Supporting Information

A hybrid terpyridine-based bis(diphenylphosphino)amine ligand, terpy-C$_6$H$_4$N(PPh$_2$)$_2$: Synthesis, coordination chemistry and photoluminescence studies

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Table of contents:

1 Materials and Physical Measurements
2 Experimental Section
3 Single Crystal X-ray Diffraction Analyses
4 Crystal data for compounds 1, 2, 3 and 4
5 References
6 NMR spectra
7 Bond lengths and bond angles for compounds 1, 2, 3 and 4
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 \([\text{CpRu(PPH}_3\text{)}_2\text{Cl}]\), \([\text{Pd(COD)Cl}_2]\), \([\text{AuCl(SMe}_2\text{)}]^3\) and 4’-(p-aminophenyl)terpyridine were prepared according to published procedures. The \(^1\text{H}\) and \(^{31}\text{P}\{^1\text{H}\} \text{NMR (}\delta\text{ 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\(_3\)PO\(_4\) were used as internal and external standards for \(^1\text{H}\) and \(^{31}\text{P}\{^1\text{H}\} \text{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\(_2\)P)\(_2\)NC\(_6\)H\(_4\))}-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. \(^{31}\text{P}\{^1\text{H}\} \text{NMR (CDCl}_3\): 69.3 ppm (s). \(^1\text{H}\) NMR (CDCl\(_3\)) \(\delta\): 6.74 (d, H7’, 2H, \(3J_{HH} = 8.5\) Hz), 7.30-7.42 (m, ArH, H5,5’, 22H), 7.51 (d,
H8,8’, 2H, \( J_{HH} = 8.5 \) Hz), 7.85 (td, H4,4”, 2H, \( J_{HH} = 7.1 \) Hz, \( J_{HH} = 1.8 \) Hz), 8.60 (s, H3’,5’, 2H), 8.63 (d, H3,3”, 2H, \( J_{HH} = 7.9 \) Hz), 8.69 (d, H6,6”, 2H, \( J_{HH} = 4.0 \) Hz). ESI(MS): m/z = 693.23 [M+H]⁺. Anal. Calcd. for C₄₅H₃₄N₄P₂: C, 78.00; H, 4.95; N, 8.09 %. Found: C, 78.14; H, 4.57; N, 8.07 %.

**Synthesis of [(Ru(PPh₃)(Cp){4′-{p-(Ph₂P)₂NC₆H₄}-2,2’:6’2’’-terpy}]Cl (2)**

A toluene solution (5 mL) of [CpRu(PPh₃)₂Cl] (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.). \(^{31}P\) NMR (CDCl₃) \( \delta \): 44.2 (t, PPh₃, 1P) and 79.4 (d, PPh₂, 2P) (\( J_{PP} = 32.5 \) Hz). \(^1H\) NMR (CDCl₃) \( \delta \): 4.48 (s, C⁵H⁵, 5H) 6.60 (d, H7,7′, 2H, \( J_{HH} = 8.6 \) Hz), 7.11-7.34 (m, ArH, H5,5′, 22H), 7.48 (d, H8,8′, 2H, \( J_{HH} = 8.6 \) Hz), 7.59 (dt, H4,4′, 2H, \( J_{HH} = 20.9, 6.6 \) 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 C₆₈H₅₄N₄P₃RuCl: C, 70.61; H, 4.70; N, 4.84 %. Found: C, 70.77; H, 4.45; N, 4.65 %.

**Synthesis of cis-[PdCl₂{4′-{p-(Ph₂P)₂NC₆H₄}-2,2’:6’2’’-terpy}] (3)**

A solution of [Pd(COD)Cl₂] (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. \(^{31}P\) NMR (CDCl₃) \( \delta \): 34.9 (s). \(^1H\) NMR (CDCl₃) \( \delta \): 6.67 (d, H7,7′, 2H, \( J_{HH} = 7.9 \) Hz), 7.36-7.62 (m, ArH, H5,5’, 22H), 7.66 (d, H8,8′, 2H, \( J_{HH} = 7.9 \) Hz), 7.94 (t, H4,4′, 2H, \( J_{HH} = 7.9 \) 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 C₆₈H₅₄N₄P₂PdCl₂: C, 62.01; H, 3.94; N, 6.44 %. Found: C, 62.01; H, 3.63; N, 6.25 %.

**Synthesis of [(AuCl)₂{4′-{p-(Ph₂P)₂NC₆H₄}-2,2’:6’2’’-terpy}] (4)**
A solution of \([\text{AuCl(SMe}_2\text{)}]\) (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 °C. Yield: 78 % (0.038 g). MP: 192-194 °C (dec.).

\(^{31}\text{P}\{^1\text{H}\} \text{ NMR (CDCl}_3\} \delta: 88.3 \text{ (s)}. \)

\(^1\text{H} \text{ NMR (CDCl}_3\} \delta: 6.40 \text{ (d, H7,7′, 2H, } \text{J}_{HH} = 8.5 \text{ Hz)}, 7.35-7.72 \text{ (m, ArH, H5,5′, H8,8′, 24H)}, 7.88 \text{ (td, H4,4′, 2H, } \text{J}_{HH} = 7.1 \text{ Hz, } \text{J}_{HH} = 1.8 \text{ Hz)}, 8.49 \text{ (s, H3′,5′, 2H)}, 8.63 \text{ (d, H3,3′, 2H, } \text{J}_{HH} = 7.9 \text{ Hz)}, 8.67 \text{ (d, H6,6′, 2H, } \text{J}_{HH} = 4.0 \text{ Hz)}. \text{ ESI(MS): m/z = 1179.09 [M+Na}^+\text{]. Anal. Calcd. for C}_45\text{H}_34\text{N}_4\text{P}_2\text{Au}_2\text{Cl}_2: C, 46.69; H, 2.96; N, 4.84 %. Found: C, 46.76; H, 2.86; N, 4.42 %.

\textbf{Synthesis of [Au}\{^4′-\{p-(\text{Ph}_2\text{P})_2\text{NC}_6\text{H}_4\}_2-2,2′:6′2′′-\text{terpy}\}\}{\text{2(OTf)}_2 (5)}\text{ }

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. \(^{31}\text{P}\{^1\text{H}\} \text{ NMR (CDCl}_3\} \delta: 104.3 \text{ (s)}. \)

\(^1\text{H} \text{ NMR (CDCl}_3\} \delta: 6.46 \text{ (d, H7,7′, 2H, } \text{J}_{HH} = 8.0 \text{ Hz)}, 7.36-7.67 \text{ (m, ArH, H5,5′, H8,8′, 24H)}, 8.02 \text{ (br s, H4,4′, 2H)}, 8.61 \text{ (s, H3′,5′, 2H)}, 8.74 \text{ (br s, H3,3′, 2H)}, 8.81 \text{ (br s, H6,6′, 2H)}. \text{ Anal. Calcd. for C}_92\text{H}_68\text{N}_8\text{P}_4\text{Au}_2\text{S}_2\text{F}_6\text{O}_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 %.

\textbf{Synthesis of [(AuCl)_2}\{^4′-\{p-(\text{Ph}_2\text{P})_2\text{NC}_6\text{H}_4\}_2-2,2′:6′2′′-\text{terpy}\}\}{\text{Zn(OTf)}_2 (6)}\text{ }

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$_6$) $\delta$: 86.2 (s). $^1$H NMR (DMSO-d$_6$) $\delta$: 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), 9.11 (s, H3′,5′, 2H). Anal. Calcd for C$_{92}$H$_{68}$N$_8$P$_4$Au$_4$Cl$_4$F$_6$O$_6$S$_2$Zn: 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 ($\lambda_\alpha$ = 0.71073 Å) with the $\omega$-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.

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5. References.


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{H} NMR spectrum of 3 in CDCl$_3$. 
Figure S7. $^{31}$P{¹H} NMR spectrum of 4 in CDCl$_3$. 
**Figure S8.** $^{31}$P{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

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C72  H72  0.998
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C73  H73  1
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\text{P1} & \quad \text{N3} & \quad \text{P1}^1 & \quad 99.3(2) \\
\text{C12} & \quad \text{N3} & \quad \text{P1} & \quad 130.36(12) \\
\text{C12} & \quad \text{N3} & \quad \text{P1}^1 & \quad 130.36(12) \\
\text{C6}^1 & \quad \text{N2} & \quad \text{C6} & \quad 117.0(5) \\
\text{C1} & \quad \text{N1} & \quad \text{C5} & \quad 118.3(4) \\
\text{C11}^1 & \quad \text{C12} & \quad \text{N3} & \quad 120.4(3) \\
\text{C11} & \quad \text{C12} & \quad \text{N3} & \quad 120.4(3) \\
\text{C11} & \quad \text{C12} & \quad \text{C11}^1 & \quad 119.2(5) \\
\text{C8} & \quad \text{C7} & \quad \text{C6} & \quad 119.7(4) \\
\text{C11} & \quad \text{C10} & \quad \text{C9}^1 & \quad 121.6(4) \\
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\text{C4} & \quad \text{C5} & \quad \text{N1} & \quad 121.8(4) \\
\text{C4} & \quad \text{C5} & \quad \text{C6} & \quad 121.9(4) \\
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\text{C7} & \quad \text{C6} & \quad \text{N2} & \quad 123.1(4) \\
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\text{C8} & \quad \text{C9} & \quad \text{C10} & \quad 121.2(3) \\
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\text{C10} & \quad \text{C11} & \quad \text{C121} & \quad 119.9(4) \\
\text{C71} & \quad \text{C8} & \quad \text{C7} & \quad 117.4(6) \\
\text{C9} & \quad \text{C8} & \quad \text{C7} & \quad 121.3(3) \\
\text{C9} & \quad \text{C8} & \quad \text{C71} & \quad 121.3(3) \\
\text{C20} & \quad \text{C19} & \quad \text{P1} & \quad 119.4(3)
\end{align*}
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C17  C18  C13  119.9(5)
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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)
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C16  C15  C14  120.2(5)

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