Supporting Information

A hybrid terpyridine-based bis(diphenylphosphino)amine ligand, terpy-$C_6H_4N(PPh_2)_2$: Synthesis, coordination chemistry and photoluminescence studies

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1. Materials and Physical Measurements

All experimental manipulations were performed under inert atmosphere of dry nitrogen or argon, using standard Schlenk line techniques. All the solvents were purified by conventional procedures and distilled prior to use. Other reagents were obtained from commercial sources and used as received without further purification. Metal reagents $[CpRu(PPh_3)_2Cl]$,[1] $[Pd(COD)Cl_2]$,[2] $[AuCl(SMe_2)]$[3] and 4′-(*p*-aminophenyl)terpyridine[4] were prepared according to published procedures. The ^1H and $^{31}P\{^1H\}$ NMR (δ in ppm) spectra were obtained from either Bruker Avance-400 MHz or Bruker Avance- 500 MHz spectrometer. The spectra were recorded in $CDCl_3$ (or DMSO-d_6) solutions with $CDCl_3$ (or DMSO-d_6) as an internal lock; TMS and 85% H_3PO_4 were used as internal and external standards for ^1H and $^{31}P\{^1H\}$ NMR, respectively. Positive values indicate downfield shifts. The UV-Vis and Fluorescence spectra were recorded at 298 K on Perkin-Elmer UV-Vis and fluorescence spectrometers, respectively, using a quartz cell (1 cm width). Mass spectra were recorded on BRUKER mass spectrometer using Electro-spray ionization mass spectrometry (ESI-MS) method. Microanalysis were carried out on a Carlo Erba (model 1106) elemental analyzer. Melting points of all compounds were determined on a Veego melting point apparatus and are uncorrected.

2. Experimental Section

Synthesis of 4′-{*p*-$(Ph_2P)_2NC_6H_4$}-2,2′:6′2′′-terpy (1)

A solution of chlorodiphenylphosphine (3.57 g, 2.9 mL 16.2 mmol) in dichloromethane (10 mL) was added dropwise to the suspension of 4′-(*p*-aminophenyl)-2,2′:6’,2′′-terpyridine (2.5 g, 7.30 mmol) and triethylamine (7.8 g, 77.1 mmol) in dichloromethane (40 mL) at 0 ˚C. The dark brown colored solution thus obtained was stirred at room temperature overnight. The reaction mixture was quenched with degassed water and the organic phase was separated, dried with sodium sulphate. The solvent was evaporated under reduced pressure and the residue obtained was washed with diethyl ether (3× 50 mL). The crude residue was passed through neutral alumina using dichloromethane as eluent to get colorless solid product. Analytically pure X-ray quality crystals of **1** were obtained by crystallizing from a 1:1 mixture of dichloromethane and acetonitrile. Yield: 48% (2.42 g) MP: 170-171 ˚C. $^{31}P\{^1H\}$ NMR ($CDCl_3$): 69.3 ppm (s). ^1H NMR ($CDCl_3$) δ: 6.74 (d, H7,7′, 2H, $^3J_{HH}$ = 8.5 Hz), 7.30-7.42 (m, ArH, H5,5′, 22H), 7.51 (d,

H8,8′, 2H, $^{3}J_{HH}$ = 8.5 Hz), 7.85 (td, H4,4″, 2H, $^{3}J_{HH}$ = 7.1 Hz, $^{4}J_{HH}$ = 1.8 Hz), 8.60 (s, H3′,5′, 2H), 8.63 (d, H3,3″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 8.69 (d, H6,6″, 2H, $^{3}J_{HH}$ = 4.0 Hz). ESI(MS): m/z = 693.23 $[M+H]^{+}$. Anal. Calcd. for $C_{45}H_{34}N_4P_2$: C, 78.00; H, 4.95; N, 8.09 %. Found: C, 78.14; H, 4.57; N, 8.07 %.

Synthesis of [(Ru(PPh$_3$)(Cp){4′-{*p*-(Ph$_2$P)$_2$NC$_6$H$_4$}-2,2′:6′2″-terpy}]Cl (2)

A toluene solution (5 mL) of [CpRu(PPh$_3$)$_2$Cl] (0.021g, 0.028 mmol) was added to a stirred solution **1** (0.020 g, 0.028 mmol) also in toluene (5 mL). The color of the reaction mixture changed from white to yellow. Further, reaction mixture was allowed to reflux for 4 h. The solvent was removed under vacuum and residue was washed with petroleum ether, resulting in the pure compound **2**. Crystals suitable for X-ray analysis were grown from the saturated solution of chloroform. Yield: 82 % (0.026 g). MP: 220 ˚C (dec.). $^{31}P\{^{1}H\}$ NMR ($CDCl_3$) δ: 44.2 (t, PPh_3, 1P) and 79.4 (d, PPh_2, 2P) ($^{2}J_{PP}$ = 32.5 Hz). ^{1}H NMR ($CDCl_3$) δ: 4.48 (s, C_5H_5, 5H) 6.60 (d, H7,7′, 2H, $^{3}J_{HH}$ = 8.6 Hz), 7.11-7.34 (m, ArH, H5,5″, 22H), 7.48 (d, H8,8′, 2H, $^{3}J_{HH}$ = 8.6 Hz), 7.59 (dt, H4,4″, 2H, $^{3}J_{HH}$ = 20.9, 6.6 Hz), 7.88 – 7.82(m, 15H), 8.54 (s, H3′,5′, 2H), 8.65 – 8.61 (br t, H3,3″, H6,6″, 4H). ESI(MS): m/z = 1121.26 $[M-Cl]^{+}$. Anal. Calcd. for $C_{68}H_{54}N_4P_3RuCl$: C, 70.61; H, 4.70; N, 4.84 %. Found: C, 70.77; H, 4.45; N, 4.65 %.

Synthesis of *cis*-[PdCl$_2${4′-{*p*-(Ph$_2$P)$_2$NC$_6$H$_4$}-2,2′:6′2″-terpy}] (3)

A solution of [Pd(COD)Cl_2] (0.012 g, 0.043 mmol) in toluene (5 mL) was added dropwise to the solution of **1** (0.030 g, 0.043 mmol) also in toluene (5 mL) and the reaction mixture was stirred for 5 h at ambient temperature. The solvent was removed under reduced pressure and the residue obtained was washed form petroleum ether to get analytically pure product **3** as an orange solid. Crystals of **3** suitable for single crystal X-ray diffraction were grown by the slow adding petroleum ether into the saturated solution of chloroform. Yield: 79 % (0.029 g). MP: 215-218 ˚C. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$) δ: 34.9 (s). ^{1}H NMR ($CDCl_3$) δ: 6.67 (d, H7,7′, 2H, $^{3}J_{HH}$ = 7.9 Hz), 7.36-7.62 (m, ArH, H5,5″, 22H), 7.66 (d, H8,8′, 2H, $^{3}J_{HH}$ = 7.9 Hz), 7.94 (t, H4,4″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 8.58 (s, H3′,5′, 2H), 8.65 (br t, H3,3″, H6,6″, 4H). ESI(MS): m/z = 830.15 $[M-Cl]^{+}$ Anal. Calcd. for $C_{45}H_{34}N_4P_2PdCl_2$: C, 62.12; H, 3.94; N, 6.44 %. Found: C, 62.01; H, 3.63; N, 6.25 %.

Synthesis of [(AuCl)$_2${4′-{*p*-(Ph$_2$P)$_2$NC$_6$H$_4$}-2,2′:6′2″-terpy}] (4)

A solution of [AuCl(SMe_2)] (0.025 g, 0.086 mmol) in dichloromethane (5 mL) was added dropwise to the solution of **1** (0.030 g, 0.043 mmol) also in dichloromethane (5 mL). The resulting solution was stirred at room temperature for 5 h, in the minimum exposure of light. During which its color changed from white to yellow. The solvent was evaporated under reduced pressure and residue was washed form petroleum ether (5 mL). Crystals of **4** suitable for single crystal X-ray diffraction were obtained from a 1:1 mixture of dichloromethane and toluene at 0 ^{o}C. Yield: 78 % (0.038 g). MP: 192-194 ˚C (dec.). $^{31}P\{^{1}H\}$ NMR ($CDCl_3$) δ: 88.3 (s). ^{1}H NMR ($CDCl_3$) δ: 6.40 (d, H7,7′, 2H, $^{3}J_{HH}$ = 8.5 Hz), 7.35-7.72 (m, ArH, H5,5″, H8,8′, 24H), 7.88 (td, H4,4″, 2H, $^{3}J_{HH}$ = 7.1 Hz, $^{4}J_{HH}$ = 1.8 Hz), 8.49 (s, H3′,5′, 2H), 8.63 (d, H3,3″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 8.67 (d, H6,6″, 2H, $^{3}J_{HH}$ = 4.0 Hz). ESI(MS): m/z = 1179.09 $[M+Na]^{+}$. Anal. Calcd. for $C_{45}H_{34}N_4P_2Au_2Cl_2$: C, 46.69; H, 2.96; N, 4.84 %. Found: C, 46.76; H, 2.86; N, 4.42 %.

Synthesis of [Au{4′-{*p*-$(Ph_2P)_2NC_6H_4$}-2,2′:6′2″-terpy}]$_2(OTf)_2$ (5)

To the solution of **4** (0.020 g, 0.017 mmol) in dichloromethane (10 mL) was added AgOTf (0.008 g, 0.034 mmol) and the reaction mixture was stirred for 1 h at room temperature. The AgCl precipitate formed was filtered through celite and the filtrate was added dropwise to the solution of **1** (0.011 g, 0.017 mmol). The yellow color reaction mixture was further stirred for 2 h and the solution was concentrated to 2 mL, added petroleum ether to afford yellow color precipitate. The precipitate was separated and dried under reduced pressure to get analytically pure product **5**. Yield: 80 % (0.028 g). MP: 148-150 ˚C. $^{31}P\{^{1}H\}$ NMR ($CDCl_3$) δ: 104.3 (s). ^{1}H NMR ($CDCl_3$) δ: 6.46 (d, H7,7′, 2H, $^{3}J_{HH}$ = 8.0 Hz), 7.36-7.67 (m, ArH, H5,5″, H8,8′, 24H), 8.02 (br s, H4,4″, 2H), 8.61 (s, H3′,5′, 2H), 8.74 (br s, H3,3″, 2H), 8.81 (br s, H6,6″, 2H). Anal. Calcd. for $C_{92}H_{68}N_8P_4Au_2S_2F_6O_6$: C, 53.19; H, 3.30; N, 5.39; S, 3.09 %. Found: C, 53.23; H, 3.66; N, 5.18; S, 3.19 %.

Synthesis of [$(AuCl)_2${4′-{*p*-$(Ph_2P)_2NC_6H_4$}-2,2′:6′2″-terpy}Zn](OTf)$_2$ (6)

It was prepared by using $Zn(OTf)_2$ (0.0115 g, 0.0318 mmol) in tetrahydrofuran (5 mL) and **4** (0.0736 g, 0.0636 mmol) in dichloromethane (5 mL).The turbid yellow color solution was stirred at room temperature for 5 h. The solvent was evaporated under reduced pressure and the residue obtained was dissolved in 5 mL of dichloromethane and diluted with 1 mL of petroleum ether to get analytically product of **6** as microcrystalline solid. Yield: 73 % (0.062 g). MP: 238-239 ˚C

(decomp). $^{31}P\{^{1}H\}$ NMR (DMSO-d_6) δ: 86.2 (s). ^{1}H NMR (DMSO-d_6) δ: 6.80 (d, H7,7″, 2H, $^{3}J_{HH}$ = 8.5 Hz), 7.39-7.80 (m, ArH, H5,5″, 22H), 7.82 (d, H6,6″, 2H, $^{3}J_{HH}$ = 8.0 Hz), 7.88 (d, H8,8″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 8.19 (t, H4,4″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 8.95 (d, H3,3″, 2H, $^{3}J_{HH}$ = 7.9 Hz), 9.11 (s, H3′,5′, 2H). Anal. Calcd for $C_{92}H_{68}N_8P_4Au_4Cl_4F_6O_6S_2Zn$: C, 41.25; H, 2.56; N, 4.18; S, 2.39 %. Found: C, 41.65; H, 2.56; N, 3.90; S, 2.34 %.

3. X-ray Crystallography.

A crystal of each of the compounds in the present work suitable for single-crystal X-ray diffraction studies was mounted in a cryoloop with a drop of paratone oil and placed in the cold nitrogen stream of the kryoflex attachment of the Bruker APEX CCD diffractometer for complex **1**, **2** and Rigaku Saturn724 diffractometer for complex **3** and **4**. Data were collected at 100 K using graphite-monochromated Mo-Kα radiation (λα = 0.71073 Å) with the ω-scan technique. The data were reduced by using Crystal Clear- SMExpert 2.1 b24 software. Crystal data and summary of data collection for compounds **1**, **2**, **3** and **4** are given in Table S1. The structures were solved by direct methods and refined by least-squares against F2 utilizing the software packages SHELXL-97/2013,[5] SIR-92[6] and WINGX.[7] All non-hydrogen atoms were refined anisotropically. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1501300 (**1**), 1501301 (**2**), 1501302 (**3**) and 1501303 (**4**).

4. **Table S1.** Crystallographic Data for Compounds **1**, **2**, **3** and **4**.

	1	**2**	**3**	**4**
Emp. formula	$C_{45}H_{34}N_4P_2{\cdot}CH_2Cl_2$	$C_{68}H_{54}N_4P_3RuCl{\cdot}5(CHCl_3)$	$C_{45}H_{34}Cl_2N_4P_2Pd{\cdot}2(CHCl_3)$	$C_{45}H_{34}Au_2Cl_2N_4P_2{\cdot}C_7H_8$
fw	777.63	1753.42	1108.74	1249.67
Cryst. Sys.	Monoclinic	Triclinic	monoclinic	Triclinic
space group	$P2_1/n$	P-1	C2/c	P-1
a, Å	15.467(2)	10.247(3)	14.826(11)	12.903(6)
b, Å	9.3663(12)	13.871(4)	18.064(10)	13.059(6)
c, Å	26.864(3)	27.160(8)	18.267(14)	16.715(6)
α, deg	90	96.116(4)	90	98.626(3)
β, deg	100.924(2)	101.187(4)	99.056(7)	92.793(3)
γ, deg	90	92.193(4)	90	97.092(4)
V, Å^3	3821.2(8)	3758.63	4831.7(6)	2757.0(2)
Z	4	2	4	2
$D_{calc,}$ g cm^{-3}	1.352	1.549	1.524	1.5053
μ(MoKa), mm^{-1}	0.294	0.887	0.931	5.505
F (000)	1616	1772	2232.0	1208.0
T (K)	100	100	150	150
2θ range, deg	2.3-28.4	2.2-26.3	4.4-50	4.3-50
Total no. reflns	115450	68342	15799	53561
No.of indep reflns	9448 [R_{int} = 0.106]	14677 [R_{int} = 0.104]	4246 [R_{int} = 0.1070]	9681 [R_{int} = 0.0474]
S	1.03	1.08	1.05	1.03
R_1	0.0660	0.0821	0.0527	0.0347
wR_2	0.1992	0.2059	0.1082	0.0875

5. References.

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6. NMR Spectra

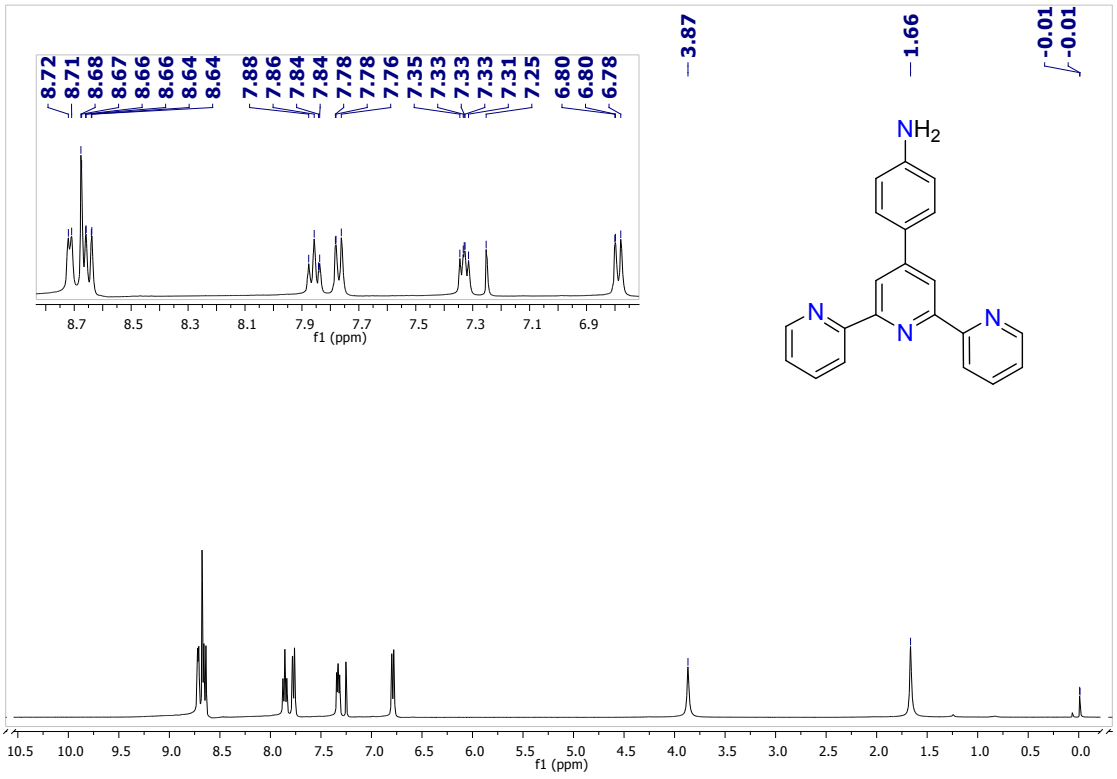

Figure S1.[1]H NMR spectrum of 4′-(*p*-aminophenyl)terpyridine in $CDCl_3$. Expanded view of aromatic region shown in inset.

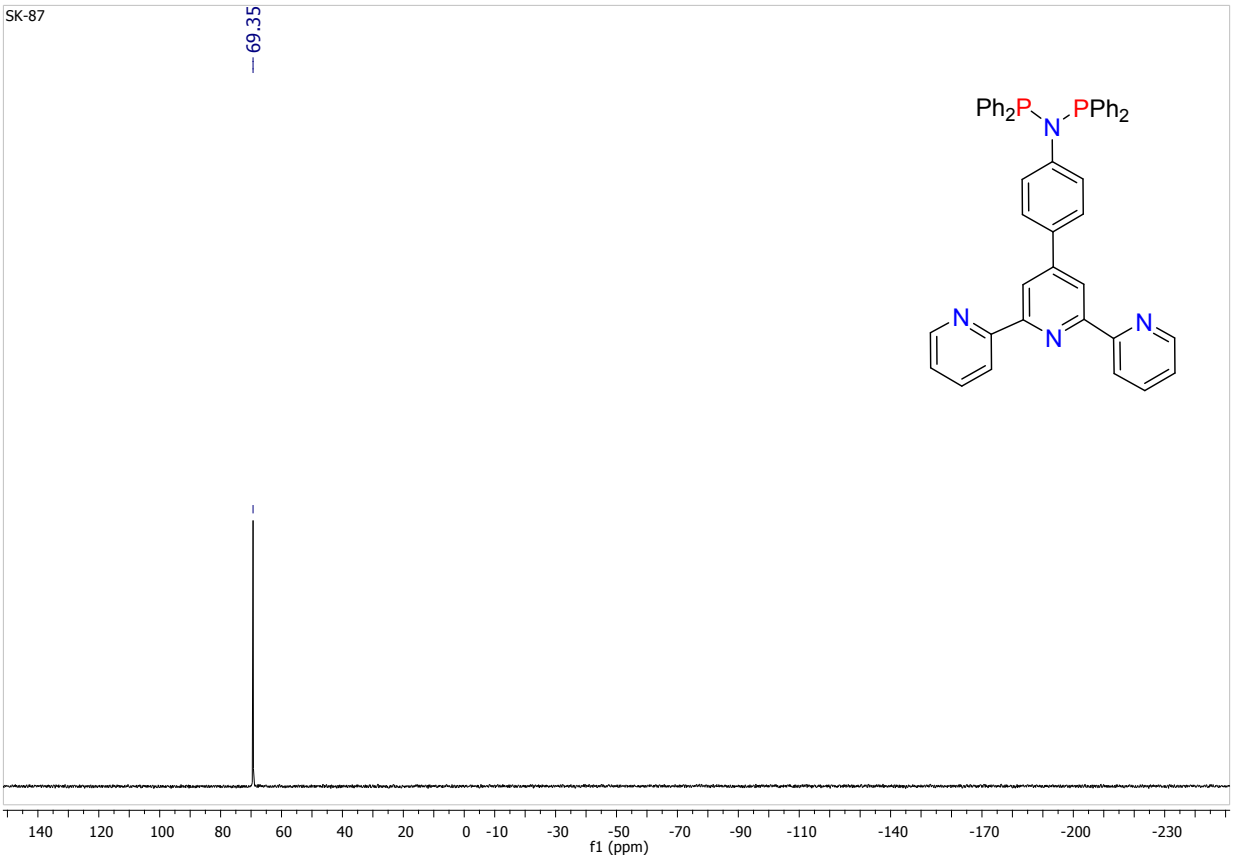

Figure S2.$^{31}P\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$.

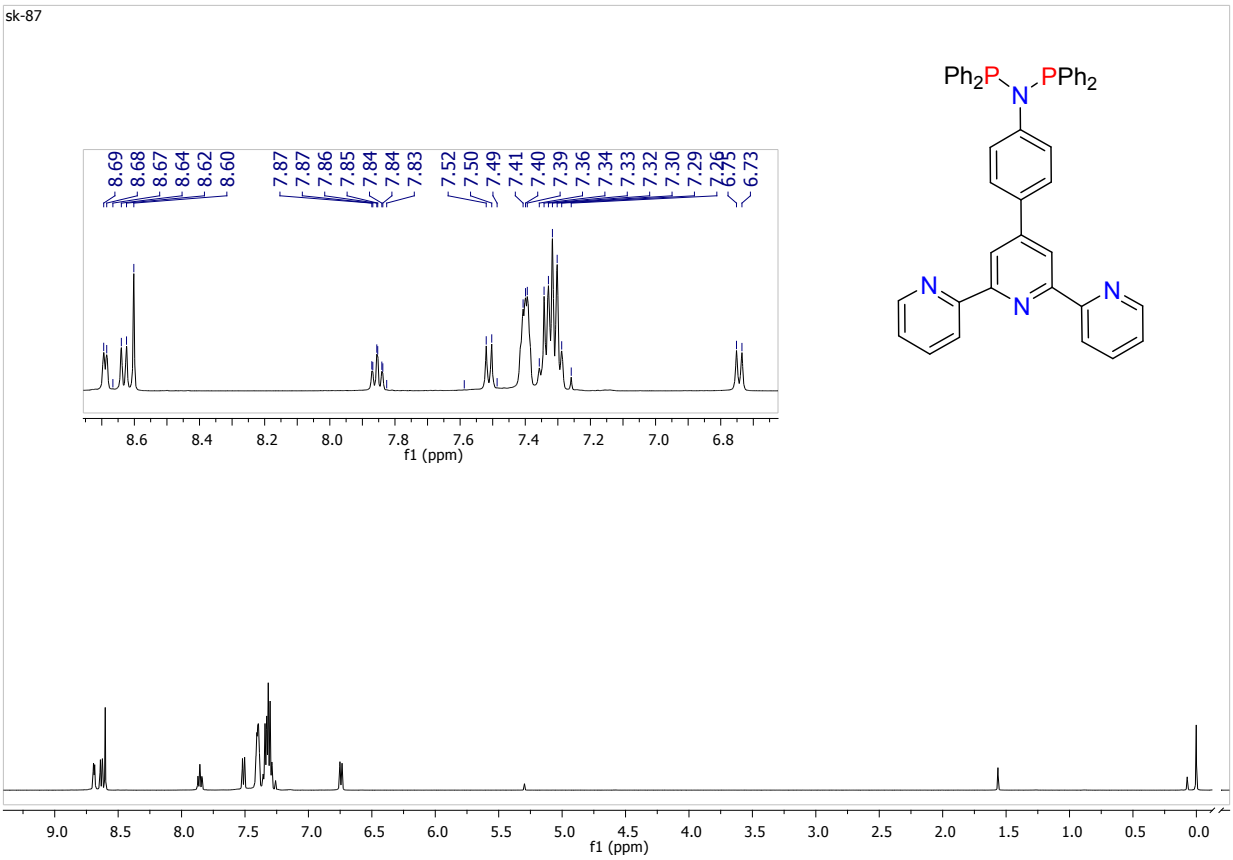

Figure S3.[1]H NMR spectrum of **1** in $CDCl_3$.

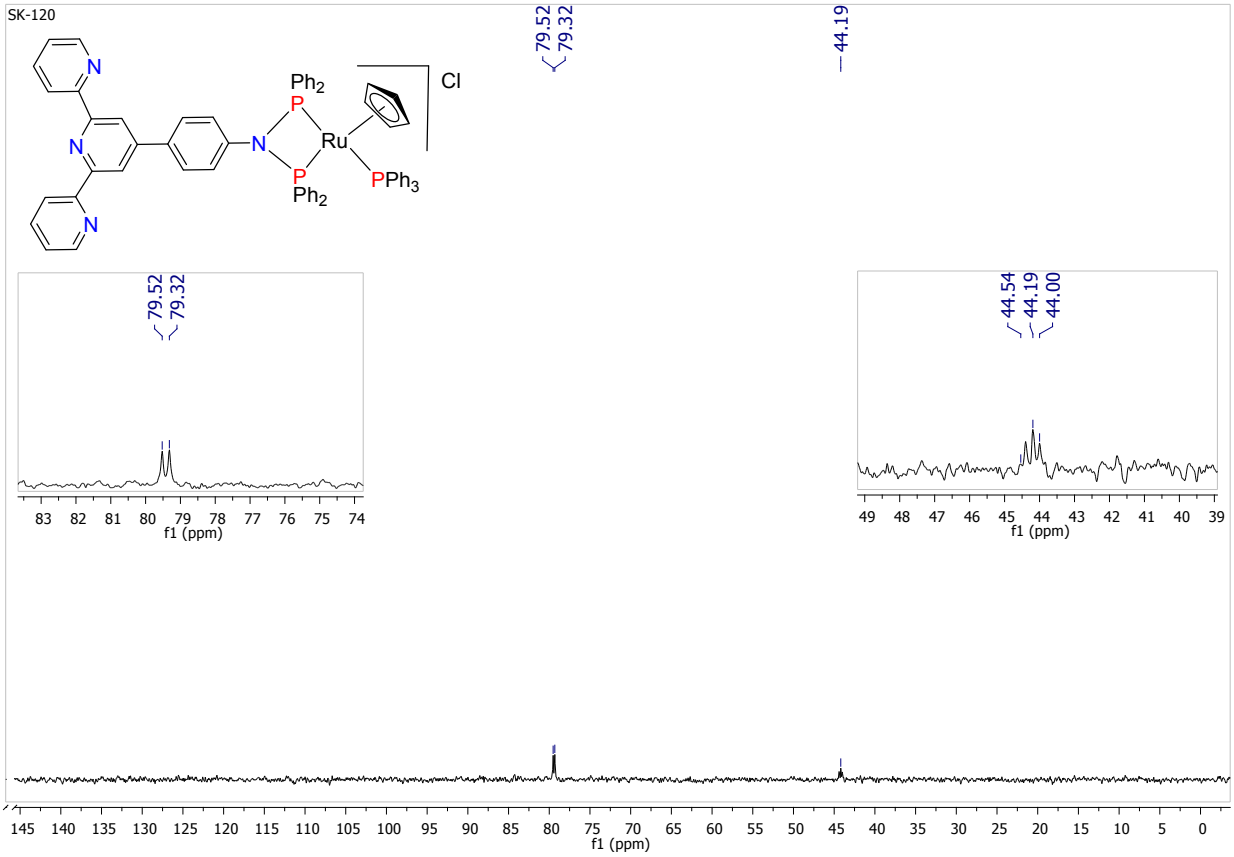

Figure S4.$^{31}P\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$. Expanded view of doublet (PPh_2) and triplet (PPh_3) peaks are shown in inset.

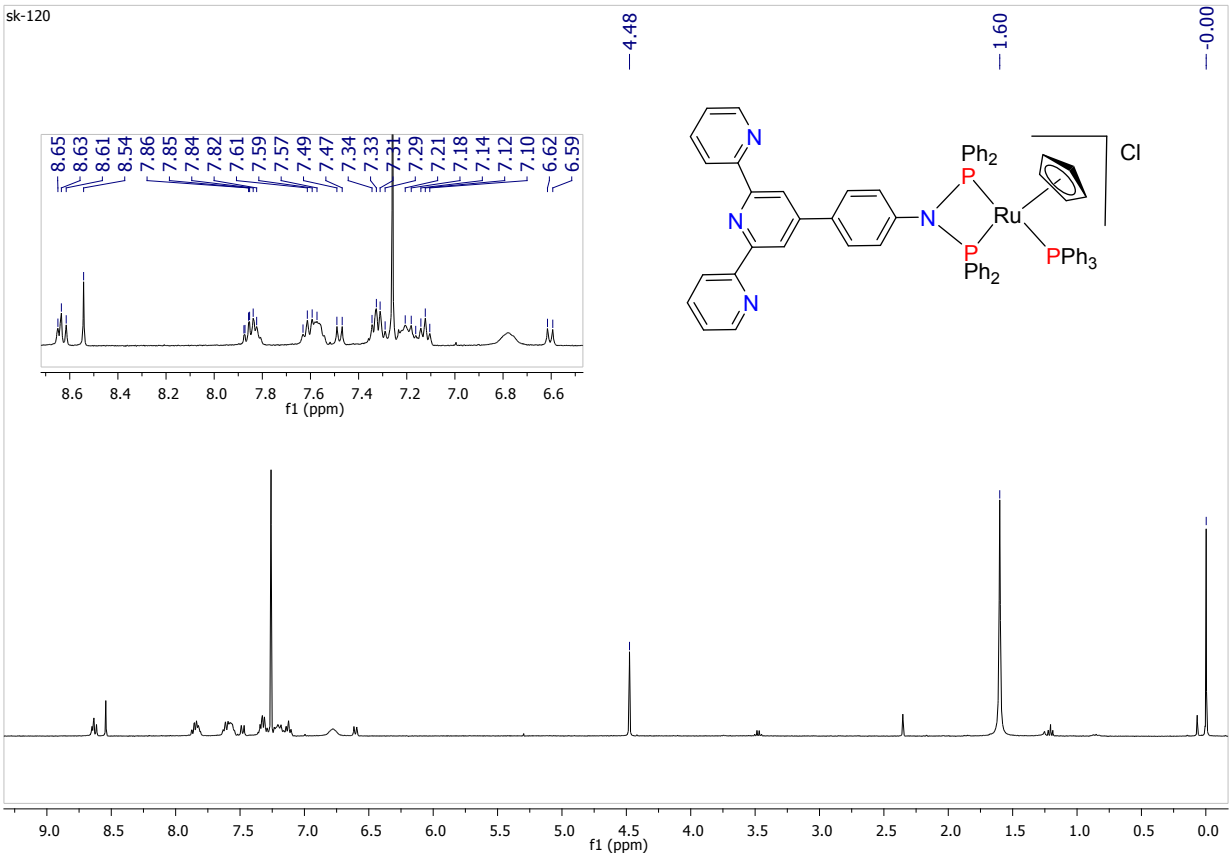

Figure S5. ^{1}H NMR spectrum of **2** in $CDCl_3$.

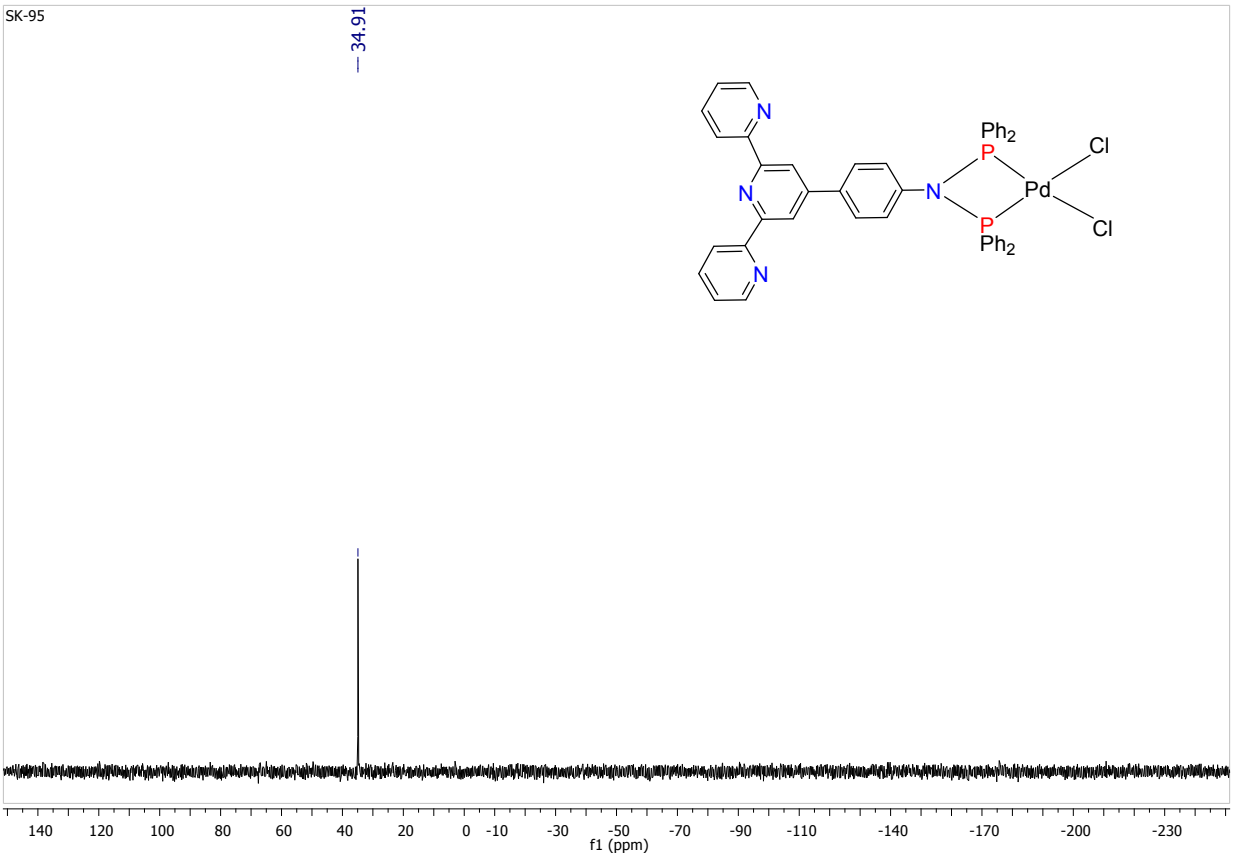

Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$.

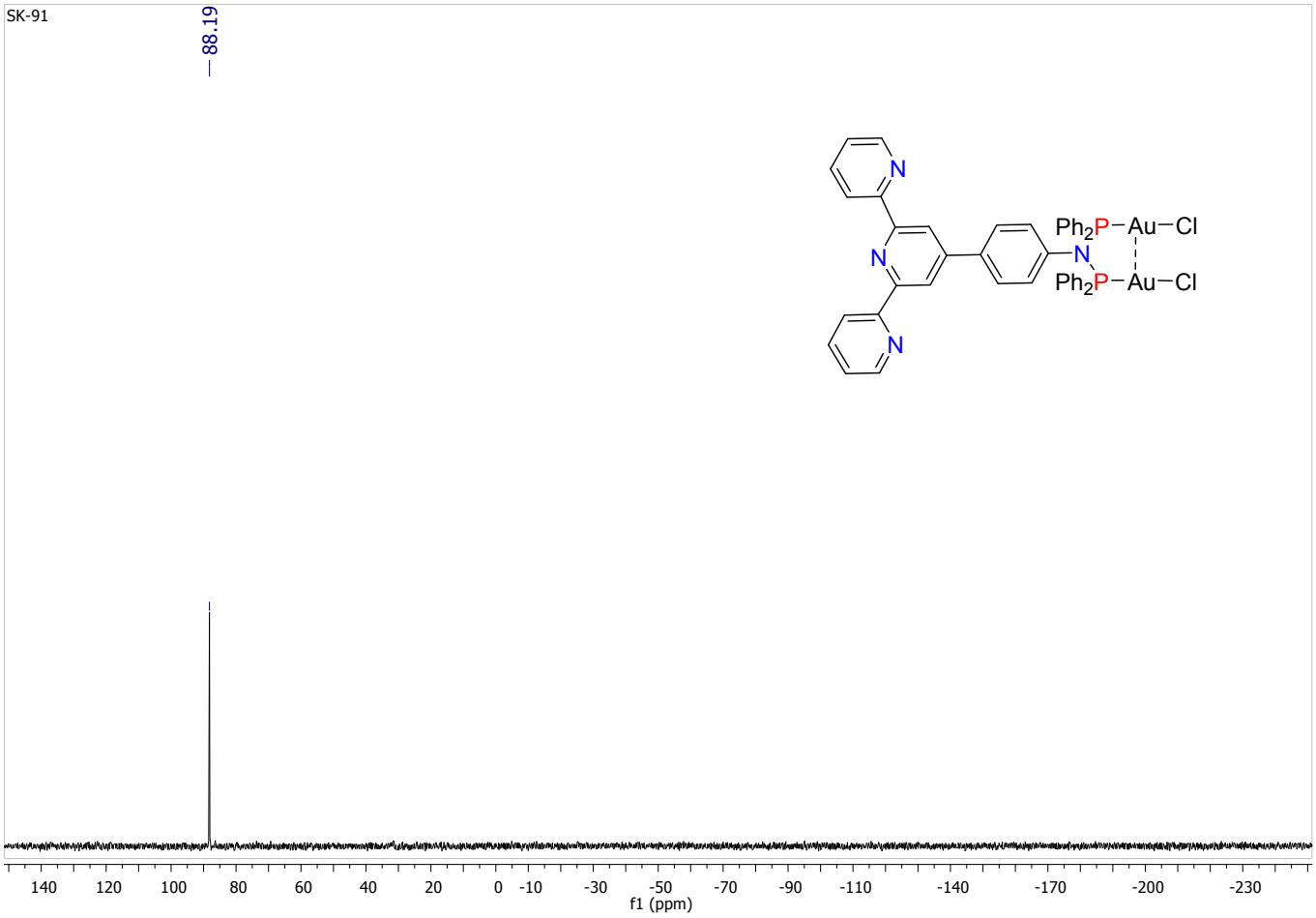

Figure S7. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$.

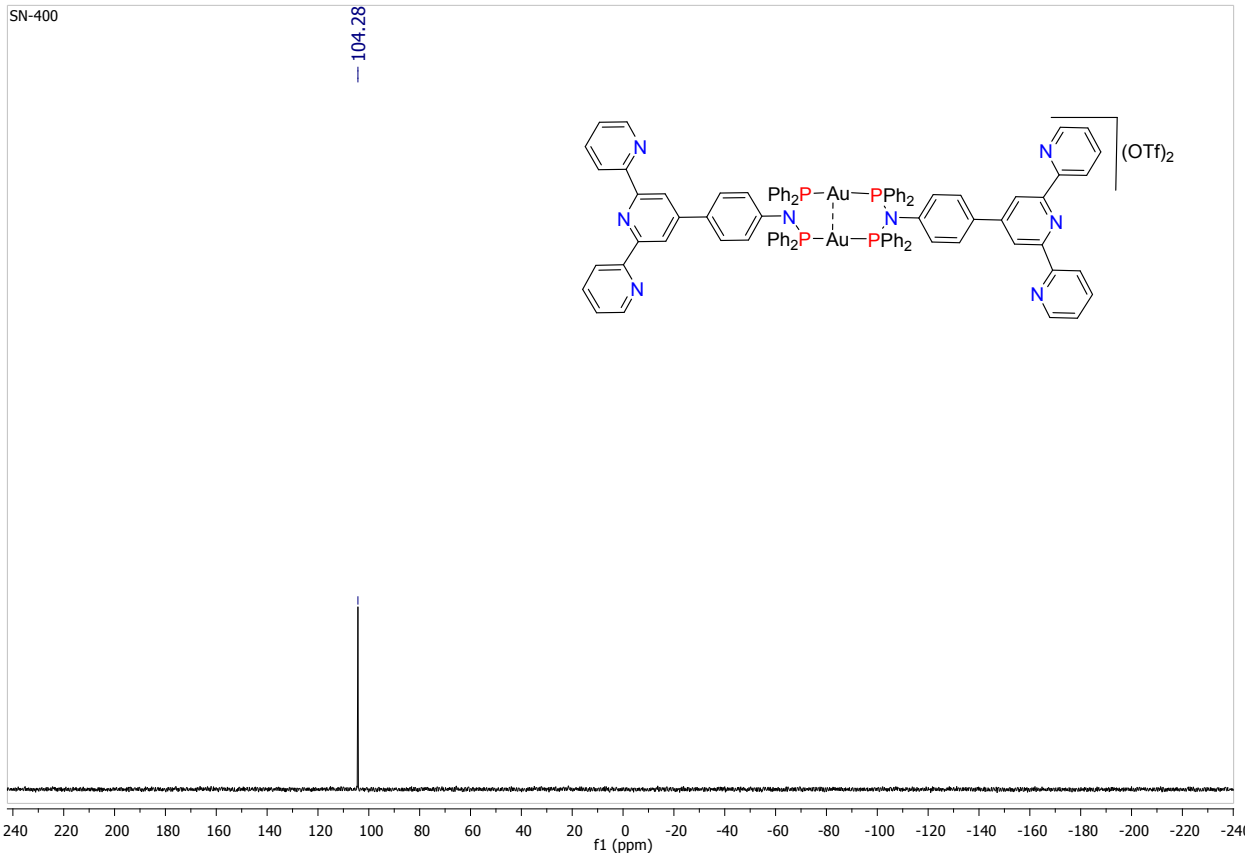

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of **5** in $CDCl_3$.

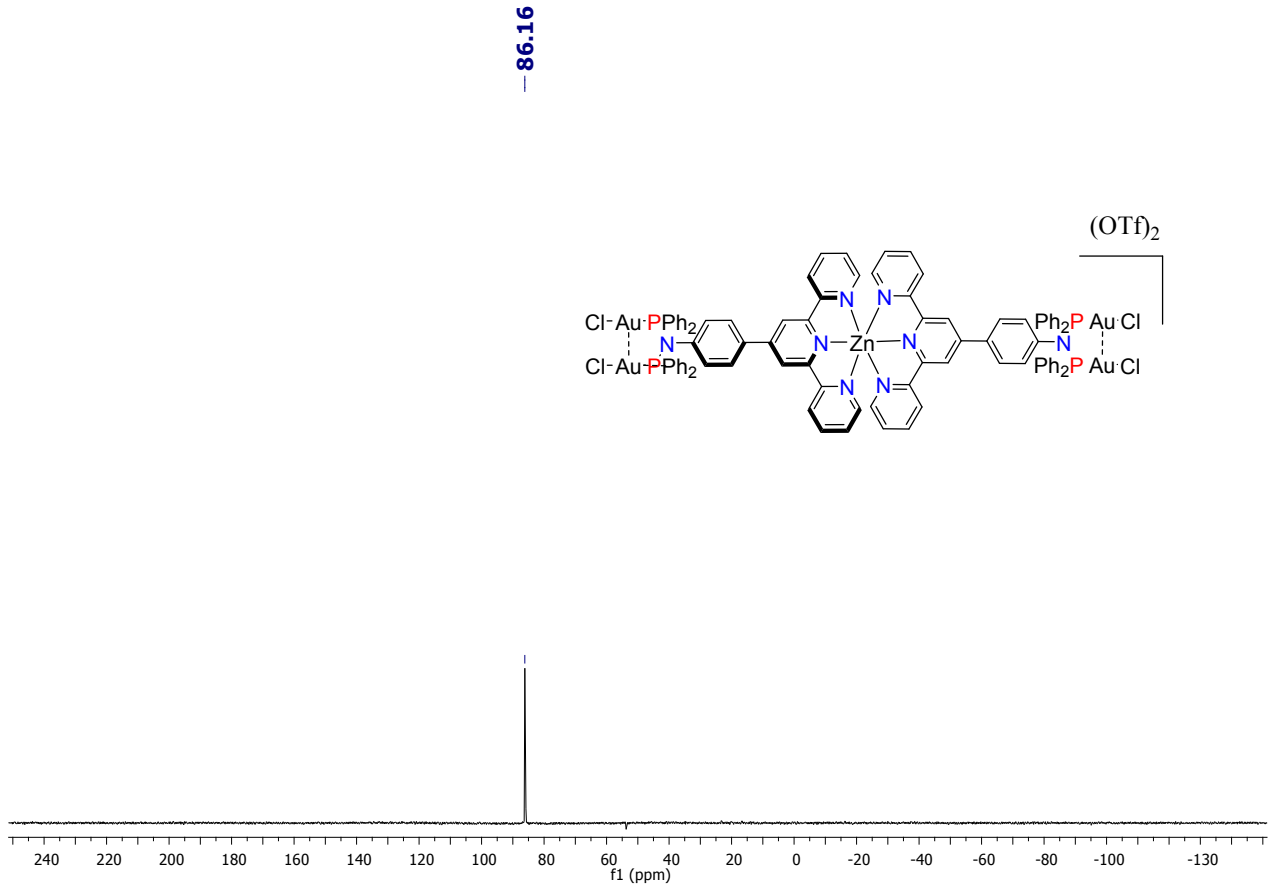

Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum of **6** in DMSO-d_6.

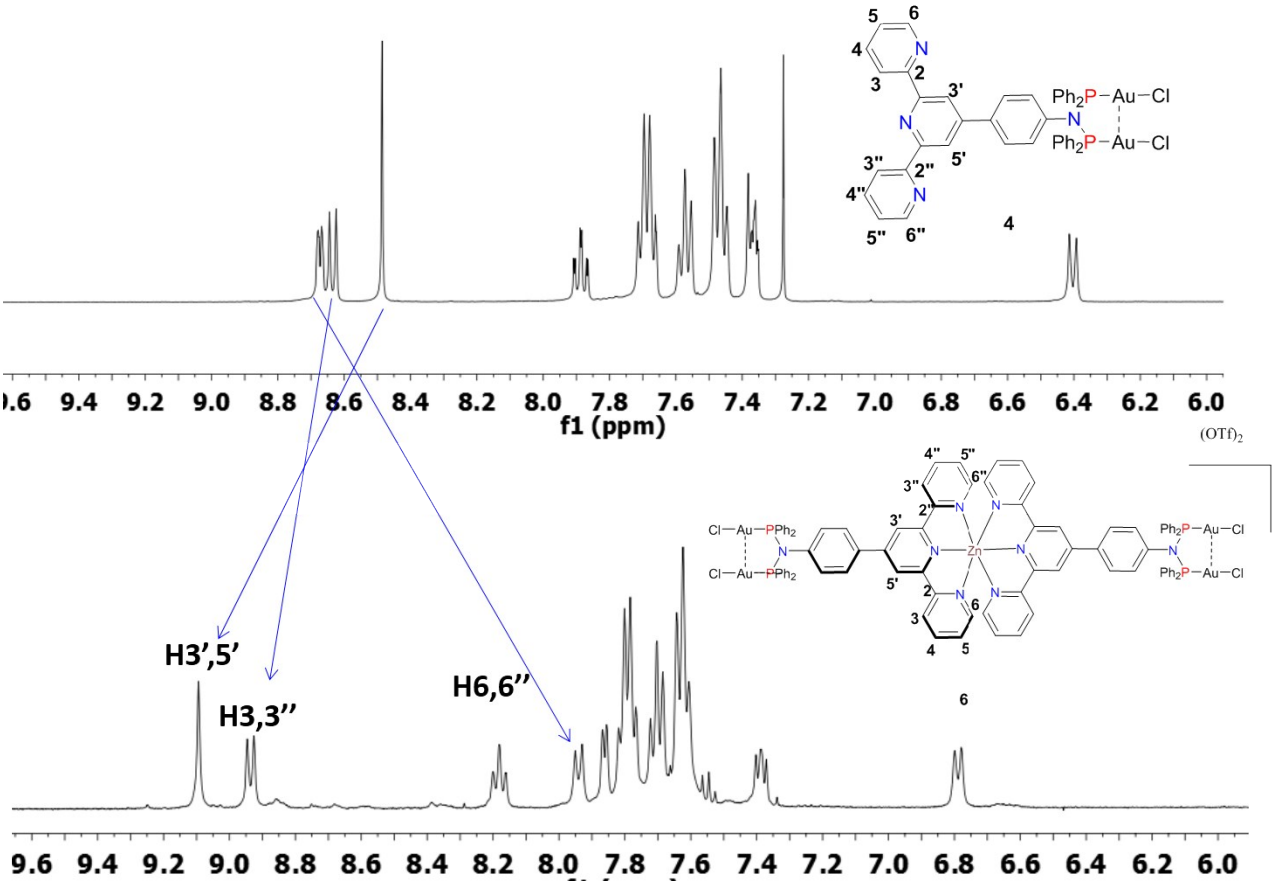

Figure S10. Comparative ^{1}H NMR spectra of complexes **4** and **6**.

7. Bond lengths (Å) and bond angles (˚) for **1**

P1	N4	1.731(2)
P1	C22	1.826(3)
P1	C28	1.836(3)
P2	N4	1.721(2)
P2	C34	1.835(3)
P2	C40	1.833(3)
N1	C1	1.337(4)
N1	C5	1.345(4)
N2	C6	1.339(4)
N2	C10	1.341(4)
N3	C11	1.339(4)
N3	C15	1.335(5)
N4	C19	1.440(3)
C1	H1	0.95
C1	C2	1.382(4)
C2	H2	0.951
C2	C3	1.377(4)
C3	H3	0.95
C3	C4	1.388(5)
C4	H4	0.949
C4	C5	1.397(4)
C5	C6	1.491(4)
C6	C7	1.401(4)
C7	H7	0.951
C7	C8	1.396(4)
C8	C9	1.402(4)
C8	C16	1.483(3)
C9	H9	0.95
C9	C10	1.395(4)

C10	C11	1.493(4)
C11	C12	1.387(4)
C12	H12	0.951
C12	C13	1.394(4)
C13	H13	0.949
C13	C14	1.376(5)
C14	H14	0.95
C14	C15	1.387(4)
C15	H15	0.95
C16	C17	1.405(4)
C16	C21	1.392(4)
C17	H17	0.95
C17	C18	1.390(4)
C18	H18	0.951
C18	C19	1.389(4)
C19	C20	1.395(4)
C20	H20	0.951
C20	C21	1.389(4)
C21	H21	0.95
C22	C23	1.401(4)
C22	C27	1.402(5)
C23	H23	0.949
C23	C24	1.394(5)
C24	H24	0.949
C24	C25	1.403(7)
C25	H25	0.95
C25	C26	1.381(7)
C26	H26	0.95
C26	C27	1.385(5)
C27	H27	0.951

C28	C29	1.394(4)
C28	C33	1.406(4)
C29	H29	0.95
C29	C30	1.400(5)
C30	H30	0.949
C30	C31	1.380(4)
C31	H31	0.951
C31	C32	1.393(4)
C32	H32	0.95
C32	C33	1.385(4)
C33	H33	0.95
C34	C35	1.395(4)
C34	C39	1.402(4)
C35	H35	0.95
C35	C36	1.394(4)
C36	H36	0.951
C36	C37	1.387(5)
C37	H37	0.949
C37	C38	1.385(4)
C38	H38	0.949
C38	C39	1.398(4)
C39	H39	0.95
C40	C41	1.404(4)
C40	C45	1.391(4)
C41	H41	0.95
C41	C42	1.382(4)
C42	H42	0.95
C42	C43	1.397(4)
C43	H43	0.949
C43	C44	1.375(4)

C44	H44	0.95
C44	C45	1.399(4)
C45	H45	0.949
C46	H46A	0.99
C46	H46B	0.989
C46	Cl1	1.758(5)
C46	Cl2	1.752(5)

N4	P1	C22	104.0(1)
N4	P1	C28	104.5(1)
C22	P1	C28	102.7(1)
N4	P2	C34	103.3(1)
N4	P2	C40	105.4(1)
C34	P2	C40	101.1(1)
C1	N1	C5	117.1(3)
C6	N2	C10	117.9(2)
C11	N3	C15	117.3(3)
P1	N4	P2	114.5(1)
P1	N4	C19	122.3(2)
P2	N4	C19	123.0(2)
N1	C1	H1	117.8
N1	C1	C2	124.5(3)
H1	C1	C2	117.7
C1	C2	H2	121
C1	C2	C3	118.0(3)
H2	C2	C3	121.1
C2	C3	H3	120.4
C2	C3	C4	119.2(3)
H3	C3	C4	120.3
C3	C4	H4	120.7
C3	C4	C5	118.8(3)

H4	C4	C5	120.6
N1	C5	C4	122.4(3)
N1	C5	C6	116.4(2)
C4	C5	C6	121.1(2)
N2	C6	C5	116.8(2)
N2	C6	C7	122.9(3)
C5	C6	C7	120.3(2)
C6	C7	H7	120.4
C6	C7	C8	119.3(3)
H7	C7	C8	120.3
C7	C8	C9	117.4(2)
C7	C8	C16	121.7(2)
C9	C8	C16	120.8(2)
C8	C9	H9	120.4
C8	C9	C10	119.3(2)
H9	C9	C10	120.3
N2	C10	C9	123.0(3)
N2	C10	C11	116.6(2)
C9	C10	C11	120.4(2)
N3	C11	C10	116.0(2)
N3	C11	C12	122.9(3)
C10	C11	C12	121.1(2)
C11	C12	H12	120.7
C11	C12	C13	118.8(3)
H12	C12	C13	120.6
C12	C13	H13	120.6
C12	C13	C14	118.8(3)
H13	C13	C14	120.7
C13	C14	H14	120.8
C13	C14	C15	118.3(3)

H14	C14	C15	120.8
N3	C15	C14	123.9(3)
N3	C15	H15	118
C14	C15	H15	118.1
C8	C16	C17	121.7(2)
C8	C16	C21	120.2(2)
C17	C16	C21	118.1(2)
C16	C17	H17	119.8
C16	C17	C18	120.5(2)
H17	C17	C18	119.7
C17	C18	H18	119.6
C17	C18	C19	120.8(2)
H18	C18	C19	119.5
N4	C19	C18	120.3(2)
N4	C19	C20	120.8(2)
C18	C19	C20	118.9(2)
C19	C20	H20	119.8
C19	C20	C21	120.3(3)
H20	C20	C21	119.9
C16	C21	C20	121.3(3)
C16	C21	H21	119.3
C20	C21	H21	119.4
P1	C22	C23	125.4(2)
P1	C22	C27	115.3(2)
C23	C22	C27	119.2(3)
C22	C23	H23	120.2
C22	C23	C24	119.5(3)
H23	C23	C24	120.2
C23	C24	H24	119.9
C23	C24	C25	120.1(4)

H24	C24	C25	120
C24	C25	H25	119.7
C24	C25	C26	120.6(4)
H25	C25	C26	119.6
C25	C26	H26	120.4
C25	C26	C27	119.2(4)
H26	C26	C27	120.4
C22	C27	C26	121.2(3)
C22	C27	H27	119.4
C26	C27	H27	119.4
P1	C28	C29	124.0(2)
P1	C28	C33	117.2(2)
C29	C28	C33	118.0(3)
C28	C29	H29	119.6
C28	C29	C30	120.8(3)
H29	C29	C30	119.6
C29	C30	H30	119.9
C29	C30	C31	120.2(3)
H30	C30	C31	119.9
C30	C31	H31	120
C30	C31	C32	119.8(3)
H31	C31	C32	120.2
C31	C32	H32	120
C31	C32	C33	120.1(3)
H32	C32	C33	120
C28	C33	C32	121.1(3)
C28	C33	H33	119.5
C32	C33	H33	119.5
P2	C34	C35	118.9(2)
P2	C34	C39	122.2(2)

C35	C34	C39	118.3(2)
C34	C35	H35	119.5
C34	C35	C36	121.1(3)
H35	C35	C36	119.4
C35	C36	H36	120
C35	C36	C37	120.0(3)
H36	C36	C37	120
C36	C37	H37	120.2
C36	C37	C38	119.6(3)
H37	C37	C38	120.2
C37	C38	H38	119.7
C37	C38	C39	120.6(3)
H38	C38	C39	119.7
C34	C39	C38	120.3(3)
C34	C39	H39	119.8
C38	C39	H39	119.9
P2	C40	C41	125.0(2)
P2	C40	C45	116.5(2)
C41	C40	C45	118.5(2)
C40	C41	H41	119.8
C40	C41	C42	120.3(3)
H41	C41	C42	119.9
C41	C42	H42	119.7
C41	C42	C43	120.5(3)
H42	C42	C43	119.7
C42	C43	H43	120.2
C42	C43	C44	119.8(3)
H43	C43	C44	120.1
C43	C44	H44	120
C43	C44	C45	119.9(3)

H44	C44	C45	120.1
C40	C45	C44	121.0(3)
C40	C45	H45	119.5
C44	C45	H45	119.5
H46A	C46	H46B	107.8
H46A	C46	Cl1	109
H46A	C46	Cl2	109
H46B	C46	Cl1	108.9
H46B	C46	Cl2	109
Cl1	C46	Cl2	113.1(3)

Bond lengths (Å) and bond angles (˚) for **2**

Ru1	P1	2.291(2)
Ru1	P2	2.254(2)
Ru1	P3	2.359(2)
Ru1	C1	2.244(6)
Ru1	C2	2.262(6)
Ru1	C3	2.247(7)
Ru1	C4	2.212(6)
Ru1	C5	2.229(5)
P1	N1	1.740(5)
P1	C6	1.831(5)
P1	C12	1.826(6)
P2	N1	1.731(5)
P2	C18	1.811(6)
P2	C24	1.843(5)
P3	C51	1.809(6)
P3	C57	1.831(6)
P3	C63	1.835(6)

N1	C30	1.426(8)
N2	C41	1.342(7)
N2	C45	1.344(9)
N3	C38	1.340(7)
N3	C39	1.346(8)
N4	C46	1.355(8)
N4	C50	1.340(7)
C1	H1	0.95
C1	C2	1.421(8)
C1	C5	1.416(8)
C2	H2	0.95
C2	C3	1.419(9)
C3	H3	0.95
C3	C4	1.422(8)
C4	H4	0.951
C4	C5	1.411(9)
C5	H5	0.951
C6	C7	1.368(9)
C6	C11	1.417(8)
C7	H7	0.949
C7	C8	1.394(8)
C8	H8	0.951
C8	C9	1.389(8)
C9	H9	0.949
C9	C10	1.39(1)
C10	H10	0.951
C10	C11	1.373(7)
C11	H11	0.95
C12	C13	1.395(8)
C12	C17	1.401(8)

C13	H13	0.951
C13	C14	1.397(9)
C14	H14	0.949
C14	C15	1.39(1)
C15	H15	0.95
C15	C16	1.38(1)
C16	H16	0.951
C16	C17	1.392(9)
C17	H17	0.95
C18	C19	1.398(8)
C18	C23	1.387(9)
C19	H19	0.95
C19	C20	1.379(9)
C20	H20	0.95
C20	C21	1.37(1)
C21	H21	0.951
C21	C22	1.38(1)
C22	H22	0.95
C22	C23	1.39(1)
C23	H23	0.949
C24	C25	1.401(8)
C24	C29	1.379(9)
C25	H25	0.949
C25	C26	1.410(7)
C26	H26	0.95
C26	C27	1.38(1)
C27	H27	0.948
C27	C28	1.378(9)
C28	H28	0.949
C28	C29	1.408(7)

C29	H29	0.95
C30	C31	1.404(8)
C30	C35	1.398(8)
C31	H31	0.95
C31	C32	1.375(9)
C32	H32	0.95
C32	C33	1.401(8)
C33	C34	1.397(9)
C33	C36	1.471(8)
C34	H34	0.95
C34	C35	1.379(9)
C35	H35	0.95
C36	C37	1.418(8)
C36	C40	1.382(7)
C37	H37	0.949
C37	C38	1.388(8)
C38	C41	1.501(8)
C39	C40	1.396(8)
C39	C46	1.483(7)
C40	H40	0.95
C41	C42	1.385(9)
C42	H42	0.95
C42	C43	1.40(1)
C43	H43	0.951
C43	C44	1.375(9)
C44	H44	0.95
C44	C45	1.383(9)
C45	H45	0.95
C46	C47	1.387(9)
C47	H47	0.951

C47	C48	1.392(8)
C48	H48	0.951
C48	C49	1.39(1)
C49	H49	0.951
C49	C50	1.368(9)
C50	H50	0.95
C51	C52	1.404(9)
C51	C56	1.405(9)
C52	H52	0.95
C52	C53	1.38(1)
C53	H53	0.95
C53	C54	1.393(9)
C54	H54	0.949
C54	C55	1.38(1)
C55	H55	0.949
C55	C56	1.40(1)
C56	H56	0.95
C57	C58	1.412(8)
C57	C62	1.394(8)
C58	H58	0.95
C58	C59	1.383(9)
C59	H59	0.95
C59	C60	1.382(9)
C60	H60	0.95
C60	C61	1.393(8)
C61	H61	0.951
C61	C62	1.379(9)
C62	H62	0.95
C63	C64	1.403(7)
C63	C68	1.392(8)

C64	H64	0.95
C64	C65	1.388(8)
C65	H65	0.949
C65	C66	1.39(1)
C66	H66	0.951
C66	C67	1.393(8)
C67	H67	0.95
C67	C68	1.397(8)
C68	H68	0.95
C69	H69	1
C69	Cl2	1.753(7)
C69	Cl3	1.741(8)
C69	Cl4	1.755(6)
C70	H70	1
C70	Cl5	1.761(9)
C70	Cl6	1.756(9)
C70	Cl7	1.761(7)
C71	H71	1.001
C71	Cl8	1.771(8)
C71	Cl9	1.763(7)
C71	Cl10	1.740(8)
C72	H72	0.998
C72	Cl11	1.773(9)
C72	Cl13	1.759(8)
C72	Cl15	1.731(8)
Cl12	C73	1.760(7)
C73	H73	1
C73	Cl14	1.726(9)
C73	Cl16	1.758(9)

P1	Ru1	P2	96.95(3)
P1	Ru1	P3	97.30(5)
P1	Ru1	C1	161.6(2)
P1	Ru1	C2	134.4(2)
P1	Ru1	C3	103.0(2)
P1	Ru1	C4	99.8(2)
P1	Ru1	C5	128.7(2)
P2	Ru1	P3	103.62(5)
P2	Ru1	C1	115.5(2)
P2	Ru1	C2	152.0(2)
P2	Ru1	C3	141.9(2)
P2	Ru1	C4	105.5(2)
P2	Ru1	C5	93.0(2)
P3	Ru1	C1	98.3(2)
P3	Ru1	C2	88.6(1)
P3	Ru1	C3	114.5(2)
P3	Ru1	C4	149.9(2)
P3	Ru1	C5	134.0(2)
C1	Ru1	C2	36.8(2)
C1	Ru1	C3	61.4(2)
C1	Ru1	C4	61.9(2)
C1	Ru1	C5	36.9(2)
C2	Ru1	C3	36.7(2)
C2	Ru1	C4	61.8(2)
C2	Ru1	C5	61.5(2)
C3	Ru1	C4	37.2(2)
C3	Ru1	C5	61.5(2)
C4	Ru1	C5	37.1(2)
Ru1	P1	N1	95.9(2)
Ru1	P1	C6	127.3(2)

Ru1	P1	C12	115.8(2)
N1	P1	C6	104.9(3)
N1	P1	C12	109.4(3)
C6	P1	C12	102.0(3)
Ru1	P2	N1	97.4(2)
Ru1	P2	C18	123.8(2)
Ru1	P2	C24	114.9(2)
N1	P2	C18	111.6(3)
N1	P2	C24	104.4(2)
C18	P2	C24	103.3(2)
Ru1	P3	C51	126.3(2)
Ru1	P3	C57	111.1(2)
Ru1	P3	C63	112.2(2)
C51	P3	C57	101.1(3)
C51	P3	C63	101.4(3)
C57	P3	C63	101.6(3)
P1	N1	P2	96.9(3)
P1	N1	C30	133.3(4)
P2	N1	C30	128.2(4)
C41	N2	C45	117.3(5)
C38	N3	C39	117.7(5)
C46	N4	C50	117.1(5)
Ru1	C1	H1	122.4
Ru1	C1	C2	72.3(3)
Ru1	C1	C5	71.0(3)
H1	C1	C2	126
H1	C1	C5	126
C2	C1	C5	108.0(5)
Ru1	C2	C1	70.9(3)
Ru1	C2	H2	123.5

Ru1	C2	C3	71.1(3)
C1	C2	H2	126.2
C1	C2	C3	107.7(5)
H2	C2	C3	126.1
Ru1	C3	C2	72.2(3)
Ru1	C3	H3	123.4
Ru1	C3	C4	70.1(3)
C2	C3	H3	126
C2	C3	C4	108.1(5)
H3	C3	C4	125.9
Ru1	C4	C3	72.8(4)
Ru1	C4	H4	120.9
Ru1	C4	C5	72.1(3)
C3	C4	H4	126.1
C3	C4	C5	107.9(5)
H4	C4	C5	126.1
Ru1	C5	C1	72.1(3)
Ru1	C5	C4	70.8(3)
Ru1	C5	H5	122.9
C1	C5	C4	108.3(5)
C1	C5	H5	125.8
C4	C5	H5	125.8
P1	C6	C7	122.7(5)
P1	C6	C11	119.1(4)
C7	C6	C11	118.2(5)
C6	C7	H7	119.3
C6	C7	C8	121.3(6)
H7	C7	C8	119.4
C7	C8	H8	119.8
C7	C8	C9	120.2(6)

H8	C8	C9	120
C8	C9	H9	120.5
C8	C9	C10	119.0(6)
H9	C9	C10	120.5
C9	C10	H10	119.6
C9	C10	C11	120.7(6)
H10	C10	C11	119.7
C6	C11	C10	120.5(5)
C6	C11	H11	119.8
C10	C11	H11	119.7
P1	C12	C13	117.4(4)
P1	C12	C17	124.1(4)
C13	C12	C17	118.5(5)
C12	C13	H13	119.7
C12	C13	C14	120.7(5)
H13	C13	C14	119.7
C13	C14	H14	120.1
C13	C14	C15	119.9(6)
H14	C14	C15	120
C14	C15	H15	120.1
C14	C15	C16	119.8(6)
H15	C15	C16	120.1
C15	C16	H16	119.6
C15	C16	C17	120.8(6)
H16	C16	C17	119.6
C12	C17	C16	120.2(5)
C12	C17	H17	120
C16	C17	H17	119.9
P2	C18	C19	114.2(4)
P2	C18	C23	127.0(4)

C19	C18	C23	118.8(5)
C18	C19	H19	119.7
C18	C19	C20	120.5(6)
H19	C19	C20	119.8
C19	C20	H20	119.9
C19	C20	C21	120.2(6)
H20	C20	C21	119.9
C20	C21	H21	119.8
C20	C21	C22	120.5(6)
H21	C21	C22	119.7
C21	C22	H22	120.2
C21	C22	C23	119.6(6)
H22	C22	C23	120.3
C18	C23	C22	120.5(6)
C18	C23	H23	119.7
C22	C23	H23	119.8
P2	C24	C25	122.7(4)
P2	C24	C29	118.1(4)
C25	C24	C29	119.2(5)
C24	C25	H25	120.4
C24	C25	C26	119.3(5)
H25	C25	C26	120.2
C25	C26	H26	119.7
C25	C26	C27	120.7(6)
H26	C26	C27	119.6
C26	C27	H27	120
C26	C27	C28	120.0(6)
H27	C27	C28	120
C27	C28	H28	120.2
C27	C28	C29	119.6(6)

H28	C28	C29	120.2
C24	C29	C28	121.2(6)
C24	C29	H29	119.3
C28	C29	H29	119.5
N1	C30	C31	122.9(5)
N1	C30	C35	119.8(5)
C31	C30	C35	117.3(5)
C30	C31	H31	119.4
C30	C31	C32	121.1(5)
H31	C31	C32	119.5
C31	C32	H32	119.1
C31	C32	C33	121.9(6)
H32	C32	C33	119
C32	C33	C34	116.7(5)
C32	C33	C36	123.3(5)
C34	C33	C36	119.9(5)
C33	C34	H34	119.1
C33	C34	C35	121.8(6)
H34	C34	C35	119.1
C30	C35	C34	121.2(6)
C30	C35	H35	119.4
C34	C35	H35	119.4
C33	C36	C37	121.9(5)
C33	C36	C40	120.8(5)
C37	C36	C40	117.2(5)
C36	C37	H37	120.6
C36	C37	C38	118.8(5)
H37	C37	C38	120.6
N3	C38	C37	123.5(5)
N3	C38	C41	115.2(5)

C37	C38	C41	121.3(5)
N3	C39	C40	122.6(5)
N3	C39	C46	116.2(5)
C40	C39	C46	121.2(5)
C36	C40	C39	120.2(5)
C36	C40	H40	120
C39	C40	H40	119.8
N2	C41	C38	116.9(5)
N2	C41	C42	123.3(6)
C38	C41	C42	119.7(5)
C41	C42	H42	120.8
C41	C42	C43	118.5(6)
H42	C42	C43	120.7
C42	C43	H43	120.8
C42	C43	C44	118.4(6)
H43	C43	C44	120.8
C43	C44	H44	120.5
C43	C44	C45	119.2(6)
H44	C44	C45	120.2
N2	C45	C44	123.3(6)
N2	C45	H45	118.3
C44	C45	H45	118.4
N4	C46	C39	116.2(5)
N4	C46	C47	122.5(6)
C39	C46	C47	121.3(5)
C46	C47	H47	120.6
C46	C47	C48	118.7(6)
H47	C47	C48	120.6
C47	C48	H48	120.5
C47	C48	C49	118.9(6)

H48	C48	C49	120.5
C48	C49	H49	121
C48	C49	C50	118.1(6)
H49	C49	C50	120.9
N4	C50	C49	124.5(6)
N4	C50	H50	117.7
C49	C50	H50	117.8
P3	C51	C52	120.0(4)
P3	C51	C56	123.1(4)
C52	C51	C56	116.6(5)
C51	C52	H52	118.7
C51	C52	C53	122.4(6)
H52	C52	C53	118.8
C52	C53	H53	120.2
C52	C53	C54	119.5(6)
H53	C53	C54	120.3
C53	C54	H54	120.3
C53	C54	C55	119.7(6)
H54	C54	C55	120
C54	C55	H55	119.8
C54	C55	C56	120.4(6)
H55	C55	C56	119.9
C51	C56	C55	121.3(6)
C51	C56	H56	119.3
C55	C56	H56	119.3
P3	C57	C58	118.6(4)
P3	C57	C62	123.9(4)
C58	C57	C62	117.4(5)
C57	C58	H58	119.7
C57	C58	C59	120.7(5)

H58	C58	C59	119.6
C58	C59	H59	119.4
C58	C59	C60	121.0(6)
H59	C59	C60	119.5
C59	C60	H60	120.6
C59	C60	C61	118.7(6)
H60	C60	C61	120.7
C60	C61	H61	119.7
C60	C61	C62	120.6(6)
H61	C61	C62	119.7
C57	C62	C61	121.5(6)
C57	C62	H62	119.1
C61	C62	H62	119.4
P3	C63	C64	122.5(4)
P3	C63	C68	118.3(4)
C64	C63	C68	119.1(5)
C63	C64	H64	119.7
C63	C64	C65	120.7(5)
H64	C64	C65	119.6
C64	C65	H65	120.1
C64	C65	C66	119.7(6)
H65	C65	C66	120.1
C65	C66	H66	119.9
C65	C66	C67	120.2(6)
H66	C66	C67	119.9
C66	C67	H67	120
C66	C67	C68	120.0(6)
H67	C67	C68	120.1
C63	C68	C67	120.2(5)
C63	C68	H68	119.9

C67	C68	H68	119.9
H69	C69	Cl2	108.5
H69	C69	Cl3	108.5
H69	C69	Cl4	108.5
Cl2	C69	Cl3	109.8(4)
Cl2	C69	Cl4	109.1(4)
Cl3	C69	Cl4	112.3(4)
H70	C70	Cl5	108.4
H70	C70	Cl6	108.5
H70	C70	Cl7	108.5
Cl5	C70	Cl6	110.4(5)
Cl5	C70	Cl7	111.1(5)
Cl6	C70	Cl7	110.0(5)
H71	C71	Cl8	108.4
H71	C71	Cl9	108.3
H71	C71	Cl10	108.3
Cl8	C71	Cl9	110.8(4)
Cl8	C71	Cl10	111.0(4)
Cl9	C71	Cl10	109.9(4)
H72	C72	Cl11	108.5
H72	C72	Cl13	108.4
H72	C72	Cl15	108.5
Cl11	C72	Cl13	108.5(4)
Cl11	C72	Cl15	111.2(5)
Cl13	C72	Cl15	111.8(5)
Cl12	C73	H73	107.8
Cl12	C73	Cl14	111.5(4)
Cl12	C73	Cl16	110.3(4)
H73	C73	Cl14	107.7
H73	C73	Cl16	107.7

Cl14	C73	Cl16	111.6(4)

Bond lengths (Å) and bond angles (˚) for **3**

Pd1	Cl1	2.3538(12)
Pd1	Cl1[1]	2.3538(12)
Pd1	P1[1]	2.2070(12)
Pd1	P1	2.2070(12)
P1	P1[1]	2.607(2)
P1	N3[1]	1.711(3)
P1	C13	1.808(4)
P1	C19	1.785(5)
Cl3	C25	1.775(5)
Cl2	C25	1.772(6)
Cl4	C25	1.760(5)
N3	C12	1.439(7)
N2	C6	1.345(5)
N2	C6[1]	1.345(5)
N1	C5	1.346(6)
N1	C1	1.328(6)
C12	C11	1.389(5)
C12	C11[1]	1.389(5)
C7	C6	1.391(6)
C7	C8	1.388(5)
C10	C91	1.387(5)
C10	C11	1.384(6)
C5	C6	1.487(6)
C5	C4	1.394(6)
C1	C2	1.384(6)

C9	C8	1.499(8)
C13	C18	1.399(6)
C13	C14	1.382(6)
C19	C20	1.392(6)
C19	C24	1.393(6)
C2	C3	1.378(6)
C18	C17	1.385(7)
C3	C4	1.385(6)
C14	C15	1.383(6)
C20	C21	1.379(7)
C24	C23	1.382(7)
C21	C22	1.377(7)
C23	C22	1.368(7)
C16	C17	1.385(8)
C16	C15	1.377(8)

Cl1	Pd1	$Cl1^1$	95.34(6)
$P1^1$	Pd1	Cl1	96.16(4)
$P1^1$	Pd1	$Cl1^1$	168.32(4)
P1	Pd1	$Cl1^1$	96.16(4)
P1	Pd1	Cl1	168.32(4)
$P1^1$	Pd1	P1	72.42(6)
$P1^1$	P1	$Pd1^1$	53.79(3)
$N3^1$	P1	$Pd1^1$	94.15(13)
C13	P1	$Pd1^1$	116.09(14)
C13	P1	$N3^1$	110.97(16)
C19	P1	$Pd1^1$	117.03(14)
C19	P1	$N3^1$	108.28(16)

C19	P1	C13	109.1(2)
P1	N3	P1[1]	99.3(2)
C12	N3	P1	130.36(12)
C12	N3	P1[1]	130.36(12)
C6[1]	N2	C6	117.0(5)
C1	N1	C5	118.3(4)
C11[1]	C12	N3	120.4(3)
C11	C12	N3	120.4(3)
C11	C12	C11[1]	119.2(5)
C8	C7	C6	119.7(4)
C11	C10	C9[1]	121.6(4)
C6	C5	N1	116.3(4)
C4	C5	N1	121.8(4)
C4	C5	C6	121.9(4)
C2	C1	N1	123.5(5)
C7	C6	N2	123.1(4)
C5	C6	N2	117.3(4)
C5	C6	C7	119.6(4)
C10	C9	C101	117.7(5)
C8	C9	C101	121.2(3)
C8	C9	C10	121.2(3)
C18	C13	P1	116.8(3)
C14	C13	P1	123.8(4)
C14	C13	C18	119.3(4)
C10	C11	C121	119.9(4)
C71	C8	C7	117.4(6)
C9	C8	C7	121.3(3)
C9	C8	C71	121.3(3)
C20	C19	P1	119.4(3)

C24	C19	P1	121.7(4)
C24	C19	C20	118.6(5)
C3	C2	C1	118.3(5)
C17	C18	C13	119.9(5)
C4	C3	C2	119.1(4)
C3	C4	C5	119.0(4)
C15	C14	C13	120.4(5)
C21	C20	C19	121.0(4)
C23	C24	C19	118.9(5)
C22	C21	C20	120.3(5)
C22	C23	C24	122.7(5)
C15	C16	C17	120.1(5)
C16	C17	C18	120.1(6)
C23	C22	C21	118.5(5)
Cl2	C25	Cl3	110.6(3)
Cl4	C25	Cl3	110.3(3)
Cl4	C25	Cl2	109.6(3)
C16	C15	C14	120.2(5)

Bond lengths (Å) and bond angles (˚) for **4**

Au1	Au2	2.9667(9)
Au1	P1	2.234(2)
Au1	Cl1	2.294(2)
Au2	Cl2	2.291(2)
Au2	P2	2.229(2)
P1	N4	1.714(5)
P1	C22	1.807(7)
P1	C28	1.818(7)

P2	N4	1.704(5)
P2	C34	1.816(7)
P2	C40	1.812(7)
N4	C19	1.478(9)
N1	C5	1.34(1)
N1	C1	1.36(1)
C27	H27	0.951
C27	C22	1.397(9)
C27	C26	1.39(1)
N2	C6	1.33(1)
N2	C10	1.34(1)
C12	H12	0.951
C12	C11	1.35(1)
C12	C13	1.38(1)
C34	C39	1.41(1)
C34	C35	1.37(1)
C22	C23	1.403(9)
C19	C18	1.39(1)
C19	C20	1.38(1)
C28	C29	1.40(1)
C28	C33	1.39(1)
C18	H18	0.95
C18	C17	1.39(1)
C40	C41	1.39(1)
C40	C45	1.39(1)
C21	H21	0.951
C21	C16	1.39(1)
C21	C20	1.39(1)
C16	C17	1.40(1)
C16	C8	1.49(1)

C20	H20	0.949
C17	H17	0.95
C31	H31	0.95
C31	C32	1.39(1)
C31	C30	1.38(1)
C6	C7	1.40(1)
C6	C5	1.489(9)
C39	H39	0.951
C39	C38	1.38(1)
C41	H41	0.95
C41	C42	1.40(1)
C4	H4	0.95
C4	C3	1.39(1)
C4	C5	1.40(1)
C25	H25	0.95
C25	C24	1.37(1)
C25	C26	1.387(9)
C23	H23	0.95
C23	C24	1.40(1)
C24	H24	0.95
C8	C7	1.410(9)
C8	C9	1.39(1)
C7	H7	0.951
C26	H26	0.949
C9	H9	0.95
C9	C10	1.39(1)
C3	H3	0.951
C3	C2	1.37(1)
C29	H29	0.95
C29	C30	1.37(1)

C10	C11	1.48(1)
C32	H32	0.95
C32	C33	1.38(1)
C38	H38	0.949
C38	C37	1.38(1)
C15	H15	0.95
C15	N3	1.43(2)
C15	C14	1.34(2)
N3	C11	1.30(1)
C14	H14	0.95
C14	C13	1.32(2)
C33	H33	0.951
C2	H2	0.949
C2	C1	1.39(1)
C1	H1	0.949
C35	H35	0.95
C35	C36	1.39(1)
C13	H13	0.949
C37	H37	0.949
C37	C36	1.39(1)
C36	H36	0.95
C45	H45	0.951
C45	C44	1.43(1)
C42	H42	0.95
C42	C43	1.38(1)
C30	H30	0.951
C43	H43	0.951
C43	C44	1.36(2)
C44	H44	0.951
Cl6	C1S	1.67(2)

Cl5	C1S		1.67(1)
C1S	H1SA		0.99
C1S	H1SB		0.99
Au2	Au1	P1	85.43(4)
Au2	Au1	Cl1	95.02(4)
P1	Au1	Cl1	178.83(6)
Au1	Au2	Cl2	99.96(5)
Au1	Au2	P2	84.86(4)
Cl2	Au2	P2	175.17(6)
Au1	P1	N4	111.5(2)
Au1	P1	C22	113.1(2)
Au1	P1	C28	114.7(2)
N4	P1	C22	106.6(3)
N4	P1	C28	104.5(3)
C22	P1	C28	105.8(3)
Au2	P2	N4	111.2(2)
Au2	P2	C34	111.6(2)
Au2	P2	C40	113.6(2)
N4	P2	C34	105.9(3)
N4	P2	C40	106.8(3)
C34	P2	C40	107.2(3)
P1	N4	P2	122.5(3)
P1	N4	C19	118.3(4)
P2	N4	C19	119.2(4)
C5	N1	C1	116.4(7)
H27	C27	C22	120.1
H27	C27	C26	119.9
C22	C27	C26	120.0(6)
C6	N2	C10	118.5(7)
H12	C12	C11	119.7

H12	C12	C13	119.6
C11	C12	C13	120.7(8)
P2	C34	C39	121.4(5)
P2	C34	C35	120.1(6)
C39	C34	C35	118.4(7)
P1	C22	C27	121.6(5)
P1	C22	C23	118.6(5)
C27	C22	C23	119.7(6)
N4	C19	C18	119.2(6)
N4	C19	C20	119.8(6)
C18	C19	C20	121.0(6)
P1	C28	C29	121.9(5)
P1	C28	C33	118.3(5)
C29	C28	C33	119.7(7)
C19	C18	H18	120.2
C19	C18	C17	119.6(6)
H18	C18	C17	120.3
P2	C40	C41	120.7(6)
P2	C40	C45	119.2(6)
C41	C40	C45	119.9(7)
H21	C21	C16	119.4
H21	C21	C20	119.4
C16	C21	C20	121.2(6)
C21	C16	C17	118.7(6)
C21	C16	C8	120.5(6)
C17	C16	C8	120.8(6)
C19	C20	C21	119.1(6)
C19	C20	H20	120.5
C21	C20	H20	120.4
C18	C17	C16	120.4(6)

C18	C17	H17	119.8
C16	C17	H17	119.8
H31	C31	C32	119.8
H31	C31	C30	119.7
C32	C31	C30	120.5(9)
N2	C6	C7	123.1(6)
N2	C6	C5	117.2(6)
C7	C6	C5	119.7(6)
C34	C39	H39	120.1
C34	C39	C38	119.8(7)
H39	C39	C38	120.1
C40	C41	H41	119.2
C40	C41	C42	121.5(8)
H41	C41	C42	119.4
H4	C4	C3	121.1
H4	C4	C5	121.1
C3	C4	C5	117.8(7)
H25	C25	C24	119.4
H25	C25	C26	119.3
C24	C25	C26	121.4(7)
C22	C23	H23	120.2
C22	C23	C24	119.7(6)
H23	C23	C24	120.1
C25	C24	C23	119.5(7)
C25	C24	H24	120.2
C23	C24	H24	120.3
C16	C8	C7	120.7(6)
C16	C8	C9	122.5(6)
C7	C8	C9	116.8(6)
C6	C7	C8	118.7(6)

C6	C7	H7	120.7
C8	C7	H7	120.6
C27	C26	C25	119.7(6)
C27	C26	H26	120.2
C25	C26	H26	120.1
C8	C9	H9	119.5
C8	C9	C10	121.0(7)
H9	C9	C10	119.5
C4	C3	H3	120.3
C4	C3	C2	119.6(7)
H3	C3	C2	120.2
C28	C29	H29	120.1
C28	C29	C30	119.8(7)
H29	C29	C30	120
N1	C5	C6	116.8(6)
N1	C5	C4	123.9(7)
C6	C5	C4	119.3(6)
N2	C10	C9	121.7(7)
N2	C10	C11	115.9(7)
C9	C10	C11	122.3(7)
C31	C32	H32	120.3
C31	C32	C33	119.5(8)
H32	C32	C33	120.2
C39	C38	H38	119.9
C39	C38	C37	120.4(7)
H38	C38	C37	119.7
H15	C15	N3	120
H15	C15	C14	120
N3	C15	C14	120(1)
C15	N3	C11	118(1)

C15	C14	H14	120
C15	C14	C13	121(1)
H14	C14	C13	119
C28	C33	C32	120.2(7)
C28	C33	H33	119.9
C32	C33	H33	119.8
C3	C2	H2	120.7
C3	C2	C1	118.8(7)
H2	C2	C1	120.6
N1	C1	C2	123.5(7)
N1	C1	H1	118.3
C2	C1	H1	118.2
C34	C35	H35	118.8
C34	C35	C36	122.4(7)
H35	C35	C36	118.8
C12	C11	C10	122.4(8)
C12	C11	N3	121.3(9)
C10	C11	N3	116.3(8)
C12	C13	C14	118.7(9)
C12	C13	H13	120.6
C14	C13	H13	120.7
C38	C37	H37	119.6
C38	C37	C36	120.7(8)
H37	C37	C36	119.7
C35	C36	C37	118.1(8)
C35	C36	H36	121
C37	C36	H36	120.9
C40	C45	H45	121.1
C40	C45	C44	117.9(8)
H45	C45	C44	121

C41	C42	H42	120.9
C41	C42	C43	118.0(9)
H42	C42	C43	121
C31	C30	C29	120.1(8)
C31	C30	H30	120
C29	C30	H30	119.9
C42	C43	H43	119
C42	C43	C44	122(1)
H43	C43	C44	119
C45	C44	C43	120.7(9)
C45	C44	H44	120
C43	C44	H44	120
Cl6	C1S	Cl5	113.8(9)
Cl6	C1S	H1SA	109
Cl6	C1S	H1SB	109
Cl5	C1S	H1SA	109
Cl5	C1S	H1SB	109
H1SA	C1S	H1SB	108