 90°
Volume	3844.94(6) Å^3	
Z	4	
Density (calculated)	1.919 Mg/m^3	
Absorption coefficient	6.351 mm^{-1}	
F(000)	2128	
Crystal size	0.25 x 0.15 x 0.1 mm^3	
Theta range for data collection	2.09 to 25.03°.	
Index ranges	–22<=h<=17, –11<=k<=12, –19<=l<=25	
Reflections collected	21160	
Independent reflections	6777 [R(int) = 0.0416]	
Completeness to theta = 25.03°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4596 and 0.2654	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6777 / 0 / 523	
Goodness-of-fit on F^2	1.197	
Final R indices [$I > 2\sigma(I)$]	$R1$ = 0.0263, $wR2$ = 0.0651	
R indices (all data)	$R1$ = 0.0350, $wR2$ = 0.0738	
Largest diff. peak and hole	1.164 and -2.175 e.Å^{-3}	

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

	x	y	z	U(eq)
Re(1)	-1485(1)	4086(1)	2731(1)	36(1)
Re(2)	1736(1)	3872(1)	3236(1)	37(1)
O(1)	-2376(2)	5485(4)	3435(2)	74(1)
O(2)	-3016(2)	3523(4)	1487(2)	66(1)
O(3)	-1777(2)	1618(3)	3346(2)	61(1)
O(4)	2525(2)	1723(4)	4258(2)	93(2)
O(5)	2553(3)	2906(5)	2356(2)	86(1)
O(6)	3200(2)	5422(4)	4089(2)	77(1)
N(1)	-312(2)	4564(3)	3534(2)	38(1)
N(2)	-695(2)	3133(3)	2344(2)	36(1)
N(3)	606(2)	2940(3)	2587(2)	37(1)
N(4)	975(2)	4455(3)	3741(2)	37(1)
N(5)	1174(2)	5530(3)	2586(2)	39(1)
N(6)	767(2)	7536(3)	2329(2)	45(1)
N(7)	-1071(2)	7936(3)	2226(2)	48(1)
N(8)	-1270(2)	5866(3)	2288(2)	43(1)
C(1)	-2041(3)	4970(5)	3164(3)	48(1)
C(2)	-2436(3)	3743(4)	1947(3)	46(1)
C(3)	-1652(3)	2537(5)	3123(2)	44(1)
C(4)	2211(3)	2506(5)	3859(3)	55(1)
C(5)	2251(3)	3292(5)	2692(3)	53(1)
C(6)	2641(3)	4853(5)	3767(2)	49(1)
C(7)	105(3)	5364(4)	4089(2)	40(1)
C(8)	-138(3)	6171(4)	4483(3)	50(1)
C(9)	417(4)	6873(5)	4984(3)	63(2)
C(10)	1205(4)	6786(5)	5116(3)	63(2)
C(11)	1462(3)	5996(5)	4741(3)	55(1)
C(12)	900(3)	5281(4)	4216(2)	39(1)
C(13)	239(3)	4098(4)	3369(2)	36(1)

C(14)	49(2)	3348(4)	2767(2)	35(1)
C(15)	-624(3)	2462(4)	1812(2)	36(1)
C(16)	-1187(3)	1968(4)	1205(2)	44(1)
C(17)	-931(4)	1372(4)	761(2)	53(1)
C(18)	-137(4)	1242(4)	914(3)	51(1)
C(19)	426(3)	1721(4)	1509(2)	46(1)
C(20)	180(3)	2342(4)	1960(2)	38(1)
C(21)	984(3)	5733(4)	1893(2)	40(1)
C(22)	1008(3)	4926(5)	1392(2)	48(1)
C(23)	802(3)	5421(6)	747(3)	59(1)
C(24)	573(4)	6688(6)	597(3)	68(2)
C(25)	537(3)	7501(5)	1077(3)	62(2)
C(26)	737(3)	6994(4)	1732(2)	43(1)
C(27)	1031(3)	6639(4)	2814(2)	42(1)
C(28)	672(4)	8906(4)	2416(3)	59(2)
C(29)	592(3)	9245(4)	3066(3)	52(1)
C(30)	1264(3)	9436(5)	3658(3)	67(2)
C(31)	1218(4)	9761(6)	4267(3)	78(2)
C(32)	510(4)	9953(6)	4280(3)	73(2)
C(33)	-162(3)	9779(5)	3696(3)	64(2)
C(34)	-132(3)	9422(4)	3082(3)	50(1)
C(35)	-891(3)	9280(4)	2461(3)	59(2)
C(36)	-1291(3)	7459(4)	1570(3)	47(1)
C(37)	-1391(3)	8033(5)	958(3)	62(2)
C(38)	-1593(3)	7250(6)	394(3)	68(2)
C(39)	-1706(3)	5947(5)	437(3)	58(1)
C(40)	-1624(3)	5377(5)	1033(2)	49(1)
C(41)	-1411(3)	6155(4)	1616(2)	40(1)
C(42)	-1071(3)	6957(4)	2629(3)	47(1)

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

Re(1)-C(1)	1.904(5)
Re(1)-C(3)	1.913(5)
Re(1)-C(2)	1.912(5)
Re(1)-N(8)	2.206(4)
Re(1)-N(1)	2.218(3)
Re(1)-N(2)	2.220(3)
Re(2)-C(5)	1.900(6)
Re(2)-C(6)	1.908(5)
Re(2)-C(4)	1.908(5)
Re(2)-N(5)	2.203(3)
Re(2)-N(4)	2.211(4)
Re(2)-N(3)	2.226(3)
O(1)-C(1)	1.153(6)
O(2)-C(2)	1.150(6)
O(3)-C(3)	1.143(6)
O(4)-C(4)	1.154(6)
O(5)-C(5)	1.160(6)
O(6)-C(6)	1.156(6)
N(1)-C(13)	1.321(5)
N(1)-C(7)	1.399(5)
N(2)-C(14)	1.332(5)
N(2)-C(15)	1.392(5)
N(3)-C(14)	1.329(5)
N(3)-C(20)	1.394(5)
N(4)-C(13)	1.333(6)
N(4)-C(12)	1.388(5)
N(5)-C(27)	1.331(6)
N(5)-C(21)	1.391(6)
N(6)-C(27)	1.336(6)
N(6)-C(26)	1.379(6)
N(6)-C(28)	1.468(6)
N(7)-C(42)	1.341(6)
N(7)-C(36)	1.383(6)

N(7)-C(35)	1.487(6)
N(8)-C(42)	1.324(6)
N(8)-C(41)	1.385(6)
C(7)-C(8)	1.400(6)
C(7)-C(12)	1.409(6)
C(8)-C(9)	1.360(7)
C(9)-C(10)	1.393(8)
C(10)-C(11)	1.374(8)
C(11)-C(12)	1.399(6)
C(13)-C(14)	1.424(6)
C(15)-C(16)	1.391(6)
C(15)-C(20)	1.417(7)
C(16)-C(17)	1.383(7)
C(17)-C(18)	1.398(8)
C(18)-C(19)	1.371(7)
C(19)-C(20)	1.393(6)
C(21)-C(22)	1.383(6)
C(21)-C(26)	1.396(6)
C(22)-C(23)	1.371(7)
C(23)-C(24)	1.392(8)
C(24)-C(25)	1.359(8)
C(25)-C(26)	1.399(7)
C(28)-C(29)	1.504(8)
C(29)-C(30)	1.383(8)
C(29)-C(34)	1.391(8)
C(30)-C(31)	1.386(9)
C(31)-C(32)	1.361(8)
C(32)-C(33)	1.372(8)
C(33)-C(34)	1.390(8)
C(34)-C(35)	1.501(7)
C(36)-C(37)	1.382(7)
C(36)-C(41)	1.395(6)
C(37)-C(38)	1.377(8)
C(38)-C(39)	1.391(7)
C(39)-C(40)	1.360(7)

C(40)-C(41)	1.404(7)
C(1)-Re(1)-C(3)	88.58(19)
C(1)-Re(1)-C(2)	90.9(2)
C(3)-Re(1)-C(2)	87.77(19)
C(1)-Re(1)-N(8)	91.98(18)
C(3)-Re(1)-N(8)	179.04(17)
C(2)-Re(1)-N(8)	93.00(17)
C(1)-Re(1)-N(1)	94.81(17)
C(3)-Re(1)-N(1)	98.31(16)
C(2)-Re(1)-N(1)	171.72(18)
N(8)-Re(1)-N(1)	80.86(14)
C(1)-Re(1)-N(2)	172.49(17)
C(3)-Re(1)-N(2)	92.34(16)
C(2)-Re(1)-N(2)	96.55(17)
N(8)-Re(1)-N(2)	87.01(14)
N(1)-Re(1)-N(2)	77.68(13)
C(5)-Re(2)-C(6)	88.9(2)
C(5)-Re(2)-C(4)	88.9(2)
C(6)-Re(2)-C(4)	86.8(2)
C(5)-Re(2)-N(5)	95.60(18)
C(6)-Re(2)-N(5)	91.55(17)
C(4)-Re(2)-N(5)	175.24(19)
C(5)-Re(2)-N(4)	171.50(17)
C(6)-Re(2)-N(4)	99.11(17)
C(4)-Re(2)-N(4)	94.27(19)
N(5)-Re(2)-N(4)	81.56(13)
C(5)-Re(2)-N(3)	94.31(18)
C(6)-Re(2)-N(3)	173.41(17)
C(4)-Re(2)-N(3)	98.94(17)
N(5)-Re(2)-N(3)	82.43(13)
N(4)-Re(2)-N(3)	77.41(13)
C(13)-N(1)-C(7)	103.0(4)
C(13)-N(1)-Re(1)	110.3(3)
C(7)-N(1)-Re(1)	145.1(3)

C(14)-N(2)-C(15)	102.2(4)
C(14)-N(2)-Re(1)	110.3(3)
C(15)-N(2)-Re(1)	147.3(3)
C(14)-N(3)-C(20)	102.6(4)
C(14)-N(3)-Re(2)	110.0(3)
C(20)-N(3)-Re(2)	144.7(3)
C(13)-N(4)-C(12)	102.5(4)
C(13)-N(4)-Re(2)	110.7(3)
C(12)-N(4)-Re(2)	144.7(3)
C(27)-N(5)-C(21)	104.9(4)
C(27)-N(5)-Re(2)	125.0(3)
C(21)-N(5)-Re(2)	129.7(3)
C(27)-N(6)-C(26)	106.9(4)
C(27)-N(6)-C(28)	127.9(4)
C(26)-N(6)-C(28)	124.2(4)
C(42)-N(7)-C(36)	107.3(4)
C(42)-N(7)-C(35)	124.5(4)
C(36)-N(7)-C(35)	128.1(4)
C(42)-N(8)-C(41)	105.8(4)
C(42)-N(8)-Re(1)	123.6(3)
C(41)-N(8)-Re(1)	130.0(3)
O(1)-C(1)-Re(1)	178.6(5)
O(2)-C(2)-Re(1)	178.2(5)
O(3)-C(3)-Re(1)	177.9(4)
O(4)-C(4)-Re(2)	176.6(5)
O(5)-C(5)-Re(2)	178.0(5)
O(6)-C(6)-Re(2)	178.3(5)
N(1)-C(7)-C(8)	131.8(5)
N(1)-C(7)-C(12)	107.6(4)
C(8)-C(7)-C(12)	120.5(4)
C(9)-C(8)-C(7)	117.8(5)
C(8)-C(9)-C(10)	121.9(5)
C(11)-C(10)-C(9)	121.6(5)
C(10)-C(11)-C(12)	117.4(5)
N(4)-C(12)-C(11)	130.6(5)

N(4)-C(12)-C(7)	108.7(4)
C(11)-C(12)-C(7)	120.7(4)
N(1)-C(13)-N(4)	118.2(4)
N(1)-C(13)-C(14)	121.2(4)
N(4)-C(13)-C(14)	120.3(4)
N(3)-C(14)-N(2)	118.7(4)
N(3)-C(14)-C(13)	120.7(4)
N(2)-C(14)-C(13)	120.4(4)
N(2)-C(15)-C(16)	131.1(4)
N(2)-C(15)-C(20)	108.6(4)
C(16)-C(15)-C(20)	120.3(4)
C(17)-C(16)-C(15)	117.6(5)
C(16)-C(17)-C(18)	121.9(5)
C(19)-C(18)-C(17)	121.3(5)
C(18)-C(19)-C(20)	117.8(5)
C(19)-C(20)-N(3)	130.9(4)
C(19)-C(20)-C(15)	121.2(4)
N(3)-C(20)-C(15)	107.9(4)
C(22)-C(21)-C(26)	120.1(4)
C(22)-C(21)-N(5)	131.2(4)
C(26)-C(21)-N(5)	108.7(4)
C(23)-C(22)-C(21)	117.7(5)
C(22)-C(23)-C(24)	121.6(5)
C(25)-C(24)-C(23)	122.1(5)
C(24)-C(25)-C(26)	116.4(5)
N(6)-C(26)-C(21)	106.2(4)
N(6)-C(26)-C(25)	131.6(4)
C(21)-C(26)-C(25)	122.1(5)
N(6)-C(27)-N(5)	113.2(4)
N(6)-C(28)-C(29)	114.5(4)
C(30)-C(29)-C(34)	119.3(5)
C(30)-C(29)-C(28)	118.6(5)
C(34)-C(29)-C(28)	122.1(5)
C(29)-C(30)-C(31)	120.5(6)
C(32)-C(31)-C(30)	120.1(6)

C(33)-C(32)-C(31)	120.0(6)
C(32)-C(33)-C(34)	121.0(5)
C(29)-C(34)-C(33)	119.1(5)
C(29)-C(34)-C(35)	123.1(5)
C(33)-C(34)-C(35)	117.8(5)
N(7)-C(35)-C(34)	113.2(4)
C(37)-C(36)-N(7)	132.2(4)
C(37)-C(36)-C(41)	122.1(5)
N(7)-C(36)-C(41)	105.7(4)
C(38)-C(37)-C(36)	116.9(5)
C(37)-C(38)-C(39)	121.4(5)
C(40)-C(39)-C(38)	122.2(5)
C(39)-C(40)-C(41)	117.4(5)
N(8)-C(41)-C(36)	108.8(4)
N(8)-C(41)-C(40)	131.2(4)
C(36)-C(41)-C(40)	120.1(4)
N(8)-C(42)-N(7)	112.4(4)

Symmetry transformations used to generate equivalent atoms:

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Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **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)	31(1)	33(1)	46(1)	-1(1)	18(1)	-3(1)
Re(2)	29(1)	37(1)	44(1)	5(1)	13(1)	3(1)
O(1)	60(2)	78(3)	94(3)	-25(2)	43(2)	4(2)
O(2)	42(2)	68(2)	70(3)	-10(2)	6(2)	-7(2)
O(3)	75(3)	40(2)	73(2)	6(2)	37(2)	-12(2)
O(4)	65(3)	73(3)	115(4)	50(3)	12(3)	10(2)
O(5)	61(3)	122(4)	84(3)	-7(3)	39(2)	31(3)
O(6)	51(2)	86(3)	82(3)	-9(2)	15(2)	-28(2)
N(1)	36(2)	38(2)	41(2)	-3(2)	16(2)	-3(2)
N(2)	31(2)	38(2)	39(2)	-3(2)	14(2)	-3(2)
N(3)	34(2)	37(2)	41(2)	-1(2)	16(2)	1(2)
N(4)	34(2)	41(2)	36(2)	-1(2)	14(2)	-4(2)
N(5)	39(2)	38(2)	40(2)	6(2)	16(2)	3(2)
N(6)	47(2)	35(2)	54(2)	8(2)	22(2)	4(2)
N(7)	37(2)	31(2)	64(3)	5(2)	9(2)	-3(2)
N(8)	36(2)	34(2)	55(3)	2(2)	14(2)	-4(2)
C(1)	42(3)	41(3)	60(3)	-5(2)	20(2)	-7(2)
C(2)	41(3)	36(2)	61(3)	0(2)	21(3)	-1(2)
C(3)	39(3)	51(3)	46(3)	-10(2)	22(2)	-3(2)
C(4)	37(3)	50(3)	69(3)	11(3)	12(3)	-1(2)
C(5)	39(3)	58(3)	59(3)	2(2)	16(3)	8(2)
C(6)	48(3)	50(3)	52(3)	7(2)	23(2)	3(3)
C(7)	49(3)	38(2)	35(2)	2(2)	21(2)	-3(2)
C(8)	58(3)	47(3)	50(3)	-4(2)	29(3)	0(2)
C(9)	92(5)	50(3)	53(3)	-14(2)	37(3)	-8(3)
C(10)	79(4)	63(3)	43(3)	-14(2)	20(3)	-22(3)
C(11)	53(3)	65(3)	41(3)	-2(2)	14(3)	-15(3)
C(12)	46(3)	40(2)	31(2)	2(2)	16(2)	-7(2)
C(13)	35(3)	35(2)	38(3)	2(2)	16(2)	-2(2)
C(14)	36(2)	29(2)	43(2)	-1(2)	18(2)	-3(2)

C(15)	42(3)	25(2)	42(2)	3(2)	18(2)	-1(2)
C(16)	49(3)	33(2)	47(3)	-2(2)	17(2)	-7(2)
C(17)	78(4)	37(2)	40(3)	-1(2)	20(3)	-10(3)
C(18)	80(4)	33(2)	48(3)	2(2)	33(3)	2(3)
C(19)	59(3)	32(2)	55(3)	1(2)	32(3)	2(2)
C(20)	46(3)	28(2)	42(3)	5(2)	22(2)	1(2)
C(21)	33(2)	47(2)	38(3)	5(2)	14(2)	-4(2)
C(22)	44(3)	54(3)	46(3)	-1(2)	18(2)	-5(2)
C(23)	64(4)	74(4)	40(3)	-2(3)	22(3)	-3(3)
C(24)	74(4)	79(4)	45(3)	14(3)	19(3)	1(3)
C(25)	64(4)	59(3)	60(3)	23(3)	23(3)	12(3)
C(26)	37(3)	42(2)	49(3)	10(2)	15(2)	2(2)
C(27)	46(3)	36(2)	46(3)	2(2)	23(2)	-1(2)
C(28)	70(4)	36(3)	83(4)	14(2)	42(3)	10(2)
C(29)	54(3)	31(2)	69(4)	0(2)	22(3)	0(2)
C(30)	40(3)	57(3)	98(5)	-9(3)	21(3)	-5(3)
C(31)	64(4)	71(4)	80(4)	-11(3)	12(3)	-10(3)
C(32)	75(4)	71(4)	77(4)	-19(3)	36(4)	-10(3)
C(33)	53(3)	51(3)	95(4)	-12(3)	39(3)	-3(3)
C(34)	39(3)	31(2)	79(4)	0(2)	23(3)	-2(2)
C(35)	43(3)	33(2)	80(4)	0(2)	6(3)	-4(2)
C(36)	32(2)	37(2)	59(3)	9(2)	8(2)	-2(2)
C(37)	46(3)	50(3)	74(4)	19(3)	9(3)	-5(3)
C(38)	58(4)	78(4)	60(4)	29(3)	15(3)	2(3)
C(39)	51(3)	65(3)	54(3)	6(2)	20(3)	1(3)
C(40)	44(3)	47(3)	54(3)	2(2)	19(2)	-2(2)
C(41)	31(2)	38(2)	50(3)	7(2)	14(2)	1(2)
C(42)	39(3)	41(3)	55(3)	4(2)	14(2)	0(2)

Table S5. Crystal data and structure refinement for **2**.

Identification code	i6014	
Empirical formula	$C_{53}\ H_{34}\ N_4\ O_{10}\ Re_2$	
Formula weight	1259.24	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 13.3125(15) Å	α = 73.052(9)°.
	b = 13.6261(18) Å	β = 91.069(8)°.
	c = 15.5143(13) Å	γ = 119.326(11)°.
Volume	2320.9(4) Å^3	
Z	2	
Density (calculated)	1.802 Mg/m^3	
Absorption coefficient	5.277 mm^{-1}	
F(000)	1220	
Crystal size	0.40 x 0.30 x 0.20 mm^3	
Theta range for data collection	1.39 to 24.97°.	
Index ranges	0<=h<=15, -16<=k<=14, -18<=l<=18	
Reflections collected	8543	
Independent reflections	8153 [R(int) = 0.0326]	
Completeness to theta = 24.97°	100.0 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.4184 and 0.2267	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8153 / 0 / 587	
Goodness-of-fit on F^2	0.994	
Final R indices [I>2σ(I)]	$R1$ = 0.0340, $wR2$ = 0.0769	
R indices (all data)	$R1$ = 0.0993, $wR2$ = 0.0949	
Largest diff. peak and hole	1.127 and -0.736 e.Å^{-3}	

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	4341(1)	1587(1)	3988(1)	27(1)
Re(2)	-1048(1)	120(1)	7970(1)	33(1)
C(1)	4797(8)	2187(10)	2712(7)	47(3)
C(2)	5774(8)	1634(8)	4020(6)	35(2)
C(3)	3622(8)	9(8)	3913(6)	35(2)
C(4)	-1232(8)	-255(9)	9245(7)	43(2)
C(5)	-2297(9)	416(10)	8041(7)	47(3)
C(6)	-2193(9)	-1516(9)	8156(6)	42(2)
C(11)	3028(7)	803(7)	5923(6)	25(2)
C(12)	3064(7)	365(7)	6897(6)	30(2)
C(13)	3974(8)	196(8)	7194(6)	37(2)
C(14)	4014(9)	-220(10)	8098(7)	55(3)
C(15)	3131(10)	-492(11)	8736(7)	66(3)
C(16)	2202(8)	-359(8)	8459(6)	42(2)
C(17)	2153(7)	76(7)	7531(6)	30(2)
C(18)	1172(7)	222(7)	7240(6)	27(2)
C(19)	1179(7)	730(7)	6307(6)	27(2)
C(20)	247(7)	906(7)	6018(6)	25(2)
C(21)	256(7)	1426(7)	5050(6)	26(2)
C(22)	-625(8)	1664(8)	4737(6)	35(2)
C(23)	-608(8)	2143(8)	3828(6)	36(2)
C(24)	293(8)	2435(8)	3203(6)	36(2)
C(25)	1170(8)	2214(8)	3489(6)	32(2)
C(26)	1163(7)	1700(7)	4402(6)	25(2)
C(27)	2079(7)	1439(7)	4690(6)	25(2)
C(28)	2121(7)	1015(7)	5628(6)	24(2)
C(31)	5028(7)	4266(8)	3561(6)	34(2)
C(32)	5843(7)	3829(8)	4707(6)	33(2)
C(33)	6227(8)	3283(8)	5428(6)	42(2)
C(34)	7032(9)	4004(9)	5865(6)	47(3)

C(35)	7445(9)	5235(9)	5587(7)	55(3)
C(36)	7097(8)	5786(8)	4872(7)	45(2)
C(37)	6262(7)	5039(7)	4437(6)	31(2)
C(38)	5991(9)	6494(8)	3158(6)	44(2)
C(39)	5727(8)	6634(8)	2181(7)	40(2)
C(40)	5019(10)	7090(10)	1916(9)	70(4)
C(41)	4781(14)	7304(15)	1033(11)	105(6)
C(42)	5259(14)	7096(16)	416(10)	110(6)
C(43)	5983(10)	6631(11)	670(7)	65(3)
C(44)	6217(8)	6375(8)	1562(7)	41(2)
C(45)	6990(8)	5845(9)	1763(7)	45(3)
C(51)	8720(8)	7697(8)	1875(6)	38(2)
C(52)	9599(8)	6993(8)	2834(6)	38(2)
C(53)	10352(9)	6819(10)	3393(7)	52(3)
C(54)	10049(10)	5680(10)	3853(8)	63(3)
C(55)	9003(11)	4705(11)	3781(8)	65(3)
C(56)	8237(9)	4855(9)	3232(7)	51(3)
C(57)	8562(8)	6024(8)	2769(6)	35(2)
C(61)	9784(17)	5841(17)	929(13)	130(6)
C(62)	8894(15)	4878(15)	799(11)	98(5)
C(63)	8102(17)	4744(18)	196(13)	133(7)
C(64)	8360(16)	5876(17)	-392(12)	124(6)
C(65)	9182(17)	6865(18)	-291(13)	133(7)
C(66)	9912(15)	6935(16)	333(12)	118(6)
C(67)	8620(20)	3730(20)	1445(18)	256(14)
N(1)	5072(6)	3359(6)	4124(5)	29(2)
N(2)	5746(6)	5307(6)	3694(5)	33(2)
N(3)	9656(6)	8027(7)	2266(5)	37(2)
N(4)	8026(6)	6516(6)	2159(5)	37(2)
O(1)	5143(7)	2599(8)	1938(5)	70(2)
O(2)	6676(5)	1687(6)	4042(5)	53(2)
O(3)	3214(6)	-925(6)	3857(5)	52(2)
O(4)	-1366(7)	-500(7)	10031(5)	66(2)
O(5)	-3030(7)	602(9)	8153(6)	86(3)
O(6)	-2875(7)	-2491(6)	8319(5)	63(2)

O(7)	3902(5)	1017(5)	5406(4)	31(1)
O(8)	2809(5)	1667(5)	4029(4)	28(1)
O(9)	-641(5)	676(5)	6533(4)	32(1)
O(10)	386(5)	-98(5)	7901(4)	33(2)

Table S7. Bond lengths [Å] and angles [°] for **2**.

Re(1)-C(2)	1.878(9)
Re(1)-C(1)	1.890(10)
Re(1)-C(3)	1.918(10)
Re(1)-O(7)	2.096(6)
Re(1)-O(8)	2.097(5)
Re(1)-N(1)	2.194(7)
Re(2)-C(4)	1.882(10)
Re(2)-C(5)	1.905(10)
Re(2)-C(6)	1.922(11)
Re(2)-O(10)	2.079(5)
Re(2)-O(9)	2.120(5)
Re(2)-N(3)#1	2.201(7)
C(1)-O(1)	1.158(11)
C(2)-O(2)	1.167(10)
C(3)-O(3)	1.144(10)
C(4)-O(4)	1.158(11)
C(5)-O(5)	1.149(11)
C(6)-O(6)	1.133(11)
C(11)-O(7)	1.283(9)
C(11)-C(28)	1.413(11)
C(11)-C(12)	1.463(11)
C(12)-C(13)	1.387(11)
C(12)-C(17)	1.395(11)
C(13)-C(14)	1.361(12)
C(13)-H(13)	0.9300
C(14)-C(15)	1.380(13)
C(14)-H(14)	0.9300
C(15)-C(16)	1.379(13)
C(15)-H(15)	0.9300
C(16)-C(17)	1.401(12)
C(16)-H(16)	0.9300
C(17)-C(18)	1.460(11)
C(18)-O(10)	1.293(9)

C(18)-C(19)	1.408(11)
C(19)-C(20)	1.416(11)
C(19)-C(28)	1.472(10)
C(20)-O(9)	1.288(9)
C(20)-C(21)	1.460(11)
C(21)-C(22)	1.406(11)
C(21)-C(26)	1.411(11)
C(22)-C(23)	1.366(12)
C(22)-H(22)	0.9300
C(23)-C(24)	1.374(12)
C(23)-H(23)	0.9300
C(24)-C(25)	1.378(11)
C(24)-H(24)	0.9300
C(25)-C(26)	1.383(11)
C(25)-H(25)	0.9300
C(26)-C(27)	1.458(11)
C(27)-O(8)	1.285(9)
C(27)-C(28)	1.412(11)
C(31)-N(1)	1.316(10)
C(31)-N(2)	1.342(10)
C(31)-H(31)	0.9300
C(32)-C(37)	1.382(11)
C(32)-C(33)	1.390(12)
C(32)-N(1)	1.394(10)
C(33)-C(34)	1.379(12)
C(33)-H(33)	0.9300
C(34)-C(35)	1.409(13)
C(34)-H(34)	0.9300
C(35)-C(36)	1.358(13)
C(35)-H(35)	0.9300
C(36)-C(37)	1.412(12)
C(36)-H(36)	0.9300
C(37)-N(2)	1.380(10)
C(38)-N(2)	1.457(11)
C(38)-C(39)	1.529(13)

C(38)-H(38A)	0.9700
C(38)-H(38B)	0.9700
C(39)-C(40)	1.362(14)
C(39)-C(44)	1.384(13)
C(40)-C(41)	1.380(18)
C(40)-H(40)	0.9300
C(41)-C(42)	1.32(2)
C(41)-H(41)	0.9300
C(42)-C(43)	1.388(18)
C(42)-H(42)	0.9300
C(43)-C(44)	1.394(13)
C(43)-H(43)	0.9300
C(44)-C(45)	1.504(12)
C(45)-N(4)	1.476(11)
C(45)-H(45A)	0.9700
C(45)-H(45B)	0.9700
C(51)-N(3)	1.305(11)
C(51)-N(4)	1.334(11)
C(51)-H(51)	0.9300
C(52)-C(53)	1.377(13)
C(52)-N(3)	1.394(11)
C(52)-C(57)	1.395(12)
C(53)-C(54)	1.354(14)
C(53)-H(53)	0.9300
C(54)-C(55)	1.409(15)
C(54)-H(54)	0.9300
C(55)-C(56)	1.369(15)
C(55)-H(55)	0.9300
C(56)-C(57)	1.381(12)
C(56)-H(56)	0.9300
C(57)-N(4)	1.388(11)
C(61)-C(62)	1.34(2)
C(61)-C(66)	1.44(2)
C(61)-H(61)	0.9300
C(62)-C(63)	1.38(2)

C(62)-C(67)	1.46(3)
C(63)-C(64)	1.41(2)
C(63)-H(63)	0.9300
C(64)-C(65)	1.31(2)
C(64)-H(64)	0.9300
C(65)-C(66)	1.35(2)
C(65)-H(65)	0.9300
C(66)-H(66)	0.9300
C(67)-H(67A)	0.9600
C(67)-H(67B)	0.9600
C(67)-H(67C)	0.9600
N(3)-Re(2)#1	2.201(7)

C(2)-Re(1)-C(1)	84.0(4)
C(2)-Re(1)-C(3)	89.3(4)
C(1)-Re(1)-C(3)	88.6(4)
C(2)-Re(1)-O(7)	95.2(3)
C(1)-Re(1)-O(7)	176.8(4)
C(3)-Re(1)-O(7)	94.6(3)
C(2)-Re(1)-O(8)	173.8(3)
C(1)-Re(1)-O(8)	98.9(3)
C(3)-Re(1)-O(8)	96.2(3)
O(7)-Re(1)-O(8)	81.6(2)
C(2)-Re(1)-N(1)	93.3(3)
C(1)-Re(1)-N(1)	93.7(4)
C(3)-Re(1)-N(1)	176.7(3)
O(7)-Re(1)-N(1)	83.2(2)
O(8)-Re(1)-N(1)	81.1(2)
C(4)-Re(2)-C(5)	84.7(4)
C(4)-Re(2)-C(6)	87.4(4)
C(5)-Re(2)-C(6)	88.0(4)
C(4)-Re(2)-O(10)	94.6(3)
C(5)-Re(2)-O(10)	176.4(4)
C(6)-Re(2)-O(10)	95.5(3)
C(4)-Re(2)-O(9)	173.6(3)

C(5)-Re(2)-O(9)	99.1(3)
C(6)-Re(2)-O(9)	97.9(3)
O(10)-Re(2)-O(9)	81.3(2)
C(4)-Re(2)-N(3)#1	93.6(4)
C(5)-Re(2)-N(3)#1	95.4(4)
C(6)-Re(2)-N(3)#1	176.6(3)
O(10)-Re(2)-N(3)#1	81.2(3)
O(9)-Re(2)-N(3)#1	81.0(2)
O(1)-C(1)-Re(1)	175.9(10)
O(2)-C(2)-Re(1)	178.5(8)
O(3)-C(3)-Re(1)	178.6(8)
O(4)-C(4)-Re(2)	178.8(10)
O(5)-C(5)-Re(2)	174.4(9)
O(6)-C(6)-Re(2)	176.0(8)
O(7)-C(11)-C(28)	125.8(8)
O(7)-C(11)-C(12)	114.0(7)
C(28)-C(11)-C(12)	120.2(7)
C(13)-C(12)-C(17)	119.7(8)
C(13)-C(12)-C(11)	120.7(7)
C(17)-C(12)-C(11)	119.6(8)
C(14)-C(13)-C(12)	121.3(8)
C(14)-C(13)-H(13)	119.3
C(12)-C(13)-H(13)	119.3
C(13)-C(14)-C(15)	119.8(9)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(16)-C(15)-C(14)	120.1(10)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(17)	120.7(9)
C(15)-C(16)-H(16)	119.7
C(17)-C(16)-H(16)	119.7
C(12)-C(17)-C(16)	118.4(8)
C(12)-C(17)-C(18)	121.0(8)
C(16)-C(17)-C(18)	120.6(8)

O(10)-C(18)-C(19)	126.3(7)
O(10)-C(18)-C(17)	114.2(7)
C(19)-C(18)-C(17)	119.5(7)
C(18)-C(19)-C(20)	120.0(7)
C(18)-C(19)-C(28)	119.9(7)
C(20)-C(19)-C(28)	120.0(7)
O(9)-C(20)-C(19)	126.6(8)
O(9)-C(20)-C(21)	113.7(7)
C(19)-C(20)-C(21)	119.7(7)
C(22)-C(21)-C(26)	118.4(8)
C(22)-C(21)-C(20)	121.5(7)
C(26)-C(21)-C(20)	120.0(7)
C(23)-C(22)-C(21)	120.8(8)
C(23)-C(22)-H(22)	119.6
C(21)-C(22)-H(22)	119.6
C(22)-C(23)-C(24)	120.5(8)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(24)-C(25)	120.0(8)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
C(24)-C(25)-C(26)	121.0(8)
C(24)-C(25)-H(25)	119.5
C(26)-C(25)-H(25)	119.5
C(25)-C(26)-C(21)	119.2(7)
C(25)-C(26)-C(27)	120.3(7)
C(21)-C(26)-C(27)	120.5(7)
O(8)-C(27)-C(28)	126.3(8)
O(8)-C(27)-C(26)	114.0(7)
C(28)-C(27)-C(26)	119.7(7)
C(27)-C(28)-C(11)	120.6(7)
C(27)-C(28)-C(19)	119.8(7)
C(11)-C(28)-C(19)	119.5(7)
N(1)-C(31)-N(2)	113.6(8)
N(1)-C(31)-H(31)	123.2

N(2)-C(31)-H(31)	123.2
C(37)-C(32)-C(33)	121.4(8)
C(37)-C(32)-N(1)	108.1(8)
C(33)-C(32)-N(1)	130.5(8)
C(34)-C(33)-C(32)	116.7(9)
C(34)-C(33)-H(33)	121.6
C(32)-C(33)-H(33)	121.6
C(33)-C(34)-C(35)	121.3(9)
C(33)-C(34)-H(34)	119.3
C(35)-C(34)-H(34)	119.3
C(36)-C(35)-C(34)	122.6(9)
C(36)-C(35)-H(35)	118.7
C(34)-C(35)-H(35)	118.7
C(35)-C(36)-C(37)	115.7(9)
C(35)-C(36)-H(36)	122.2
C(37)-C(36)-H(36)	122.2
N(2)-C(37)-C(32)	107.3(7)
N(2)-C(37)-C(36)	130.5(8)
C(32)-C(37)-C(36)	122.2(8)
N(2)-C(38)-C(39)	115.0(7)
N(2)-C(38)-H(38A)	108.5
C(39)-C(38)-H(38A)	108.5
N(2)-C(38)-H(38B)	108.5
C(39)-C(38)-H(38B)	108.5
H(38A)-C(38)-H(38B)	107.5
C(40)-C(39)-C(44)	120.1(10)
C(40)-C(39)-C(38)	116.8(10)
C(44)-C(39)-C(38)	123.1(8)
C(39)-C(40)-C(41)	120.8(13)
C(39)-C(40)-H(40)	119.6
C(41)-C(40)-H(40)	119.6
C(42)-C(41)-C(40)	120.7(14)
C(42)-C(41)-H(41)	119.6
C(40)-C(41)-H(41)	119.6
C(41)-C(42)-C(43)	119.5(13)

C(41)-C(42)-H(42)	120.3
C(43)-C(42)-H(42)	120.3
C(42)-C(43)-C(44)	121.2(12)
C(42)-C(43)-H(43)	119.4
C(44)-C(43)-H(43)	119.4
C(39)-C(44)-C(43)	117.6(10)
C(39)-C(44)-C(45)	125.8(9)
C(43)-C(44)-C(45)	116.5(10)
N(4)-C(45)-C(44)	114.3(8)
N(4)-C(45)-H(45A)	108.7
C(44)-C(45)-H(45A)	108.7
N(4)-C(45)-H(45B)	108.7
C(44)-C(45)-H(45B)	108.7
H(45A)-C(45)-H(45B)	107.6
N(3)-C(51)-N(4)	111.8(8)
N(3)-C(51)-H(51)	124.1
N(4)-C(51)-H(51)	124.1
C(53)-C(52)-N(3)	131.6(9)
C(53)-C(52)-C(57)	120.4(9)
N(3)-C(52)-C(57)	108.0(8)
C(54)-C(53)-C(52)	117.1(11)
C(54)-C(53)-H(53)	121.4
C(52)-C(53)-H(53)	121.4
C(53)-C(54)-C(55)	122.1(11)
C(53)-C(54)-H(54)	119.0
C(55)-C(54)-H(54)	119.0
C(56)-C(55)-C(54)	121.9(11)
C(56)-C(55)-H(55)	119.1
C(54)-C(55)-H(55)	119.1
C(55)-C(56)-C(57)	115.1(10)
C(55)-C(56)-H(56)	122.4
C(57)-C(56)-H(56)	122.4
C(56)-C(57)-N(4)	131.6(9)
C(56)-C(57)-C(52)	123.4(9)
N(4)-C(57)-C(52)	105.1(8)

C(62)-C(61)-C(66)	113.0(18)
C(62)-C(61)-H(61)	123.5
C(66)-C(61)-H(61)	123.5
C(61)-C(62)-C(63)	132.3(19)
C(61)-C(62)-C(67)	116(2)
C(63)-C(62)-C(67)	111.1(19)
C(62)-C(63)-C(64)	109.6(18)
C(62)-C(63)-H(63)	125.2
C(64)-C(63)-H(63)	125.2
C(65)-C(64)-C(63)	122(2)
C(65)-C(64)-H(64)	118.9
C(63)-C(64)-H(64)	118.9
C(64)-C(65)-C(66)	125(2)
C(64)-C(65)-H(65)	117.5
C(66)-C(65)-H(65)	117.5
C(65)-C(66)-C(61)	117.6(19)
C(65)-C(66)-H(66)	121.2
C(61)-C(66)-H(66)	121.2
C(62)-C(67)-H(67A)	109.5
C(62)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(62)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(31)-N(1)-C(32)	105.2(7)
C(31)-N(1)-Re(1)	126.1(6)
C(32)-N(1)-Re(1)	127.8(6)
C(31)-N(2)-C(37)	105.7(7)
C(31)-N(2)-C(38)	128.5(8)
C(37)-N(2)-C(38)	125.7(7)
C(51)-N(3)-C(52)	106.9(8)
C(51)-N(3)-Re(2)#1	125.3(6)
C(52)-N(3)-Re(2)#1	127.8(6)
C(51)-N(4)-C(57)	108.2(8)
C(51)-N(4)-C(45)	125.5(8)

C(57)-N(4)-C(45)	125.4(8)
C(11)-O(7)-Re(1)	133.0(5)
C(27)-O(8)-Re(1)	132.6(5)
C(20)-O(9)-Re(2)	131.6(5)
C(18)-O(10)-Re(2)	133.1(5)

Symmetry transformations used to generate equivalent atoms:

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

Table S8. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2**. 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)	24(1)	30(1)	27(1)	-11(1)	0(1)	13(1)
Re(2)	26(1)	41(1)	27(1)	-9(1)	3(1)	16(1)
C(1)	37(6)	64(7)	41(6)	-21(5)	-3(5)	23(6)
C(2)	32(5)	28(5)	36(5)	-14(4)	0(4)	7(4)
C(3)	30(5)	44(6)	36(5)	-15(5)	1(4)	21(5)
C(4)	36(6)	49(6)	45(6)	-15(5)	4(5)	23(5)
C(5)	40(6)	70(8)	33(6)	-14(5)	-1(5)	32(6)
C(6)	48(6)	45(6)	27(5)	-9(5)	-2(5)	21(5)
C(11)	24(4)	19(4)	36(5)	-11(4)	-2(4)	14(4)
C(12)	29(5)	32(5)	21(5)	-6(4)	-2(4)	11(4)
C(13)	30(5)	48(6)	29(5)	-8(4)	2(4)	19(5)
C(14)	52(7)	93(9)	38(6)	-7(6)	-5(5)	57(7)
C(15)	63(8)	97(10)	38(7)	-4(6)	-7(6)	52(8)
C(16)	40(6)	57(7)	23(5)	-8(5)	3(4)	23(5)
C(17)	27(5)	31(5)	38(5)	-13(4)	-5(4)	17(4)
C(18)	27(5)	32(5)	25(5)	-11(4)	-4(4)	17(4)
C(19)	22(4)	32(5)	25(5)	-9(4)	3(4)	12(4)
C(20)	25(5)	22(4)	34(5)	-17(4)	-5(4)	11(4)
C(21)	28(5)	26(5)	30(5)	-14(4)	-7(4)	16(4)
C(22)	36(5)	40(5)	38(6)	-11(4)	-5(4)	25(5)
C(23)	38(5)	42(6)	35(6)	-8(4)	-10(4)	28(5)
C(24)	47(6)	44(6)	28(5)	-13(4)	-11(4)	29(5)
C(25)	37(5)	40(5)	31(5)	-14(4)	-4(4)	27(5)
C(26)	21(4)	18(4)	35(5)	-10(4)	-5(4)	9(4)
C(27)	21(4)	15(4)	31(5)	-10(4)	1(4)	2(4)
C(28)	26(5)	18(4)	28(5)	-7(4)	-4(4)	11(4)
C(31)	33(5)	43(6)	29(5)	-12(4)	-5(4)	21(5)
C(32)	32(5)	38(5)	33(5)	-21(4)	-3(4)	15(4)
C(33)	49(6)	40(6)	45(6)	-21(5)	-14(5)	25(5)
C(34)	63(7)	53(7)	34(6)	-14(5)	-23(5)	35(6)

C(35)	59(7)	51(7)	58(7)	-31(6)	-29(6)	22(6)
C(36)	53(6)	32(5)	50(6)	-20(5)	-10(5)	19(5)
C(37)	37(5)	22(5)	35(5)	-9(4)	-5(4)	16(4)
C(38)	53(6)	35(6)	47(6)	-14(5)	-8(5)	26(5)
C(39)	34(5)	33(5)	47(6)	-5(5)	-9(5)	16(5)
C(40)	64(8)	64(8)	68(9)	0(7)	-2(7)	35(7)
C(41)	95(12)	125(14)	90(12)	0(11)	-36(10)	72(11)
C(42)	92(12)	146(16)	42(9)	11(9)	-29(8)	48(11)
C(43)	54(7)	75(8)	36(6)	-16(6)	-7(6)	13(7)
C(44)	29(5)	44(6)	43(6)	-12(5)	-4(4)	14(5)
C(45)	42(6)	50(6)	46(6)	-24(5)	0(5)	21(5)
C(51)	35(5)	43(6)	35(5)	-8(5)	-5(4)	21(5)
C(52)	32(5)	40(6)	39(6)	-11(5)	6(4)	16(5)
C(53)	52(7)	59(7)	49(7)	-9(6)	-13(5)	35(6)
C(54)	66(8)	61(8)	67(8)	-10(7)	-16(7)	42(7)
C(55)	74(9)	60(8)	55(8)	-1(6)	14(7)	38(7)
C(56)	55(7)	37(6)	57(7)	-13(5)	2(6)	22(5)
C(57)	44(6)	36(5)	30(5)	-7(4)	-3(4)	25(5)
N(1)	28(4)	27(4)	31(4)	-10(3)	-3(3)	12(3)
N(2)	38(4)	35(4)	28(4)	-13(3)	-4(3)	19(4)
N(3)	38(5)	40(5)	32(4)	-10(4)	-3(4)	20(4)
N(4)	26(4)	34(4)	38(4)	-9(4)	6(3)	8(4)
O(1)	67(5)	107(7)	26(4)	-9(4)	9(4)	42(5)
O(2)	30(4)	62(5)	75(5)	-29(4)	-3(4)	27(4)
O(3)	55(5)	46(4)	67(5)	-35(4)	-13(4)	25(4)
O(4)	77(6)	91(6)	27(4)	-6(4)	9(4)	46(5)
O(5)	65(6)	135(9)	88(7)	-34(6)	-3(5)	73(6)
O(6)	64(5)	45(5)	59(5)	-13(4)	10(4)	13(4)
O(7)	27(3)	37(4)	31(3)	-9(3)	-5(3)	19(3)
O(8)	28(3)	36(3)	21(3)	-6(3)	3(3)	17(3)
O(9)	24(3)	42(4)	26(3)	-9(3)	1(3)	16(3)
O(10)	28(3)	43(4)	24(3)	-1(3)	7(3)	20(3)