

SUPPORTING INFORMATION FOR

**“Dendritic Ir(III) Complexes Functionalized with Triphenylsilylphenyl Groups: Synthesis, DFT
Calculation and Comprehensive Structure-Property Correlation”**

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Characterization Data of cyclometalating ligand for Ir(ppyTPS)₃, 2-Phenyl-4-(4-(triphenylsilyl)phenyl)pyridine (1').

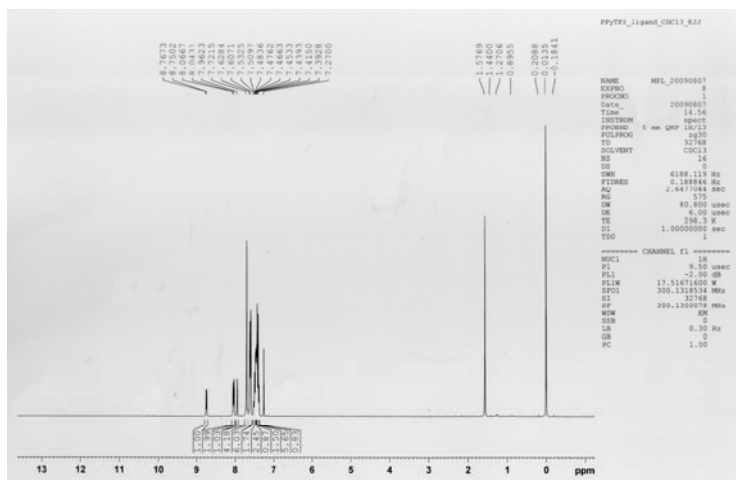


Figure S1 ¹H NMR (CDCl₃, 300 MHz) of cyclometalating ligand for Ir(ppyTPS)₃

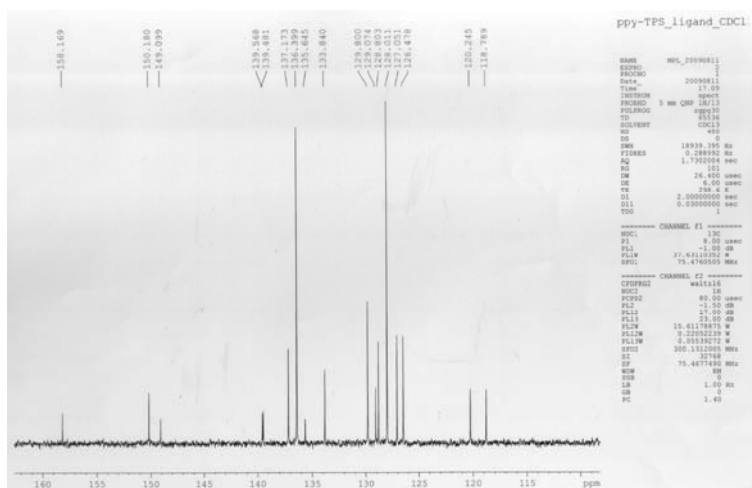


Figure S2 ¹³C NMR (CDCl₃, 75 MHz) of cyclometalating ligand for Ir(ppyTPS)₃

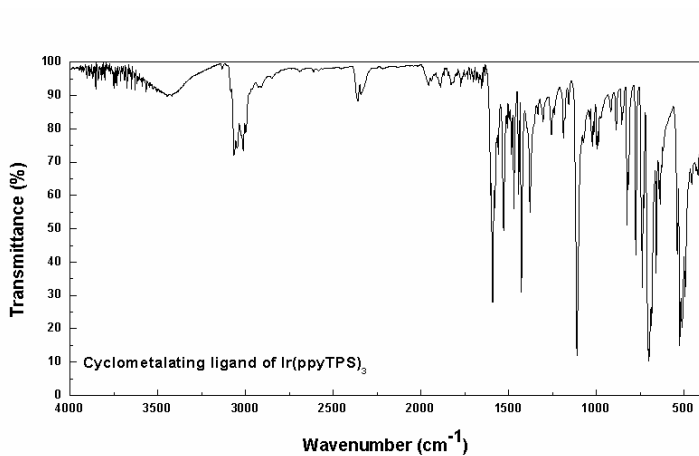


Figure S3 FT-IR spectrum of cyclometalating ligand for Ir(ppyTPS)₃ in KBr disk

Characterization Data of Ir(ppyTPS)₃, Ir(III) Tris(2-phenyl-4-(4-(triphenylsilyl)phenyl)pyridinato-N,C^{3'}) (1).

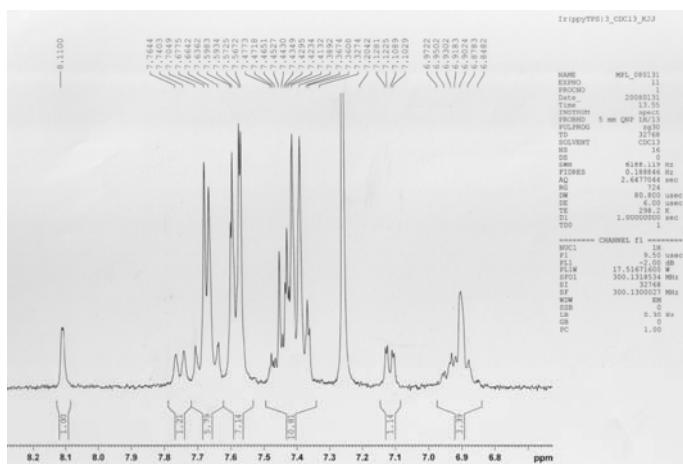


Figure S4 ¹H NMR (CDCl₃, 300 MHz) of Ir(ppyTPS)₃

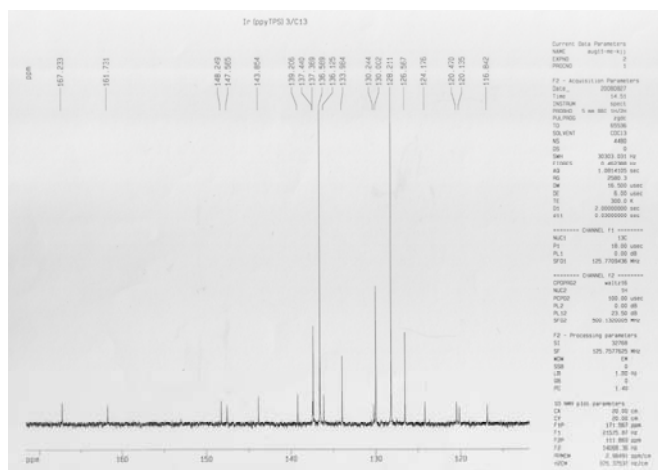


Figure S5 ¹³C NMR (CDCl₃, 125 MHz) of Ir(ppyTPS)₃

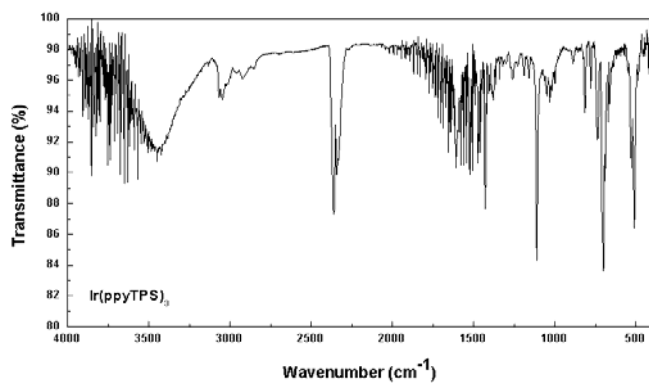


Figure S6 FT-IR spectrum of Ir(ppyTPS)₃ in KBr disk

Characterization Data of cyclometalating ligand for Ir(TPSppyTPS)₃, 2-(4'-(Triphenylsilyl)biphenyl-3-yl)-4-(4-(triphenylsilyl)phenyl)pyridine (2').

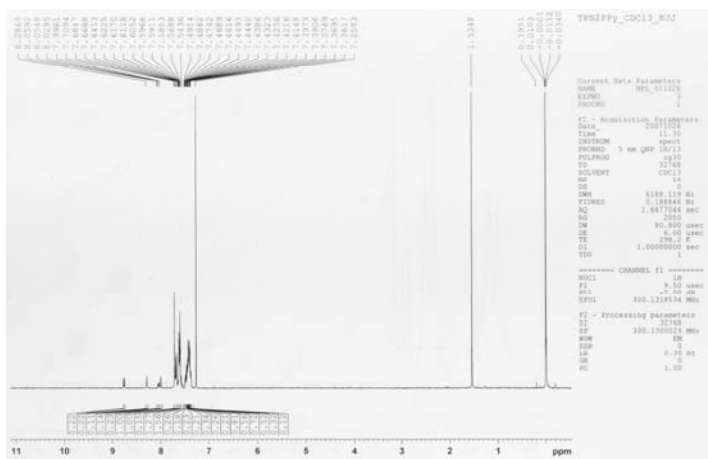


Figure S7 ¹H NMR (CDCl₃, 300 MHz) of cyclometalating ligand for Ir(TPSppyTPS)₃

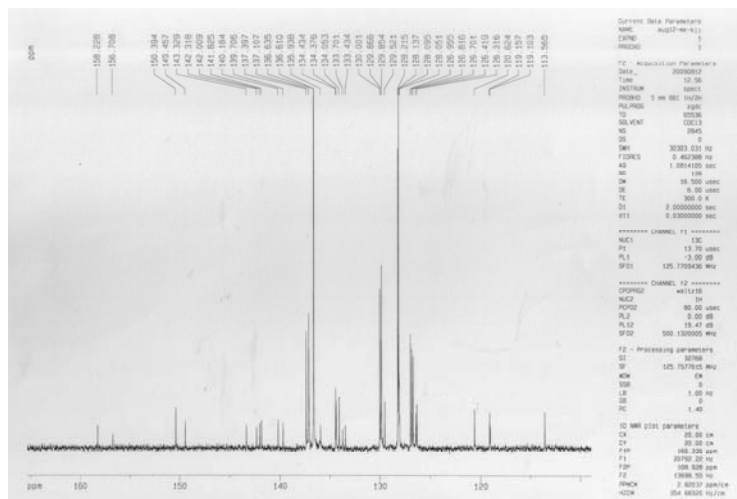


Figure S8 ¹³C NMR (CDCl₃, 125 MHz) of cyclometalating ligand for Ir(TPSppyTPS)₃

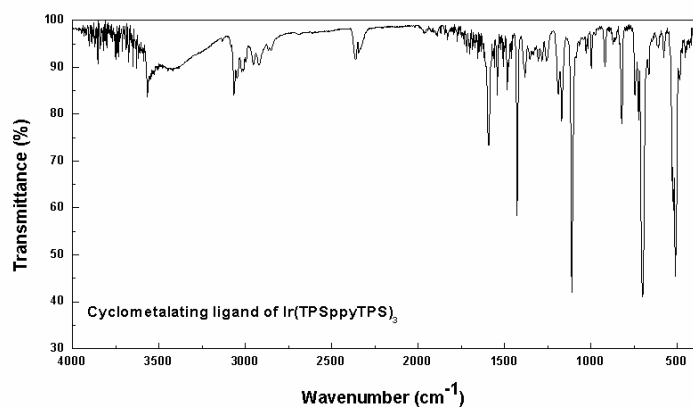


Figure S9 FT-IR spectrum of cyclometalating ligand for Ir(TPSppyTPS)₃ in KBr disk

Characterization Data of Ir(TPSPpyTPS)₃, Ir(III) tris(2-(4'-(triphenylsilyl)biphenyl-3-yl)-4-(triphenylsilyl)phenyl)pyridinato-*N,C*^{3'}) (2).

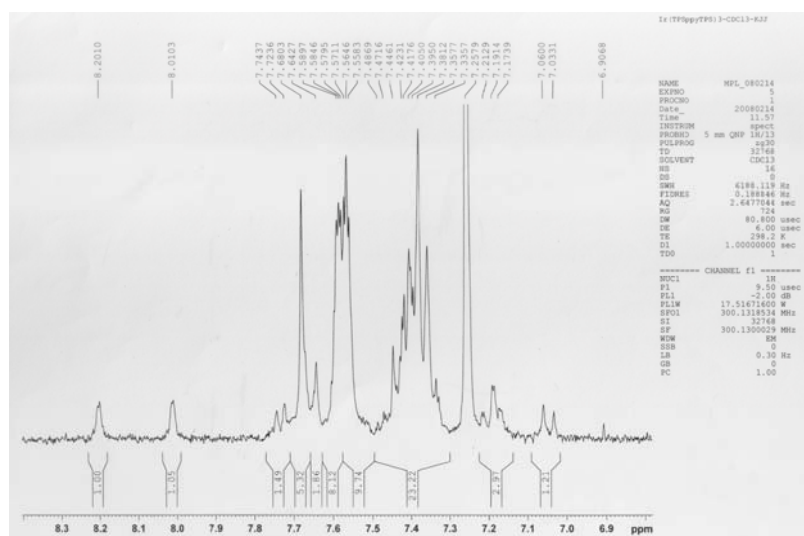


Figure S10 ¹H NMR (CDCl₃, 300 MHz) of Ir(TPSPpyTPS)₃

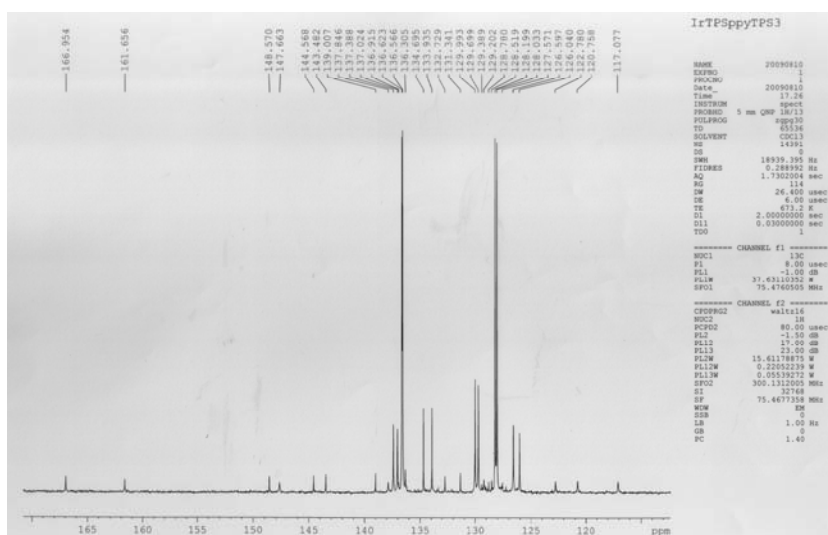


Figure S11 ¹³C NMR (CDCl₃, 75 MHz) of Ir(TPSPpyTPS)₃

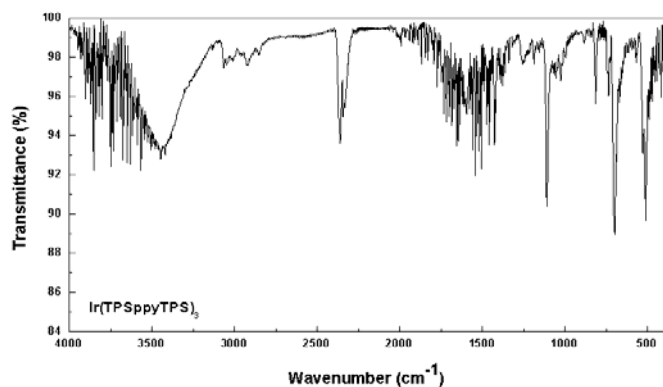


Figure S12 FT-IR spectrum of Ir(TPSPpyTPS)₃ in KBr disk

Characterization Data of Ir(TPSPpy)₃, Ir(III) tris(2-(4'-(triphenylsilyl)biphenyl-3-yl)pyridinato-N,C^{3'}) (4).

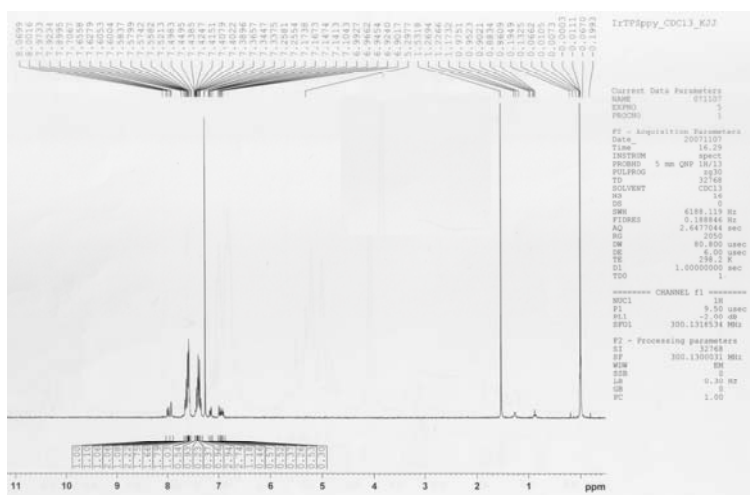


Figure S13 ¹H NMR (CDCl₃, 300 MHz) of Ir(TPSPpy)₃

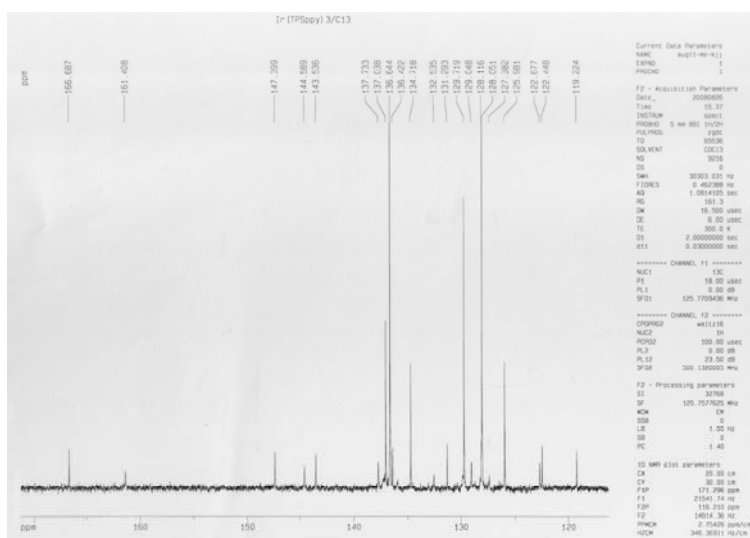


Figure S14 ¹³C NMR (CDCl₃, 125 MHz) of Ir(TPSPpy)₃

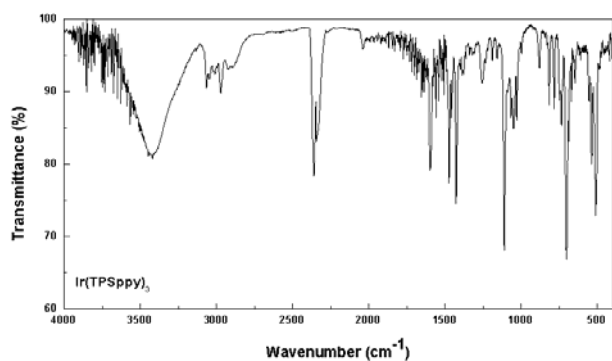


Figure S15 FT-IR spectrum of Ir(TPSPpy)₃ in KBr disk

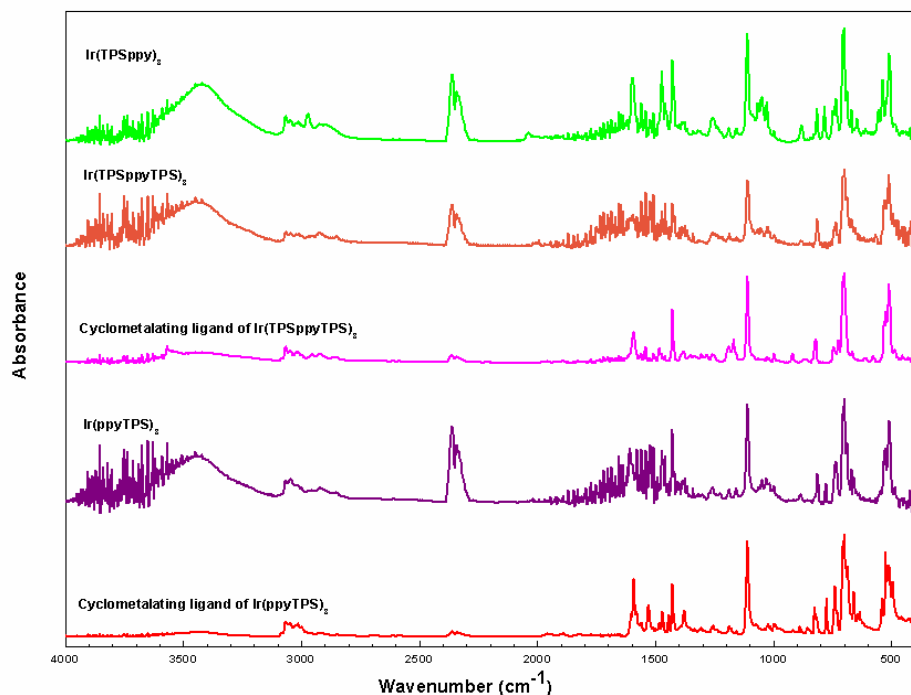


Figure S16 FT-IR spectra of newly synthesized Ir(III) complexes, corresponding ligands and reference in KBr disk

Phenyl-silicon compounds have a strong, characteristic band at about 1100 cm^{-1} which often splits into two when two phenyl groups are attached to the one silicon atom, but appears as a single band in the case of three phenyl groups.¹

Solvatochromic Behavior

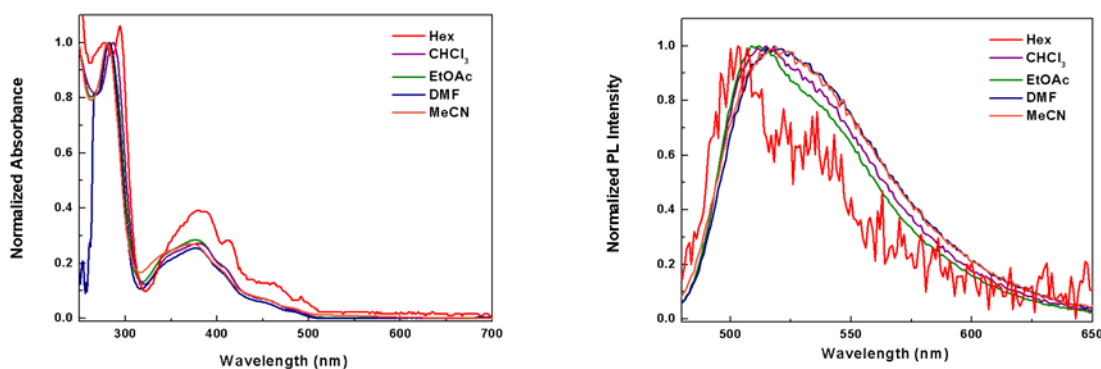


Figure S17 Normalized UV-vis absorption and photoluminescence spectra of Ir(ppy)₃ in the solution state (1.0×10^{-5} M in solvents which show different polarity, excitation wavelength = 340 nm)

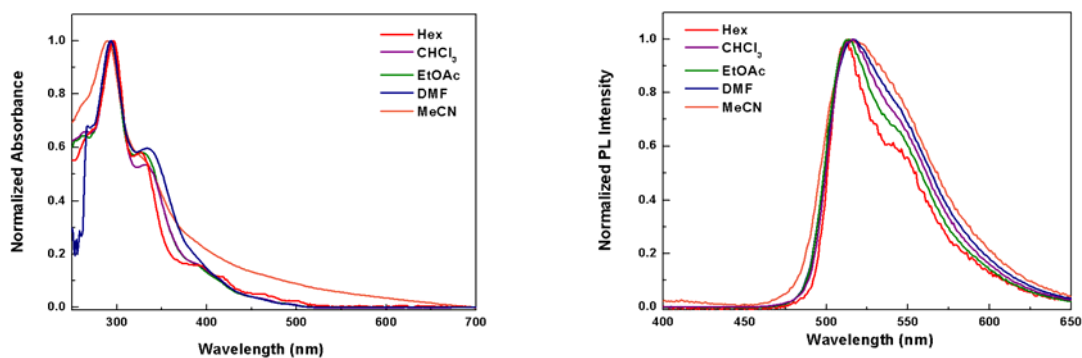


Figure S18 Normalized UV-vis absorption and photoluminescence spectra of Ir(TPSppy)₃ in the solution state (1.0×10^{-5} M in solvents which show different polarity, excitation wavelength = 340 nm)

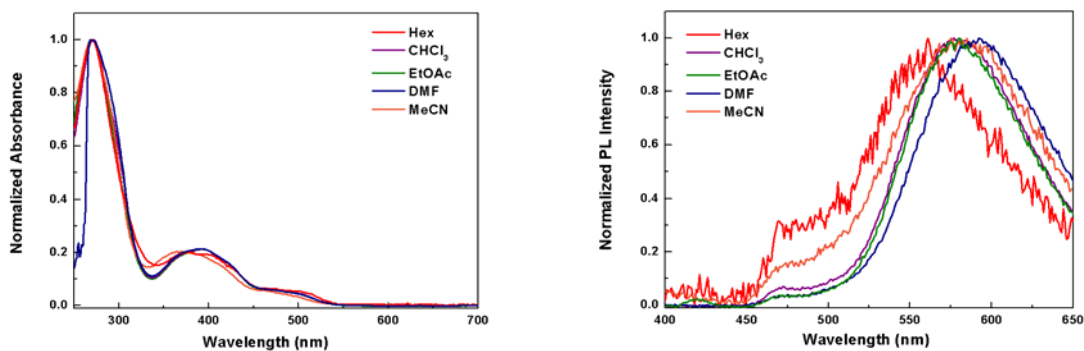


Figure S19 Normalized UV-vis absorption and photoluminescence spectra of Ir(ppyTPS)₃ in the solution state (1.0×10^{-5} M in solvents which show different polarity, excitation wavelength = 340 nm)

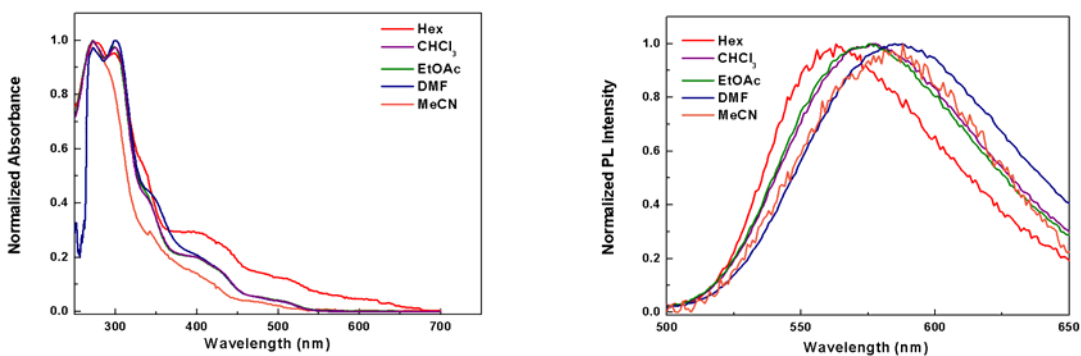


Figure S20 Normalized UV-vis absorption and photoluminescence spectra of Ir(TPSpyTPS)₃ in the solution state (1.0×10^{-5} M in solvents which show different polarity, excitation wavelength = 340 nm)

Enhanced Thermal Property

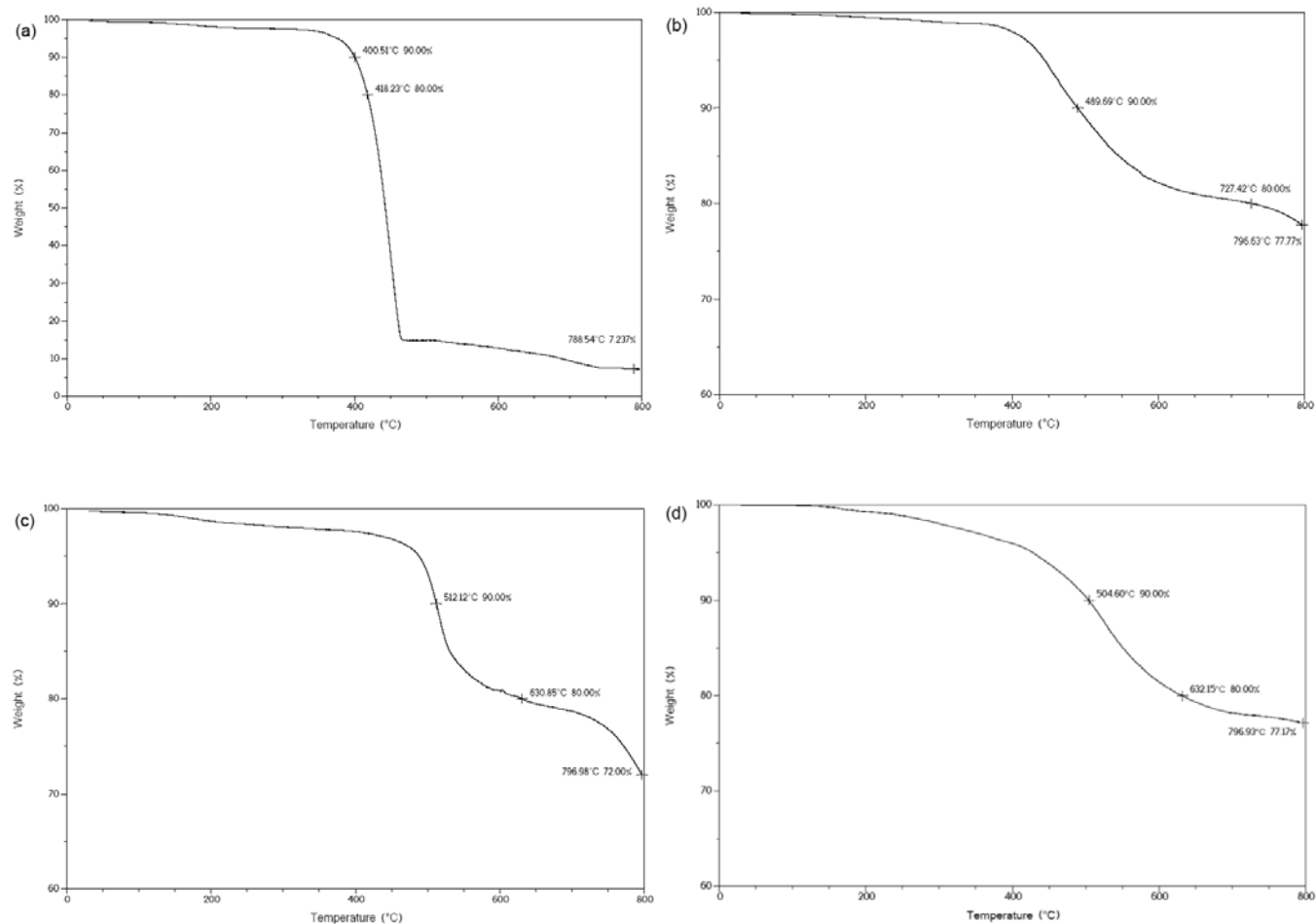


Figure S21 Thermal gravimetric analysis of Ir(III) complexes (a) Ir(ppy)₃, (b) Ir(TPSppy)₃, (c) Ir(ppyTPS)₃, and (d) Ir(TPSppyTPS)₃

Reference

1. George Socrates, *Infrared Characteristic Group Frequencies*, John Wiley & Sons, Chichester, 2nd edn., 1994, ch. 18, pp. 188-194.