Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Tetrazole Iridium(III) complexes as class of phosphorescent emitters for high-efficiency OLEDs

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Figure 1. TGA data complexes (IrTz1, IrTz2, IrTz3)

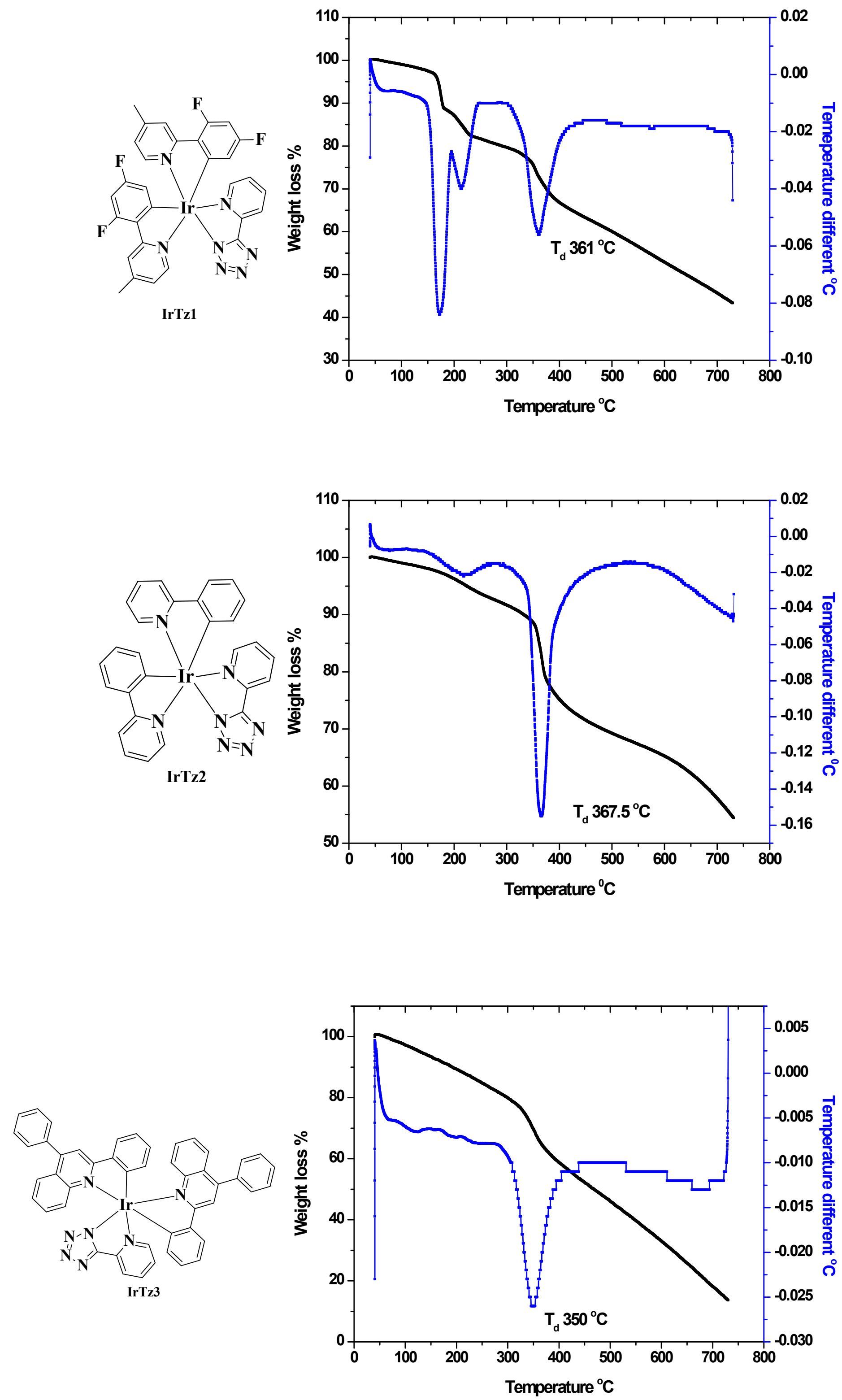


Figure 2. Molecular orbitals of phosphor complexes

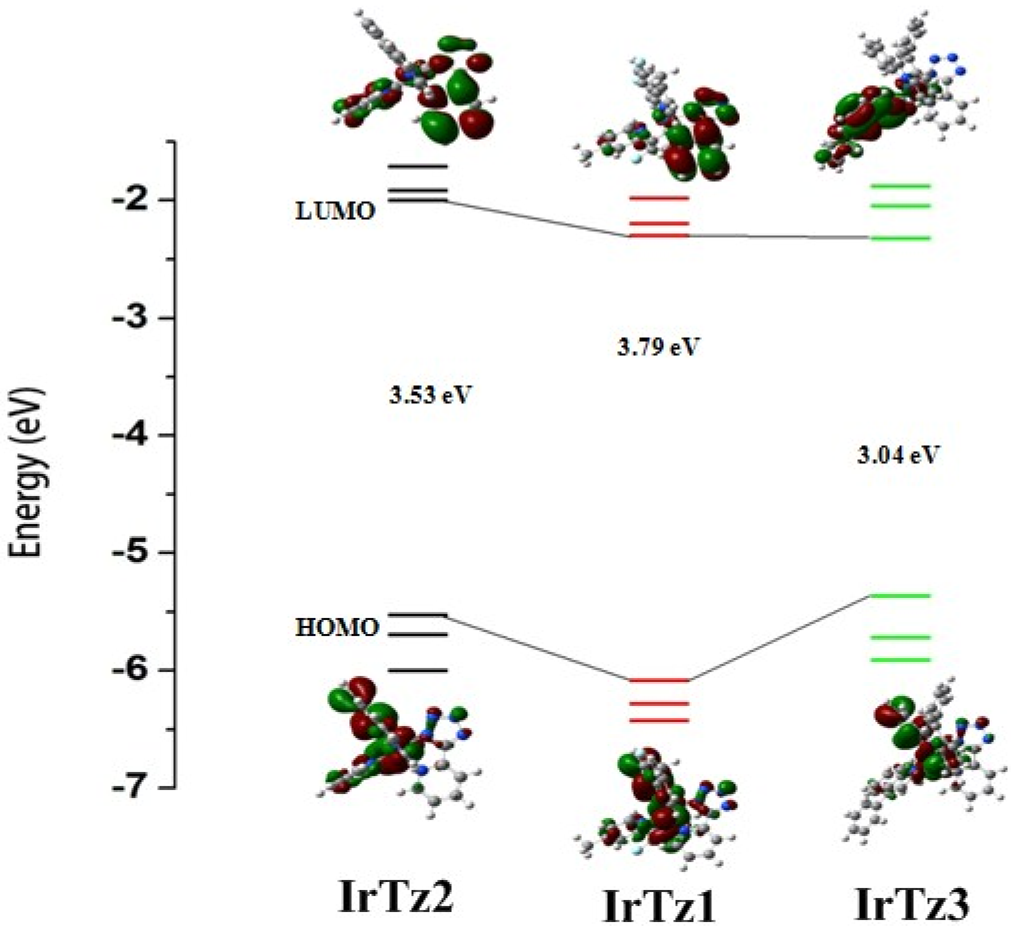


Figure 3. Cyclic voltammograms of phosphor complexes.

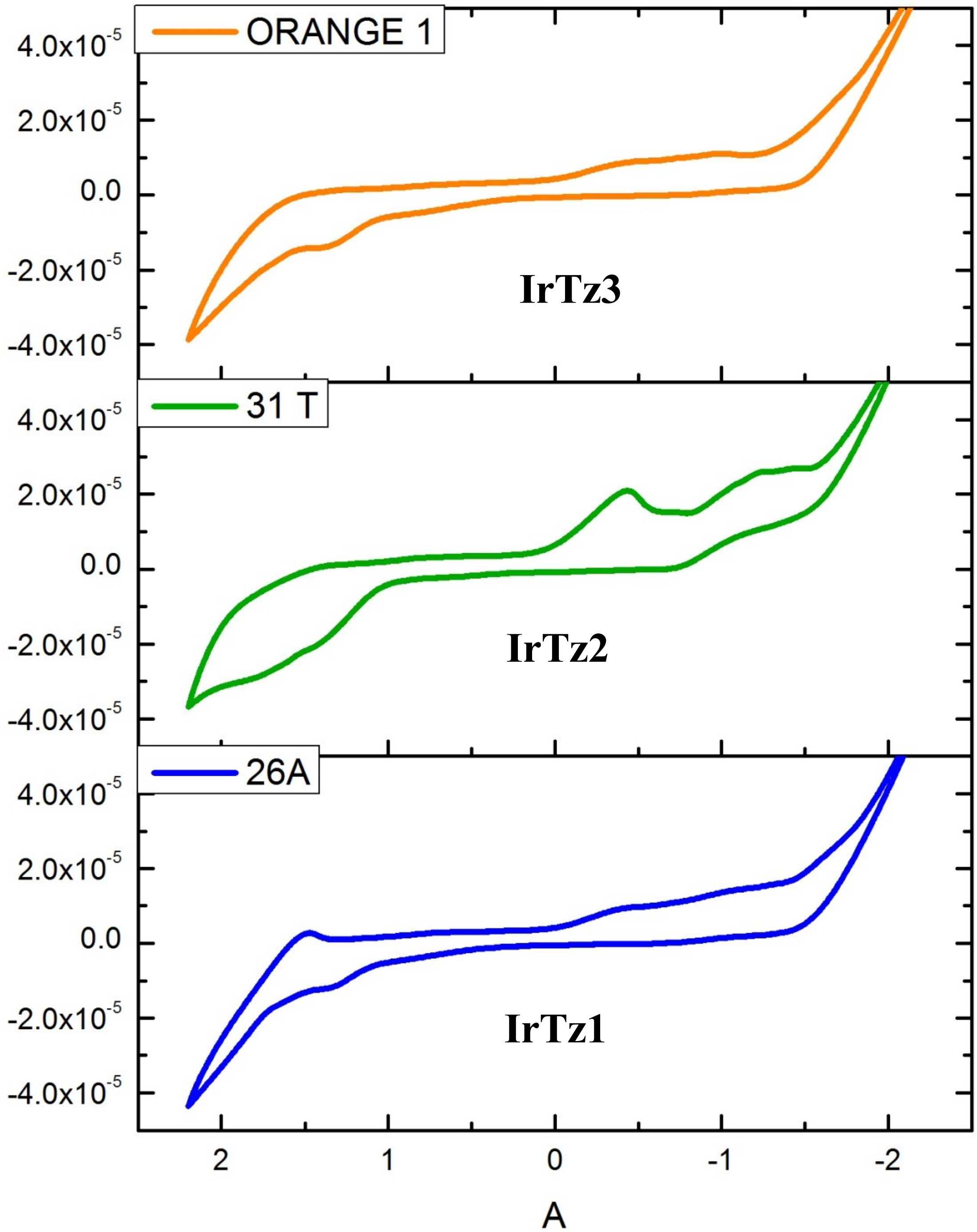


Figure 4. PL excitation spectra of thin films (60 nm thick) of an Ir complex (8 wt%) in BCPO matrix**: IrTz1** (blue, λ_{em} = 520 nm), **IrTz2** (green, λ_{em} = 530 nm) and **IrTz3** (orange, λ_{em} = 600 nm) and bare **BCPO** thin film (black, λ_{em} = 420 nm).

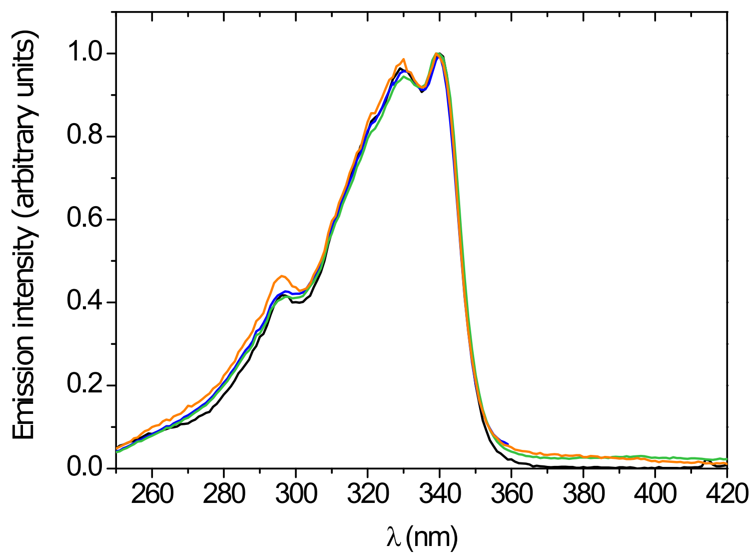


Figure 5. Corrected PL emission (λ_{ex} = 350 nm)spectra of thin films (60 nm thick) of an Ir complex (8 wt%) in BCPO matrix**: IrTz1** (blue) , **IrTz2** (green) and **IrTz3** (orange,) and bare **BCPO** thin film (black).

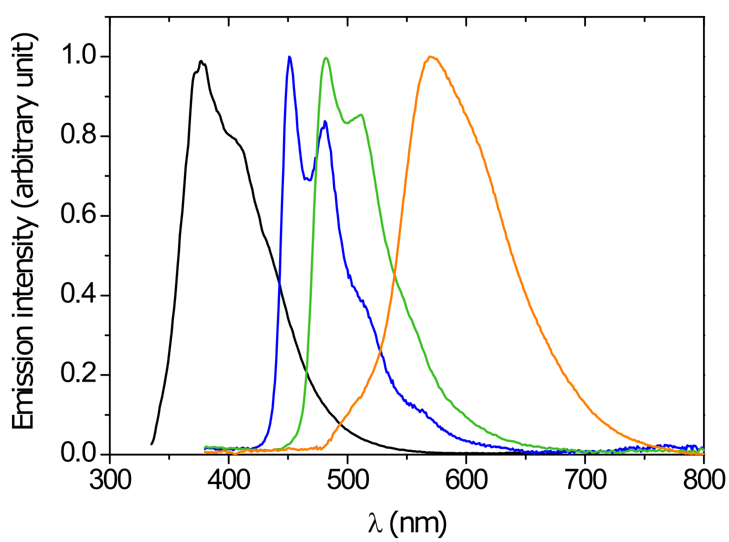


Figure 6. Schematic representation of the layered structure used in the investigated OLEDs.

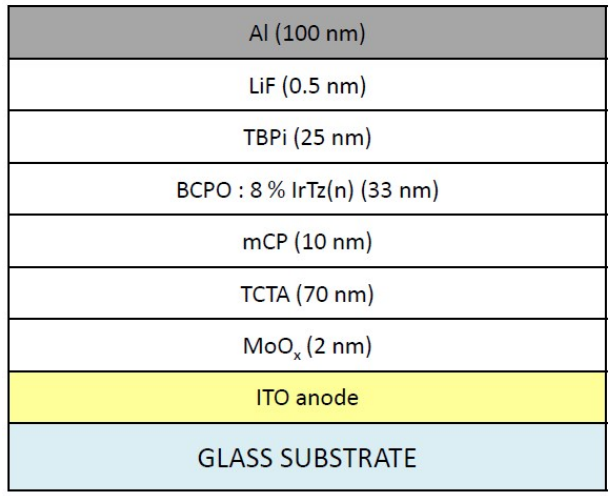


Figure 7. The energy diagrams of the studied OLED devices having Ir complexes as phosphors in the emitting layer.

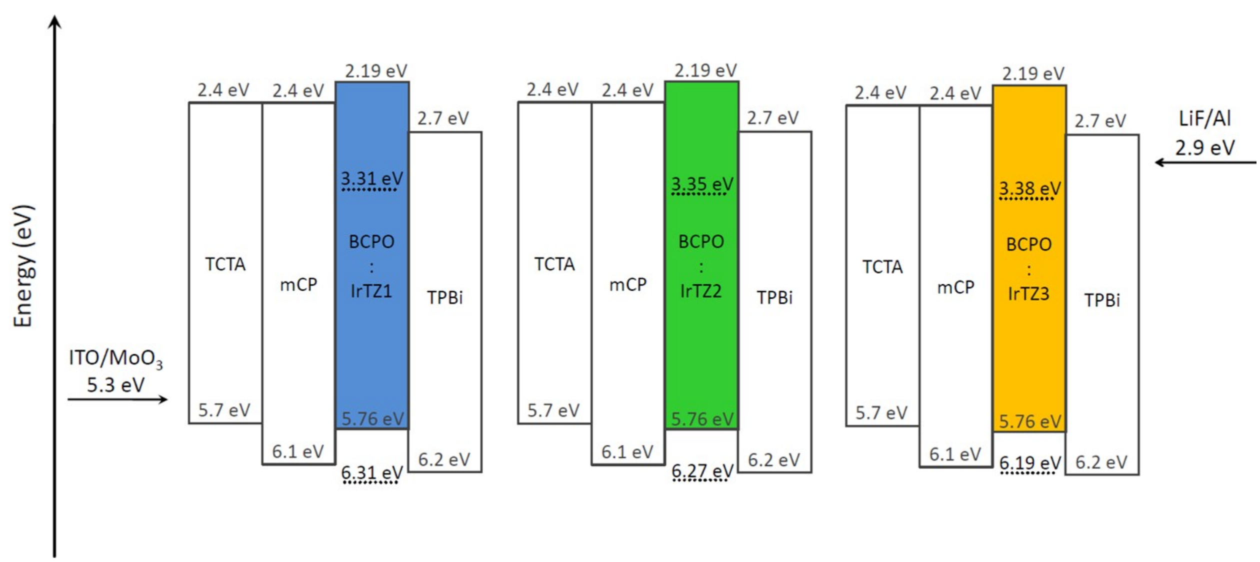


Figure 8. Luminance versus applied voltage for the investigated OLEDs**: IrTz1** (blue), **IrTz2** (green) and **IrTz3** (orange).

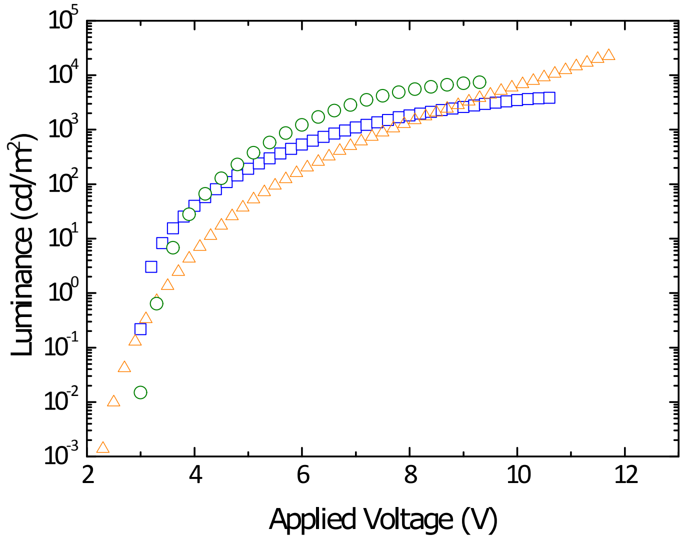


Figure 9. Current density versus applied voltage for the investigated OLEDs**: IrTz1** (blue), **IrTz2** (green) and **IrTz3** (orange).

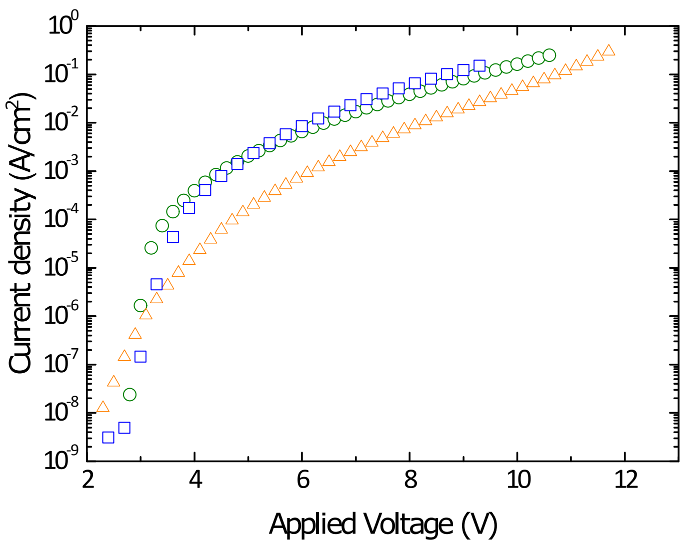


Figure 10. External quantum efficiency versus current density for the investigated OLEDs**:** **IrTz1** (blue), **IrTz2** (green) and **IrTz3** (orange).

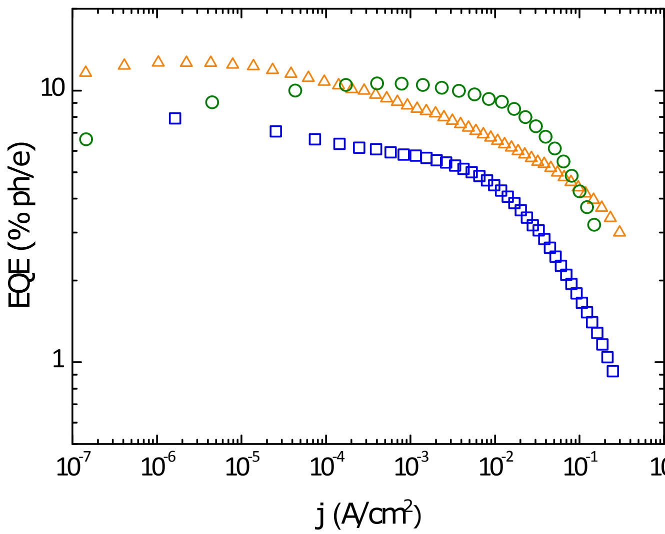


Table 1. Electrochemical properties and molecular orbital energy levels of complexes.

Ir	$^{a}E_{1/2}$ ^{ox} [V]	$^{a}E_{1/2}$ ^{red} [V]	HOMO[b] [eV]	LUMO[b] [eV]	E_g [c] [eV]	HOMO[d] [eV]	LUMO[d] [eV]	E_g [e] [eV]
Tz1	1.51	-1.49	-6.31	-3.31	3.00	-6.08	-2.29	3.79
Tz2	1.47	-0.81, -1.45	-6.27	-3.35	2.92	-5.52	-1.99	3.53
Tz3	1.39	-1.42	-6.19	-3.38	2.81	-5.36	-2.32	3.04

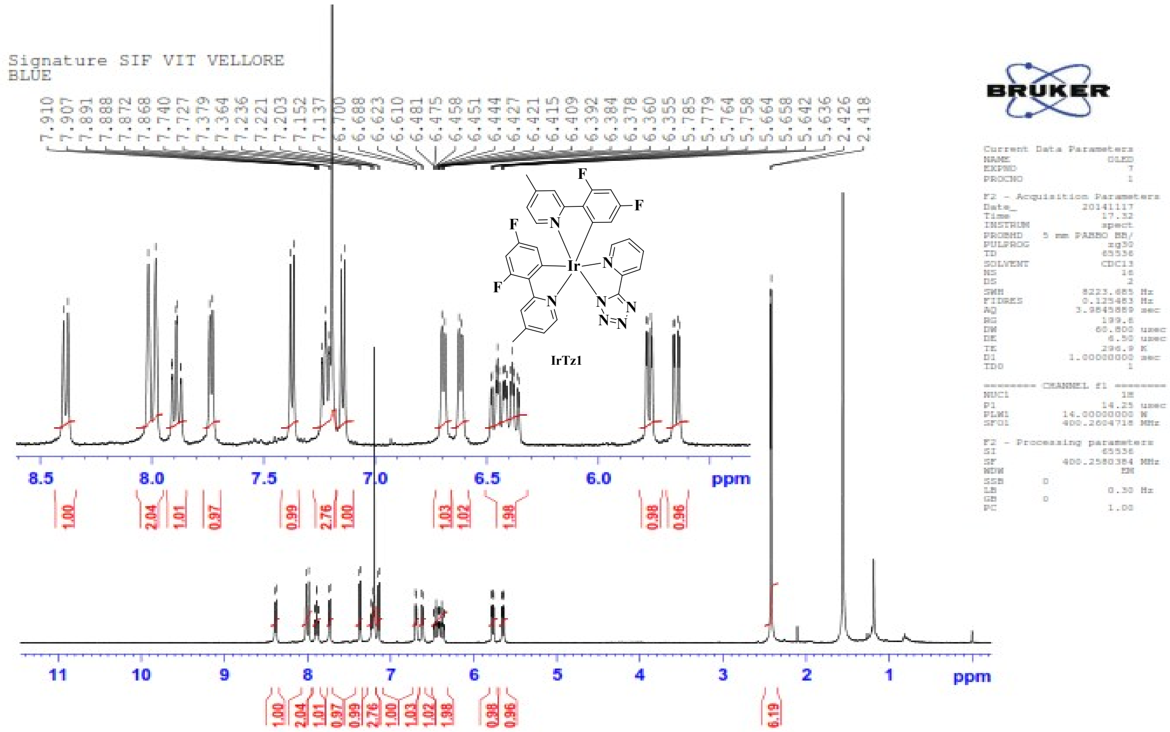
a) The redox potential of compounds obtained from cyclic voltammetry using glassy carbon as working electrode with reference to Fc/Fc+ couple. 0.1 M Tetrabutylmmonium hexafluorophosphate was used as a supporting electrolyte; b) HOMO, LUMO energy calculated using $E_{HOMO} = -(Eox + 4.8)$ eV and $E_{LUMO} = -(E_{red} + 4.8)$ eV; c) HOMO–LUMO energy gap; d) HOMO, LUMO energy calculated using Gaussian 03 programme at B3LYP/6-31G level; e) Computed HOMO–LUMO energy gap.

Table 2. Photophysical properties of of thin films (60 nm thick) of an Ir complex (8 wt%) in BCPO matrix**:**

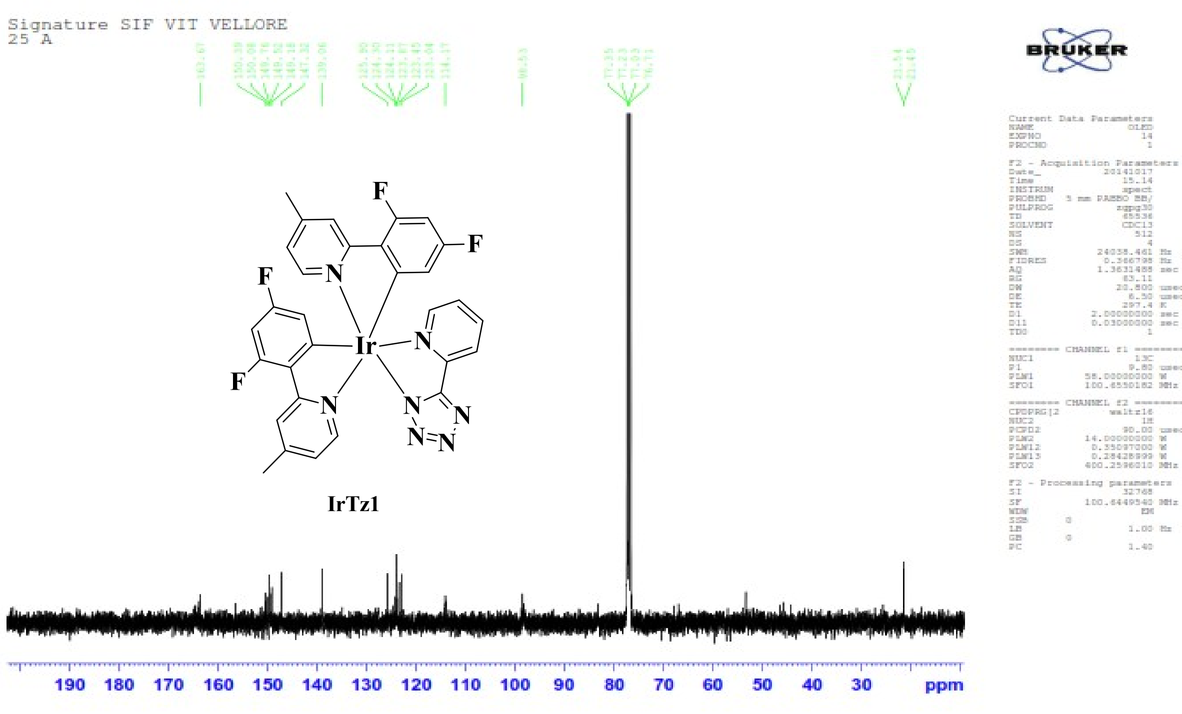
Ir complex	$\lambda_{em\ max}$ (nm)	Φ_{PL} (%)*	τ (μs)	k_r	k_{nr}
IrTz1	451	44	1.4	0.31	0.40
IrTz2	482	60	1.9	0.34	0.19
IrTz3	569	65	1.9	0.32	0.20

* Estimated measurement uncertainty ±10%.

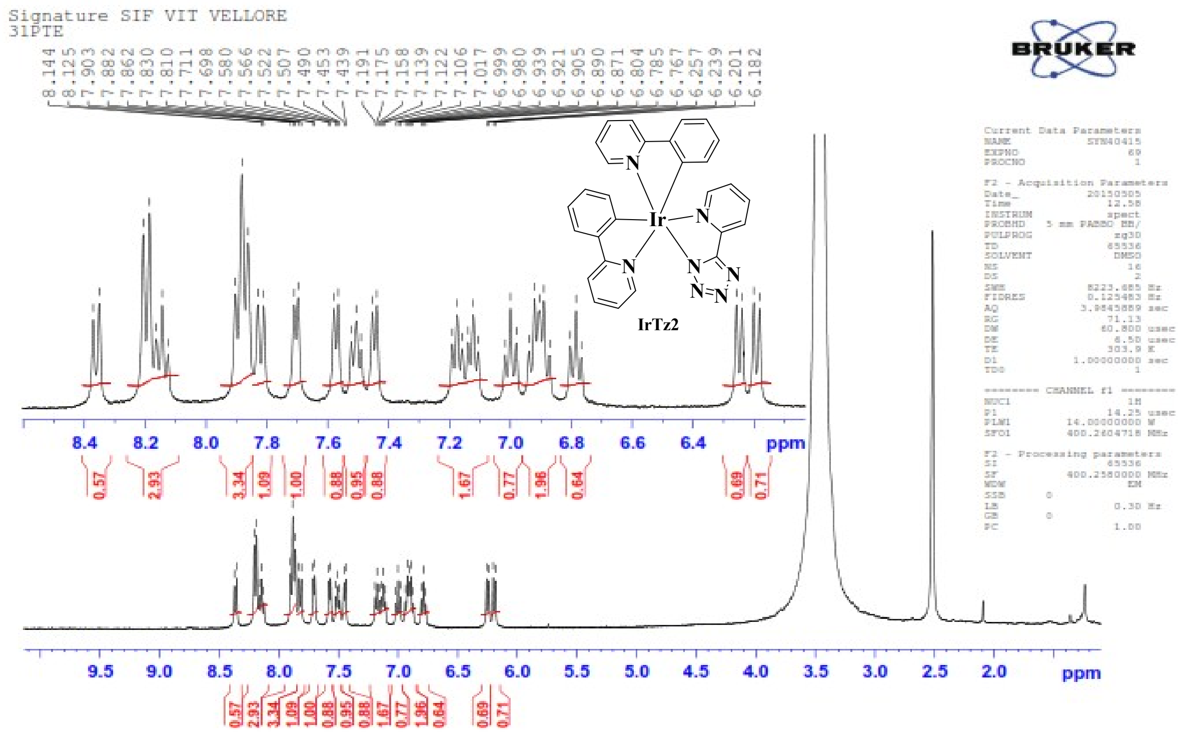
^{1}H-NMR spectrum of IrTz1



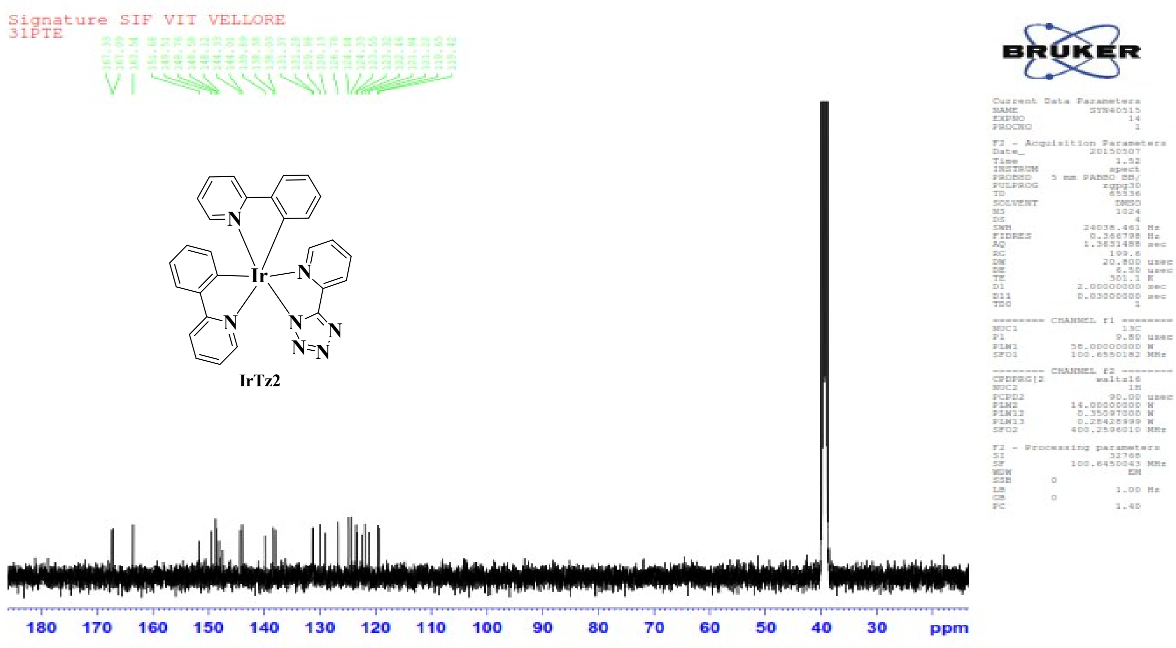
^{13}C-NMR spectrum of IrTz1



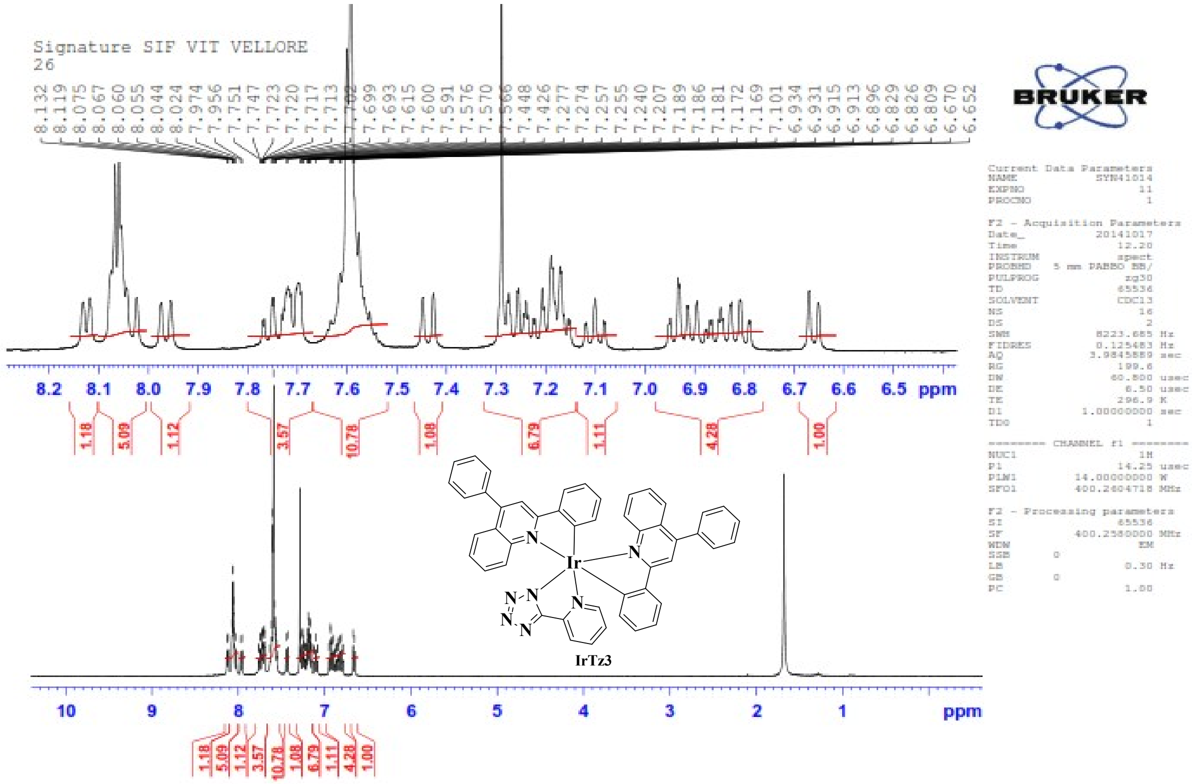
[1]H-NMR spectrum of IrTz2



[13]C-NMR spectrum of IrTz2



[1]H-NMR spectrum of IrTz3



[13]C-NMR spectrum of IrTz3