Electronic Supplementary Information (ESI)

Synthesis of New Terpyridine-like ligands based on Triazolopyridines and Benzotriazoles

M. Cabrero-Antonino\textsuperscript{a}, R. Ballesteros-Garrido\textsuperscript{a,b,*}, L. Chiassai\textsuperscript{a}, E. Escrivà\textsuperscript{c}, C. Ramirez de Arellano\textsuperscript{a,d}, R. Ballesteros\textsuperscript{a} and B. Abarca\textsuperscript{a}.

S1: Materials and Methods
S2: NMR Spectra
S3: Fluorescence Spectra
S4 Ortep for \textit{TPT} and \textit{Ru(TPT)}\textsubscript{2}
S5: HRMS and NMR Spectra of \textit{Ru(TPT)}\textsubscript{2}

\textit{\textsuperscript{a)} Universitat de Valencia, Facultat de Farmacia Dpto Química Organica, Vicente Andres Estellés s/n 46100 Burjassot, Spain}
\textit{\textsuperscript{b)} ICMol, Universitat de Valencia Catedrático José Beltrán Martínez nº 2 46980 Paterna, Spain}
\textit{\textsuperscript{c)} Universitat de Valencia, Facultat de Farmacia Dpto Química Inorganica, Vicente Andres Estellés s/n 46100 Burjassot, Spain}
\textit{\textsuperscript{d)} Centro de Innovación en Química Avanzada (ORFEO–CINQA), E-46100, Valencia, Spain}
Starting materials, if commercially available, were purchased and used as such. The solvents used were of spectroscopic or equivalent grade. When known compounds had to be prepared by literature procedures, pertinent references are given. Melting points or ranges (m.p.) given were determined on a Büchi B-545 heated stage. \(^1\)H and (\(^1\)H decoupled) \(^{13}\)C nuclear magnetic resonance (NMR) spectra were recorded at 300 and 75 MHz. Chemical shifts are reported in δ units, parts per million (ppm), and were measured relative to the signals for residual deuterated water or deuterated methanol. Coupling constants (J) are given in Hz. Coupling patterns are abbreviated as, for example, s (singlet), d (doublet), t (triplet), q (quartet), td (triplet of doublets), m (multiplet), app. s (apparent singlet) and br. (broad). COSY and DEPT/ed-HSQC experiments were performed for all compounds. IR spectra were recorded using FT-IR ATR. HRMS were recorded using TOF electro-spray ionization (ESI-positive). UV-Visible spectra were measured on an Agilent 8453 spectrometer equipped with a Peltier temperature controller system (±0.1 °C). The emission spectra were recorded with a PTI MO- 5020 spectrofluorimeter in the 300–700 nm range. Quantum yield was determined with a Hamamatsu-PHA equipment. The absorbance of the excitation wavelength was maintained lower than 0.15. \(10^{-5}\) M solutions of ligands were prepared using 98/2 ethanol/water v/v as solvent. \(M^{2+}\) solutions were prepared solving the corresponding perchlorate in 98/2 ethanol/water v/v \(10^{-3}\) mol dm\(^{-3}\) concentration. Working solutions were obtained mixing 2 mL of the solution of ligands with the corresponding amounts of the solutions of the metals.
S2: NMR Spectra
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Mar27-2015
ab8050
cosyg CDCl3 /opt/topspin ABAR 45
S2: NMR Spectra

Mar27-2015
ab8050
hsqced CDCl3 /opt/topspin ABAR 45
S2: NMR Spectra
S2: NMR Spectra
S2: NMR Spectra

AB$_2$ system

Mar13-2014
ab8023
cosygpcDCl3 /opt/topspin ABAR 53
S2: NMR Spectra
S2: NMR Spectra
S2: NMR Spectra
S2: NMR Spectra

Mar27-2015
ab8058
hsqc CCl3 /opt/topspin ABAR 46
S3: Fluorescence Spectra

Fluorescence Spectra of TPT (5), BPT (6), and BPB (7) with and without Zn.

Emission (a.a.) vs Wavelength (nm)

- TPT (5): Blue line for TPT, Red line for TPT[Zn]
- BPT (6): Blue line for BPT, Red line for BPT[Zn]
- BPB (7): Blue line for BPB, Red line for BPB[Zn]
S4 Ortep for TPT and Ru(TPT)$_2$

**TPT CDCC-1537651**

**Ru(TPT)$_2$ CDCC-1537650**
S5: HRMS and NMR Spectra of Ru(TPT)$_2$

**Chemical Formula:** C$_{33}$H$_{22}$N$_{14}$Ru$^{2+}$

**Exact Mass:** 743.1419

$m/z^2$ [C$_{33}$H$_{22}$N$_{14}$Ru$^{2+}$] calc: 365.0670 found: 365.0610

**Found elemental compositions**

**MS Details**

**Isotope cluster details**

**Compound Details**

**MS result summary for RuC$_{21}$H$_{24}$N$_{14}$F$_6$, [M+2H]$$^{++}$$**
S5: HRMS and NMR Spectra of Ru(TPT)$_2$
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