Supporting information

Aromatic amine *N*-oxide organometallic compounds: searching for prospective agents against infectious diseases

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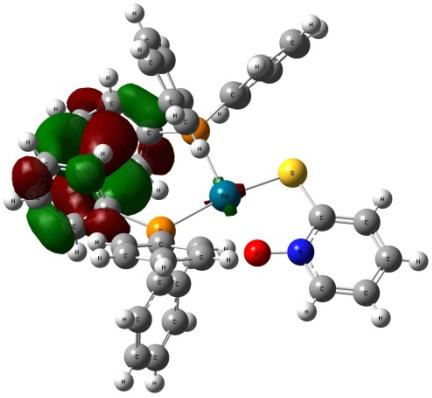
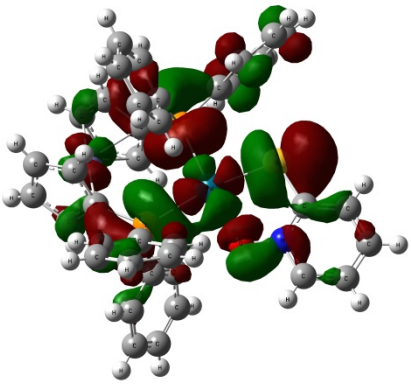
Figure S1. B89/6-31+G(d)/LANL2DZ Kohn-Sham frontier orbitals for the M-dppf-mpo (M=Pd, Pt) species, represented as 0.02 a.u. isosurfaces.

Pd-dppf-mpo

HOMO ε = -7.40 eV

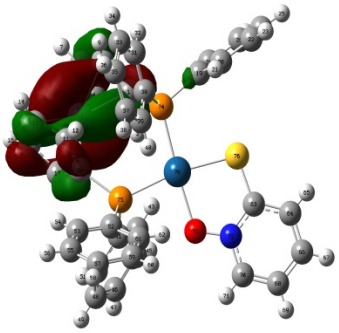


LUMO ε = -5.45 eV



Pt-dppf-mpo

HOMO ε = -7.39 Ev



LUMO ε = -4.95 eV

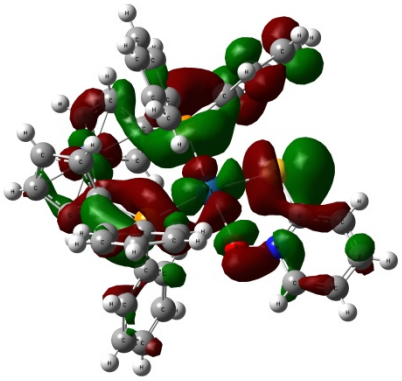
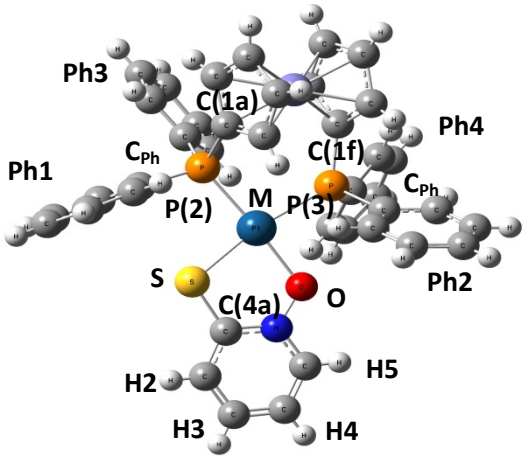


Table S1. Wiberg bond indices (WBI, a.u.) as calculated for the species $[M(mpo)(dppf)]^+$ (M=Pd, Pt) at the BP86/6-31+G(d)/LANL2DZ level. Atom numbering scheme is shown in the figure.



Bonding interaction	$[Pd(mpo)(dppf)]^+$	[Pt(m
M-P(2)	0.663	0.7
M-P(3)	0.580	0.6
M-S	0.665[0.710][a]	0.7
M-O	0.391 [0.412][a]	0.4
S-C(4a)	1.206 [1.220][a]	1.2
O-N	1.102 [1.119] [a]	1.0
C(4a)-N	1.159 [1.148] [a]	1.1
$P(2)\text{-}C(1a)_{Cp}$	0.889	0.8
$P(3)\text{- }C(1f)_{Cp}$	0.889	0.8
$P(2)\text{-}C_{Ph1}$	0.891	0.8
$P(2)\text{-}C_{Ph3}$	0.906	0.9
$P(3)\text{-}C_{Ph2}$	0.908	0.9
$P(3)\text{-}C_{Ph4}$	0.908	0.9
***Weak inter-unit interactions*[b]**		
P(2)…O	0.083	0.1
P(2)…S	0.111	0.0
P(3)…O	0.043	0.0
P(3)…S	0.127	0.1

[a]Values between brackets correspond to the $[Pd(mpo)_2]$ complex calculated at the same level of theory. [b]NBO analysis identifies differences in bonding patterns, with 3 units for Pd-dppd-mpo($C_{17}H_{14}PFePd//C_{17}H_{14}P//C_5H_4NOS$) and 2 units for Pt-dppf-mpo ($C_{34}H_{28}PFePt//C_5H_4NOS$) being a neutral mpo moiety the one shared in common in the complexes.

Table S2a. NPA atomic charges for the mpo protons and heavy atoms in the mpo moieties of $[M(mpo)(dppf)]^+$(M=Pd, Pt), $[Pd(mpo)_2]$ and in the free ligand. The strength of the principal covalent interactions among them is also reported in terms of WBI. All magnitudes are expressed in a.u.

Atom(s)	Hmpo	$[Pd(mpo)_2]$	$[Pd(mpo)(dppf)]^+$	$[Pt(mpo)(dppf)]^+$
Natural atomic charges				
H2	+0.279	+0.273	+0.229	+0.230
H3	+0.265	+0.263	+0.220	+0.220
H4	+0.269	+0.268	+0.225	+0.225
H5	+0.274	+0.273	+0.219	+0.221
C2	-0.262	-0.017	-0.209	-0.200
C3	-0.217	-0.230	-0.152	-0.152
C4	-0.304	-0.294	-0.221	-0.220
C5	+0.004	-0.005	+0.048	+0.051
M	---	+0.205	-0.167	-0.223
O	-0.535	-0.452	-0.486	-0.487
S	-0.158	+0.086	+0.097	+0.108
N	-0.041	-0.006	+0.012	+0.008
C(4a)	-0.033	-0.017	-0.009	-0.012
Wibergbond indices				
C2-H2	0.889	0.891	0.912	0.913
C3-H3	0.900	0.902	0.922	0.922
C4-H4	0.898	0.898	0.919	0.918
C5-H5	0.893	0.894	0.923	0.921
O-N	1.054	1.119	1.102	1.090
S-C(4a)	1.409	1.220	1.206	1.208
N-C(4a)	1.231	1.148	1.159	1.166
O...C(4a)	0.069	0.110	0.110	0.108
S...N	0.147	0.099	0.097	0.099
O...C5	0.068	0.102	0.091	0.084
S...C2	0.090	0.062	0.059	0.056

Table S3a. NPA atomic charges (a.u.) corresponding to the dppf moiety in $[M(mpo)(dppf)]^+$ (M=Pd, Pt).

Atom	$[Pd(mpo)(dppf)]^+$	$[Pt(mpo)(dppf)]^+$
M	-0.167	-0.223
Fe	-0.411	-0.429
P(2)	+1.293	+1.308
P(3)	+1.206	+1.236
C(1a)	-0.413	-0.392
C(1f)	-0.387	-0.389
C_{Ph1}	-0.393	-0.389
C_{Ph2}	-0.364	-0.370
C_{Ph2}	-0.396	-0.397
C_{Ph4}	-0.375	-0.382

Table S3a. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Pd(mpo)(dppf)]PF_6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1A)	5196(9)	7183(4)	1320(5)	41(2)
C(1B)	4187(9)	7496(4)	1576(5)	43(2)
C(1C)	4540(10)	8100(4)	1705(5)	56(3)
C(1D)	5766(10)	8180(4)	1532(6)	56(3)
C(1E)	6180(10)	7639(5)	1283(5)	54(3)
C(1F)	6109(10)	6915(4)	3270(6)	49(3)
C(1G)	7368(9)	6991(4)	3123(6)	52(3)
C(1H)	7797(10)	7593(5)	3302(6)	65(3)
C(1I)	6811(10)	7892(5)	3554(6)	56(3)
C(1J)	5785(9)	7476(4)	3562(5)	45(2)
C(2A)	4526(9)	6329(4)	68(5)	40(2)
C(2B)	4989(10)	5876(4)	-335(5)	50(3)
C(2C)	4385(11)	5775(5)	-1164(6)	67(3)
C(2D)	3332(12)	6137(5)	-1559(6)	62(3)
C(2E)	2904(11)	6590(5)	-1176(6)	63(3)
C(2F)	3470(9)	6690(4)	-356(6)	48(3)
C(2G)	6937(9)	6168(5)	1346(6)	52(3)
C(2H)	7836(10)	6423(5)	989(7)	59(3)
C(2I)	9158(12)	6272(6)	1205(9)	86(4)
C(2J)	9610(14)	5841(7)	1785(11)	112(6)
C(2K)	8763(14)	5540(6)	2128(9)	98(5)
C(2L)	7405(11)	5707(5)	1902(7)	72(3)
C(3A)	3688(9)	6457(4)	3504(5)	42(2)
C(3B)	2492(9)	6648(4)	2989(5)	48(3)
C(3C)	1435(11)	6838(5)	3282(6)	62(3)
C(3D)	1567(12)	6832(5)	4078(6)	64(3)
C(3E)	2743(13)	6655(5)	4596(6)	73(4)
C(3F)	3820(12)	6476(5)	4329(6)	63(3)
C(3G)	6112(10)	5708(5)	3767(6)	60(3)
C(3H)	7212(11)	5865(5)	4379(7)	93(5)
C(3I)	7987(15)	5433(7)	4863(9)	136(7)
C(3J)	7723(18)	4860(6)	4742(10)	170(9)
C(3K)	6640(20)	4686(7)	4108(12)	241(14)
C(3L)	5832(17)	5114(6)	3645(9)	169(9)
C(4A)	1981(9)	4903(4)	1084(5)	43(2)
C(4B)	1070(10)	4484(5)	659(6)	55(3)
C(4C)	405(10)	4099(5)	1017(7)	60(3)
C(4D)	684(10)	4096(4)	1843(7)	63(3)
C(4E)	1581(9)	4502(4)	2265(6)	50(3)
N(4)	2223(7)	4895(3)	1899(4)	44(2)
O(4)	3017(6)	5297(3)	2377(3)	53(2)
P(2)	5207(2)	6405(1)	1150(2)	40(1)
P(3)	5078(3)	6256(1)	3098(1)	45(1)
S(4)	2800(3)	5418(1)	661(1)	50(1)
Fe	5975(1)	7553(1)	2421(1)	44(1)
Pd	4060(1)	5861(1)	1824(1)	41(1)
F(41)	966(9)	7391(4)	6023(6)	154(4)
F(42)	-1103(8)	7120(4)	5518(5)	149(3)
F(43)	-853(11)	6383(4)	6359(5)	153(4)
F(44)	1254(10)	6693(6)	6880(6)	213(6)
F(45)	485(11)	6488(4)	5585(6)	160(4)
F(46)	-381(9)	7281(4)	6815(5)	154(4)
P(4)	75(3)	6885(2)	6209(2)	69(1)

Table S3b. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Pt(mpo)(dppf)]PF_6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
C(1A)	5191(6)	7202(3)	1309(3)	39(2)
C(1B)	4168(6)	7498(3)	1559(3)	46(2)
C(1C)	4519(7)	8110(3)	1696(4)	57(2)
C(1D)	5757(8)	8193(3)	1534(4)	58(2)
C(1E)	6175(7)	7641(3)	1283(4)	55(2)
C(1F)	6073(7)	6916(3)	3241(3)	44(2)
C(1G)	7358(7)	7004(3)	3090(4)	55(2)
C(1H)	7758(7)	7604(3)	3276(4)	59(2)
C(1I)	6758(8)	7891(3)	3556(4)	58(2)
C(1J)	5708(7)	7474(3)	3526(4)	53(2)
C(2A)	4538(6)	6325(3)	57(4)	41(2)
C(2B)	4964(7)	5856(3)	-338(4)	51(2)
C(2C)	4354(8)	5768(3)	-1141(4)	66(2)
C(2D)	3325(8)	6122(4)	-1562(4)	64(2)
C(2E)	2890(7)	6593(3)	-1166(4)	60(2)
C(2F)	3487(7)	6687(3)	-368(4)	49(2)
C(2G)	6947(6)	6185(3)	1334(4)	49(2)
C(2H)	7795(7)	6452(3)	956(5)	70(2)
C(2I)	9148(9)	6300(4)	1156(7)	93(4)
C(2J)	9620(10)	5873(5)	1727(8)	118(5)
C(2K)	8785(10)	5579(4)	2087(6)	99(3)
C(2L)	7443(8)	5735(3)	1893(5)	64(2)
C(3A)	3684(7)	6451(3)	3487(4)	48(2)
C(3B)	2484(7)	6658(3)	2995(4)	54(2)
C(3C)	1449(8)	6827(3)	3294(4)	60(2)
C(3D)	1579(10)	6811(4)	4095(5)	75(2)
C(3E)	2750(10)	6621(4)	4590(5)	80(3)
C(3F)	3825(9)	6438(4)	4314(4)	73(2)
C(3G)	6110(8)	5708(3)	3729(5)	70(2)
C(3H)	7154(10)	5874(4)	4358(5)	101(3)
C(3I)	8002(11)	5448(5)	4841(7)	144(5)
C(3J)	7789(14)	4873(5)	4686(7)	184(7)
C(3K)	6800(15)	4691(4)	4028(8)	205(8)
C(3L)	5958(11)	5109(4)	3558(6)	135(5)
C(4A)	1986(6)	4905(3)	1088(4)	41(2)
C(4B)	1055(7)	4490(3)	658(4)	55(2)
C(4C)	426(8)	4102(3)	1030(5)	66(2)
C(4D)	701(8)	4111(3)	1851(5)	64(2)
C(4E)	1586(7)	4515(3)	2272(4)	53(2)
N(4)	2209(5)	4906(2)	1898(3)	41(1)
O(4)	3026(4)	5306(2)	2369(2)	51(1)
P(2)	5209(2)	6411(1)	1136(1)	39(1)
P(3)	5049(2)	6253(1)	3068(1)	46(1)
S(4)	2792(2)	5417(1)	651(1)	46(1)
Fe	5945(1)	7558(1)	2406(1)	45(1)
Pt	4066(1)	5867(1)	1804(1)	39(1)
F(41)	944(6)	7393(3)	6031(4)	143(2)
F(42)	-1113(6)	7117(3)	5541(3)	145(2)
F(43)	-840(8)	6364(3)	6377(3)	157(3)
F(44)	1255(8)	6670(4)	6905(4)	203(4)
F(45)	485(7)	6480(2)	5600(4)	153(3)
F(46)	-410(6)	7264(3)	6826(3)	147(3)
P(4)	79(2)	6868(1)	6223(1)	67(1)

Table S4a. Full bond lengths [Å] and angles [°] for $[Pd(mpo)(dppf)]PF_6$.

C(1A)-C(1B)	1.426(11)	F(44)-P(4)	1.493(8)
C(1A)-C(1E)	1.454(12)	F(45)-P(4)	1.545(8)
C(1A)-P(2)	1.763(10)	F(46)-P(4)	1.543(8)
C(1A)-Fe	2.026(8)		
C(1B)-C(1C)	1.398(11)	C(1B)-C(1A)-C(1E)	104.7(8)
C(1B)-Fe	2.016(9)	C(1B)-C(1A)-P(2)	125.1(7)
C(1C)-C(1D)	1.394(12)	C(1E)-C(1A)-P(2)	130.2(7)
C(1C)-Fe	2.050(9)	C(1B)-C(1A)-Fe	69.0(5)
C(1D)-C(1E)	1.389(12)	C(1E)-C(1A)-Fe	69.9(5)
C(1D)-Fe	2.046(10)	P(2)-C(1A)-Fe	122.7(5)
C(1E)-Fe	2.048(10)	C(1C)-C(1B)-C(1A)	109.9(9)
C(1F)-C(1G)	1.405(12)	C(1C)-C(1B)-Fe	71.2(5)
C(1F)-C(1J)	1.424(12)	C(1A)-C(1B)-Fe	69.7(5)
C(1F)-P(3)	1.793(10)	C(1B)-C(1C)-C(1D)	107.6(9)
C(1F)-Fe	2.023(9)	C(1B)-C(1C)-Fe	68.6(5)
C(1G)-C(1H)	1.421(12)	C(1D)-C(1C)-Fe	70.0(6)
C(1G)-Fe	2.037(9)	C(1E)-C(1D)-C(1C)	109.5(9)
C(1H)-C(1I)	1.387(13)	C(1E)-C(1D)-Fe	70.3(6)
C(1H)-Fe	2.068(9)	C(1C)-C(1D)-Fe	70.2(6)
C(1I)-C(1J)	1.413(12)	C(1D)-C(1E)-C(1A)	108.3(9)
C(1I)-Fe	2.053(9)	C(1D)-C(1E)-Fe	70.1(6)
C(1J)-Fe	2.046(9)	C(1A)-C(1E)-Fe	68.3(5)
C(2A)-C(2B)	1.387(11)	C(1G)-C(1F)-C(1J)	106.3(8)
C(2A)-C(2F)	1.390(11)	C(1G)-C(1F)-P(3)	127.4(8)
C(2A)-P(2)	1.814(9)	C(1J)-C(1F)-P(3)	126.3(8)
C(2B)-C(2C)	1.413(12)	C(1G)-C(1F)-Fe	70.3(6)
C(2C)-C(2D)	1.375(13)	C(1J)-C(1F)-Fe	70.4(5)
C(2D)-C(2E)	1.349(13)	P(3)-C(1F)-Fe	122.7(5)
C(2E)-C(2F)	1.394(12)	C(1F)-C(1G)-C(1H)	108.9(9)
C(2G)-C(2H)	1.375(13)	C(1F)-C(1G)-Fe	69.2(5)
C(2G)-C(2L)	1.401(13)	C(1H)-C(1G)-Fe	70.9(5)
C(2G)-P(2)	1.805(10)	C(1I)-C(1H)-C(1G)	108.1(10)
C(2H)-C(2I)	1.355(14)	C(1I)-C(1H)-Fe	69.7(5)
C(2I)-C(2J)	1.374(18)	C(1G)-C(1H)-Fe	68.6(5)
C(2J)-C(2K)	1.365(18)	C(1H)-C(1I)-C(1J)	107.9(9)
C(2K)-C(2L)	1.399(14)	C(1H)-C(1I)-Fe	70.9(6)
C(3A)-C(3B)	1.374(11)	C(1J)-C(1I)-Fe	69.6(5)
C(3A)-C(3F)	1.398(11)	C(1I)-C(1J)-C(1F)	108.8(9)
C(3A)-P(3)	1.824(9)	C(1I)-C(1J)-Fe	70.1(6)
C(3B)-C(3C)	1.393(12)	C(1F)-C(1J)-Fe	68.7(5)
C(3C)-C(3D)	1.347(12)	C(2B)-C(2A)-C(2F)	119.2(8)
C(3D)-C(3E)	1.352(13)	C(2B)-C(2A)-P(2)	119.8(7)
C(3E)-C(3F)	1.378(13)	C(2F)-C(2A)-P(2)	120.8(7)
C(3G)-C(3L)	1.361(13)	C(2A)-C(2B)-C(2C)	120.7(9)
C(3G)-C(3H)	1.366(12)	C(2D)-C(2C)-C(2B)	118.4(10)
C(3G)-P(3)	1.813(10)	C(2E)-C(2D)-C(2C)	121.3(10)
C(3H)-C(3I)	1.377(14)	C(2D)-C(2E)-C(2F)	121.2(10)
C(3I)-C(3J)	1.313(16)	C(2A)-C(2F)-C(2E)	119.2(10)
C(3J)-C(3K)	1.388(17)	C(2H)-C(2G)-C(2L)	117.7(10)
C(3K)-C(3L)	1.371(17)	C(2H)-C(2G)-P(2)	123.7(9)
C(4A)-N(4)	1.362(10)	C(2L)-C(2G)-P(2)	118.6(8)
C(4A)-C(4B)	1.385(11)	C(2I)-C(2H)-C(2G)	122.1(12)
C(4A)-S(4)	1.710(9)	C(2H)-C(2I)-C(2J)	119.1(14)
C(4B)-C(4C)	1.354(12)	C(2K)-C(2J)-C(2I)	122.2(14)
C(4C)-C(4D)	1.377(13)	C(2J)-C(2K)-C(2L)	117.7(14)
C(4D)-C(4E)	1.355(12)	C(2G)-C(2L)-C(2K)	121.0(12)
C(4E)-N(4)	1.359(11)	C(3B)-C(3A)-C(3F)	117.8(9)
N(4)-O(4)	1.335(8)	C(3B)-C(3A)-P(3)	119.4(6)
O(4)-Pd	2.059(6)	C(3F)-C(3A)-P(3)	122.6(8)
P(2)-Pd	2.240(3)	C(3A)-C(3B)-C(3C)	121.0(9)
P(3)-Pd	2.335(2)	C(3D)-C(3C)-C(3B)	120.2(10)
S(4)-Pd	2.293(2)	C(3C)-C(3D)-C(3E)	119.7(11)
F(41)-P(4)	1.547(8)	C(3D)-C(3E)-C(3F)	121.6(9)
F(42)-P(4)	1.542(8)	C(3E)-C(3F)-C(3A)	119.6(10)
F(43)-P(4)	1.544(8)	C(3L)-C(3G)-C(3H)	117.7(10)

C(3L)-C(3G)-P(3)	119.7(8)	C(1G)-Fe-C(1E)	112.7(4)
C(3H)-C(3G)-P(3)	122.6(9)	C(1D)-Fe-C(1E)	39.6(3)
C(3G)-C(3H)-C(3I)	120.7(12)	C(1C)-Fe-C(1E)	67.3(4)
C(3J)-C(3I)-C(3H)	121.6(13)	C(1F)-Fe-C(1J)	41.0(3)
C(3I)-C(3J)-C(3K)	119.1(13)	C(1A)-Fe-C(1J)	138.8(4)
C(3L)-C(3K)-C(3J)	119.5(14)	C(1B)-Fe-C(1J)	112.3(4)
C(3G)-C(3L)-C(3K)	121.4(12)	C(1G)-Fe-C(1J)	67.3(4)
N(4)-C(4A)-C(4B)	116.2(9)	C(1D)-Fe-C(1J)	140.0(4)
N(4)-C(4A)-S(4)	118.9(7)	C(1C)-Fe-C(1J)	112.7(4)
C(4B)-C(4A)-S(4)	124.9(7)	C(1E)-Fe-C(1J)	179.3(4)
C(4C)-C(4B)-C(4A)	122.9(9)	C(1F)-Fe-C(1I)	68.9(4)
C(4B)-C(4C)-C(4D)	119.5(9)	C(1A)-Fe-C(1I)	177.3(4)
C(4E)-C(4D)-C(4C)	118.0(10)	C(1B)-Fe-C(1I)	140.6(4)
N(4)-C(4E)-C(4D)	122.1(9)	C(1G)-Fe-C(1I)	67.6(4)
O(4)-N(4)-C(4E)	116.2(7)	C(1D)-Fe-C(1I)	113.2(4)
O(4)-N(4)-C(4A)	122.4(8)	C(1C)-Fe-C(1I)	113.5(4)
C(4E)-N(4)-C(4A)	121.2(8)	C(1E)-Fe-C(1I)	139.0(4)
N(4)-O(4)-Pd	115.7(5)	C(1J)-Fe-C(1I)	40.3(3)
C(1A)-P(2)-C(2A)	104.2(4)	C(1F)-Fe-C(1H)	68.3(4)
C(1A)-P(2)-C(2G)	108.0(5)	C(1A)-Fe-C(1H)	138.7(4)
C(2A)-P(2)-C(2G)	104.2(4)	C(1B)-Fe-C(1H)	178.5(4)
C(1A)-P(2)-Pd	114.7(3)	C(1G)-Fe-C(1H)	40.5(3)
C(2A)-P(2)-Pd	112.2(3)	C(1D)-Fe-C(1H)	114.1(4)
C(2G)-P(2)-Pd	112.6(4)	C(1C)-Fe-C(1H)	141.0(4)
C(1F)-P(3)-C(3G)	103.3(4)	C(1E)-Fe-C(1H)	112.8(5)
C(1F)-P(3)-C(3A)	103.3(5)	C(1J)-Fe-C(1H)	66.8(4)
C(3G)-P(3)-C(3A)	107.9(5)	C(1I)-Fe-C(1H)	39.3(4)
C(1F)-P(3)-Pd	123.9(3)	O(4)-Pd-P(2)	174.86(19)
C(3G)-P(3)-Pd	112.2(4)	O(4)-Pd-S(4)	84.38(17)
C(3A)-P(3)-Pd	105.1(3)	P(2)-Pd-S(4)	91.73(9)
C(4A)-S(4)-Pd	98.1(3)	O(4)-Pd-P(3)	87.02(17)
C(1F)-Fe-C(1A)	108.9(4)	P(2)-Pd-P(3)	97.03(9)
C(1F)-Fe-C(1B)	110.2(4)	S(4)-Pd-P(3)	170.86(10)
C(1A)-Fe-C(1B)	41.3(3)	F(44)-P(4)-F(41)	88.1(6)
C(1F)-Fe-C(1G)	40.5(3)	F(44)-P(4)-F(45)	93.2(6)
C(1A)-Fe-C(1G)	109.8(4)	F(41)-P(4)-F(45)	88.7(5)
C(1B)-Fe-C(1G)	138.3(4)	F(44)-P(4)-F(43)	94.1(6)
C(1F)-Fe-C(1D)	177.5(4)	F(41)-P(4)-F(43)	177.6(5)
C(1A)-Fe-C(1D)	68.9(4)	F(45)-P(4)-F(43)	90.4(5)
C(1B)-Fe-C(1D)	67.4(4)	F(44)-P(4)-F(42)	176.6(7)
C(1G)-Fe-C(1D)	141.1(4)	F(41)-P(4)-F(42)	88.7(5)
C(1F)-Fe-C(1C)	138.6(4)	F(45)-P(4)-F(42)	88.0(5)
C(1A)-Fe-C(1C)	69.1(4)	F(43)-P(4)-F(42)	89.1(5)
C(1B)-Fe-C(1C)	40.2(3)	F(44)-P(4)-F(46)	88.5(6)
C(1G)-Fe-C(1C)	178.5(4)	F(41)-P(4)-F(46)	92.1(5)
C(1D)-Fe-C(1C)	39.8(4)	F(45)-P(4)-F(46)	178.2(6)
C(1F)-Fe-C(1E)	139.4(4)	F(43)-P(4)-F(46)	88.8(5)
C(1A)-Fe-C(1E)	41.8(3)	F(42)-P(4)-F(46)	90.4(5)
C(1B)-Fe-C(1E)	68.2(4)		

Table S4b. Full bond lengths [Å] and angles [°] for [Pt(mpo)(dppf)]PF_6.

C(1A)-C(1B)	1.418(7)	F(44)-P(4)	1.510(6)
C(1A)-C(1E)	1.426(8)	F(45)-P(4)	1.537(5)
C(1A)-P(2)	1.794(6)	F(46)-P(4)	1.560(5)
C(1A)-Fe	2.014(6)		
C(1B)-C(1C)	1.417(9)	C(1B)-C(1A)-C(1E)	106.9(5)
C(1B)-Fe	2.016(6)	C(1B)-C(1A)-P(2)	123.8(5)
C(1C)-C(1D)	1.400(9)	C(1E)-C(1A)-P(2)	129.2(5)
C(1C)-Fe	2.052(7)	C(1B)-C(1A)-Fe	69.5(3)
C(1D)-C(1E)	1.417(9)	C(1E)-C(1A)-Fe	70.5(4)
C(1D)-Fe	2.048(7)	P(2)-C(1A)-Fe	122.0(3)
C(1E)-Fe	2.042(6)	C(1A)-C(1B)-C(1C)	108.9(6)
C(1F)-C(1J)	1.431(8)	C(1A)-C(1B)-Fe	69.3(4)
C(1F)-C(1G)	1.442(8)	C(1C)-C(1B)-Fe	71.0(4)
C(1F)-P(3)	1.798(6)	C(1D)-C(1C)-C(1B)	107.6(6)
C(1F)-Fe	2.020(6)	C(1D)-C(1C)-Fe	69.9(4)
C(1G)-C(1H)	1.413(9)	C(1B)-C(1C)-Fe	68.3(4)
C(1G)-Fe	2.030(7)	C(1C)-C(1D)-C(1E)	108.8(6)
C(1H)-C(1I)	1.417(9)	C(1C)-C(1D)-Fe	70.2(4)
C(1H)-Fe	2.058(7)	C(1E)-C(1D)-Fe	69.5(4)
C(1I)-C(1J)	1.422(9)	C(1A)-C(1E)-C(1D)	107.9(6)
C(1I)-Fe	2.079(6)	C(1A)-C(1E)-Fe	68.4(3)
C(1J)-Fe	2.039(7)	C(1D)-C(1E)-Fe	70.0(4)
C(2A)-C(2F)	1.391(9)	C(1J)-C(1F)-C(1G)	106.9(6)
C(2A)-C(2B)	1.392(8)	C(1J)-C(1F)-P(3)	125.2(5)
C(2A)-P(2)	1.821(6)	C(1G)-C(1F)-P(3)	127.9(5)
C(2B)-C(2C)	1.377(9)	C(1J)-C(1F)-Fe	70.1(4)
C(2C)-C(2D)	1.366(10)	C(1G)-C(1F)-Fe	69.5(4)
C(2D)-C(2E)	1.399(9)	P(3)-C(1F)-Fe	123.2(3)
C(2E)-C(2F)	1.368(9)	C(1H)-C(1G)-C(1F)	108.3(6)
C(2G)-C(2H)	1.373(9)	C(1H)-C(1G)-Fe	70.9(4)
C(2G)-C(2L)	1.394(9)	C(1F)-C(1G)-Fe	68.8(4)
C(2G)-P(2)	1.808(6)	C(1I)-C(1H)-C(1G)	108.2(6)
C(2H)-C(2I)	1.389(11)	C(1I)-C(1H)-Fe	70.7(4)
C(2I)-C(2J)	1.365(13)	C(1G)-C(1H)-Fe	68.7(4)
C(2J)-C(2K)	1.370(14)	C(1H)-C(1I)-C(1J)	108.4(6)
C(2K)-C(2L)	1.381(11)	C(1H)-C(1I)-Fe	69.2(4)
C(3A)-C(3B)	1.377(9)	C(1J)-C(1I)-Fe	68.3(4)
C(3A)-C(3F)	1.405(8)	C(1I)-C(1J)-C(1F)	108.1(6)
C(3A)-P(3)	1.819(7)	C(1I)-C(1J)-Fe	71.3(4)
C(3B)-C(3C)	1.369(8)	C(1F)-C(1J)-Fe	68.6(3)
C(3C)-C(3D)	1.362(9)	C(2F)-C(2A)-C(2B)	119.0(6)
C(3D)-C(3E)	1.345(11)	C(2F)-C(2A)-P(2)	120.2(5)
C(3E)-C(3F)	1.392(10)	C(2B)-C(2A)-P(2)	120.4(5)
C(3G)-C(3H)	1.359(11)	C(2C)-C(2B)-C(2A)	119.3(7)
C(3G)-C(3L)	1.370(10)	C(2D)-C(2C)-C(2B)	121.9(7)
C(3G)-P(3)	1.820(8)	C(2C)-C(2D)-C(2E)	118.9(7)
C(3H)-C(3I)	1.404(12)	C(2F)-C(2E)-C(2D)	119.8(7)
C(3I)-C(3J)	1.320(12)	C(2E)-C(2F)-C(2A)	121.0(7)
C(3J)-C(3K)	1.368(14)	C(2H)-C(2G)-C(2L)	119.2(7)
C(3K)-C(3L)	1.381(12)	C(2H)-C(2G)-P(2)	121.6(6)
C(4A)-N(4)	1.363(7)	C(2L)-C(2G)-P(2)	119.3(5)
C(4A)-C(4B)	1.396(8)	C(2G)-C(2H)-C(2I)	120.7(9)
C(4A)-S(4)	1.715(6)	C(2J)-C(2I)-C(2H)	118.9(9)
C(4B)-C(4C)	1.354(9)	C(2I)-C(2J)-C(2K)	121.6(9)
C(4C)-C(4D)	1.375(9)	C(2L)-C(2K)-C(2J)	119.3(10)
C(4D)-C(4E)	1.349(9)	C(2K)-C(2L)-C(2G)	120.1(8)
C(4E)-N(4)	1.355(7)	C(3B)-C(3A)-C(3F)	117.4(6)
N(4)-O(4)	1.342(6)	C(3B)-C(3A)-P(3)	120.1(5)
O(4)-Pt	2.071(4)	C(3F)-C(3A)-P(3)	122.4(6)
P(2)-Pt	2.2388(15)	C(3A)-C(3B)-C(3C)	121.6(6)
P(3)-Pt	2.3159(17)	C(3B)-C(3C)-C(3D)	121.1(8)
S(4)-Pt	2.3026(17)	C(3E)-C(3D)-C(3C)	118.5(8)
F(41)-P(4)	1.568(6)	C(3D)-C(3E)-C(3F)	122.5(7)
F(42)-P(4)	1.557(6)	C(3E)-C(3F)-C(3A)	118.9(8)
F(43)-P(4)	1.545(5)	C(3H)-C(3G)-C(3L)	117.4(8)

C(3H)-C(3G)-P(3)	122.0(6)
C(3L)-C(3G)-P(3)	120.3(6)
C(3G)-C(3H)-C(3I)	121.3(9)
C(3J)-C(3I)-C(3H)	119.9(10)
C(3I)-C(3J)-C(3K)	120.3(10)
C(3J)-C(3K)-C(3L)	119.6(10)
C(3G)-C(3L)-C(3K)	121.2(9)
N(4)-C(4A)-C(4B)	116.5(6)
N(4)-C(4A)-S(4)	119.7(5)
C(4B)-C(4A)-S(4)	123.8(5)
C(4C)-C(4B)-C(4A)	121.5(6)
C(4B)-C(4C)-C(4D)	120.0(7)
C(4E)-C(4D)-C(4C)	119.0(7)
N(4)-C(4E)-C(4D)	121.0(7)
O(4)-N(4)-C(4A)	121.8(5)
O(4)-N(4)-C(4E)	116.1(5)
C(4A)-N(4)-C(4E)	122.0(6)
N(4)-O(4)-Pt	116.0(3)
C(1A)-P(2)-C(2G)	107.5(3)
C(1A)-P(2)-C(2A)	105.0(3)
C(2G)-P(2)-C(2A)	103.9(3)
C(1A)-P(2)-Pt	114.63(19)
C(2G)-P(2)-Pt	113.0(2)
C(2A)-P(2)-Pt	111.9(2)
C(1F)-P(3)-C(3A)	102.8(3)
C(1F)-P(3)-C(3G)	102.9(3)
C(3A)-P(3)-C(3G)	108.0(3)
C(1F)-P(3)-Pt	123.3(2)
C(3A)-P(3)-Pt	106.6(2)
C(3G)-P(3)-Pt	112.2(2)
C(4A)-S(4)-Pt	97.8(2)
C(1A)-Fe-C(1F)	109.3(2)
C(1A)-Fe-C(1B)	41.2(2)
C(1F)-Fe-C(1B)	110.0(3)
C(1A)-Fe-C(1G)	109.8(3)
C(1F)-Fe-C(1G)	41.7(2)
C(1B)-Fe-C(1G)	138.6(3)
C(1A)-Fe-C(1E)	41.2(2)
C(1F)-Fe-C(1E)	138.7(3)
C(1B)-Fe-C(1E)	68.5(3)
C(1G)-Fe-C(1E)	111.0(3)
C(1A)-Fe-C(1C)	69.1(3)
C(1F)-Fe-C(1C)	138.7(3)
C(1B)-Fe-C(1C)	40.8(2)
C(1G)-Fe-C(1C)	178.9(3)
C(1E)-Fe-C(1C)	68.1(3)
C(1A)-Fe-C(1J)	138.6(3)
C(1F)-Fe-C(1J)	41.3(2)
C(1B)-Fe-C(1J)	111.3(3)
C(1G)-Fe-C(1J)	69.1(3)
C(1E)-Fe-C(1J)	179.8(3)
C(1C)-Fe-C(1J)	111.9(3)
C(1A)-Fe-C(1D)	68.9(3)
C(1F)-Fe-C(1D)	177.9(3)
C(1B)-Fe-C(1D)	68.0(3)
C(1G)-Fe-C(1D)	139.6(3)
C(1E)-Fe-C(1D)	40.5(2)
C(1C)-Fe-C(1D)	39.9(3)
C(1J)-Fe-C(1D)	139.5(3)
C(1A)-Fe-C(1H)	138.5(3)
C(1F)-Fe-C(1H)	69.1(3)
C(1B)-Fe-C(1H)	179.0(3)
C(1G)-Fe-C(1H)	40.4(2)
C(1E)-Fe-C(1H)	111.8(3)
C(1C)-Fe-C(1H)	140.2(3)
C(1J)-Fe-C(1H)	68.4(3)
C(1D)-Fe-C(1H)	112.9(3)
C(1A)-Fe-C(1I)	177.6(3)
C(1F)-Fe-C(1I)	68.6(3)
C(1B)-Fe-C(1I)	140.2(3)
C(1G)-Fe-C(1I)	67.8(3)
C(1E)-Fe-C(1I)	139.8(3)
C(1C)-Fe-C(1I)	113.2(3)
C(1J)-Fe-C(1I)	40.4(2)
C(1D)-Fe-C(1I)	113.2(3)
C(1H)-Fe-C(1I)	40.0(2)
O(4)-Pt-P(2)	175.51(12)
O(4)-Pt-S(4)	84.35(12)
P(2)-Pt-S(4)	92.42(6)
O(4)-Pt-P(3)	85.72(12)
P(2)-Pt-P(3)	97.68(6)
S(4)-Pt-P(3)	169.51(6)
F(44)-P(4)-F(45)	93.9(4)
F(44)-P(4)-F(43)	92.9(5)
F(45)-P(4)-F(43)	90.8(3)
F(44)-P(4)-F(42)	176.1(5)
F(45)-P(4)-F(42)	88.8(4)
F(43)-P(4)-F(42)	89.8(4)
F(44)-P(4)-F(41)	90.2(5)
F(45)-P(4)-F(41)	89.2(3)
F(43)-P(4)-F(41)	176.9(4)
F(42)-P(4)-F(41)	87.1(4)
F(44)-P(4)-F(46)	88.9(4)
F(45)-P(4)-F(46)	177.0(4)
F(43)-P(4)-F(46)	88.1(3)
F(42)-P(4)-F(46)	88.4(4)
F(41)-P(4)-F(46)	91.8(4)

Table S5a. Anisotropic displacement parameters ($Å^2$ x 10^3) for [Pd(mpo)(dppf)]PF_6. The anisotropicdisplacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	37(6)	52(7)	38(5)	-2(5)	17(4)	1(5)
C(1B)	44(6)	44(7)	41(5)	4(5)	9(5)	2(5)
C(1C)	62(7)	42(7)	55(6)	-5(5)	2(6)	22(5)
C(1D)	60(7)	35(7)	75(7)	0(6)	24(6)	-5(5)
C(1E)	55(7)	53(7)	58(6)	6(6)	20(6)	2(6)
C(1F)	48(6)	37(6)	56(6)	8(5)	4(5)	-1(5)
C(1G)	40(6)	48(7)	60(6)	0(5)	-2(5)	2(5)
C(1H)	35(6)	46(7)	99(9)	-4(6)	-7(6)	-2(5)
C(1I)	59(7)	44(7)	56(6)	-11(5)	2(6)	9(6)
C(1J)	43(6)	29(6)	59(6)	5(5)	10(5)	-3(5)
C(2A)	35(5)	37(6)	49(5)	-1(5)	16(5)	-5(4)
C(2B)	50(6)	56(7)	44(5)	0(6)	13(5)	-1(5)
C(2C)	63(8)	78(9)	64(7)	-13(7)	24(6)	-2(7)
C(2D)	78(9)	55(8)	53(6)	-2(6)	18(7)	-17(7)
C(2E)	70(8)	47(8)	71(7)	7(6)	18(7)	-9(6)
C(2F)	45(6)	43(7)	58(6)	-1(5)	19(5)	-10(5)
C(2G)	36(6)	70(8)	50(6)	-23(6)	9(5)	-2(5)
C(2H)	46(6)	50(7)	89(8)	-28(6)	30(6)	-2(5)
C(2I)	50(8)	83(11)	130(12)	-56(9)	32(8)	-8(7)
C(2J)	44(8)	94(13)	189(18)	-63(12)	20(10)	5(8)
C(2K)	67(9)	87(11)	121(12)	-32(9)	-1(9)	37(8)
C(2L)	54(7)	62(9)	98(9)	-15(7)	18(7)	12(6)
C(3A)	35(5)	66(7)	23(4)	0(5)	4(4)	-9(5)
C(3B)	50(6)	51(7)	46(5)	0(5)	19(5)	-3(5)
C(3C)	50(7)	87(9)	48(6)	-7(6)	15(6)	-3(6)
C(3D)	72(8)	77(9)	50(6)	4(6)	31(6)	0(7)
C(3E)	102(10)	87(10)	41(6)	1(6)	41(7)	-4(8)
C(3F)	69(8)	73(9)	41(6)	3(6)	8(6)	-1(6)
C(3G)	62(7)	50(8)	49(6)	13(6)	-16(5)	-7(6)
C(3H)	78(9)	57(9)	108(10)	8(8)	-33(8)	-17(7)
C(3I)	143(14)	62(11)	141(13)	34(10)	-65(11)	-6(10)
C(3J)	214(19)	42(10)	159(15)	24(10)	-102(14)	-2(11)
C(3K)	260(20)	66(12)	240(20)	31(13)	-180(20)	-41(13)
C(3L)	199(17)	43(9)	159(14)	42(9)	-128(13)	-34(10)
C(4A)	36(5)	44(6)	47(5)	-13(5)	7(5)	-3(4)
C(4B)	53(7)	62(8)	43(6)	-9(5)	3(5)	-17(6)
C(4C)	55(7)	46(7)	77(8)	0(6)	13(6)	-13(5)
C(4D)	63(7)	38(7)	87(8)	13(7)	19(7)	-16(6)
C(4E)	45(6)	58(7)	48(6)	19(5)	16(5)	-3(5)
N(4)	34(5)	53(6)	38(4)	8(4)	2(4)	2(4)
O(4)	45(4)	65(5)	45(4)	-12(3)	8(3)	-27(4)
P(2)	32(1)	38(2)	53(2)	-9(1)	12(1)	-2(1)
P(3)	45(2)	42(2)	43(1)	0(1)	1(1)	-4(1)
S(4)	51(2)	52(2)	45(1)	-6(1)	11(1)	-12(1)
Fe	39(1)	38(1)	56(1)	-5(1)	13(1)	-1(1)
Pd	38(1)	39(1)	43(1)	-4(1)	7(1)	-4(1)
F(41)	115(7)	171(9)	179(9)	1(7)	48(7)	-66(6)
F(42)	98(7)	224(10)	107(6)	16(6)	-2(5)	12(7)
F(43)	243(11)	141(8)	113(6)	-30(5)	112(7)	-98(8)
F(44)	123(8)	345(16)	140(9)	84(9)	-13(7)	90(9)
F(45)	240(11)	107(7)	207(9)	-20(6)	185(9)	13(7)
F(46)	136(8)	201(10)	148(8)	-102(7)	76(7)	-20(7)
P(4)	50(2)	96(3)	62(2)	-8(2)	18(2)	1(2)

Table S5b. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Pt(mpo)(dppf)]PF_6$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	34(4)	42(4)	45(4)	-2(3)	15(3)	2(3)
C(1B)	34(4)	54(5)	49(4)	0(3)	11(3)	5(3)
C(1C)	60(5)	42(4)	68(5)	4(4)	16(4)	15(4)
C(1D)	64(5)	38(4)	70(5)	1(4)	17(4)	-12(4)
C(1E)	53(5)	55(5)	63(4)	-7(4)	24(4)	-9(4)
C(1F)	47(4)	34(4)	43(4)	-4(3)	2(3)	-2(3)
C(1G)	40(4)	48(4)	70(5)	-13(4)	3(4)	1(3)
C(1H)	30(4)	56(5)	83(5)	-16(4)	4(4)	-16(4)
C(1I)	67(5)	46(4)	59(4)	-20(4)	11(4)	-4(4)
C(1J)	44(4)	44(4)	65(4)	-4(4)	5(4)	1(3)
C(2A)	36(4)	42(4)	47(4)	6(3)	14(3)	-4(3)
C(2B)	45(4)	60(5)	47(4)	-13(4)	11(3)	2(4)
C(2C)	70(6)	73(6)	54(5)	-11(4)	17(5)	-8(5)
C(2D)	69(6)	74(6)	44(4)	1(4)	7(4)	-24(5)
C(2E)	54(5)	57(5)	64(5)	17(4)	9(4)	-11(4)
C(2F)	48(4)	51(4)	47(4)	-2(3)	9(4)	-2(4)
C(2G)	33(4)	44(4)	67(5)	-20(4)	7(4)	7(3)
C(2H)	43(5)	70(6)	103(6)	-35(5)	29(5)	-8(4)
C(2I)	44(6)	85(7)	162(10)	-73(7)	45(7)	-19(5)
C(2J)	34(5)	105(9)	198(13)	-79(9)	3(7)	19(6)
C(2K)	60(6)	80(7)	134(9)	-36(6)	-9(6)	31(6)
C(2L)	52(5)	46(5)	89(6)	-18(4)	10(5)	12(4)
C(3A)	56(5)	49(4)	37(4)	-2(3)	10(4)	-14(4)
C(3B)	58(5)	65(5)	40(4)	-5(3)	17(4)	-12(4)
C(3C)	55(5)	72(5)	57(5)	-10(4)	24(4)	-5(4)
C(3D)	82(7)	85(6)	66(6)	-10(5)	35(6)	-14(5)
C(3E)	85(7)	108(7)	51(5)	8(5)	28(5)	-14(6)
C(3F)	71(6)	97(7)	43(4)	15(4)	-1(4)	-4(5)
C(3G)	75(6)	36(4)	74(5)	1(4)	-20(5)	-3(4)
C(3H)	106(8)	57(5)	99(7)	7(5)	-40(6)	-4(6)
C(3I)	124(10)	76(8)	155(10)	17(7)	-86(8)	-7(7)
C(3J)	208(15)	50(7)	182(12)	19(7)	-128(10)	11(8)
C(3K)	255(18)	41(6)	194(13)	17(7)	-142(12)	-17(8)
C(3L)	165(11)	49(6)	112(7)	6(5)	-91(7)	-5(6)
C(4A)	38(4)	38(4)	46(4)	-5(3)	7(3)	9(3)
C(4B)	52(5)	51(5)	59(4)	-7(4)	10(4)	-12(4)
C(4C)	52(5)	55(5)	81(6)	-9(4)	0(4)	-21(4)
C(4D)	62(5)	49(5)	81(6)	14(4)	19(5)	-9(4)
C(4E)	53(5)	47(4)	61(5)	11(4)	19(4)	-3(4)
N(4)	36(3)	31(3)	50(3)	-2(3)	4(3)	-3(2)
O(4)	52(3)	52(3)	43(3)	-4(2)	5(2)	-21(2)
P(2)	27(1)	38(1)	50(1)	-6(1)	10(1)	-2(1)
P(3)	44(1)	38(1)	46(1)	-2(1)	-4(1)	-2(1)
S(4)	46(1)	46(1)	46(1)	-6(1)	11(1)	-10(1)
Fe	36(1)	37(1)	62(1)	-7(1)	12(1)	-1(1)
Pt	33(1)	37(1)	43(1)	-3(1)	4(1)	-3(1)
F(41)	90(5)	153(6)	186(6)	13(5)	37(5)	-35(4)
F(42)	93(5)	216(7)	112(4)	29(5)	5(4)	14(5)
F(43)	233(8)	143(5)	133(5)	-34(4)	116(6)	-99(5)
F(44)	123(6)	314(10)	142(6)	83(7)	-11(5)	89(7)
F(45)	228(8)	114(5)	177(6)	-12(4)	158(6)	17(5)
F(46)	108(5)	209(7)	129(5)	-91(5)	41(4)	-16(5)
P(4)	48(1)	91(2)	62(1)	-4(1)	18(1)	3(1)

Table S6a. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for[Pd(mpo)(dppf)]PF_6.

Aom	x	y	z	U(eq)
H(1B)	3409	7324	1647	52
H(1C)	4046	8395	1875	67
H(1D)	6235	8540	1576	67
H(1E)	6955	7579	1121	65
H(1G)	7842	6696	2939	63
H(1H)	8600	7757	3259	78
H(1I)	6823	8295	3692	67
H(1J)	5024	7555	3731	54
H(2B)	5704	5637	-57	60
H(2C)	4693	5471	-1435	80
H(2D)	2907	6068	-2100	75
H(2E)	2219	6839	-1465	75
H(2F)	3145	6995	-95	57
H(2H)	7528	6708	588	71
H(2I)	9750	6457	963	104
H(2J)	10525	5752	1950	134
H(2K)	9077	5236	2499	117
H(2L)	6804	5508	2124	86
H(3B)	2388	6650	2438	57
H(3C)	636	6969	2925	74
H(3D)	853	6949	4271	76
H(3E)	2828	6655	5145	87
H(3F)	4628	6368	4697	75
H(3H)	7440	6267	4470	112
H(3I)	8715	5550	5287	164
H(3J)	8255	4575	5076	204
H(3K)	6460	4281	3998	289
H(3L)	5078	4997	3238	203
H(4B)	908	4466	104	66
H(4C)	-235	3838	708	73
H(4D)	270	3823	2104	76
H(4E)	1762	4512	2822	60

Table S6b. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [Pt(mpo)(dppf)]PF_6.

Atom	x	y	z	U(eq)
H(1B)	3393	7321	1623	55
H(1C)	4019	8402	1863	68
H(1D)	6227	8552	1583	69
H(1E)	6954	7577	1130	66
H(1G)	7842	6716	2903	66
H(1H)	8542	7779	3223	70
H(1I)	6783	8285	3730	70
H(1J)	4922	7550	3667	64
H(2B)	5652	5604	-62	62
H(2C)	4652	5458	-1405	79
H(2D)	2919	6052	-2103	77
H(2E)	2198	6842	-1445	71
H(2F)	3186	6996	-106	59
H(2H)	7461	6737	563	84
H(2I)	9723	6486	905	112
H(2J)	10531	5780	1874	142
H(2K)	9119	5277	2457	118
H(2L)	6869	5539	2137	77
H(3B)	2373	6682	2447	64
H(3C)	644	6956	2944	72
H(3D)	875	6928	4295	90
H(3E)	2845	6612	5137	96
H(3F)	4623	6309	4671	88
H(3H)	7310	6279	4472	121
H(3I)	8712	5571	5269	172
H(3J)	8315	4591	5026	220
H(3K)	6694	4287	3899	246
H(3L)	5276	4983	3117	162
H(4B)	862	4479	103	66
H(4C)	-192	3829	732	80
H(4D)	282	3843	2112	77
H(4E)	1772	4526	2826	64

Table S7. ^{13}C NMR chemical shift values (δ, in ppm) of the ligand and the complexes in DMSO-d_6.

Ligand	Carbon	Free Ligand	**[Pd(mpo)(dppf)](PF$_6$)**	**Δδ[a]**	**[Pt(mpo)(dppf)](PF$_6$)**	**Δδ[a]**
mpo	**1**	167.91	154.9	-13.01	151.8	-16.11
	2	132.32	127.5	-4.82	128.2	-4.12
	3	124.02	132.1	8.08	132.1	8.08
	4	114.66	120.1	5.44	120.7	6.04
	5	139.04	138.1	-0.94	139.1	0.06
dppf (Cp)	-	-	C-H$_a$ 78.01 C-H$_b$ 75.85 C-H$_c$ 74.48 C-H$_d$ 74.48 C-P 78.13	-	C-H$_a$ 76.89 C-H$_b$ 75.85 C-H$_c$ 75.39 C-H$_d$ 75.02 C-P *	-

[a] $\Delta\delta = (\delta_{complex} - \delta_{ligand})$

* not assigned