Supplementary Material for Dalton Transactions

Norharmane Rhenium(I) polypyridyl complexes: Synthesis, structural and spectroscopic characterization

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List of Contents

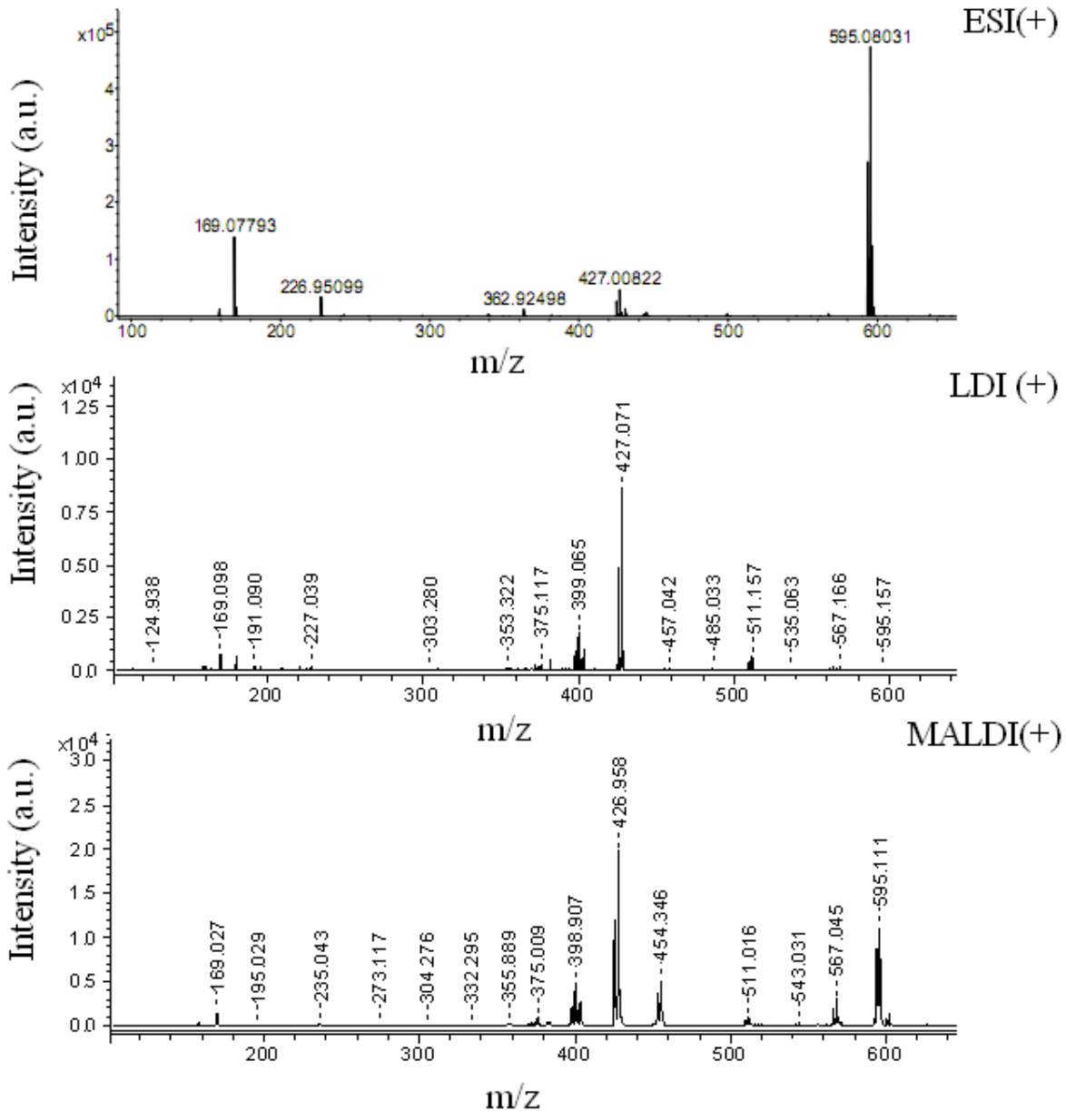

Fig. S1 Positive ion mass spectra of complex $[Re(CO)_3(bpy)(nHo)]^+$ $[CF_3SO_3]^-$ MW = 743.68 detected as $[M^+]$, exact mass = 595.078. a) ESI mass spectrum. b) LDI mass spectrum. c) MALDI mass spectrum acquired with DCTB as MALDI matrix.

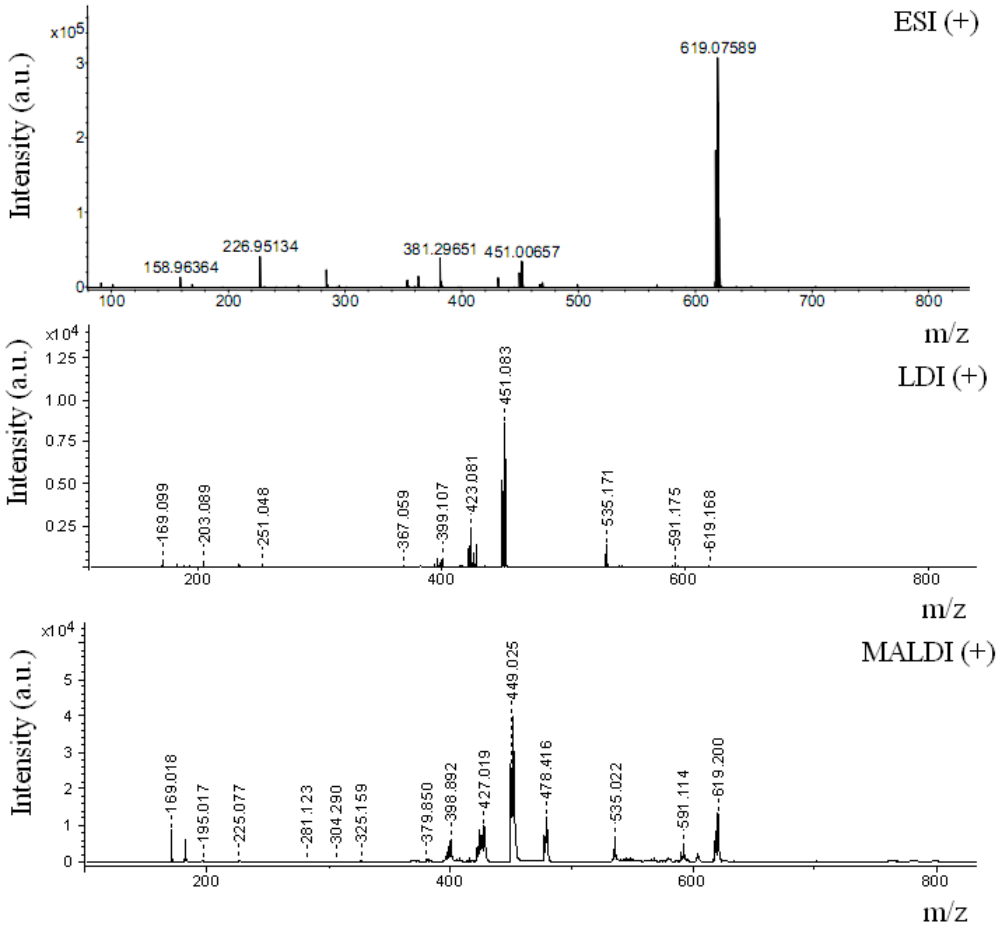

Fig. S2: Positive ion mass spectra of complex $[Re(CO)_3(phen)(nHo)]^+ [CF_3SO_3]^-$ MW = 767.71 detected as $[M^+]$, exact mass = 619.078. a) ESI mass spectrum. b) LDI mass spectrum. c) MALDI mass spectrum acquired with DCTB as MALDI matrix.

Table S1: ^{1}H-NMR signals (ppm) and coupling constant J (Hz) for nHo and $[Re(CO)_3(bpy)(nHo)]CF_3SO_3$.

	^{1}H-NMR															
	H-C1	**H-C3**	**H-C4**	**H-C5**	**H-C6**	**H-C7**	**H-C8**	**H-C9**	**H-C3´**	**H-C4´**	**H-C5´**	**H-C6´**	**H-C3´´**	**H-C4´´**	**H-C5´´**	**H-C6´´**
nHo	8,920 (s)	8,347 (d, J 5,2)	8,106 (d, J 5,2)	8,249 (d J 7,8)	7,248 (t, J 7,5)	7,549 (t, J 7,5)	7,607 (d, J 8,1)	11,620 (s)	--	--	--	--	--	--	--	--
$[Re(CO)_3(bpy)(nHo)]CF_3SO_3$	8,540 (s)	8,420 (d, J 5,5)	8,142 (d, J 6)	8,249 (d J 7,5)	7,270 (t, J 7,5)	7,559 (t, J 7,5)	7,614 (d, J 7)	11,730 (s)	9,442 (d 5,5)	7,965 (t, J 7)	7,289 (t, J 7)	8,681 (d, J 8)	9,442 (d 5,5)	7,615 (t, J 7)	7,289 (t, J 7)	8,681 (d, J 8)

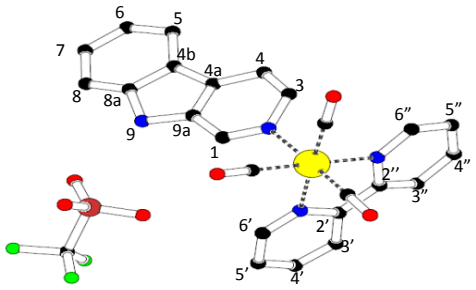

Table S2a. Results obtained by mass spectrometry using different ionization methods for the analysis of $[Re(CO)_3(bpy)(nHo)]^+[CF_3SO_3]^-$ in positive ion mode (n.d. not detected). MALDI matrix: DCTB and nHo.

Ion formula	Exact mass	ESI	LDI	MALDI	
				DCTB	nHo
$[Re(CO)_3(bpy)(nHo)]^+$	595.078			•	
$[Re(CO)_2(bpy)(nHo)]^+$	567.083	✓	✓	✓	✓
$[Re(bpy)(nHo)]^+$	511.093	n.d.	✓	✓	✓
$[Re(CO)_3(bpy)]^+$	427.009	✓	✓	✓	✓
$[Re(CO)_2(bpy)]^+$	399.014	n.d.	✓	✓	✓
$[nHo+H]^+$	169.068	✓	✓	✓	✓

Table S2b. Results obtained by mass spectrometry using different ionization methods for the analysis of $[Re(CO)_3(phen)(nHo)]^+[CF_3SO_3]^-$ in positive ion mode (n.d. not detected). MALDI matrix: DCTB and nHo.

Ion formula	Exact mass	ESI	LDI	MALDI	
				DCTB	nHo
$[Re(CO)_3(phen)(nHo)]^+$	619.078	✓	✓	✓	✓
$[Re(CO)_2(phen)(nHo)]^+$	591.083	n.d.	✓	✓	✓
$[Re(phen)(nHo)]^+$	533.093	n.d.	✓	✓	✓
$[Re(CO)_3(phen)]^+$	451.009	✓	✓	✓	✓
$[Re(CO)_2(phen)]^+$	432.014	n.d.	✓	✓	✓
$[Re(phen)]^+$	367.024	n.d.	✓	n.d.	✓
$[nHo+H]^+$	169.068	n.d.	✓	✓	✓

Table S3: Comparison of experimental absorption data of the $[Re(CO)_3(bpy)(nHo)]CF_3SO_3$ complex in MeOH with TD-DFT calculations **for Re-1 conformer (a) and Re-2 conformer (b).** Electronic transitions are computed at the PBE0-CPM/LanL2TZ(f)/6-311G/6-311G* level of theory.

(a)

λ_{exp} /nm ($\varepsilon/10^3$ $M^{-1}cm^{-1}$)	λ_{calc} /nm	f_{osc}	Major contributions
370 (6,8)	391.4	0.0668	H-1→L (95%)
307 (30,5)	308.4	0.2909	H-1→L+1 (76%)
	300.3	0.0928	H-5→L (45%), H-2→L+1 (10%), H-2→L+2 (16%), H-1→L+3 (13%)
	293.0	0.1214	H-2→L+4 (37%), H-1→L+2 (24%), H→L+4 (17%)
	285.6	0.0818	H-5→L (12%), H-3→L+1 (25%), H-3→L+4 (10%), H-2→L+5 (16%), H-1→L+3 (11%)
	280.9	0.0811	H-2→L+3 (82%)
	276.9	0.1296	H-5→L (12%), H-2→L+2 (31%), H-2→L+5 (25%)
249 (43,0)	254.6	0.0645	H-4→L+3 (60%), H-3→L+3 (21%)
	250.5	0.1952	H-6→L+1 (31%), H-1→L+6 (13%), H→L+6 (16%)
	248.3	0.3116	H-4→L+4 (29%), H-3→L+4 (12%), H-1→L+4 (12%), H→L+6 (35%)
	246.4	0.158	H-6→L+1 (36%), H→L+6 (21%)
241 (41.8)	239.9	0.0647	H-8→L (17%), H-5→L+2 (68%)
	238.3	0.2402	H→L+7 (82%)
230 (31,6)	226.1	0.0631	H-4→L+12 (10%), H-3→L+6 (15%), H-2→L+10 (10%)

(b)

λ_{exp} /nm ($\varepsilon/10^3$ $M^{-1}cm^{-1}$)	λ_{calc} /nm	f_{osc}	Major contributions
370 (6.8)	361.4	0.074	H-4→L (59%), H-2→L (39%)
355 (30.5)	345.4	0.0662	H→L+1 (94%)
319 (22.2)	317.9	0.3334	H-1→L+1 (79%)
307 (30,5)	296.6	0.0627	H-5→L (10%), H-1→L+3 (24%), H-1→L+4 (20%), H→L+4 (10%)
	296.3	0.1382	H-5→L (41%), H-4→L+1 (12%), H-1→L+5 (11%)
	292.0	0.0716	H-5→L (16%), H-4→L+1 (28%), H-2→L+3 (11%), H-1→L+2 (21%), H-1→L+5 (13%)
	268.9	0.0961	H-4→L+3 (46%), H-2→L+3 (30%)
262 (35.0)	256.4	0.098	H-4→L+4 (38%), H-3→L+3 (10%), H-2→L+6 (10%)
	253.0	0.3759	H-6→L+1 (18%), H-3→L+4 (14%), H→L+6 (37%)
249 (43.0)	247.8	0.1487	H-6→L+1 (46%), H→L+6 (27%)
	243.9	0.0512	H-3→L+4 (41%)
241 (41.8)	241.5	0.0756	H-7→L (13%), H-5→L+2 (70%)
	236.8	0.3699	H-1→L+6 (12%), H→L+7 (62%)
	235.9	0.0559	H-3→L+5 (10%), H-2→L+5 (10%), H-1→L+6 (31%), H→L+7 (14%)
230 (31.5)	230.4	0.0928	H-2→L+9 (19%), H-1→L+7 (24%), H→L+10 (11%)

The experimental spectrum was compared with the calculated spectra obtained by summing Gaussian functions centered at each calculated wavelength with the maxima related to the value of the oscillator strengths (which are also plotted) using eq. 1.

$$\varepsilon(\tilde{\upsilon}) = \frac{2.175\text{x}10^8 Lmol^{-1}cm^{-2}}{\Delta_{½}\tilde{\upsilon}}(f_{osc})\exp\left[-2.772\left(\frac{\tilde{\upsilon}-\tilde{\upsilon}_{i\to f}}{\Delta_{½}\tilde{\upsilon}}\right)^2\right]$$

This is the formula that GaussSum uses to convolute spectra (see N. O'Boyle, *GaussSum* 2.2.5 program documentation).
In this equation, the parametrical value of the fwhm of the band is given in units of cm^{-1} and is symbolized by $\Delta_{½}\tilde{\upsilon}$, f_{osc} is the oscillator strength and $\tilde{\upsilon}_{i\to f}$ is the frequency (in units of cm^{-1}) corresponding to the wavelength of the calculated electronic transition.

Table S4: HOMOs-LUMOs compositions of **Re-1** along with % composition vs. Energy plots (below)

MO (energy/eV)	Re	bpy	3 CO	nHo
H-8 (-9.15)	3.80	93.58	1.70	0.93
H-6 (-7.85)	0.32	0.33	0.27	99.08
H-5 (-7.72)	0.94	98.53	0.31	0.22
H-4 (-7.30)	45.03	4.35	19.57	31.05
H-3 (-7.22)	54.33	3.04	24.12	18.51
H-2 (-7.01)	62.90	8.06	27.77	1.27
H-1 (-6.77)	28.92	3.21	13.38	54.49
H (-6.40)	0.35	0.20	0.12	99.32
L (-3.03)	2.39	92.05	4.95	0.61
L+1 (-2.22)	1.08	8.36	3.93	86.63
L+2 (-2.01)	1.00	88.05	2.88	8.07
L+3 (-1.91)	0.41	94.43	3.83	1.33
L+4 (-1.66)	22.10	1.72	74.63	1.55
L+5 (-1.39)	17.40	6.06	74.45	2.09
L+6 (-0.99)	1.04	3.79	28.05	67.12
L+7 (-0.77)	0.74	2.67	69.87	26.72

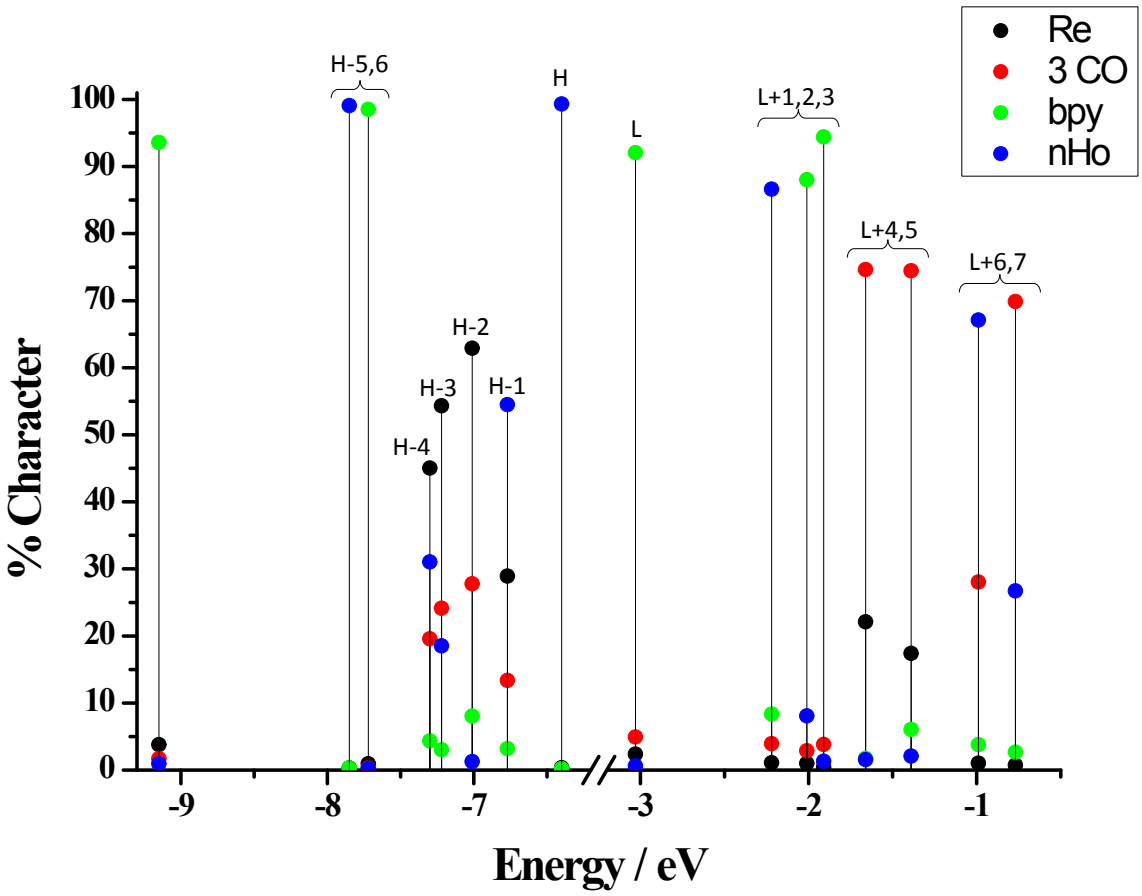

Table S5: HOMOs-LUMOs compositions of **Re-2** along with % composition vs. Energy plots (below).

MO (energy/eV)	Re	bpy	3 CO	nHo
H-7 (-8.96)	0.07	27.17	0.55	72.21
H-6 (-7.84)	0.04	1.84	0.11	98.01
H-5 (-7.72)	0.74	97.20	0.27	1.79
H-4 (-7.24)	67.27	2.47	30.10	0.15
H-3 (-7.22)	26.07	4.85	10.90	58.17
H-2 (-7.11)	63.00	9.47	26.81	0.72
H-1 (-6.71)	33.85	2.81	16.25	47.08
H (-6.39)	0.95	0.28	0.35	98.42
L (-3.05)	2.17	92.4	4.81	0.62
L+1 (-2.24)	2.98	0.79	8.70	87.53
L+2 (-2.02)	1.83	93.6	4.16	0.40
L+3 (-1.89)	0.50	92.55	5.77	1.18
L+4 (-1.59)	17.74	3.68	66.75	11.83
L+5 (-1.38)	17.13	6.91	75.05	0.92
L+6 (-0.99)	0.22	2.37	41.71	55.70
L+7 (-0.72)	0.63	0.81	57.04	41.53

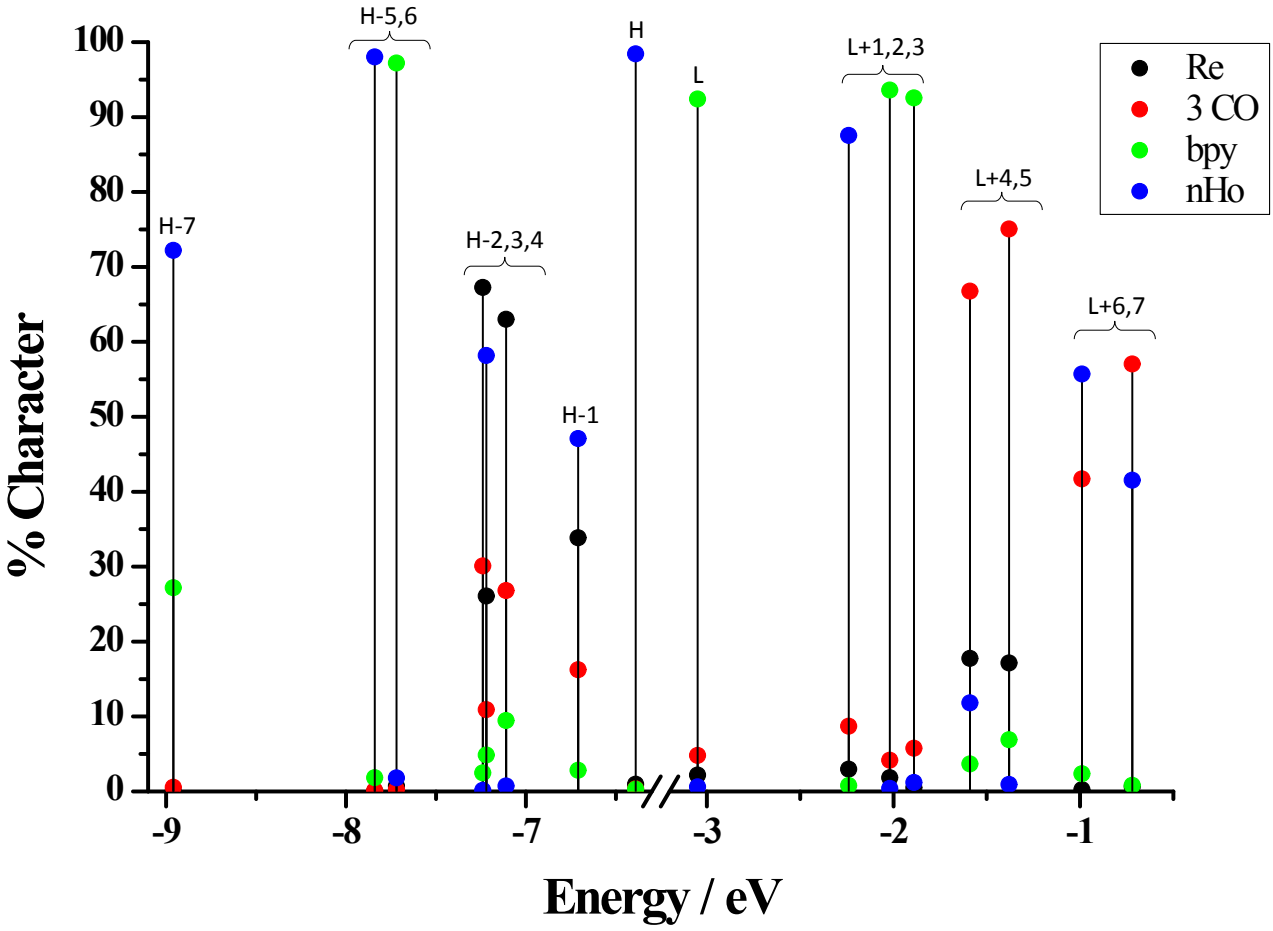

Table S6a. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *fac*-$[Re(CO)_3(phen)(nHo)]CF_3SO_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. To be deposited.

Atom	x	y	z	U(eq)
C(1)	4102(5)	4526(4)	2252(3)	61(1)
C(2)	4653(4)	4006(3)	3696(3)	40(1)
C(3)	5688(4)	3148(3)	2599(3)	44(1)
C(4)	7246(3)	319(3)	1397(3)	46(1)
C(10)	577(4)	3872(4)	3445(3)	56(1)
C(11)	2229(3)	2349(3)	1812(2)	34(1)
C(12)	1607(4)	1777(3)	1262(2)	37(1)
C(13)	2219(4)	1279(3)	733(2)	44(1)
C(14)	3374(4)	1383(3)	760(2)	50(1)
C(15)	3933(4)	1968(3)	1320(3)	47(1)
C(16)	1642(3)	2859(3)	2368(2)	35(1)
C(17)	451(4)	2818(3)	2355(2)	42(1)
C(18)	-82(4)	3345(3)	2914(3)	54(1)
C(21)	4241(4)	1104(3)	3244(3)	46(1)
C(22)	4129(4)	281(3)	3675(3)	48(1)
C(23)	3684(4)	350(3)	4372(2)	40(1)
C(24)	3435(4)	-295(3)	4975(3)	46(1)
C(25)	3528(5)	-1289(3)	5080(3)	57(1)
C(26)	3171(6)	-1686(3)	5742(4)	68(2)
C(27)	2744(5)	-1113(4)	6302(3)	69(2)
C(28)	2628(5)	-128(4)	6225(3)	59(1)
C(29)	2986(4)	277(3)	5553(3)	47(1)
C(110)	1751(4)	3883(3)	3413(2)	49(1)
C(111)	-153(4)	2260(3)	1778(3)	47(1)
C(112)	396(4)	1757(3)	1260(3)	47(1)
C(210)	3385(4)	1289(3)	4614(2)	39(1)
C(211)	3523(3)	2080(3)	4162(2)	40(1)
F(1)	8233(3)	436(2)	1825(2)	72(1)
F(2)	7251(3)	-634(2)	1193(2)	75(1)
F(3)	6439(3)	366(2)	1921(2)	75(1)
N(11)	3379(3)	2438(2)	1838(2)	37(1)
N(12)	2285(3)	3393(2)	2889(2)	37(1)
N(21)	3942(3)	1989(2)	3468(2)	38(1)
N(22)	2985(3)	1236(2)	5327(2)	47(1)
O(1)	4064(5)	5267(3)	1965(3)	102(2)
O(2)	4994(3)	4390(2)	4234(2)	57(1)
O(3)	6636(3)	3081(3)	2490(2)	65(1)
O(4)	7933(3)	942(2)	189(2)	56(1)
O(5)	7000(3)	2036(2)	998(2)	64(1)
O(6)	5912(3)	781(3)	316(2)	70(1)
Re	4112(1)	3315(1)	2786(1)	38(1)
S(1)	6995(1)	1099(1)	647(1)	39(1)

Table S6b. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for *fac*-$[Re(CO)_3(bpy)(nHo)]CF_3SO_3$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor. To be deposited.

Atom	x	y	z	U(eq)
C(1)	5840(20)	3220(20)	7354(17)	86(6)
C(2)	4372(14)	1574(17)	8463(19)	79(5)
C(3)	4434(16)	3245(19)	8970(20)	93(6)
C(4)	2200(30)	-2940(30)	6220(40)	140(10)
C(11)	4264(16)	3316(17)	4535(18)	81(5)
C(12)	4171(19)	3890(20)	3590(30)	107(8)
C(13)	4170(20)	4770(30)	3930(30)	114(8)
C(14)	4214(19)	5026(19)	5190(40)	112(9)
C(15)	4289(15)	4430(14)	6190(20)	88(5)
C(16)	4263(15)	2383(17)	4270(20)	81(5)
C(17)	4234(19)	1980(20)	3030(20)	108(8)
C(18)	4160(20)	1020(30)	2890(20)	112(8)
C(19)	4150(20)	470(20)	4030(30)	108(8)
C(21)	2140(14)	2227(16)	7300(18)	72(4)
C(22)	1106(16)	1755(15)	7296(18)	73(4)
C(23)	544(14)	695(15)	7235(16)	66(4)
C(24)	-549(17)	-99(16)	7209(16)	73(5)
C(25)	-1431(17)	-36(18)	7180(20)	87(6)
C(26)	-2272(17)	-920(20)	7190(30)	90(7)
C(27)	-2360(20)	-1930(20)	7160(20)	95(7)
C(28)	-1457(17)	-1950(20)	7190(20)	90(6)
C(29)	-551(13)	-995(16)	7191(15)	71(4)
C(110)	4219(15)	911(17)	5250(20)	90(5)
C(210)	1111(13)	189(14)	7203(15)	65(4)
C(211)	2161(14)	708(16)	7178(17)	72(4)
N(11)	4295(13)	3564(13)	5853(16)	84(4)
N(12)	4253(11)	1805(13)	5401(13)	77(4)
N(21)	2674(12)	1725(12)	7251(14)	73(4)
N(22)	443(12)	-844(12)	7171(15)	72(4)
O(1)	6711(11)	3625(14)	7410(16)	103(5)
O(2)	4363(13)	933(13)	9280(15)	97(4)
O(3)	4469(14)	3641(15)	9976(16)	111(5)
O(4)	2806(18)	-1142(17)	6860(30)	155(9)
O(5)	1033(16)	-2373(16)	7200(30)	139(8)
O(6)	2350(20)	-2400(20)	8650(20)	169(10)
F(1)	3087(12)	-2898(17)	6350(30)	177(9)
F(2)	1990(30)	-2780(40)	5020(40)	290(20)
F(3)	1494(19)	-3937(17)	6640(50)	250(20)
S(1)	2060(5)	-2113(5)	7329(8)	107(2)
Re	4372(1)	2534(1)	7340(1)	69(1)

Table S7a. Full intra-molecular lengths [Å] and angles [°] for *fac*-[Re(CO)$_3$(phen)(nHo)]CF$_3$SO$_3$. To be deposited.

C(1)-O(1)	1.142(6)	F(1)-C(4)-S(1)	116.5(3)
C(1)-Re	1.919(6)	F(2)-C(4)-S(1)	114.2(3)
C(2)-O(2)	1.132(5)	F(3)-C(4)-S(1)	113.4(3)
C(2)-Re	1.930(4)	C(18)-C(10)-C(110)	119.5(4)
C(3)-O(3)	1.151(6)	N(11)-C(11)-C(16)	117.7(3)
C(3)-Re	1.923(5)	N(11)-C(11)-C(12)	122.8(4)
C(4)-F(1)	1.348(5)	C(16)-C(11)-C(12)	119.5(4)
C(4)-F(2)	1.365(5)	C(13)-C(12)-C(11)	117.6(4)
C(4)-F(3)	1.371(5)	C(13)-C(12)-C(112)	123.6(4)
C(4)-S(1)	1.713(5)	C(11)-C(12)-C(112)	118.8(4)
C(10)-C(18)	1.377(7)	C(14)-C(13)-C(12)	119.1(4)
C(10)-C(110)	1.389(6)	C(13)-C(14)-C(15)	120.2(4)
C(11)-N(11)	1.358(5)	N(11)-C(15)-C(14)	122.3(4)
C(11)-C(16)	1.423(5)	N(12)-C(16)-C(17)	122.6(4)
C(11)-C(12)	1.413(5)	N(12)-C(16)-C(11)	117.1(4)
C(12)-C(13)	1.397(6)	C(17)-C(16)-C(11)	120.3(3)
C(12)-C(112)	1.427(6)	C(16)-C(17)-C(18)	117.6(4)
C(13)-C(14)	1.365(6)	C(16)-C(17)-C(111)	118.8(4)
C(14)-C(15)	1.401(6)	C(18)-C(17)-C(111)	123.6(4)
C(15)-N(11)	1.328(5)	C(10)-C(18)-C(17)	119.3(4)
C(16)-N(12)	1.364(5)	N(21)-C(21)-C(22)	123.8(4)
C(16)-C(17)	1.403(6)	C(23)-C(22)-C(21)	119.4(4)
C(17)-C(18)	1.407(6)	C(22)-C(23)-C(24)	136.9(4)
C(17)-C(111)	1.423(6)	C(22)-C(23)-C(210)	116.9(4)
C(21)-N(21)	1.340(5)	C(24)-C(23)-C(210)	106.2(4)
C(21)-C(22)	1.379(6)	C(25)-C(24)-C(29)	119.1(4)
C(22)-C(23)	1.368(6)	C(25)-C(24)-C(23)	134.1(4)
C(23)-C(24)	1.432(6)	C(29)-C(24)-C(23)	106.8(4)
C(23)-C(210)	1.419(6)	C(26)-C(25)-C(24)	118.7(5)
C(24)-C(25)	1.390(6)	C(25)-C(26)-C(27)	121.2(5)
C(24)-C(29)	1.419(6)	C(26)-C(27)-C(28)	122.4(5)
C(25)-C(26)	1.379(8)	C(29)-C(28)-C(27)	116.4(5)
C(26)-C(27)	1.385(8)	N(22)-C(29)-C(28)	129.2(4)
C(27)-C(28)	1.375(7)	N(22)-C(29)-C(24)	108.8(4)
C(28)-C(29)	1.399(7)	C(28)-C(29)-C(24)	122.1(4)
C(29)-N(22)	1.385(5)	N(12)-C(110)-C(10)	122.8(4)
C(110)-N(12)	1.336(5)	C(112)-C(111)-C(17)	121.4(4)
C(111)-C(112)	1.347(6)	C(111)-C(112)-C(12)	121.2(4)
C(210)-N(22)	1.371(5)	N(22)-C(210)-C(211)	129.4(4)
C(210)-C(211)	1.370(6)	N(22)-C(210)-C(23)	109.6(4)
C(211)-N(21)	1.354(5)	C(211)-C(210)-C(23)	121.0(4)
N(11)-Re	2.187(3)	N(21)-C(211)-C(210)	120.9(4)
N(12)-Re	2.176(4)	C(15)-N(11)-C(11)	118.1(3)
N(21)-Re	2.207(3)	C(15)-N(11)-Re	127.4(3)
O(4)-S(1)	1.429(3)	C(11)-N(11)-Re	114.5(2)
O(5)-S(1)	1.435(4)	C(110)-N(12)-C(16)	118.1(4)
O(6)-S(1)	1.433(3)	C(110)-N(12)-Re	126.9(3)
		C(16)-N(12)-Re	114.9(3)
O(1)-C(1)-Re	176.2(5)	C(21)-N(21)-C(211)	118.0(4)
O(2)-C(2)-Re	178.0(4)	C(21)-N(21)-Re	124.4(3)
O(3)-C(3)-Re	177.7(4)	C(211)-N(21)-Re	117.6(3)
F(1)-C(4)-F(2)	104.0(4)	C(210)-N(22)-C(29)	108.6(4)
F(1)-C(4)-F(3)	103.5(3)	C(1)-Re-C(3)	89.6(2)
F(2)-C(4)-F(3)	103.8(4)	C(1)-Re-C(2)	87.86(19)

C(3)-Re-C(2)	86.30(17)	C(2)-Re-N(21)	90.01(15)
C(1)-Re-N(12)	91.5(2)	N(12)-Re-N(21)	82.39(12)
C(3)-Re-N(12)	173.48(14)	N(11)-Re-N(21)	84.59(12)
C(2)-Re-N(12)	100.17(15)	O(4)-S(1)-O(5)	113.6(2)
C(1)-Re-N(11)	97.09(17)	O(4)-S(1)-O(6)	115.3(2)
C(3)-Re-N(11)	97.82(15)	O(5)-S(1)-O(6)	115.3(2)
C(2)-Re-N(11)	173.55(15)	O(4)-S(1)-C(4)	103.8(2)
N(12)-Re-N(11)	75.66(12)	O(5)-S(1)-C(4)	104.1(2)
C(1)-Re-N(21)	173.11(19)	O(6)-S(1)-C(4)	102.6(2)
C(3)-Re-N(21)	96.83(16)		

Table S7b: Full intra-molecular lengths [Å] and angles [°] for *fac*-[Re(CO)$_3$(bpy)(nHo)]CF$_3$SO$_3$. To be deposited

C(1)-O(1)	1.15(3)	C(12)-C(11)-C(16)	124(2)
C(1)-Re	1.93(3)	C(13)-C(12)-C(11)	120(3)
C(2)-O(2)	1.26(3)	C(14)-C(13)-C(12)	120(3)
C(2)-Re	1.84(2)	C(13)-C(14)-C(15)	120(3)
C(3)-O(3)	1.16(3)	N(11)-C(15)-C(14)	119(2)
C(3)-Re	1.93(3)	C(17)-C(16)-N(12)	117(2)
C(4)-F(2)	1.29(5)	C(17)-C(16)-C(11)	126(2)
C(4)-F(1)	1.32(4)	N(12)-C(16)-C(11)	117.1(17)
C(4)-F(3)	1.41(5)	C(16)-C(17)-C(18)	121(2)
C(4)-S(1)	1.76(4)	C(17)-C(18)-C(19)	120(2)
C(11)-N(11)	1.36(2)	C(110)-C(19)-C(18)	117(3)
C(11)-C(12)	1.34(3)	N(21)-C(21)-C(22)	123.9(19)
C(11)-C(16)	1.44(3)	C(21)-C(22)-C(23)	119.1(17)
C(12)-C(13)	1.38(4)	C(22)-C(23)-C(210)	116.1(16)
C(13)-C(14)	1.31(5)	C(22)-C(23)-C(24)	136.7(17)
C(14)-C(15)	1.39(4)	C(210)-C(23)-C(24)	107.2(16)
C(15)-N(11)	1.36(3)	C(29)-C(24)-C(23)	104.8(16)
C(16)-C(17)	1.38(3)	C(29)-C(24)-C(25)	123(2)
C(16)-N(12)	1.42(3)	C(23)-C(24)-C(25)	131.9(19)
C(17)-C(18)	1.41(4)	C(26)-C(25)-C(24)	114(2)
C(18)-C(19)	1.40(4)	C(25)-C(26)-C(27)	127(2)
C(19)-C(110)	1.37(3)	C(26)-C(27)-C(28)	117(2)
C(21)-N(21)	1.36(2)	C(29)-C(28)-C(27)	116(2)
C(21)-C(22)	1.36(3)	C(24)-C(29)-C(28)	123(2)
C(22)-C(23)	1.39(3)	C(24)-C(29)-N(22)	111.8(18)
C(23)-C(210)	1.41(3)	C(28)-C(29)-N(22)	125(2)
C(23)-C(24)	1.48(3)	N(12)-C(110)-C(19)	123(2)
C(24)-C(29)	1.36(3)	N(22)-C(210)-C(211)	129.2(17)
C(24)-C(25)	1.39(3)	N(22)-C(210)-C(23)	108.5(15)
C(25)-C(26)	1.31(3)	C(211)-C(210)-C(23)	122.3(18)
C(26)-C(27)	1.48(3)	N(21)-C(211)-C(210)	119.8(18)
C(27)-C(28)	1.38(4)	C(15)-N(11)-C(11)	119.4(18)
C(28)-C(29)	1.42(3)	C(15)-N(11)-Re	123.1(14)
C(29)-N(22)	1.41(2)	C(11)-N(11)-Re	117.5(14)
C(110)-N(12)	1.34(3)	C(110)-N(12)-C(16)	121.0(17)
C(210)-N(22)	1.38(2)	C(110)-N(12)-Re	124.3(14)
C(210)-C(211)	1.38(2)	C(16)-N(12)-Re	114.6(13)
C(211)-N(21)	1.34(3)	C(211)-N(21)-C(21)	118.7(16)
N(11)-Re	2.200(16)	C(211)-N(21)-Re	118.8(13)
N(12)-Re	2.190(15)	C(21)-N(21)-Re	122.4(13)
N(21)-Re	2.233(16)	C(210)-N(22)-C(29)	107.7(16)
O(4)-S(1)	1.41(2)	O(4)-S(1)-O(5)	117.2(15)
O(5)-S(1)	1.41(2)	O(4)-S(1)-O(6)	113.0(17)
O(6)-S(1)	1.52(2)	O(5)-S(1)-O(6)	115.8(17)
		O(4)-S(1)-C(4)	102.6(18)
O(1)-C(1)-Re	177.5(17)	O(5)-S(1)-C(4)	104.5(17)
O(2)-C(2)-Re	177.4(16)	O(6)-S(1)-C(4)	100.7(18)
O(3)-C(3)-Re	177(2)	C(2)-Re-C(1)	88.2(8)
F(2)-C(4)-F(1)	115(4)	C(2)-Re-C(3)	84.7(9)
F(2)-C(4)-F(3)	111(4)	C(1)-Re-C(3)	88.2(9)
F(1)-C(4)-F(3)	103(3)	C(2)-Re-N(12)	99.9(7)
F(2)-C(4)-S(1)	109(3)	C(1)-Re-N(12)	93.6(7)
F(1)-C(4)-S(1)	113(3)	C(3)-Re-N(12)	175.0(8)
F(3)-C(4)-S(1)	106(3)	C(2)-Re-N(11)	174.5(7)
N(11)-C(11)-C(12)	120(2)	C(1)-Re-N(11)	94.3(7)
N(11)-C(11)-C(16)	115.5(16)	C(3)-Re-N(11)	100.2(8)

N(12)-Re-N(11)	75.1(6)	C(3)-Re-N(21)	93.5(7)
C(2)-Re-N(21)	92.6(7)	N(12)-Re-N(21)	84.6(6)
C(1)-Re-N(21)	178.1(7)	N(11)-Re-N(21)	84.7(6)

Table S8a. Anisotropic displacement parameters ($Å^2$ x 10^3) for *fac*-[$Re(CO)_3$(phen)(nHo)]CF_3SO_3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$. To be deposited.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	75(4)	54(3)	52(3)	0(3)	-9(3)	-11(3)
C(2)	36(2)	37(2)	48(2)	-6(2)	8(2)	-3(2)
C(3)	48(3)	46(3)	38(2)	-8(2)	3(2)	-10(2)
C(4)	28(2)	63(3)	49(2)	-23(2)	10(2)	-17(2)
C(10)	45(3)	67(3)	55(3)	-16(3)	0(2)	15(2)
C(11)	38(2)	28(2)	37(2)	-1(2)	-2(2)	3(2)
C(12)	46(2)	30(2)	35(2)	1(2)	-4(2)	0(2)
C(13)	55(3)	36(2)	38(2)	-7(2)	-8(2)	-2(2)
C(14)	60(3)	51(3)	39(2)	-16(2)	2(2)	8(2)
C(15)	42(3)	55(3)	45(2)	-6(2)	5(2)	1(2)
C(16)	40(2)	30(2)	33(2)	1(2)	-4(2)	1(2)
C(17)	36(2)	40(2)	52(2)	-2(2)	-1(2)	1(2)
C(18)	37(2)	62(3)	64(3)	-6(3)	5(2)	9(2)
C(21)	44(3)	49(3)	44(2)	-15(2)	4(2)	7(2)
C(22)	54(3)	37(2)	51(3)	-13(2)	2(2)	8(2)
C(23)	38(2)	35(2)	47(2)	-9(2)	-3(2)	1(2)
C(24)	48(3)	36(2)	51(2)	-6(2)	-5(2)	3(2)
C(25)	74(4)	36(2)	60(3)	-10(2)	-7(3)	6(2)
C(26)	95(5)	40(3)	69(4)	3(3)	-11(3)	0(3)
C(27)	84(4)	57(3)	63(3)	11(3)	-2(3)	0(3)
C(28)	68(3)	55(3)	54(3)	2(3)	6(2)	2(3)
C(29)	46(3)	45(2)	48(2)	-3(2)	-2(2)	6(2)
C(110)	52(3)	48(3)	45(2)	-15(2)	-6(2)	11(2)
C(111)	34(2)	45(3)	61(3)	-1(2)	-5(2)	-1(2)
C(112)	47(3)	40(2)	52(3)	-3(2)	-9(2)	-10(2)
C(210)	38(2)	40(2)	40(2)	-6(2)	3(2)	3(2)
C(211)	37(2)	36(2)	47(2)	-9(2)	3(2)	5(2)
F(1)	62(2)	88(2)	62(2)	22(2)	-12(1)	-13(2)
F(2)	100(3)	44(2)	83(2)	11(2)	18(2)	-5(2)
F(3)	79(2)	90(2)	58(2)	4(2)	28(2)	-22(2)
N(11)	34(2)	40(2)	36(2)	-7(2)	3(1)	-1(2)
N(12)	37(2)	37(2)	37(2)	-9(2)	-3(2)	5(1)
N(21)	37(2)	35(2)	42(2)	-5(2)	4(2)	2(2)
N(22)	60(2)	34(2)	47(2)	-3(2)	12(2)	9(2)
O(1)	151(5)	65(3)	87(3)	25(2)	-7(3)	-16(3)
O(2)	59(2)	66(2)	45(2)	-20(2)	3(2)	-16(2)
O(3)	41(2)	90(3)	67(2)	-16(2)	14(2)	-8(2)
O(4)	54(2)	65(2)	51(2)	10(2)	19(2)	3(2)
O(5)	84(3)	41(2)	68(2)	-2(2)	17(2)	-4(2)
O(6)	51(2)	89(3)	68(2)	1(2)	-9(2)	-10(2)
Re	35(1)	40(1)	37(1)	-8(1)	-1(1)	-3(1)
S(1)	36(1)	39(1)	42(1)	-4(1)	6(1)	-5(1)

Table S8b. Anisotropic displacement parameters ($Å^2$ x 10^3) for *fac*-[$Re(CO)_3(bpy)(nHo)]CF_3SO_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$. To be deposited.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	110(18)	113(16)	52(9)	10(9)	-9(9)	68(15)
C(2)	63(9)	88(12)	79(10)	-21(9)	-6(8)	33(9)
C(3)	82(13)	114(16)	85(14)	20(12)	-7(10)	50(12)
C(11)	82(12)	94(13)	61(10)	14(9)	1(8)	40(10)
C(12)	87(14)	130(20)	87(14)	19(14)	0(11)	38(14)
C(13)	108(19)	120(20)	120(20)	35(18)	-4(15)	62(16)
C(14)	96(16)	77(13)	150(30)	30(15)	8(15)	32(12)
C(15)	84(12)	72(11)	109(14)	13(10)	8(11)	40(9)
C(16)	75(11)	94(14)	58(9)	-4(9)	-2(8)	30(10)
C(17)	99(16)	140(20)	61(11)	15(13)	7(10)	44(15)
C(18)	130(20)	140(20)	68(12)	-16(13)	7(12)	63(18)
C(19)	100(17)	120(20)	107(19)	-22(15)	17(13)	53(16)
C(21)	70(10)	80(11)	77(10)	6(8)	-2(8)	45(9)
C(22)	90(12)	83(12)	64(9)	7(9)	7(9)	55(11)
C(23)	74(10)	76(11)	49(7)	1(7)	4(7)	38(9)
C(24)	95(13)	97(13)	46(7)	-6(8)	-3(8)	63(12)
C(25)	85(13)	96(14)	73(11)	3(10)	-13(10)	41(12)
C(26)	74(12)	117(19)	77(12)	-10(11)	-3(9)	47(13)
C(27)	105(18)	99(17)	70(11)	2(11)	7(11)	43(14)
C(28)	77(13)	113(17)	63(10)	3(10)	2(9)	35(12)
C(29)	69(10)	96(13)	48(7)	6(8)	1(7)	41(9)
C(110)	78(12)	96(14)	87(12)	2(11)	11(10)	37(10)
C(210)	70(9)	81(11)	47(7)	0(7)	-3(6)	39(8)
C(211)	75(10)	88(12)	56(8)	1(8)	0(8)	43(10)
N(11)	80(9)	76(9)	83(10)	7(8)	-11(8)	28(8)
N(12)	73(8)	94(11)	53(7)	5(7)	6(6)	33(8)
N(21)	73(9)	74(9)	62(8)	10(6)	9(6)	30(7)
N(22)	77(9)	74(9)	64(8)	-4(7)	-2(7)	36(8)
O(1)	63(8)	134(13)	97(10)	1(9)	0(7)	39(8)
O(2)	108(10)	105(10)	92(9)	29(8)	0(8)	64(9)
O(3)	125(12)	141(14)	73(9)	-30(9)	1(8)	70(11)
O(4)	124(15)	101(13)	210(30)	53(15)	26(17)	35(12)
O(5)	99(12)	124(15)	210(20)	-22(15)	-36(13)	66(12)
O(6)	180(20)	220(30)	132(17)	30(17)	-17(16)	120(20)
F(1)	87(10)	179(18)	270(30)	-36(18)	13(13)	74(11)
F(2)	210(30)	480(70)	170(20)	-120(40)	-60(20)	170(40)
F(3)	117(15)	105(14)	500(70)	-70(20)	10(30)	24(12)
S(1)	92(4)	95(4)	140(5)	12(4)	6(4)	50(3)
Re	70(1)	76(1)	58(1)	5(1)	-1(1)	35(1)

Table S9a. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for *fac*-[Re(CO)$_3$(phen)(nHo)]CF$_3$SO$_3$. To be deposited.

Atom	x	y	z	U(eq)
H(10)	237	4217	3822	67
H(13)	1845	882	368	53
H(14)	3789	1064	406	60
H(15)	4720	2029	1329	57
H(18)	-870	3339	2925	65
H(21)	4541	1042	2771	55
H(22)	4353	-316	3494	57
H(25)	3825	-1678	4711	69
H(26)	3217	-2352	5814	82
H(27)	2528	-1406	6746	82
H(28)	2327	249	6601	71
H(110)	2184	4248	3772	59
H(111)	-943	2241	1758	57
H(112)	-21	1391	894	56
H(211)	3325	2689	4334	48
H(22A)	2770	1719	5590	56

Table S9b. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for *fac*-[Re(CO)$_3$(bpy)(nHo)]CF$_3$SO$_3$. To be deposited.

Atom	x	y	z	U(eq)
H(12)	4107	3698	2691	128
H(13)	4136	5182	3270	137
H(14)	4195	5611	5419	134
H(15)	4336	4622	7087	105
H(17)	4260	2344	2265	130
H(18)	4126	751	2037	135
H(19)	4105	-160	3955	130
H(21)	2504	2934	7340	87
H(22)	779	2135	7333	88
H(25)	-1424	581	7150	104
H(26)	-2878	-903	7220	108
H(27)	-2986	-2524	7129	114
H(28)	-1448	-2563	7209	108
H(110)	4240	570	6011	108
H(211)	2511	352	7110	86
H(22A)	605	-1313	7143	87