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Bimetallic Re(I)/Pt(II)/Pd(II) Complexes: Syntheses and Property Study

Supporting Information

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S1. Experimental Details

General. All reactions were performed under dry N_2 with standard Schlenk techniques unless otherwise noted. The syntheses of ligand **L1**,[1] $[PtMe_2(SMe_2)]_2$,[2] $[PtPh_2(DMSO)_2]$,[3] Pd(acac),[1] Pt(acac)[4] and Pt(dpm)[4] were achieved by methods described in the literature.

Molecular calculation: The computational calculations were performed using Gaussian09, D.01 program package.[5] The ground-state geometries were fully optimized at the B3LYP[6, 7] level using LANL2DZ basis set for platinum and rhenium as well as 6-311G(dp) basis set for all other atoms.[8] The initial geometric parameters in the calculations were employed from crystal structure data for geometry optimization. Time-dependent density function theory (TD-DFT) calculations were performed to obtain the vertical singlet and triplet excitation energies.

Synthesis of Re-L1. $Re(CO)_5Cl$ (155 mg, 0.43 mmol) and ligand **L1** (200 mg, 0.43 mmol) were dissolved in 40 mL toluene. The reaction mixture was stirred with reflux for 4 h. After cooling to room temperature, the yellow powder was filtered and washed with cold toluene and diethyl ether. A yield of 62% was obtained for this reaction. ^{1}H NMR (600 MHz, CD_2Cl_2, 298.0 K, δ, ppm): 9.16 (d, 1H, J = 5.2 Hz), 8.44 (d, 1H, J = 4.2 Hz), 8.14 (d, 1H, J = 8.2 Hz), 7.88 (td, 1H, J = 8.2 Hz, 1.3 Hz), 7.79-7.72 (m, 3H), 7.70-7.54 (m, 7H), 7.49 (d, 1H, J = 8.3 Hz), 7.35-7.32 (m, 3H), 7.27 (t, 1H, J = 7.1 Hz), 7.21 (td, 1H, J = 6.0 Hz, 1.1 Hz), 7.18 (s, 1H); ^{13}C{^{1}H} NMR (150 MHz, CD_2Cl_2, δ, ppm): 198.3, 198.1, 189.4, 155.1, 152.5, 151.7, 149.4, 147.7, 142.9, 140.8, 139.9, 139.7, 139.4, 137.9, 137.1, 132.7, 131.1, 130.8, 129.3, 128.9, 128.8, 127.8, 127.7, 126.8, 124.6, 124.4, 124.1, 122.7, 122.1, 122.0, 120.1, 112.3, 110.9, 107.2. Anal. for $C_{34}H_{21}N_5O_3ReCl$: found C 53.50, H 3.20, N 8.59, calcd C 53.09, H 2.75, N 9.10.

Synthesis of Re-Pt(dpm). This bimetallic compound was synthesized by methods described in the literature.[4] To a 20 mL screw-cap vial with a stir bar are added one equivalent of **Re-L1** (0.13 mmol, 100 mg), $[PtMe_2(SMe_2)]_2$ (37 mg, 0.065 mmol) and 3 mL of THF. The reaction is allowed to stir 1 hr at room temperature. Then a solution of HOTf (trifluoromethanesulfonic acid, 0.4 mL, 0.35 M in THF) is added dropwise.

The mixture is stirred for 30 minutes, then a solution of Na(dipivolylmethane) (Na(dpm), 0.30 mmol in 2 mL MeOH) is added. The mixture is stirred for 1.5 hr, and then partitioned between water and CH_2Cl_2. The organic layer is washed with brine, dried over $MgSO_4$, filtered, and concentrated. The residue is then purified by column chromatography using THF-CH_2Cl_2 (1:60) as eluent to give analytically pure material. Recrystallization of the yellow product in $CHCl_3$-hexane afforded **Re-Pt(dpm)** as orange-yellow crystals (yield 25%). ^{1}H NMR (600 MHz, $CDCl_3$, 298.0 K, δ, ppm): 9.23 (d, 1H, *J* = 5.7 Hz), 9.12 (d, 1H, *J* = 5.8 Hz), 8.54 (d, 1H, *J* = 7.7 Hz), 8.23 (d, 1H, *J* = 8.3 Hz), 7.85-7.78 (m, 5H), 7.66 (t, 1H, *J* = 7.7Hz), 7.59 (t, 1H, *J* = 7.4 Hz), 7.54-7.51 (m, 2H), 7.35 (t, 1H, *J* = 7.0 Hz), 7.32-7.24 (m, 4H), 6.94 (t, 1H, *J* = 6.3 Hz), 6.63 (d, 1H, *J* = 7.9 Hz), 5.94 (s, 1H), 1.40 (s, 9H), 1.33 (s, 9H); Due to the solubility issue, ^{13}C NMR was not obtained for this compound. Anal. for $C_{45}H_{39}N_5O_5RePtCl$: found C 46.67, H 3.29, N 5.89, calcd C 47.14, H 3.43, N 6.11.

Synthesis of Re-Pt. Compound **Re-Pt** was obtained using the same method as that for **Re-Pt(dpm)**. Yield 28%. ^{1}H NMR (400 MHz, CD_2Cl_2, 298.0 K, δ, ppm): 9.19 (d, 1H, *J* = 6.0 Hz), 9.03 (d, 1H, *J* = 5.3 Hz), 8.33 (d, 1H, *J* = 8.0 Hz), 8.18 (d, 1H, *J* = 8.3 Hz), 7.90-7.79 (m, 5H), 7.68 (td, 1H, *J* = 7.2 Hz, 1.2 Hz), 7.62 (td, 1H, *J* = 7.3 Hz, 0.9 Hz), 7.58-7.54 (m, 2H), 7.40 (d, 1H, *J* = 8.2 Hz), 7.34-7.28 (m, 3H), 7.20 (td, 1H, *J* = 6.6 Hz, 1.4 Hz), 6.95 (td, 1H, *J* = 6.1 Hz, 1.4 Hz), 6.69 (d, 1H, *J* = 8.0 Hz), 5.61 (s, 1H), 2.10 (s, 3H), 2.05 (s, 3H). Due to the solubility issue, ^{13}C NMR was not obtained for this compound. Anal. for $C_{39}H_{27}N_5O_5RePtCl$: found C 43.62, H 2.36, N 6.29, calcd C 44.09, H 2.56, N 6.59.

Synthesis of Re-Pt(DMSO). A mixture of **Re-L1** (0.060 g, 0.08 mmol) and $PtPh_2(DMSO)_2$ (0.039 g, 0.08 mmol) was dissolved in 30 mL of THF. The mixture was stirred at 50 ^{o}C for 6 hrs, and the solvent was removed under reduced pressure. Recrystallization from CH_2Cl_2-hexane afforded **Re-Pt(DMSO)** as an yellow solid in 57% yield. ^{1}H NMR (400 MHz, CD_2Cl_2, 298.0 K, δ, ppm): 9.68 (d, *J* = 5.4 Hz, 1H), 9.19 (d, *J* = 5.7 Hz, 1H), 8.18 (d, *J* = 7.9 Hz, 1H), 7.88 (td, *J* = 6.7 Hz, 1.3 Hz, 1H), 7.83-7.78 (m, 4H), 7.70-7.54 (m, 6H), 7.38 (d, *J*= 8.1 Hz, 1H), 7.34-7.28 (br, 1H), 7.16-7.10 (m, 6H), 6.72-6.66 (m, 2H), 5.81 (d, *J* = 8.1 Hz, 1H), 2.94 (s, 6H). Due to the

solubility issue, ^{13}C NMR was not obtained for this compound. Anal calcd for $C_{42}H_{31}N_5O_4PtReSCl$: C, 45.10; H, 2.79; N, 6.26. Found: C, 44.71; H, 2.65; N, 5.99.

Synthesis of Re-Pd. A mixture of **Re-L1** (60 mg, 0.08 mmol) and $Pd(acac)_2$ (35 mg, 0.15 mmol) was suspended in 30 mL methanol. The mixture was refluxed for 2 days, and the solvent was removed under reduced pressure. The residue was washed by diethyl ether (3 × 10 mL). Recrystallization from THF-diethyl ether afforded **Re-Pd** as a dark green solid in 92% yield. ^1H NMR (400 MHz, CD_2Cl_2, 298.0 K, δ, ppm): 9.19 (d, 1H, J = 6.0 Hz), 8.84 (d, 1H, J = 6.5 Hz), 8.33 (d, 1H, J = 7.6 Hz), 8.18 (d, 1H, J = 7.6 Hz), 7.89-7.80 (m, 5H), 7.69-7.55 (m, 4H), 7.39 (d, 1H, J = 8.1 Hz), 7.33-7.25 (m, 3H), 7.19 (t, 1H, J = 5.7 Hz), 7.03 (t, 1H, J = 5.9 Hz), 6.69 (d, 1H, J = 8.5 Hz), 5.53 (s, 1H), 2.21 (s, 3H), 2.12 (s, 3H). Due to the solubility issue, ^{13}C NMR was not obtained for this compound. Anal. for $C_{39}H_{27}N_5O_5RePdCl$: found C 48.00, H 2.78, N 7.13, calcd C 48.10, H 2.79, N 7.19.

S2. Computational Study

Table S1.TD-DFT calculated electronic transitions for **Re-Pt** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy [nm(eV)]	Oscillator Strength
Re-Pt	S1	HOMO-1→LUMO (99%)	586.09 (2.12)	0.0004
	S2	HOMO-2→LUMO (98%)	529.59 (2.34)	0.0579
	S3	HOMO→LUMO (99%)	512.16 (2.42)	0.0023
	S4	HOMO→LUMO+1 (91%) HOMO→LUMO+3 (3%)	459.35 (2.70)	0.0667
	S5	HOMO-4→LUMO (99%)	443.29 (2.80)	0.0020
	T1	HOMO-3→LUMO+1 (2%) HOMO→LUMO+1 (91%)	624.86 (1.98)	

Table S2. Primary orbitals which contribute to the calculated transitions of **Re-Pt** (iso = 0.03).

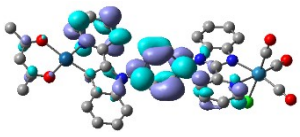
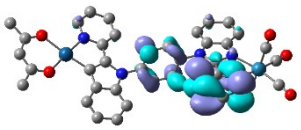
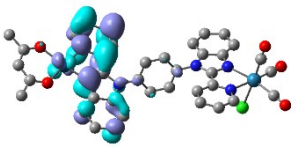
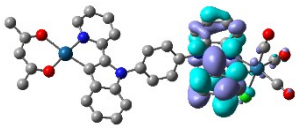
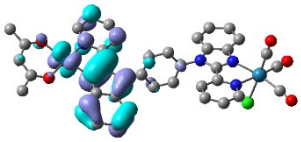
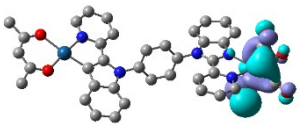
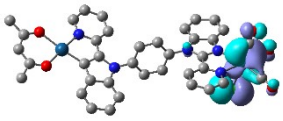
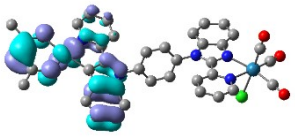
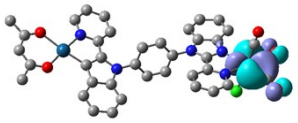
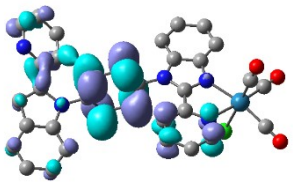
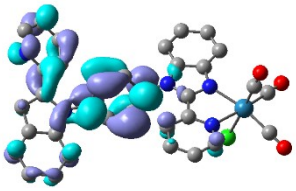
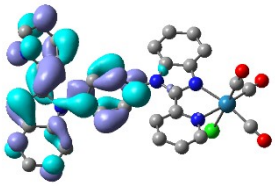
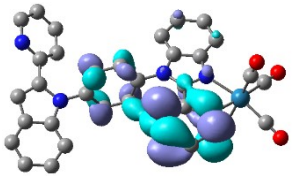
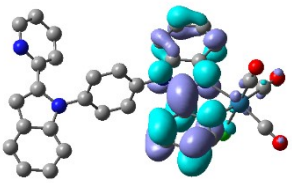
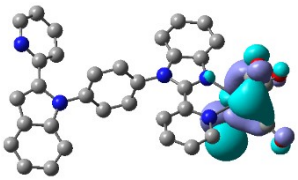
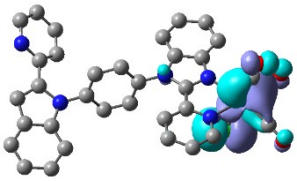
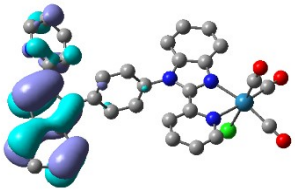
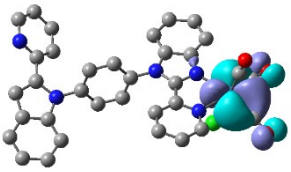
 LUMO+3	 LUMO+2	 LUMO+1
 LUMO	 HOMO	 HOMO-1
 HOMO-2	 HOMO-3	 HOMO-4

Table S3.TD-DFT calculated electronic transitions for **Re-L1** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy [nm(eV)]	Oscillator Strength
Re-L1	S1	HOMO→LUMO (99%)	586.37(2.11)	0.0003
	S2	HOMO-1→LUMO (98%)	528.33(2.35)	0.0538
	S3	HOMO-3→LUMO (99%)	444.62(2.79)	0.0027
	S4	HOMO-2→LUMO (100%)	423.86(2.93)	0.0034
	S5	HOMO→LUMO+1 (93%) HOMO→LUMO+4 (3%)	408.99(3.03)	0.0031
	T1	HOMO→LUMO (96%)	605.96(2.05)	

Table S4. Primary orbitals which contribute to the calculated transitions of **Re-L1** (iso = 0.03).

 LUMO+4	 LUMO+3	 LUMO+2
 LUMO+1	 LUMO	 HOMO
 HOMO-1	 HOMO-2	 HOMO-3

S3. Electrochemical Study

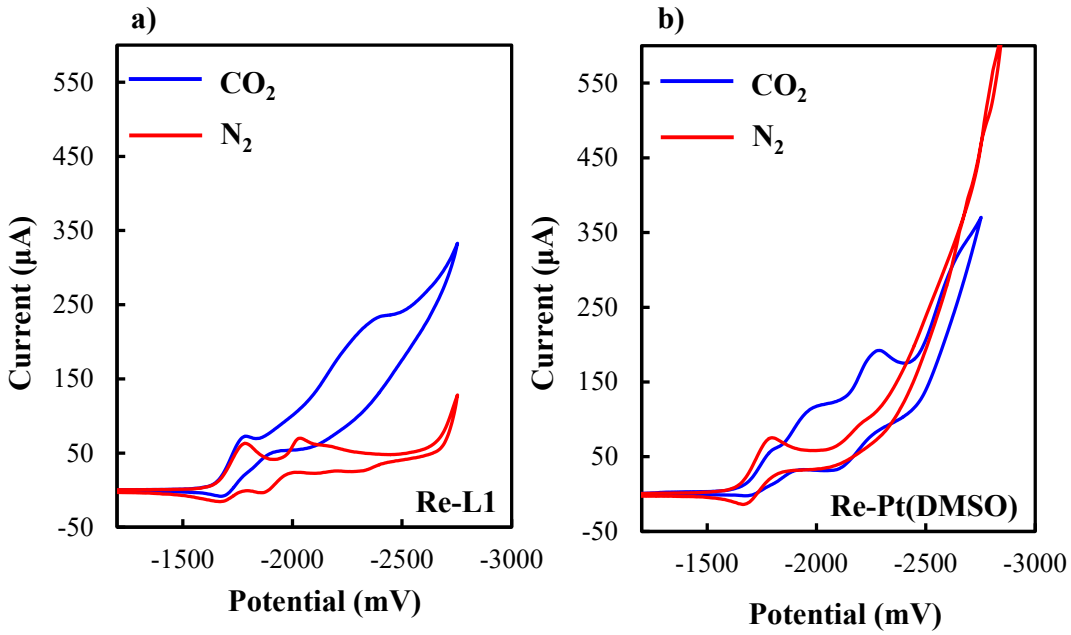


Figure S1. CV diagrams of **Re-L1** (a) and **Re-Pt(DMSO)** (b) in acetonitrile with 0.1 M NBu_4PF_6 under N_2 (red) and CO_2 (blue) at 100 mV/s at room temperature.

S4. X-ray Crystallographic Data

Table S5. Crystal data and structure refinement for **Re-Pt(dpm)**.

Identification code	Re-Pt(dpm)	
Empirical formula	C45H39ClN5O5PtRe	
Formula weight	1146.55	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 43.4528(12) Å	α= 90°
	b = 11.8801(3) Å	β= 90°
	c = 8.1619(2) Å	γ= 90°
Volume	4213.37(19) $Å^3$	
Z	4	
Density (calculated)	1.807 Mg/m^3	
Absorption coefficient	6.302 mm^{-1}	
F(000)	2216	
Crystal size	0.06 x 0.06 x 0.01 mm^3	
Theta range for data collection	1.78 to 26.50°.	
Index ranges	-54<=h<=52, -14<=k<=12, -10<=l<=10	
Reflections collected	20645	
Independent reflections	8183 [R(int) = 0.0962]	
Completeness to theta = 26.50°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9397 and 0.7036	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8183 / 2 / 492	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0747, wR2 = 0.1463	
R indices (all data)	R1 = 0.1346, wR2 = 0.1713	
Absolute structure parameter	0.05(2)	
Extinction coefficient	0.00047(9)	
Largest diff. peak and hole	2.970 and -2.025 e.$Å^{-3}$	

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

	x	y	z	U(eq)
Pt(1)	5842(1)	5658(1)	14274(1)	48(1)
Re(1)	7221(1)	10742(1)	26919(1)	36(1)
Cl(1)	6675(1)	10762(5)	27686(6)	46(1)
O(1)	7398(4)	9536(12)	30106(17)	46(4)
O(2)	7332(4)	13064(16)	28523(19)	66(5)
O(3)	7891(4)	10605(15)	25941(18)	56(4)
O(4)	5531(3)	6341(12)	12737(16)	55(4)
O(5)	5853(3)	4144(12)	13032(17)	51(4)
N(1)	7088(4)	9280(15)	25522(18)	39(4)
N(2)	7043(4)	11390(14)	24563(17)	36(4)
N(3)	6799(4)	8541(14)	23529(16)	34(4)
N(4)	6142(3)	5093(16)	15957(19)	38(4)
N(5)	6049(5)	7775(17)	18000(20)	53(5)
C(1)	7336(5)	10019(18)	28930(30)	42(6)
C(2)	7290(5)	12150(20)	27930(20)	43(6)
C(3)	7650(5)	10690(20)	26190(20)	42(5)
C(4)	7069(3)	8140(8)	25763(15)	26(4)
C(5)	7203(3)	7413(11)	26890(15)	70(6)
C(6)	7148(3)	6262(10)	26788(17)	50(5)
C(7)	6960(3)	5838(8)	25558(18)	61(7)
C(8)	6826(3)	6565(11)	24431(15)	42(5)
C(9)	6880(3)	7716(10)	24533(13)	38(5)
C(10)	6924(4)	9502(13)	24210(20)	23(4)
C(11)	6899(5)	10690(16)	23570(20)	35(5)
C(12)	6785(4)	11038(17)	22100(30)	36(5)
C(13)	6797(5)	12137(19)	21620(20)	45(5)
C(14)	6939(6)	12900(20)	22670(20)	55(7)
C(15)	7055(5)	12471(17)	24180(30)	44(5)
C(16)	6604(4)	8462(16)	22090(20)	34(4)
C(17)	6294(5)	8540(20)	22240(19)	58(7)
C(18)	6105(6)	8340(20)	20900(20)	51(7)
C(19)	6226(5)	8031(15)	19410(30)	44(5)

C(20)	6552(4)	7987(16)	19260(30)	43(5)
C(21)	6734(5)	8166(18)	20612(19)	36(5)
C(22)	5867(5)	6950(18)	15680(30)	46(6)
C(23)	5731(5)	8030(20)	15840(30)	54(7)
C(24)	5510(7)	8670(20)	14900(30)	76(9)
C(25)	5437(10)	9690(30)	15360(40)	126(16)
C(26)	5551(9)	10220(30)	16810(60)	150(18)
C(27)	5768(8)	9700(20)	17740(40)	98(12)
C(28)	5856(5)	8580(18)	17310(20)	45(6)
C(29)	6063(4)	6915(14)	17050(20)	27(4)
C(30)	6205(4)	5787(19)	17270(30)	45(6)
C(31)	6383(6)	5420(20)	18520(30)	77(9)
C(32)	6534(6)	4400(20)	18390(30)	59(7)
C(33)	6464(6)	3665(16)	17150(30)	60(7)
C(34)	6263(5)	4101(18)	15890(20)	44(6)
C(35)	5665(5)	3933(17)	11770(30)	48(5)
C(36)	5471(5)	4650(20)	11130(30)	62(8)
C(37)	5411(5)	5730(20)	11490(30)	55(6)
C(38)	5825(10)	2830(40)	9560(70)	187(19)
C(39)	5976(9)	2150(40)	12030(90)	280(40)
C(40)	5441(10)	2080(30)	11150(50)	148(16)
C(41)	5132(7)	7570(20)	11130(40)	94(10)
C(42)	4884(7)	5830(30)	10380(50)	137(16)
C(43)	5307(12)	6540(40)	8740(40)	180(20)
C(44)	5696(6)	2720(30)	11250(40)	96(12)
C(45)	5180(6)	6420(20)	10520(20)	46(6)

Table S7. Bond lengths [Å] and angles [°] for **Re-Pt(dpm)**.

Pt(1)-C(22)	1.92(2)	Re(1)-Cl(1)	2.455(6)
Pt(1)-O(4)	2.015(13)	O(1)-C(1)	1.15(2)
Pt(1)-N(4)	2.008(16)	O(2)-C(2)	1.21(3)
Pt(1)-O(5)	2.066(14)	O(3)-C(3)	1.07(2)
Re(1)-C(2)	1.88(3)	O(4)-C(37)	1.35(3)
Re(1)-C(1)	1.92(2)	O(5)-C(35)	1.33(3)
Re(1)-C(3)	1.96(2)	N(1)-C(10)	1.32(2)
Re(1)-N(1)	2.157(18)	N(1)-C(4)	1.371(19)
Re(1)-N(2)	2.212(14)	N(2)-C(11)	1.32(2)

N(2)-C(15)	1.32(2)	C(33)-C(34)	1.45(3)
N(3)-C(9)	1.326(18)	C(35)-C(36)	1.31(3)
N(3)-C(10)	1.38(2)	C(35)-C(44)	1.51(3)
N(3)-C(16)	1.45(2)	C(36)-C(37)	1.34(3)
N(4)-C(34)	1.29(2)	C(37)-C(45)	1.52(3)
N(4)-C(30)	1.38(3)	C(38)-C(44)	1.50(5)
N(5)-C(29)	1.29(2)	C(39)-C(44)	1.53(5)
N(5)-C(28)	1.39(3)	C(40)-C(44)	1.34(4)
N(5)-C(19)	1.41(3)	C(41)-C(45)	1.47(3)
C(4)-C(5)	1.3900	C(42)-C(45)	1.46(4)
C(4)-C(9)	1.3900	C(43)-C(45)	1.56(4)
C(5)-C(6)	1.3900	C(22)-Pt(1)-O(4)	95.0(8)
C(6)-C(7)	1.3900	C(22)-Pt(1)-N(4)	79.8(9)
C(7)-C(8)	1.3900	O(4)-Pt(1)-N(4)	174.6(6)
C(8)-C(9)	1.3900	C(22)-Pt(1)-O(5)	171.4(8)
C(10)-C(11)	1.51(2)	O(4)-Pt(1)-O(5)	93.4(6)
C(11)-C(12)	1.36(3)	N(4)-Pt(1)-O(5)	91.7(7)
C(12)-C(13)	1.36(3)	C(2)-Re(1)-C(1)	89.0(8)
C(13)-C(14)	1.39(3)	C(2)-Re(1)-C(3)	90.4(10)
C(14)-C(15)	1.43(3)	C(1)-Re(1)-C(3)	89.9(8)
C(16)-C(17)	1.36(3)	C(2)-Re(1)-N(1)	170.6(7)
C(16)-C(21)	1.38(2)	C(1)-Re(1)-N(1)	99.3(7)
C(17)-C(18)	1.39(3)	C(3)-Re(1)-N(1)	94.2(8)
C(18)-C(19)	1.38(3)	C(2)-Re(1)-N(2)	97.3(7)
C(19)-C(20)	1.42(2)	C(1)-Re(1)-N(2)	172.2(7)
C(20)-C(21)	1.38(3)	C(3)-Re(1)-N(2)	94.7(7)
C(22)-C(29)	1.41(3)	N(1)-Re(1)-N(2)	74.1(6)
C(22)-C(23)	1.42(3)	C(2)-Re(1)-Cl(1)	91.9(7)
C(23)-C(24)	1.44(3)	C(1)-Re(1)-Cl(1)	92.1(6)
C(23)-C(28)	1.47(3)	C(3)-Re(1)-Cl(1)	176.9(6)
C(24)-C(25)	1.30(4)	N(1)-Re(1)-Cl(1)	83.3(4)
C(25)-C(26)	1.43(4)	N(2)-Re(1)-Cl(1)	83.0(4)
C(26)-C(27)	1.36(4)	C(37)-O(4)-Pt(1)	120.8(14)
C(27)-C(28)	1.43(3)	C(35)-O(5)-Pt(1)	121.8(13)
C(29)-C(30)	1.49(3)	C(10)-N(1)-C(4)	106.4(15)
C(30)-C(31)	1.35(3)	C(10)-N(1)-Re(1)	114.5(13)
C(31)-C(32)	1.38(3)	C(4)-N(1)-Re(1)	137.4(11)
C(32)-C(33)	1.37(3)	C(11)-N(2)-C(15)	118.9(17)

C(11)-N(2)-Re(1)	118.8(12)	C(19)-C(18)-C(17)	121(2)
C(15)-N(2)-Re(1)	122.1(14)	C(18)-C(19)-N(5)	124(2)
C(9)-N(3)-C(10)	105.0(14)	C(18)-C(19)-C(20)	118(2)
C(9)-N(3)-C(16)	127.5(16)	N(5)-C(19)-C(20)	118(2)
C(10)-N(3)-C(16)	127.4(16)	C(21)-C(20)-C(19)	120(2)
C(34)-N(4)-C(30)	119.8(18)	C(20)-C(21)-C(16)	120.6(19)
C(34)-N(4)-Pt(1)	122.7(13)	C(29)-C(22)-C(23)	101.8(18)
C(30)-N(4)-Pt(1)	117.5(15)	C(29)-C(22)-Pt(1)	119.0(16)
C(29)-N(5)-C(28)	109.2(16)	C(23)-C(22)-Pt(1)	139.2(17)
C(29)-N(5)-C(19)	129.5(19)	C(22)-C(23)-C(24)	134(2)
C(28)-N(5)-C(19)	120.6(18)	C(22)-C(23)-C(28)	108.8(19)
O(1)-C(1)-Re(1)	176.5(17)	C(24)-C(23)-C(28)	117(2)
O(2)-C(2)-Re(1)	177.8(17)	C(25)-C(24)-C(23)	120(3)
O(3)-C(3)-Re(1)	172.4(19)	C(24)-C(25)-C(26)	124(3)
N(1)-C(4)-C(5)	133.1(11)	C(27)-C(26)-C(25)	120(3)
N(1)-C(4)-C(9)	106.9(10)	C(26)-C(27)-C(28)	118(3)
C(5)-C(4)-C(9)	120.0	N(5)-C(28)-C(27)	135(2)
C(6)-C(5)-C(4)	120.0	N(5)-C(28)-C(23)	104.5(19)
C(7)-C(6)-C(5)	120.0	C(27)-C(28)-C(23)	121(2)
C(6)-C(7)-C(8)	120.0	N(5)-C(29)-C(22)	115.4(18)
C(9)-C(8)-C(7)	120.0	N(5)-C(29)-C(30)	131.3(17)
N(3)-C(9)-C(8)	130.1(11)	C(22)-C(29)-C(30)	112.1(17)
N(3)-C(9)-C(4)	109.6(11)	C(31)-C(30)-N(4)	121(2)
C(8)-C(9)-C(4)	120.0	C(31)-C(30)-C(29)	128(2)
N(1)-C(10)-N(3)	112.0(15)	N(4)-C(30)-C(29)	111.1(17)
N(1)-C(10)-C(11)	120.6(17)	C(30)-C(31)-C(32)	119(2)
N(3)-C(10)-C(11)	127.3(17)	C(33)-C(32)-C(31)	121(2)
N(2)-C(11)-C(12)	121.5(18)	C(32)-C(33)-C(34)	115.4(18)
N(2)-C(11)-C(10)	110.0(16)	N(4)-C(34)-C(33)	122.8(18)
C(12)-C(11)-C(10)	128.0(18)	C(36)-C(35)-O(5)	125(2)
C(11)-C(12)-C(13)	121.9(19)	C(36)-C(35)-C(44)	124(3)
C(12)-C(13)-C(14)	117.9(18)	O(5)-C(35)-C(44)	110(2)
C(13)-C(14)-C(15)	117(2)	C(35)-C(36)-C(37)	131(2)
N(2)-C(15)-C(14)	123(2)	C(36)-C(37)-O(4)	127(2)
C(17)-C(16)-C(21)	120.1(17)	C(36)-C(37)-C(45)	122(2)
C(17)-C(16)-N(3)	120.2(16)	O(4)-C(37)-C(45)	111(2)
C(21)-C(16)-N(3)	119.1(16)	C(40)-C(44)-C(38)	108(3)
C(16)-C(17)-C(18)	120.4(17)	C(40)-C(44)-C(35)	119(3)

C(38)-C(44)-C(35)	102(3)	C(41)-C(45)-C(37)	115(2)
C(40)-C(44)-C(39)	116(4)	C(42)-C(45)-C(37)	112(2)
C(38)-C(44)-C(39)	97(3)	C(41)-C(45)-C(43)	106(3)
C(35)-C(44)-C(39)	112(2)	C(42)-C(45)-C(43)	106(3)
C(41)-C(45)-C(42)	110(3)	C(37)-C(45)-C(43)	107(2)

Table S8. Anisotropic displacement parameters ($Å^2$ x 10^3) for **Re-Pt(dpm)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	51(1)	53(1)	41(1)	-16(1)	-9(1)	-6(1)
Re(1)	42(1)	39(1)	27(1)	-8(1)	-8(1)	-1(1)
Cl(1)	54(3)	45(3)	40(2)	-5(3)	-1(2)	2(3)
O(1)	55(10)	38(10)	47(8)	16(7)	-18(7)	-13(8)
O(2)	75(13)	62(12)	61(10)	0(9)	-17(9)	-9(10)
O(3)	47(10)	62(12)	58(9)	7(8)	-8(8)	0(10)
O(4)	55(10)	50(10)	61(9)	-15(8)	25(8)	-5(9)
O(5)	48(9)	48(10)	57(8)	-16(8)	-14(7)	-13(9)
N(1)	27(9)	51(11)	39(8)	16(9)	1(7)	-4(10)
N(2)	56(11)	33(10)	20(7)	6(7)	-9(7)	1(9)
N(3)	34(10)	38(11)	29(8)	-6(7)	1(8)	1(9)
N(4)	12(8)	57(13)	46(9)	-12(9)	-1(7)	-1(9)
N(5)	67(14)	54(13)	38(9)	1(10)	-24(9)	-5(12)
C(1)	44(13)	34(13)	47(13)	-14(11)	4(10)	-32(11)
C(2)	41(14)	47(15)	41(11)	23(11)	-15(9)	10(12)
C(3)	36(12)	45(13)	47(11)	24(11)	-30(10)	-6(13)
C(6)	69(16)	37(11)	44(11)	-5(13)	5(14)	-5(11)
C(7)	73(18)	46(16)	64(14)	-25(13)	38(13)	-7(15)
C(8)	44(12)	43(13)	40(10)	-7(11)	10(11)	-3(10)
C(9)	42(12)	44(13)	29(10)	0(10)	-5(9)	-15(10)
C(10)	22(8)	9(9)	39(8)	2(8)	9(9)	6(7)
C(11)	57(14)	17(10)	32(9)	3(9)	3(9)	-16(11)
C(12)	16(9)	50(14)	40(11)	5(11)	-8(9)	-7(9)
C(13)	56(14)	61(15)	18(10)	3(10)	-5(9)	14(12)
C(14)	83(19)	49(15)	34(11)	10(11)	5(12)	17(15)

C(15)	58(14)	41(13)	33(10)	-8(11)	10(11)	-10(11)
C(16)	33(10)	46(12)	22(9)	-12(9)	-3(9)	9(9)
C(17)	68(17)	100(20)	9(9)	-5(9)	-2(8)	-7(15)
C(18)	50(15)	67(18)	36(11)	6(11)	17(10)	33(14)
C(19)	49(13)	22(10)	61(12)	-13(11)	-22(12)	-2(10)
C(20)	23(10)	52(13)	53(11)	-40(12)	-7(11)	0(10)
C(21)	44(13)	46(15)	17(8)	7(9)	1(8)	1(11)
C(22)	54(15)	30(13)	55(12)	8(11)	9(11)	-11(12)
C(23)	46(15)	67(18)	50(12)	-2(12)	-21(11)	-16(14)
C(24)	100(20)	43(16)	82(19)	-22(14)	-39(17)	28(16)
C(25)	190(40)	80(30)	110(30)	0(20)	-90(30)	40(30)
C(26)	200(40)	90(20)	160(30)	-60(30)	-100(40)	100(30)
C(27)	160(30)	51(18)	86(19)	-24(15)	-60(20)	50(20)
C(28)	57(15)	36(13)	42(11)	-8(9)	-15(10)	5(12)
C(29)	41(11)	23(10)	16(7)	-8(9)	-8(9)	6(8)
C(30)	27(11)	45(13)	63(16)	-18(12)	0(9)	-16(11)
C(31)	80(20)	90(20)	63(15)	2(15)	-51(14)	8(17)
C(32)	62(17)	40(15)	76(16)	12(13)	-43(13)	3(13)
C(33)	85(18)	5(10)	89(19)	1(12)	6(17)	6(11)
C(34)	58(15)	34(14)	39(11)	-18(10)	-8(10)	-1(11)
C(35)	38(12)	47(14)	60(13)	-8(14)	16(13)	-1(10)
C(36)	40(14)	100(20)	44(12)	-22(13)	-5(10)	-8(15)
C(38)	168	180(40)	210(50)	-70(40)	140(30)	-30(40)
C(39)	130(40)	230(50)	480(100)	-280(70)	-140(60)	100(40)
C(42)	60(20)	180(40)	170(40)	50(30)	-50(20)	-10(30)
C(43)	240(50)	220(50)	90(30)	30(30)	60(30)	70(40)
C(44)	35(15)	100(20)	150(30)	-90(20)	0(17)	10(16)
C(45)	52(15)	46(15)	41(11)	-9(10)	-15(10)	-6(12)

Table S9. Hydrogen coordinates ($x10^4$) and isotropic displacement parameters ($Å^2x10^3$) for **Re-Pt(dpm).**

	x	y	z	U(eq)
H(5A)	7332	7702	27731	85
H(6A)	7240	5765	27559	60
H(7A)	6922	5052	25489	73
H(8A)	6697	6276	23590	51

H(12A)	6695	10500	21384	43
H(13A)	6712	12373	20607	54
H(14A)	6957	13677	22392	66
H(15A)	7145	12980	24936	53
H(17A)	6205	8723	23269	70
H(18A)	5888	8422	21011	61
H(20A)	6644	7836	18224	51
H(21A)	6951	8085	20528	43
H(24A)	5419	8353	13947	91
H(25A)	5299	10101	14689	151
H(26A)	5475	10939	17122	180
H(27A)	5860	10075	18642	117
H(31A)	6403	5865	19490	92
H(32A)	6689	4214	19157	71
H(33A)	6541	2918	17131	72
H(34A)	6219	3639	14966	52
H(36A)	5351	4358	10259	75
H(38A)	6027	2467	9506	281
H(38B)	5847	3632	9283	281
H(38C)	5686	2473	8770	281
H(39A)	6071	1637	11239	420
H(39B)	5911	1725	12999	420
H(39C)	6126	2725	12357	420
H(40A)	5286	2477	10493	222
H(40B)	5361	1943	12248	222
H(40C)	5492	1364	10621	222
H(41A)	5016	7543	12153	140
H(41B)	5017	8001	10309	140
H(41C)	5332	7924	11317	140
H(42A)	4817	5581	11463	206
H(42B)	4907	5182	9652	206
H(42C)	4730	6349	9921	206
H(43A)	5294	5808	8181	271
H(43B)	5522	6783	8780	271
H(43C)	5184	7094	8141	271

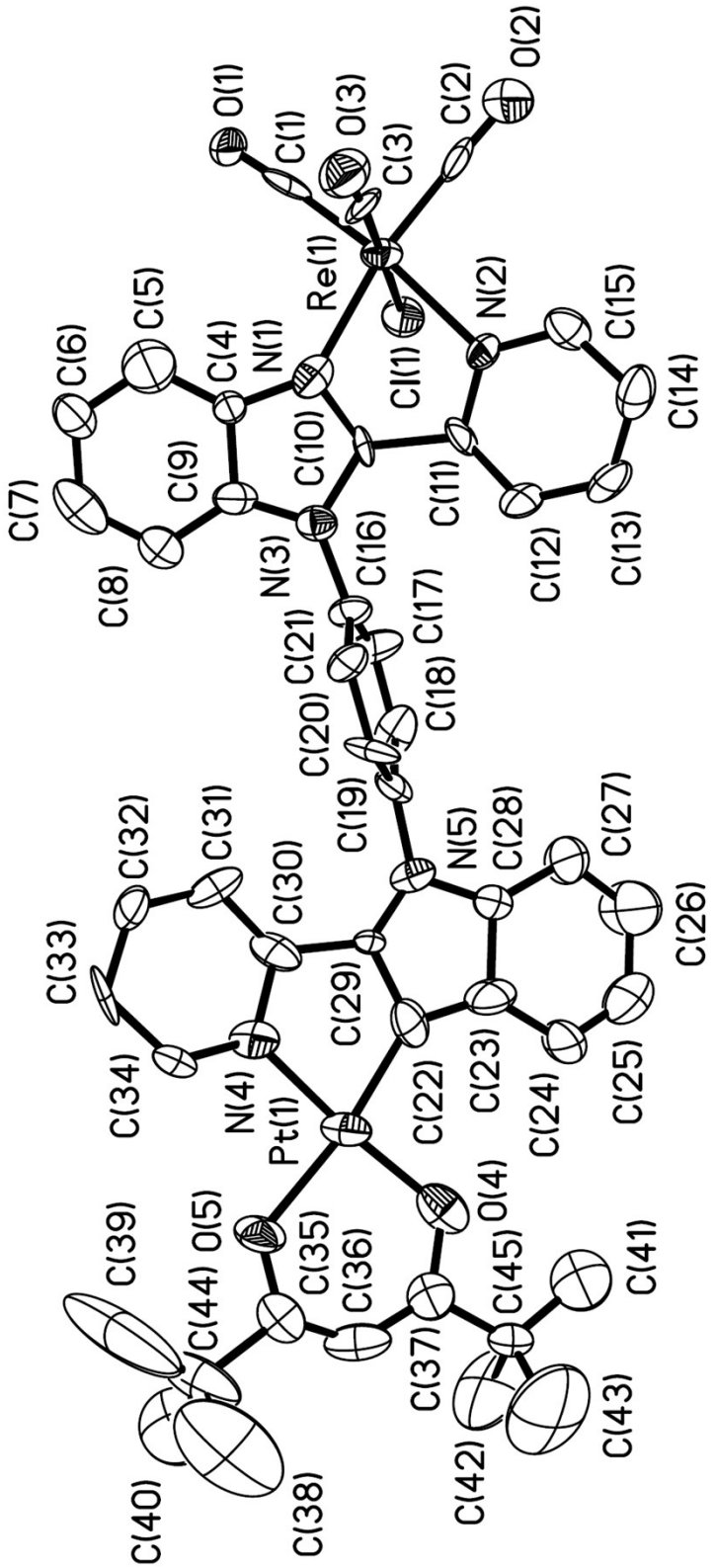


Figure S2. The structure of **Re-Pt(dpm)** showing labeling schemes and 50% thermal ellipsoids.

Table S10. Crystal data and structure refinement for **Re-Pt(dmso)**.

Identification code	**Re-Pt(dmso)**	
Empirical formula	C42H31ClN5O4PtReS	
Formula weight	1118.52	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 19.0195(5) Å	α= 90°.
	b = 8.0623(2) Å	β= 95.642(2)°
	c = 27.8363(8) Å	γ= 90°.
Volume	4247.8(2) $Å^3$	
Z	4	
Density (calculated)	1.749 Mg/m^3	
Absorption coefficient	6.294 mm^{-1}	
F(000)	2144	
Crystal size	0.10 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.73 to 26.00°.	
Index ranges	-23<=h<=19, -9<=k<=9, -34<=l<=34	
Reflections collected	36370	
Independent reflections	8313 [R(int) = 0.0795]	
Completeness to theta = 26.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7437 and 0.5718	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8313 / 1 / 429	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.1109, wR2 = 0.2899	
R indices (all data)	R1 = 0.1452, wR2 = 0.3118	
Largest diff. peak and hole	11.021 and -2.331 $e.Å^{-3}$	

Table S11. Atomic coordinates ($x10^4$) and equivalent isotropic displacement parameters ($Å^2 x 10^3$) for **Re-Pt(dmso)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	9978(1)	11428(1)	8564(1)	74(1)
Pt(1)	5231(1)	-479(1)	9071(1)	45(1)
S(1)	5032(3)	-2795(6)	9508(2)	52(1)
N(2)	9122(11)	10040(20)	8198(8)	74(6)
N(3)	8345(10)	7980(20)	8162(7)	60(5)
N(4)	6336(8)	-130(20)	9280(5)	46(4)
N(5)	6234(10)	3440(20)	8457(6)	58(5)
O(1)	5621(9)	-3645(19)	9780(7)	71(5)
Cl(1)	9056(3)	12596(11)	9021(3)	86(2)
N(1)	9719(19)	9260(40)	9093(12)	55(9)
C(1)	10020(20)	8980(40)	9523(11)	55(9)
C(2)	9820(20)	7730(40)	9769(12)	55(9)
C(3)	9330(20)	6760(40)	9585(12)	55(9)
C(4)	9030(20)	7030(40)	9156(12)	55(9)
C(5)	9220(20)	8290(40)	8909(12)	55(9)
N(1A)	9890(30)	9130(70)	8934(19)	141(12)
C(1A)	10430(30)	8910(70)	9403(19)	141(12)
C(2A)	10280(30)	7580(70)	9803(18)	141(12)
C(3A)	9590(30)	6470(70)	9730(20)	141(12)
C(4A)	9050(30)	6690(80)	9270(20)	141(12)
C(5A)	9200(30)	8020(70)	8865(19)	141(12)
C(6)	8920(12)	8700(30)	8424(7)	55(5)
C(7)	8768(12)	10230(30)	7777(8)	64(6)
C(8)	8771(11)	11410(30)	7421(9)	65(6)
C(9)	8276(14)	11070(40)	7007(9)	76(7)
C(10)	7791(16)	9810(40)	6987(11)	90(9)
C(11)	7779(13)	8720(40)	7315(9)	72(7)
C(12)	8256(14)	8800(30)	7707(9)	69(7)
C(13)	7863(11)	6690(30)	8286(8)	59(6)
C(14)	7917(12)	5160(30)	8108(10)	72(7)
C(15)	7401(12)	3980(30)	8186(7)	54(5)
C(16)	6851(11)	4430(20)	8422(8)	53(5)

C(17)	6839(12)	5990(30)	8649(9)	63(6)
C(18)	7337(15)	7180(30)	8547(10)	84(9)
C(19)	6739(11)	-1080(30)	9620(7)	52(5)
C(20)	7454(11)	-700(40)	9750(8)	72(8)
C(21)	7716(12)	510(40)	9541(8)	68(7)
C(22)	7360(11)	1430(30)	9211(8)	58(6)
C(23)	6629(11)	1150(30)	9063(7)	49(5)
C(24)	6144(12)	2010(20)	8748(7)	48(5)
C(25)	5459(12)	1540(30)	8686(6)	52(6)
C(26)	5081(12)	2690(20)	8342(7)	48(5)
C(27)	4393(15)	2880(30)	8127(6)	63(7)
C(28)	4206(11)	4130(30)	7808(8)	54(5)
C(29)	4710(20)	5250(30)	7708(9)	96(11)
C(30)	5440(14)	5080(30)	7893(9)	66(7)
C(31)	5566(11)	3780(30)	8203(7)	52(5)
C(32)	4189(6)	-373(19)	8835(5)	49(5)
C(33)	3936(10)	-1170(20)	8411(5)	86(9)
C(34)	3234(11)	-980(30)	8227(6)	97(11)
C(35)	2786(7)	20(30)	8467(8)	104(12)
C(36)	3039(8)	820(20)	8891(8)	97(11)
C(37)	3740(8)	620(20)	9075(5)	69(6)
C(38)	4410(11)	-2370(30)	9922(8)	52(5)
C(39)	4538(15)	-4290(30)	9154(8)	69(7)
O(2)	9943(15)	14720(30)	8024(11)	141(11)
O(3)	11101(13)	10260(40)	7925(12)	148(12)
O(4)	11185(12)	12700(40)	9291(11)	142(11)
C(40)	10750(20)	12290(50)	8986(13)	105(10)
C(41)	10650(20)	10630(60)	8184(15)	121(13)
C(42)	9952(16)	13500(30)	8218(9)	79(7)

Table S12. Bond lengths [Å] and angles [°] for **Re-Pt(dmso)**.

Re(1)-C(41)	1.86(5)	Re(1)-N(1)	2.37(3)
Re(1)-C(40)	1.92(4)	Re(1)-Cl(1)	2.454(7)
Re(1)-C(42)	1.927(17)	Pt(1)-C(25)	2.02(2)
Re(1)-N(1A)	2.14(5)	Pt(1)-C(32)	2.028(12)
Re(1)-N(2)	2.15(2)	Pt(1)-N(4)	2.144(15)

Pt(1)-S(1)	2.282(5)	C(16)-C(17)	1.41(3)
S(1)-O(1)	1.460(17)	C(17)-C(18)	1.40(3)
S(1)-C(38)	1.761(19)	C(19)-C(20)	1.41(3)
S(1)-C(39)	1.77(2)	C(20)-C(21)	1.27(4)
N(2)-C(7)	1.30(3)	C(21)-C(22)	1.31(3)
N(2)-C(6)	1.32(3)	C(22)-C(23)	1.43(3)
N(3)-C(6)	1.38(3)	C(23)-C(24)	1.39(3)
N(3)-C(12)	1.42(3)	C(24)-C(25)	1.35(3)
N(3)-C(13)	1.45(3)	C(25)-C(26)	1.47(3)
N(4)-C(23)	1.34(3)	C(26)-C(31)	1.36(3)
N(4)-C(19)	1.38(3)	C(26)-C(27)	1.39(3)
N(5)-C(31)	1.42(3)	C(27)-C(28)	1.37(3)
N(5)-C(16)	1.43(3)	C(28)-C(29)	1.36(4)
N(5)-C(24)	1.43(2)	C(29)-C(30)	1.44(4)
N(1)-C(5)	1.29(2)	C(30)-C(31)	1.36(3)
N(1)-C(1)	1.30(2)	C(32)-C(33)	1.3900
C(1)-C(2)	1.29(2)	C(32)-C(37)	1.3900
C(2)-C(3)	1.29(2)	C(33)-C(34)	1.3900
C(3)-C(4)	1.29(2)	C(34)-C(35)	1.3900
C(4)-C(5)	1.29(2)	C(35)-C(36)	1.3900
C(5)-C(6)	1.45(3)	C(36)-C(37)	1.3900
N(1A)-C(5A)	1.59(4)	O(2)-C(42)	1.12(3)
N(1A)-C(1A)	1.59(4)	O(3)-C(41)	1.21(4)
C(1A)-C(2A)	1.59(4)	O(4)-C(40)	1.17(4)
C(2A)-C(3A)	1.59(4)	C(41)-Re(1)-C(40)	86.6(17)
C(3A)-C(4A)	1.59(4)	C(41)-Re(1)-C(42)	90.1(16)
C(4A)-C(5A)	1.59(4)	C(40)-Re(1)-C(42)	88.4(15)
C(5A)-C(6)	1.40(5)	C(41)-Re(1)-N(1A)	94(2)
C(7)-C(8)	1.37(3)	C(40)-Re(1)-N(1A)	96.2(18)
C(7)-C(12)	1.51(4)	C(42)-Re(1)-N(1A)	174.2(17)
C(8)-C(9)	1.44(3)	C(41)-Re(1)-N(2)	94.7(15)
C(9)-C(10)	1.37(4)	C(40)-Re(1)-N(2)	167.9(13)
C(10)-C(11)	1.27(4)	C(42)-Re(1)-N(2)	103.5(10)
C(11)-C(12)	1.35(3)	N(1A)-Re(1)-N(2)	71.7(16)
C(13)-C(14)	1.34(3)	C(41)-Re(1)-N(1)	107.1(17)
C(13)-C(18)	1.35(3)	C(40)-Re(1)-N(1)	94.7(13)
C(14)-C(15)	1.40(3)	C(42)-Re(1)-N(1)	162.6(14)
C(15)-C(16)	1.34(3)	N(1A)-Re(1)-N(1)	13.7(18)

N(2)-Re(1)-N(1)	73.5(8)	C(4)-C(5)-N(1)	120.0
C(41)-Re(1)-Cl(1)	176.2(13)	C(4)-C(5)-C(6)	124(2)
C(40)-Re(1)-Cl(1)	95.2(11)	N(1)-C(5)-C(6)	116(2)
C(42)-Re(1)-Cl(1)	86.6(9)	C(5A)-N(1A)-C(1A)	120.0
N(1A)-Re(1)-Cl(1)	89.5(15)	C(5A)-N(1A)-Re(1)	122(3)
N(2)-Re(1)-Cl(1)	84.2(7)	C(1A)-N(1A)-Re(1)	115(3)
N(1)-Re(1)-Cl(1)	76.0(11)	C(2A)-C(1A)-N(1A)	119.99(9)
C(25)-Pt(1)-C(32)	92.8(8)	C(1A)-C(2A)-C(3A)	120.01(6)
C(25)-Pt(1)-N(4)	77.5(8)	C(4A)-C(3A)-C(2A)	120.00(7)
C(32)-Pt(1)-N(4)	169.7(7)	C(3A)-C(4A)-C(5A)	120.01(10)
C(25)-Pt(1)-S(1)	177.2(7)	C(6)-C(5A)-N(1A)	97(4)
C(32)-Pt(1)-S(1)	89.9(5)	C(6)-C(5A)-C(4A)	143(3)
N(4)-Pt(1)-S(1)	99.9(5)	N(1A)-C(5A)-C(4A)	120.0
O(1)-S(1)-C(38)	106.4(10)	N(2)-C(6)-N(3)	110.0(19)
O(1)-S(1)-C(39)	107.9(12)	N(2)-C(6)-C(5A)	129(3)
C(38)-S(1)-C(39)	98.2(11)	N(3)-C(6)-C(5A)	121(3)
O(1)-S(1)-Pt(1)	120.1(7)	N(2)-C(6)-C(5)	122(2)
C(38)-S(1)-Pt(1)	110.4(7)	N(3)-C(6)-C(5)	128(2)
C(39)-S(1)-Pt(1)	111.6(8)	C(5A)-C(6)-C(5)	10(3)
C(7)-N(2)-C(6)	112(2)	N(2)-C(7)-C(8)	134(3)
C(7)-N(2)-Re(1)	131.7(18)	N(2)-C(7)-C(12)	107(2)
C(6)-N(2)-Re(1)	116.1(15)	C(8)-C(7)-C(12)	119(2)
C(6)-N(3)-C(12)	107.1(19)	C(7)-C(8)-C(9)	113(2)
C(6)-N(3)-C(13)	131.3(18)	C(10)-C(9)-C(8)	124(3)
C(12)-N(3)-C(13)	121.5(19)	C(11)-C(10)-C(9)	123(3)
C(23)-N(4)-C(19)	120.3(18)	C(10)-C(11)-C(12)	119(3)
C(23)-N(4)-Pt(1)	114.5(14)	C(11)-C(12)-N(3)	135(2)
C(19)-N(4)-Pt(1)	125.2(14)	C(11)-C(12)-C(7)	121(2)
C(31)-N(5)-C(16)	124.0(19)	N(3)-C(12)-C(7)	103(2)
C(31)-N(5)-C(24)	106.6(17)	C(14)-C(13)-C(18)	124(2)
C(16)-N(5)-C(24)	129.3(19)	C(14)-C(13)-N(3)	120(2)
C(5)-N(1)-C(1)	120.0	C(18)-C(13)-N(3)	116(2)
C(5)-N(1)-Re(1)	113.0(13)	C(13)-C(14)-C(15)	119(2)
C(1)-N(1)-Re(1)	127.0(14)	C(16)-C(15)-C(14)	119(2)
C(2)-C(1)-N(1)	119.97(6)	C(15)-C(16)-C(17)	120.8(18)
C(3)-C(2)-C(1)	120.0	C(15)-C(16)-N(5)	124.5(19)
C(2)-C(3)-C(4)	120.0	C(17)-C(16)-N(5)	114.7(19)
C(5)-C(4)-C(3)	120.00(6)	C(18)-C(17)-C(16)	118.6(18)

C(13)-C(18)-C(17)	118(2)	C(29)-C(28)-C(27)	119(2)
N(4)-C(19)-C(20)	121(2)	C(28)-C(29)-C(30)	122(2)
C(21)-C(20)-C(19)	117(2)	C(31)-C(30)-C(29)	114(2)
C(20)-C(21)-C(22)	124(2)	C(26)-C(31)-C(30)	127(2)
C(21)-C(22)-C(23)	122(2)	C(26)-C(31)-N(5)	109.5(19)
N(4)-C(23)-C(24)	112.8(18)	C(30)-C(31)-N(5)	124(2)
N(4)-C(23)-C(22)	115(2)	C(33)-C(32)-C(37)	120.0
C(24)-C(23)-C(22)	132(2)	C(33)-C(32)-Pt(1)	120.1(9)
C(25)-C(24)-C(23)	120.7(18)	C(37)-C(32)-Pt(1)	119.7(9)
C(25)-C(24)-N(5)	109(2)	C(32)-C(33)-C(34)	120.0
C(23)-C(24)-N(5)	130.5(19)	C(33)-C(34)-C(35)	120.0
C(24)-C(25)-C(26)	108.0(17)	C(36)-C(35)-C(34)	120.0
C(24)-C(25)-Pt(1)	114.4(17)	C(37)-C(36)-C(35)	120.0
C(26)-C(25)-Pt(1)	137.6(15)	C(36)-C(37)-C(32)	120.0
C(31)-C(26)-C(27)	116.2(19)	O(4)-C(40)-Re(1)	171(3)
C(31)-C(26)-C(25)	107.1(19)	O(3)-C(41)-Re(1)	174(4)
C(27)-C(26)-C(25)	136.7(19)	O(2)-C(42)-Re(1)	179(3)
C(28)-C(27)-C(26)	122(2)		

Table S13. Anisotropic displacement parameters ($Å^2x10^3$) for **Re-Pt(dmso)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11}+ ...+ 2hka^*b^*U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	39(1)	57(1)	126(1)	-21(1)	3(1)	-15(1)
Pt(1)	49(1)	39(1)	48(1)	-3(1)	11(1)	-9(1)
S(1)	64(3)	35(3)	59(3)	0(2)	19(3)	-3(2)
N(2)	65(13)	44(11)	106(16)	17(11)	-24(12)	1(9)
N(3)	64(12)	44(10)	66(11)	0(9)	-18(9)	-18(9)
N(4)	32(8)	64(11)	44(8)	-26(8)	16(7)	-11(7)
N(5)	65(12)	53(11)	56(10)	-3(9)	12(9)	-20(9)
O(1)	75(11)	42(9)	98(12)	23(8)	18(9)	8(8)
Cl(1)	54(3)	110(6)	94(5)	4(4)	7(3)	-13(4)
N(1)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(1)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(2)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(3)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(4)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(5)	67(15)	34(11)	53(13)	-3(8)	-50(11)	-7(10)
C(6)	63(13)	55(13)	45(11)	-5(10)	-4(9)	-27(11)
C(7)	52(13)	76(16)	64(13)	23(12)	6(11)	27(12)
C(8)	44(12)	72(16)	80(15)	30(13)	9(11)	0(11)
C(9)	63(15)	90(20)	67(15)	19(14)	-14(12)	12(15)
C(10)	80(20)	110(20)	82(18)	19(18)	-9(15)	11(18)
C(11)	62(15)	83(18)	65(14)	-10(14)	-32(12)	-16(13)
C(12)	84(17)	59(14)	72(15)	23(12)	47(14)	8(13)
C(13)	50(12)	67(15)	61(13)	-12(11)	5(10)	-30(11)
C(14)	40(12)	75(17)	102(19)	-29(15)	11(12)	-16(11)
C(15)	77(15)	42(11)	45(10)	-2(9)	16(10)	-22(10)
C(16)	54(12)	34(10)	74(13)	-4(10)	17(10)	-18(9)
C(17)	56(13)	59(14)	79(15)	-31(12)	34(12)	-12(11)
C(18)	100(20)	56(14)	110(20)	-41(15)	61(17)	-39(14)
C(19)	60(13)	56(13)	41(10)	2(9)	11(9)	8(10)
C(20)	41(12)	120(20)	50(12)	5(14)	-2(10)	-8(14)
C(21)	50(13)	100(20)	51(12)	-16(14)	-5(10)	-30(14)
C(22)	48(12)	72(15)	54(12)	-19(11)	5(10)	-20(11)

C(23)	57(12)	53(12)	39(9)	-1(9)	16(9)	-5(10)
C(24)	70(14)	34(10)	46(10)	-4(8)	32(10)	-24(10)
C(25)	72(14)	52(12)	35(9)	-25(9)	22(9)	-36(11)
C(26)	67(14)	31(10)	45(10)	5(8)	3(10)	-1(9)
C(27)	130(20)	39(11)	23(8)	-15(8)	12(11)	3(12)
C(28)	38(11)	63(14)	63(12)	2(11)	11(9)	2(10)
C(29)	180(40)	44(14)	64(15)	30(12)	38(19)	32(19)
C(30)	70(16)	63(15)	71(14)	-8(12)	37(13)	-19(13)
C(31)	48(12)	62(14)	48(11)	7(10)	12(9)	-5(10)
C(33)	100(20)	71(18)	91(19)	8(15)	20(16)	-47(16)
C(34)	69(19)	140(30)	78(18)	15(19)	-6(15)	-40(20)
C(35)	80(20)	100(30)	120(30)	40(20)	-20(20)	-50(20)
C(36)	50(15)	120(30)	120(30)	60(20)	26(16)	19(16)
C(38)	53(12)	44(11)	62(12)	9(10)	18(10)	1(10)
C(39)	100(20)	48(13)	61(13)	-16(11)	33(13)	-20(13)
O(2)	130(20)	120(20)	160(20)	64(18)	-45(18)	-51(17)
O(3)	86(16)	150(20)	210(30)	-110(20)	2(17)	4(16)
O(4)	86(16)	120(20)	200(30)	0(20)	-72(17)	-5(14)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **Re-Pt(dmso)**.

	x	y	z	U(eq)
H(1A)	10386	9690	9657	66
H(2A)	10046	7522	10084	66
H(3A)	9183	5837	9766	66
H(4A)	8660	6321	9021	66
H(1AA)	10849	9575	9445	170
H(2AA)	10606	7455	10083	170
H(3AA)	9498	5681	9973	170
H(4AA)	8632	6026	9225	170
H(8A)	9071	12355	7445	78
H(9A)	8285	11766	6732	91
H(10A)	7449	9751	6715	108
H(11A)	7438	7856	7284	87
H(14A)	8301	4880	7929	86

H(15A)	7441	2875	8074	65
H(17A)	6499	6227	8868	75
H(18A)	7307	8288	8657	101
H(19A)	6529	-1993	9766	62
H(20A)	7731	-1338	9986	86
H(21A)	8198	774	9627	82
H(22A)	7597	2308	9066	70
H(27A)	4042	2118	8205	75
H(28A)	3736	4219	7660	65
H(29A)	4570	6180	7511	115
H(30A)	5801	5797	7805	79
H(33A)	4242	-1856	8247	103
H(34A)	3061	-1525	7937	116
H(35A)	2307	154	8341	124
H(36A)	2733	1503	9055	117
H(37A)	3913	1172	9365	83
H(38A)	4259	-3417	10060	78
H(38B)	4000	-1811	9755	78
H(38C)	4627	-1660	10180	78
H(39A)	4417	-5215	9360	104
H(39B)	4819	-4708	8903	104
H(39C)	4103	-3784	9003	104

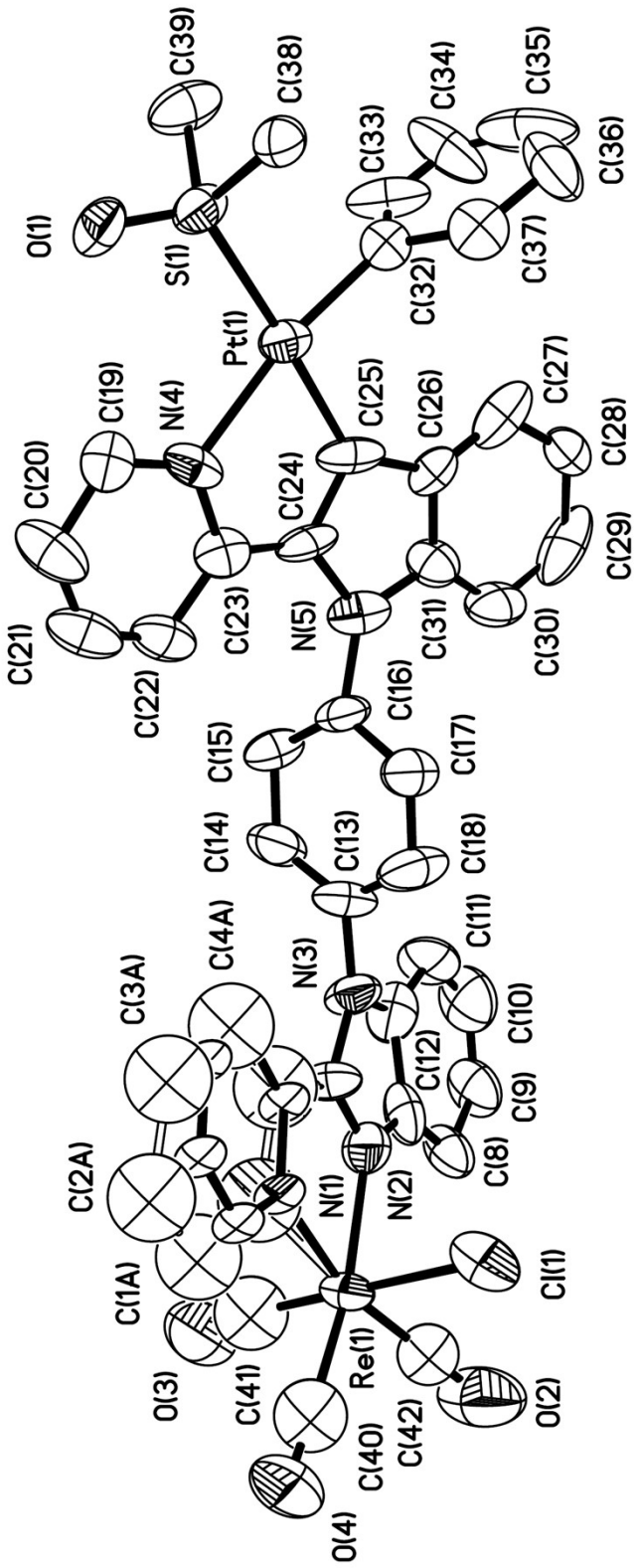


Figure S3. The structure of **Re-Pt(DMSO)** with 50% thermal ellipsoids and labeling schemes. H atoms are omitted for clarity.

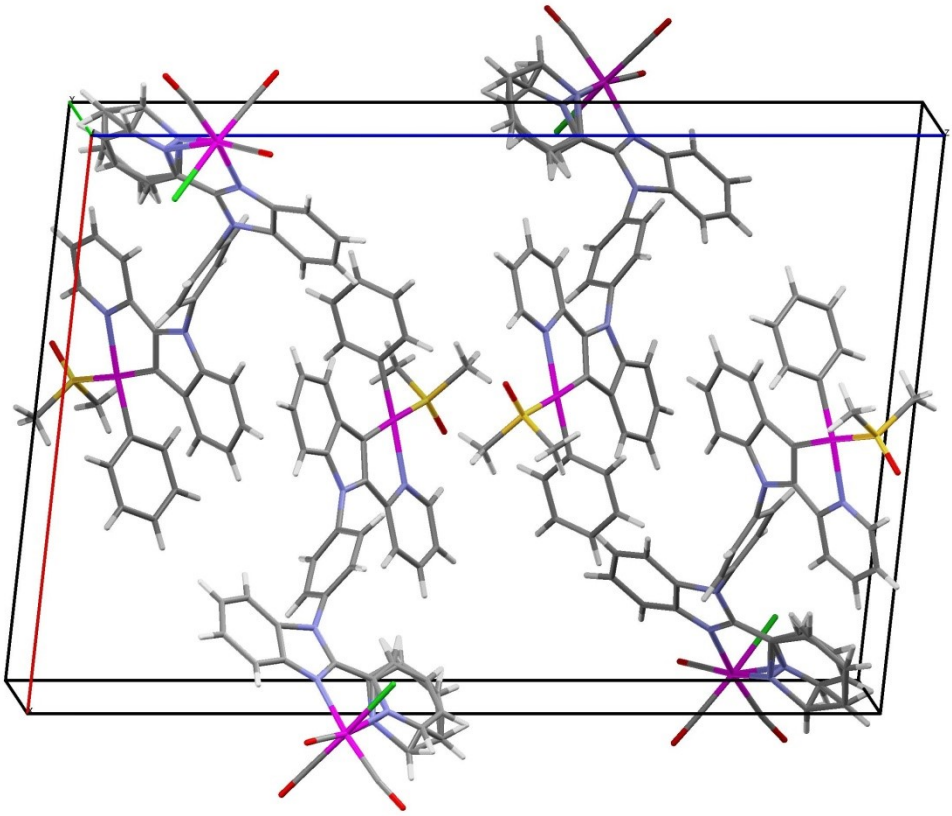


Figure S4. Unit cell pack diagram of **Re-Pt(DMSO)**, projected down the b-axis.

S5. Experimental Spectra

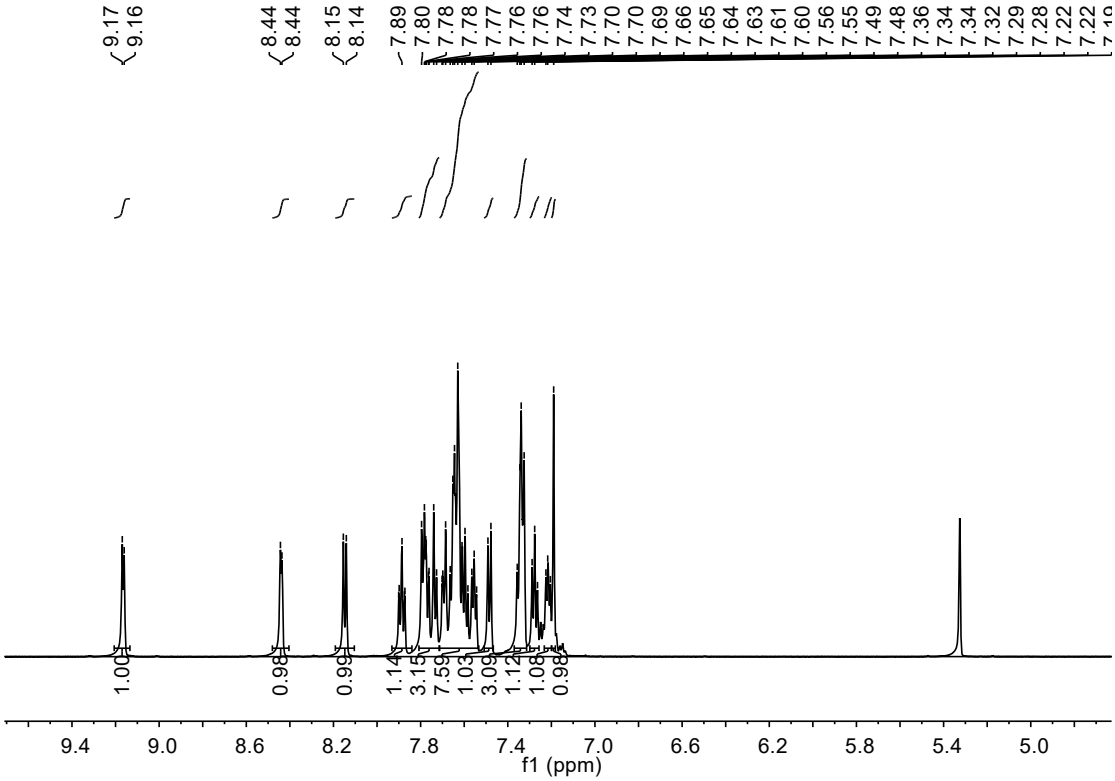


Figure S5. ^{1}H NMR spectrum of **Re-L1** in CD_2Cl_2.

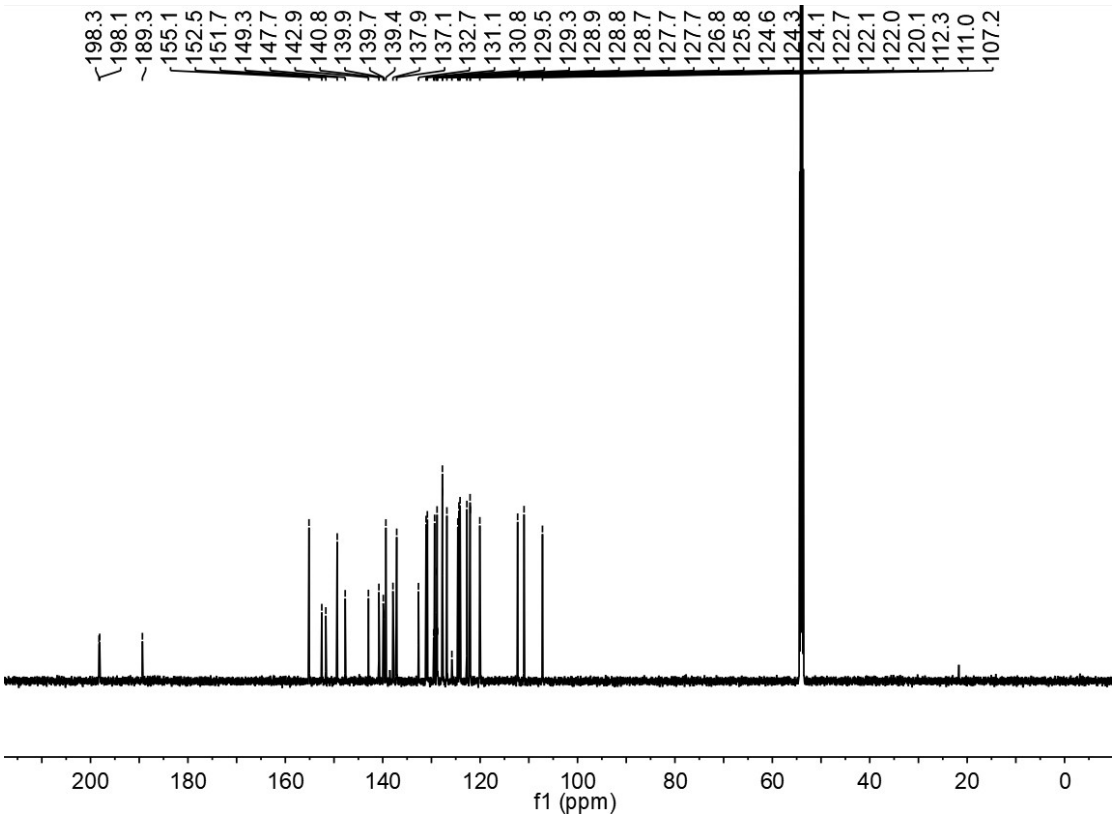


Figure S6. ^{13}C NMR spectrum of **Re-L1** in CD_2Cl_2.

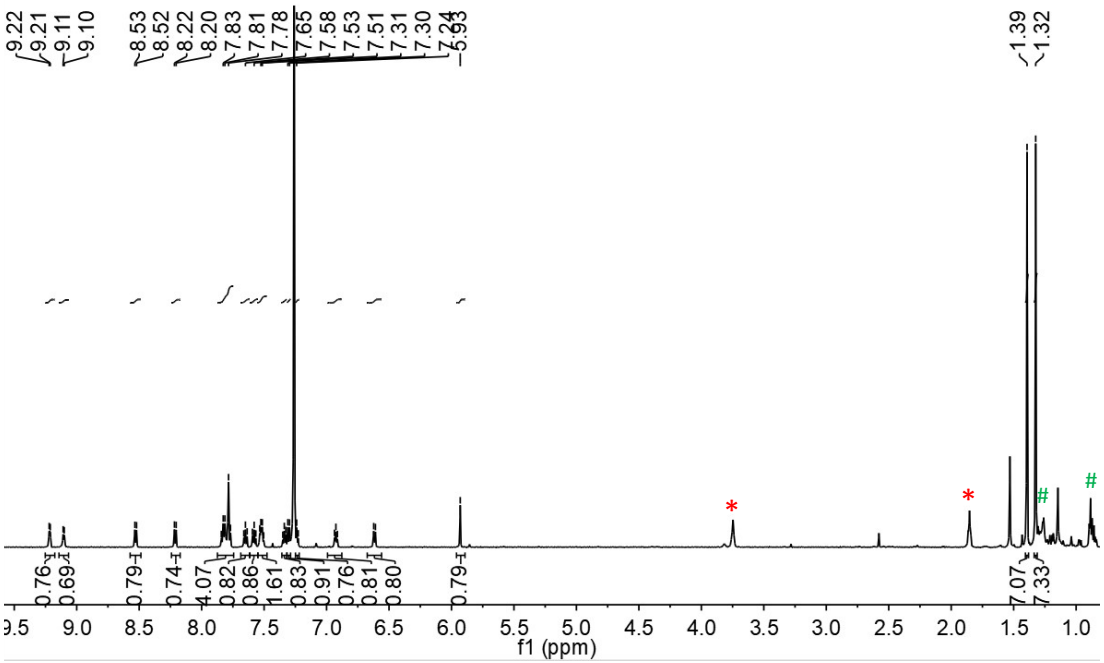


Figure S7. ^{1}H NMR spectrum of **Re-Pt(dpm)** in $CDCl_3$. (*: solvent signal from THF; #: solvent signal from hexane.)

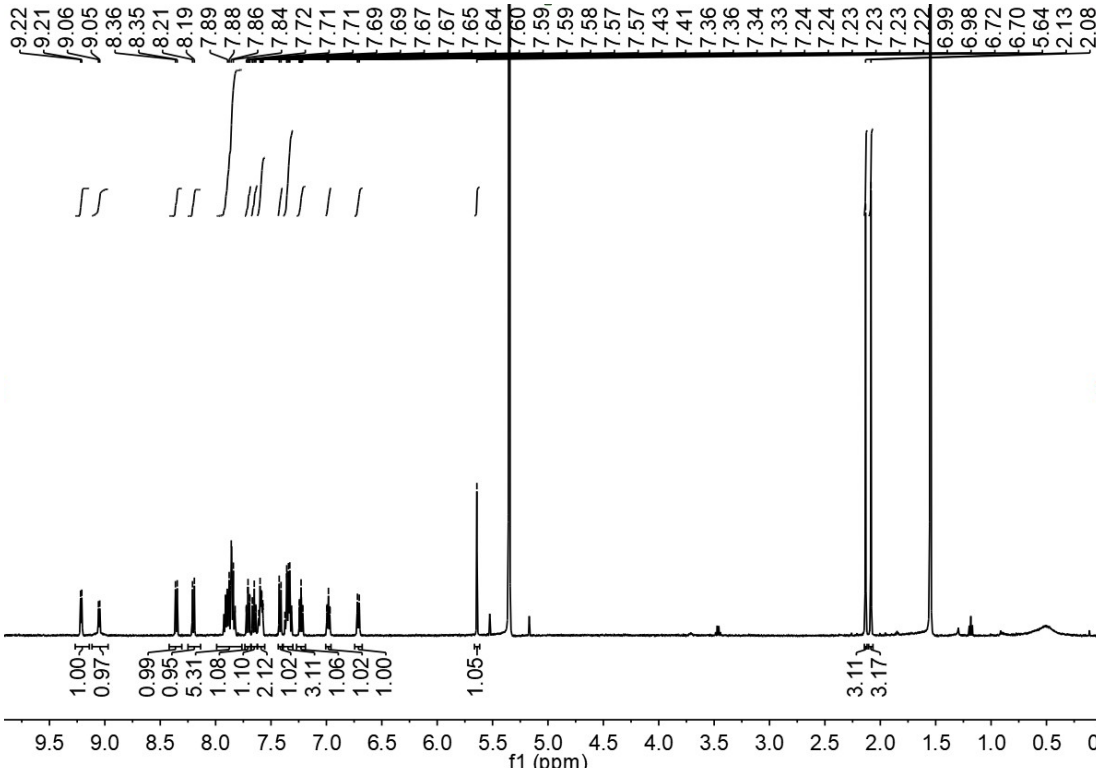


Figure S8. ^{1}H NMR spectrum of **Re-Pt** in CD_2Cl_2.

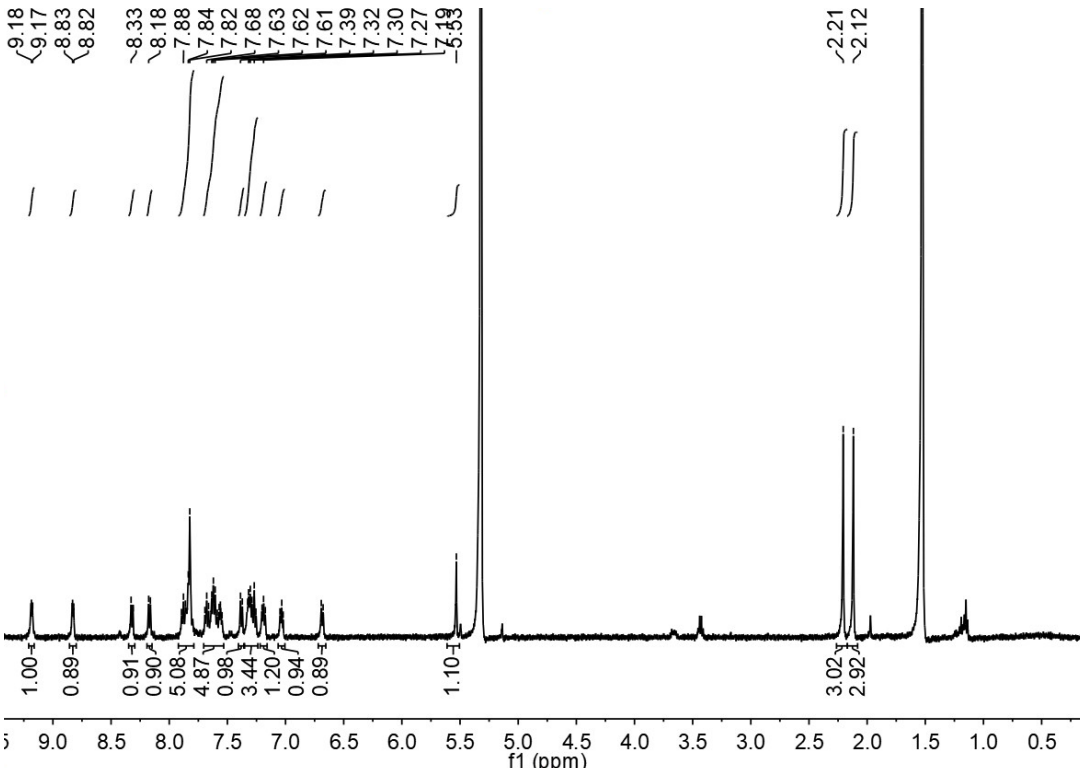


Figure S9. ^{1}H NMR spectrum of **Re-Pd** in CD_2Cl_2.

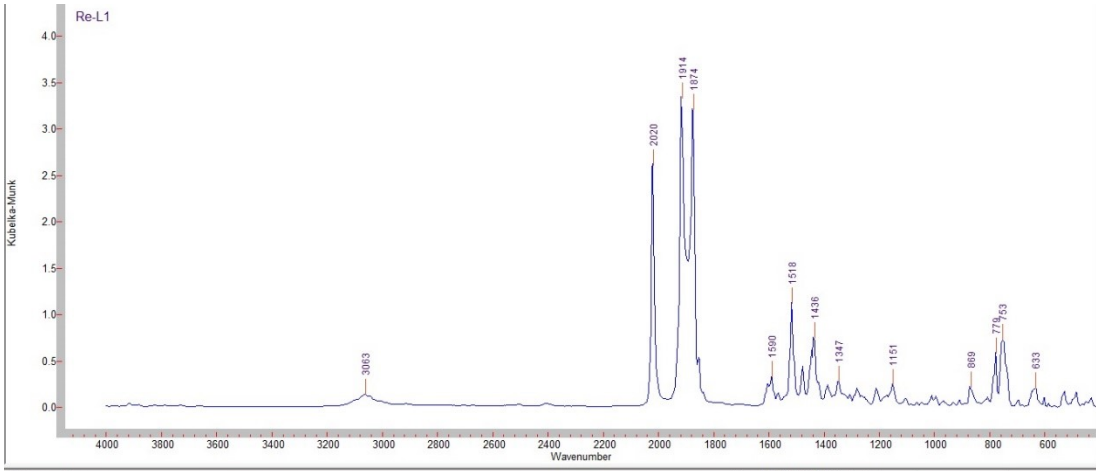


Figure S10. IR spectrum of **Re-L1**.

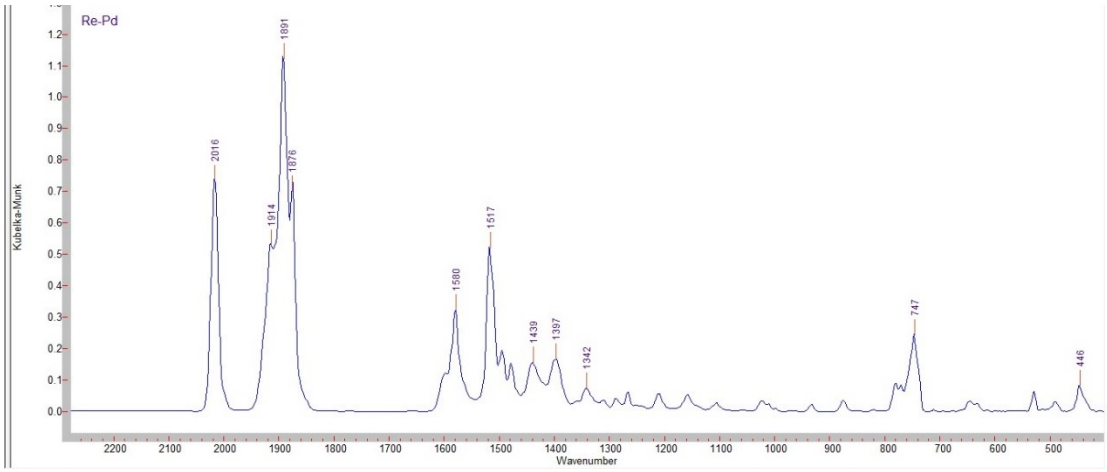


Figure S11. IR spectrum of **Re-Pd**.

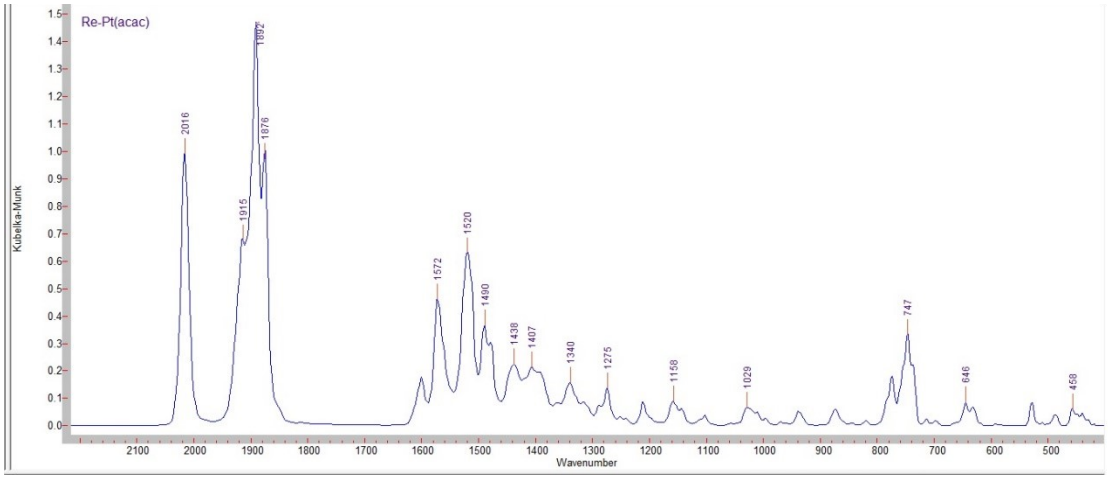


Figure S12. IR spectrum of **Re-Pt**.

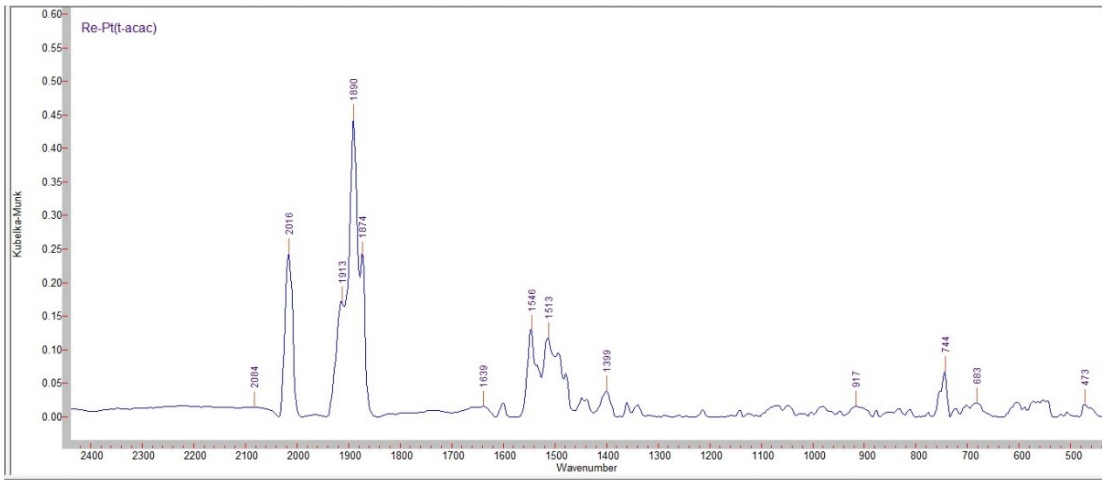


Figure S13. IR spectrum of **Re-Pt(dpm)**.

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