

Supporting Information

Zinc(II)-Heteroligand Compounds for Wet Processing OLEDs: A Study on Balancing Charge-Carrier Transport and Energy Transfer

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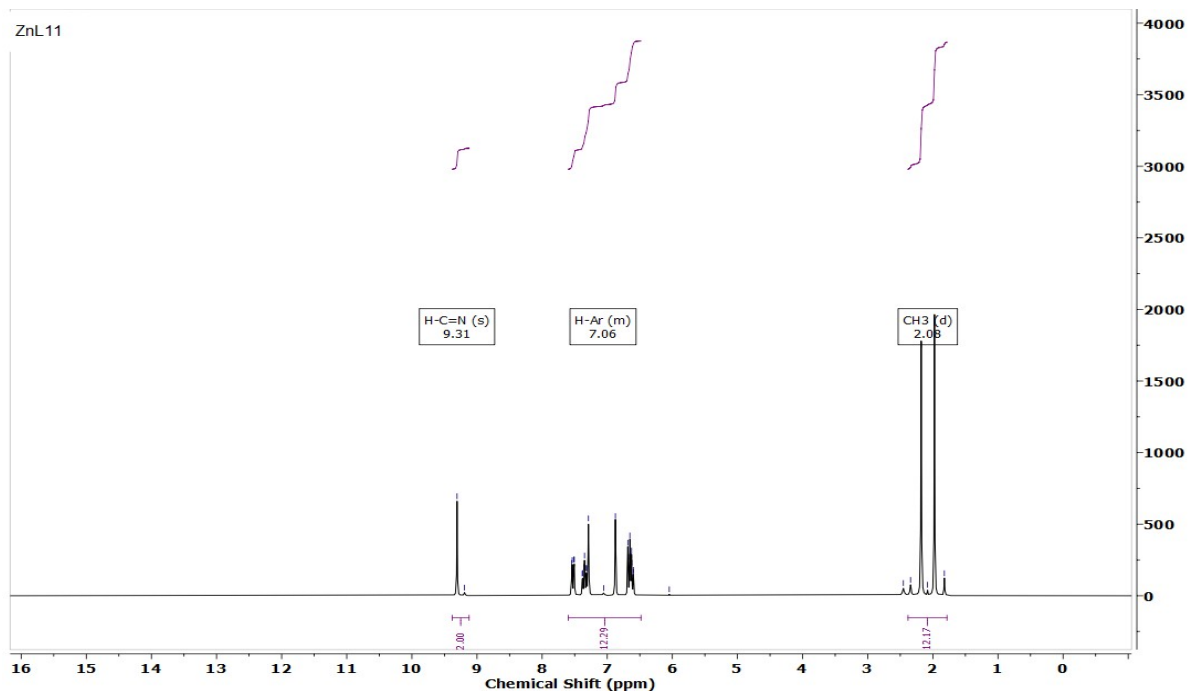


Figure S1. ^1H NMR in $\text{DMSO-}d_6$ of the complex **ZnL11**.

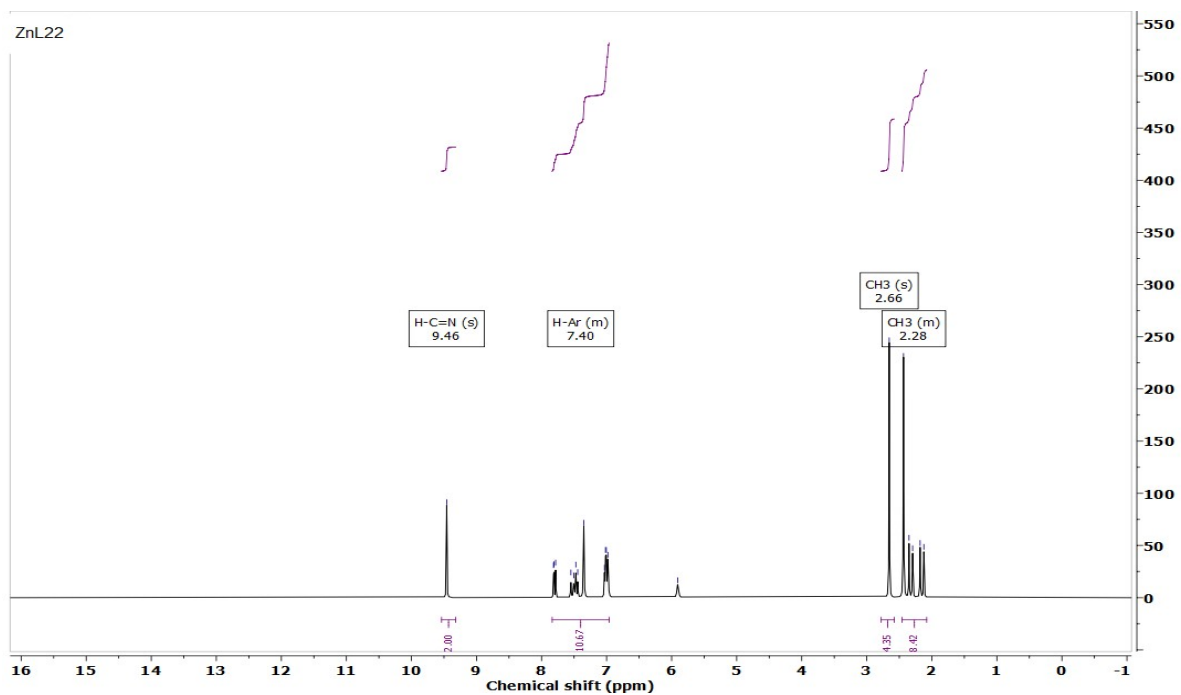


Figure S2. ^1H NMR in $\text{DMSO-}d_6$ of the complex **ZnL22**.

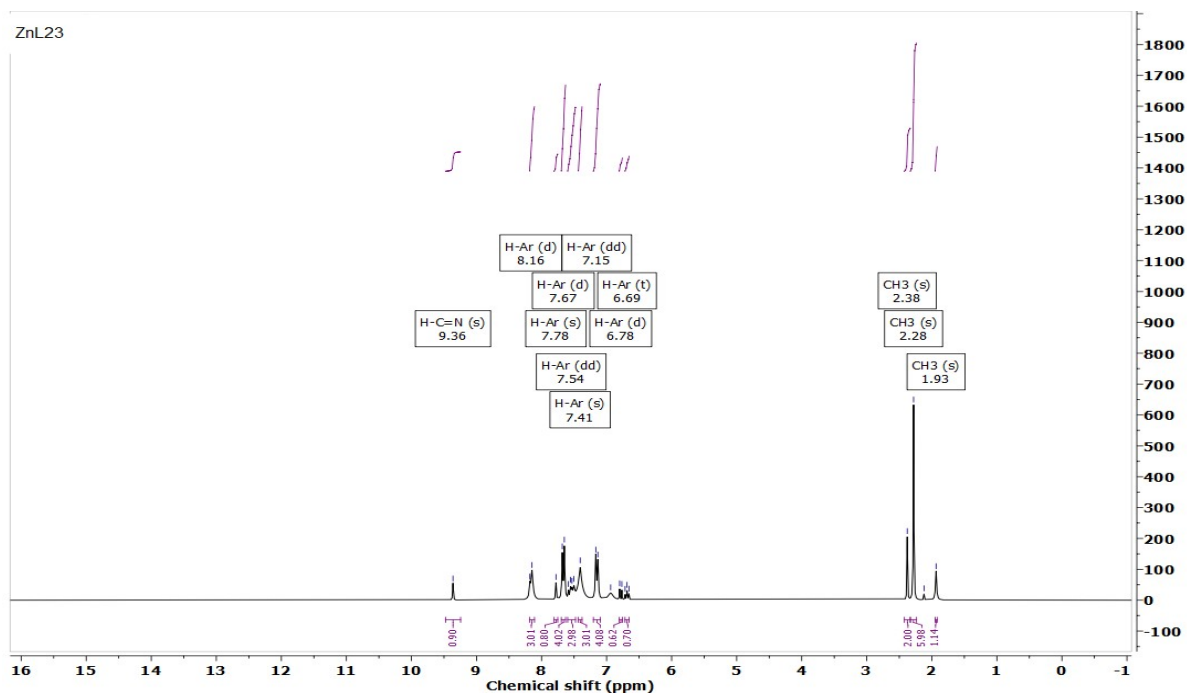


Figure S3. ^1H NMR in $\text{DMSO-}d_6$ of the complex **ZnL13**.

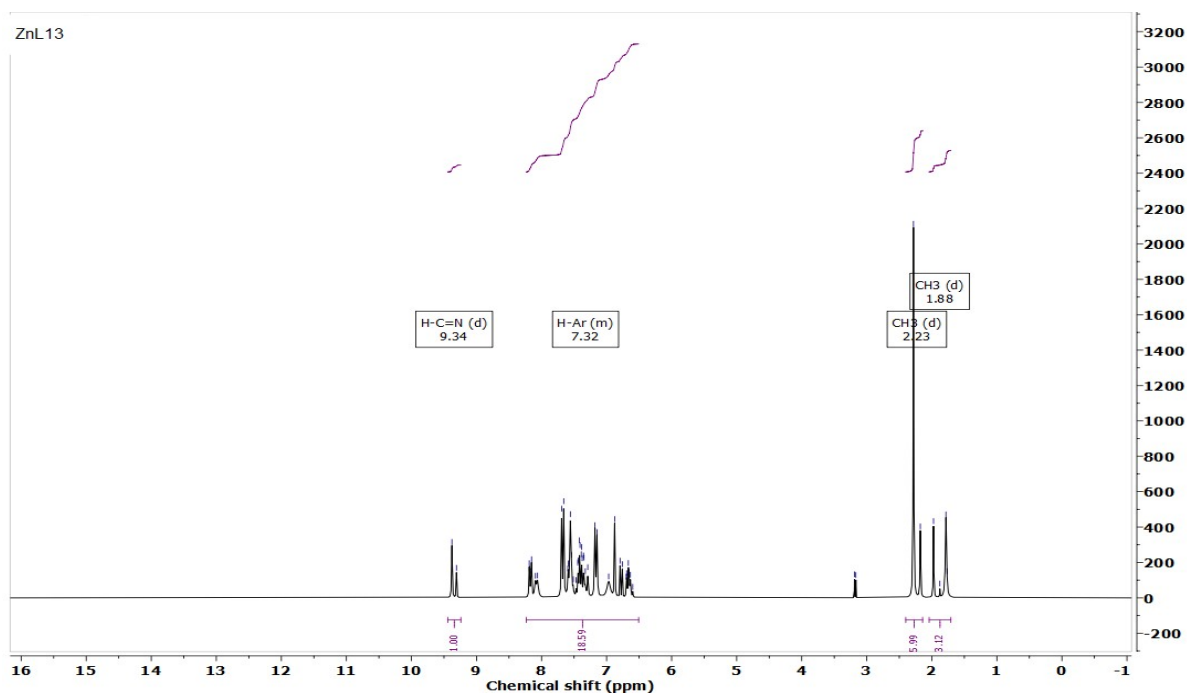


Figure S4. ^1H NMR in $\text{DMSO-}d_6$ of the complex **ZnL23**.

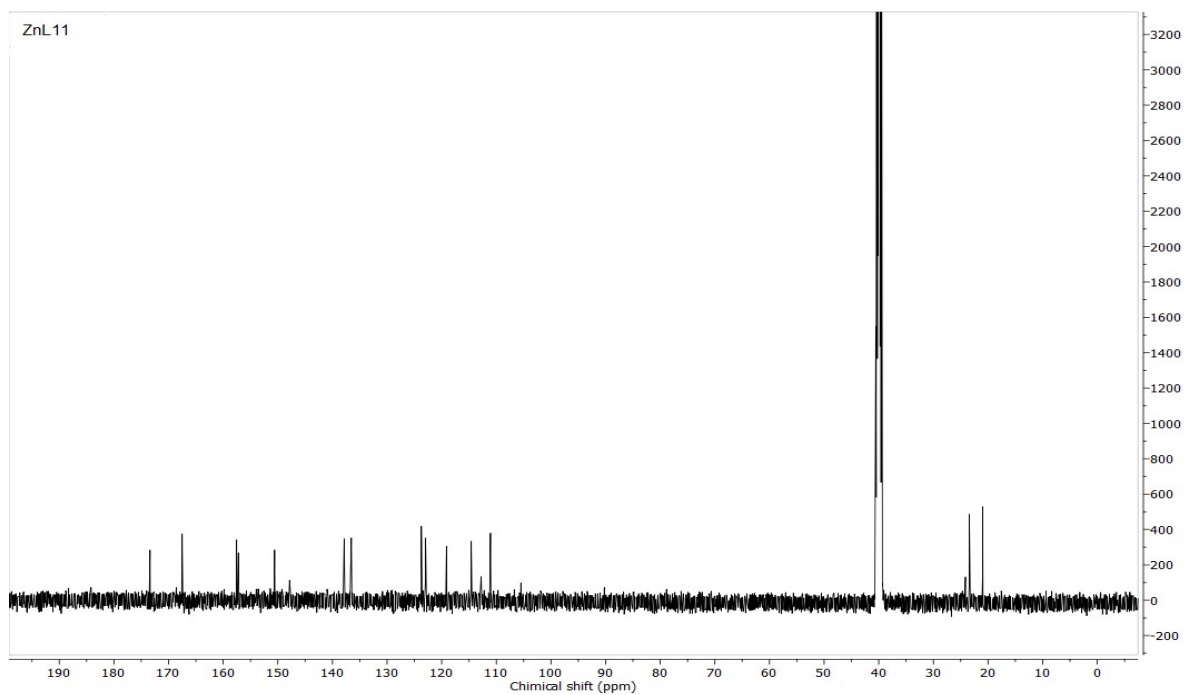


Figure S5. ^{13}C NMR in $\text{DMSO-}d_6$ of the complex **ZnL11**.

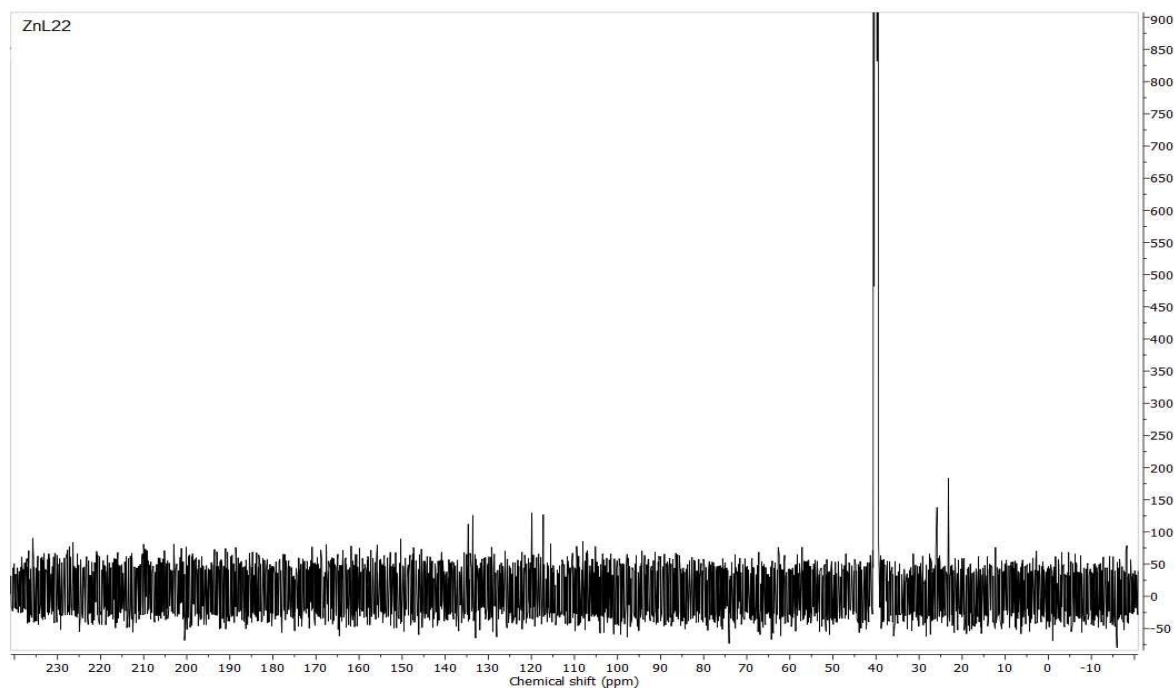


Figure S6. ^{13}C NMR in $\text{DMSO-}d_6$ of the complex **ZnL22**.

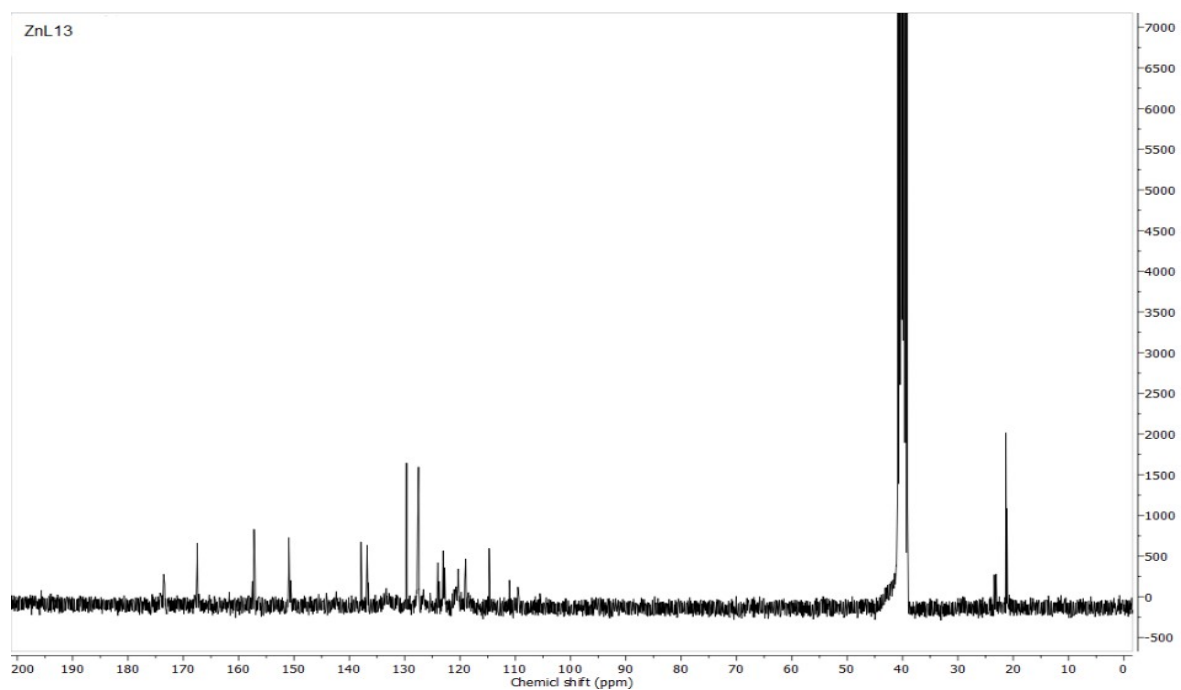


Figure S7. ^{13}C NMR in $\text{DMSO-}d_6$ of the complex **ZnL13**.

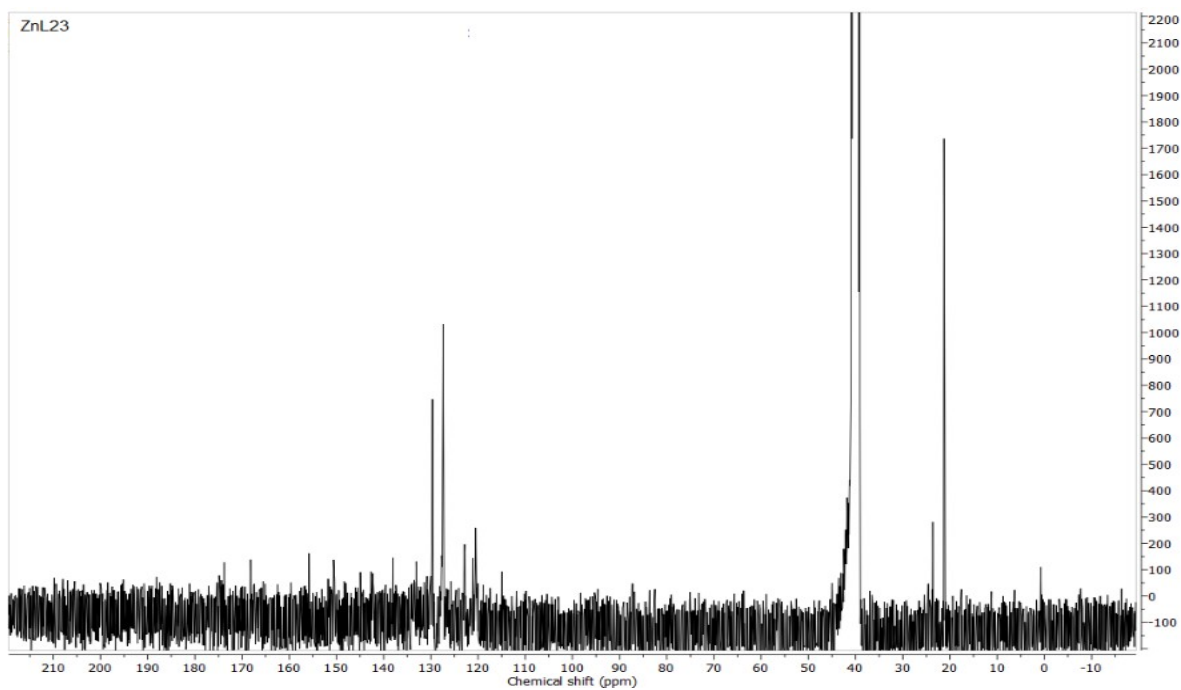


Figure S8. ^{13}C NMR in $\text{DMSO-}d_6$ of the complex **ZnL23**.

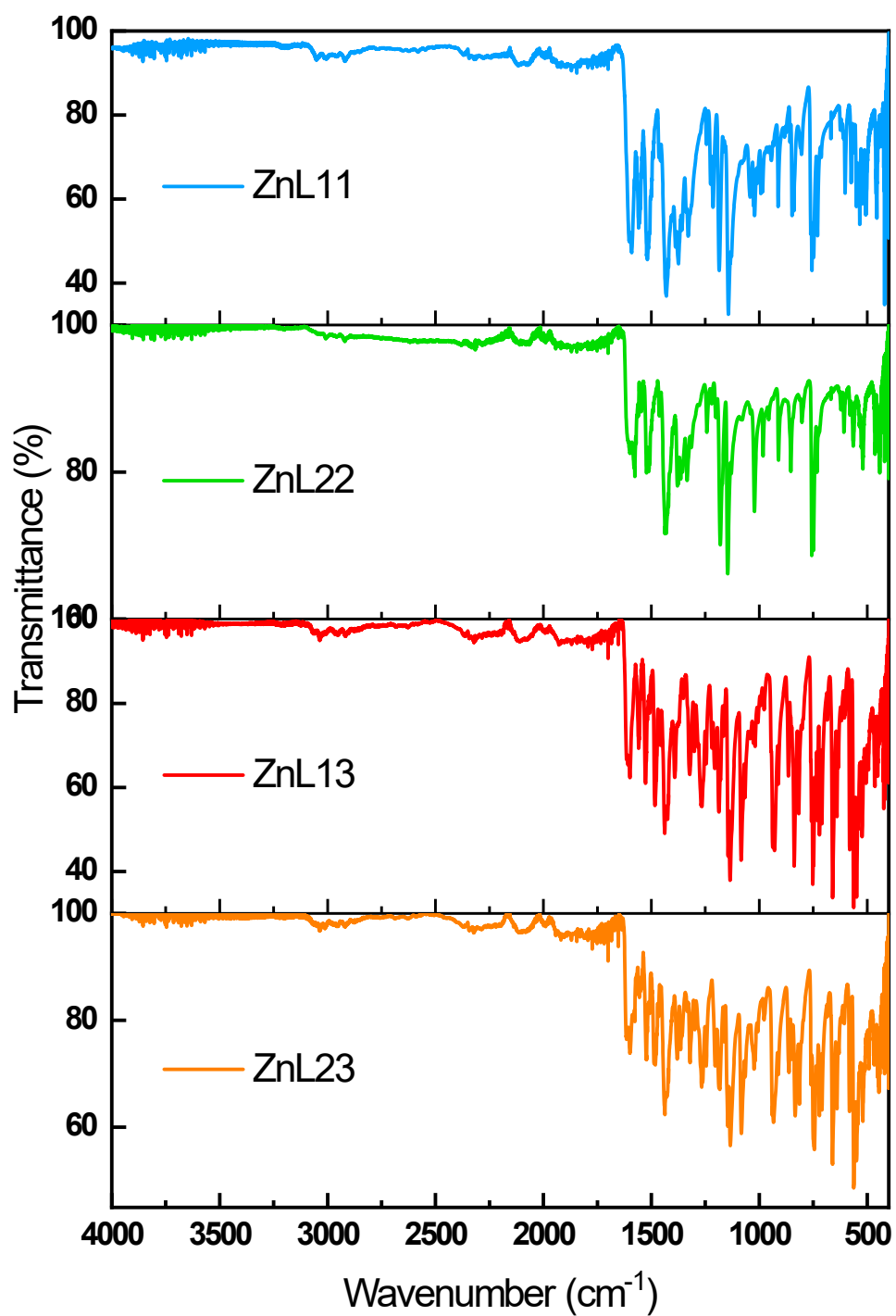


Figure S9. FTIR spectra of all Zinc(II) complexes.

Espectro completo de 100 a 1000 m/z em modo positivo

HM12-MeOH-H₂O, #18-51 RT: 0.08-0.23 AV: 34 NL: 3.20E9
T: FTMS + p ESI Full ms (100.0000-1000.0000)

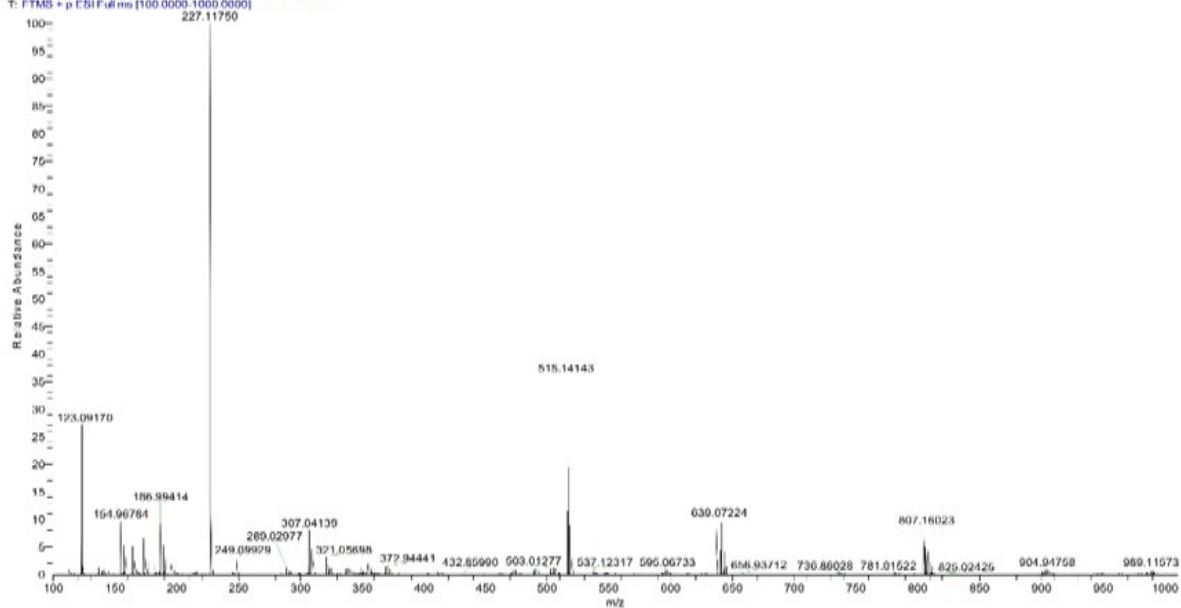


Figure S10. HRMS of the complex ZnL11.

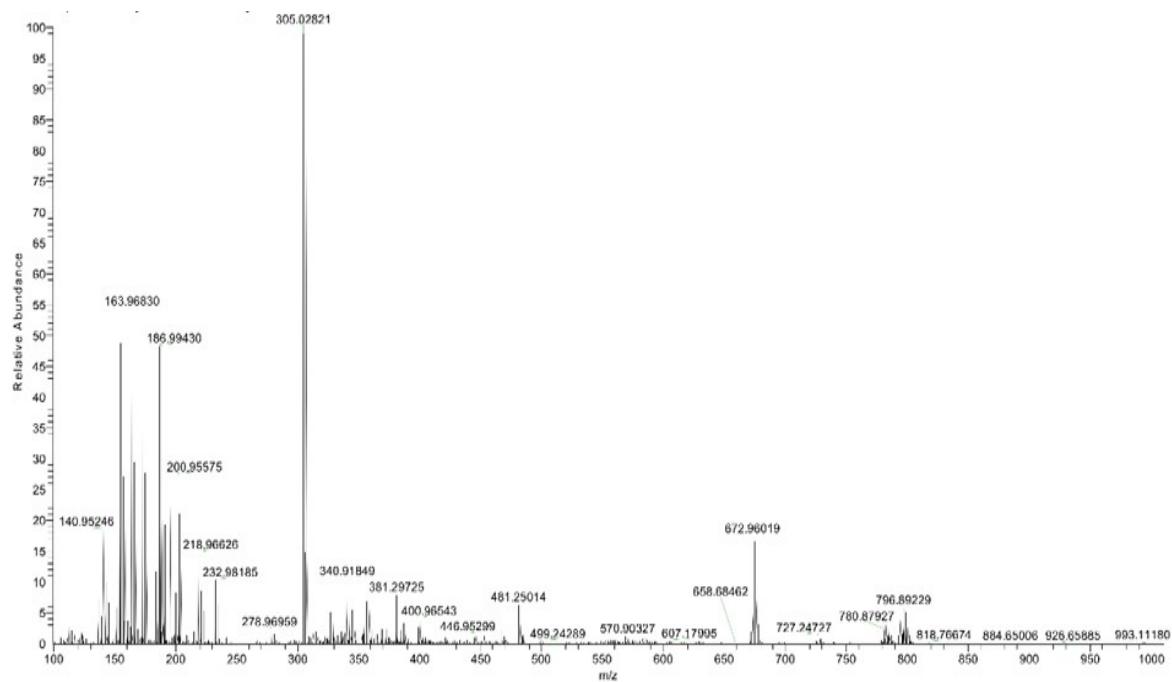


Figure S11. HRMS of the complex ZnL22.

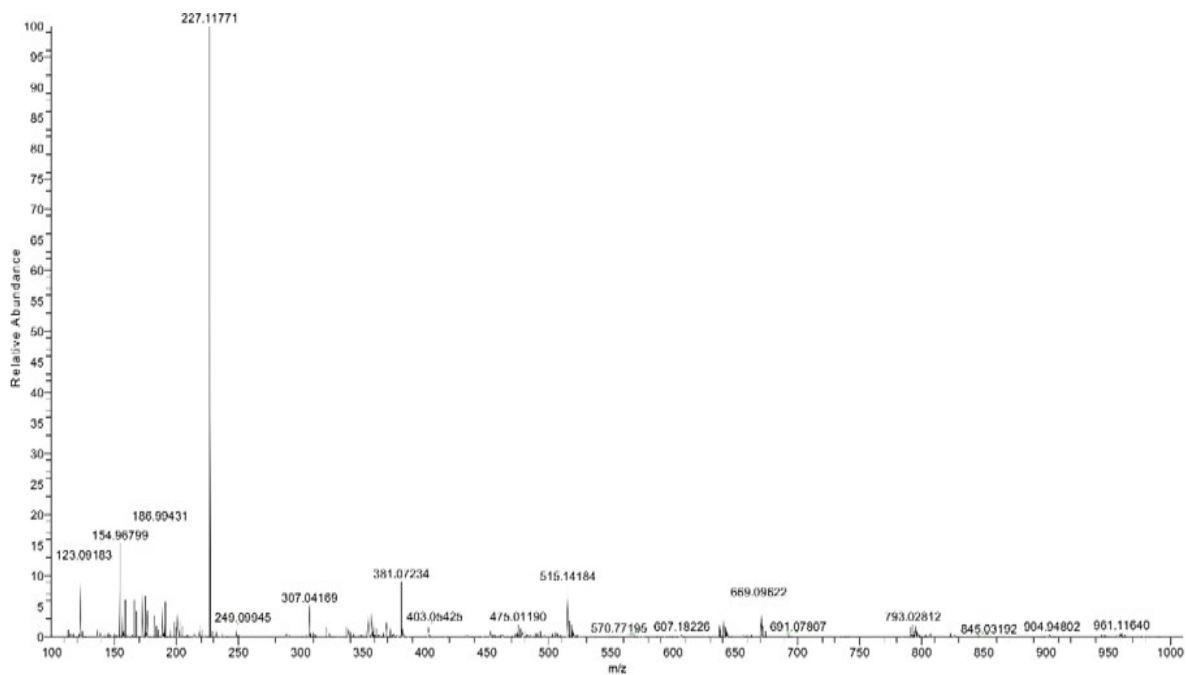


Figure S12. HRMS of the complex ZnL13.

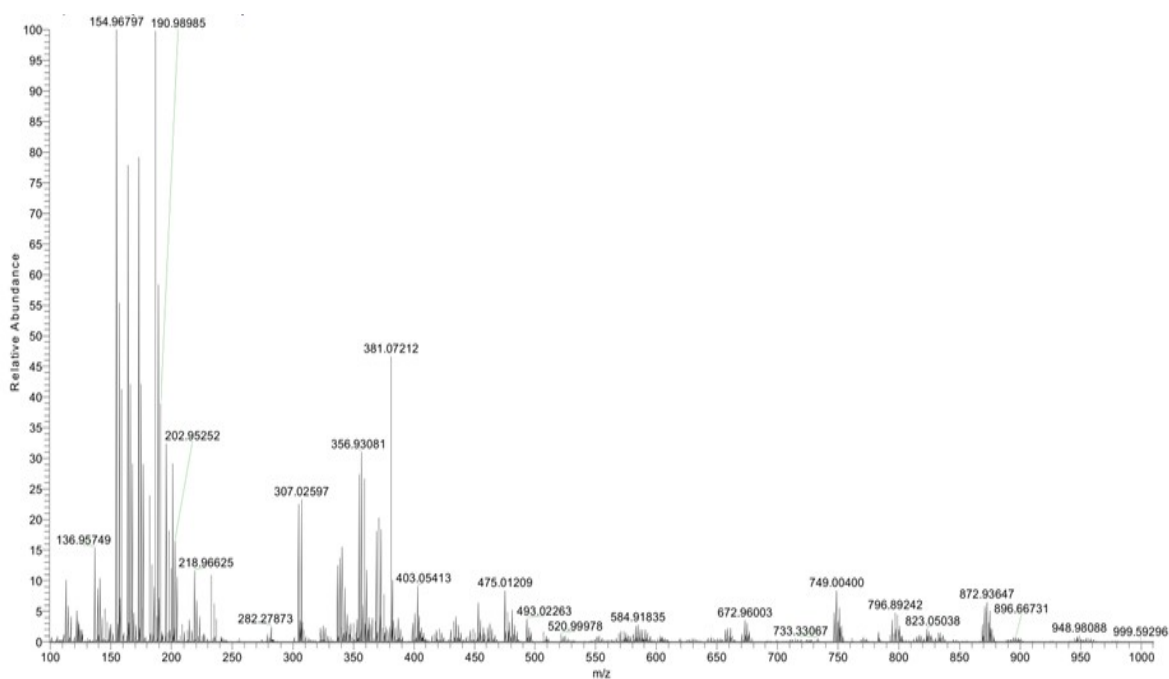


Figure S13. HRMS of the complex ZnL23.

TGA analysis

To gather information regarding the Zinc complexes chemical stability for their possible application in optoelectronics, their thermogravimetric curves are presented in Figure S14. It can also be seen in the thermograms that all complexes presented at least two main decomposition processes. The first thermal event showed a temperature of decomposition between 300 to 400 °C, depending on the complex, where the heteroligand presented the higher ones (**ZnL11**: 306 °C, **ZnL22**: 336 °C, **ZnL13**: 342 °C, and **ZnL23**: 342 °C). In this event, the complexes presented initial decomposition temperatures around 300 °C, once again with the heteroligand presenting the higher ones (**ZnL11**: 287 °C, **ZnL22**: 309 °C, **ZnL13**: 313 °C, and **ZnL23**: 317 °C). Firstly, no water or coordinated solvent, usually related to a weight loss between 100-200 °C was observed in the thermograms of the complexes.¹ In addition, around 30% and 15% weight loss could be observed in homo and heteroligands Zn complexes. The second main thermal event takes place between 500-600 °C to a final weight loss between 80-90%. The decomposition of the complexes was not completed at 700 °C, where the final solid material at this temperature is probably a mixture of carbonaceous zinc oxide.

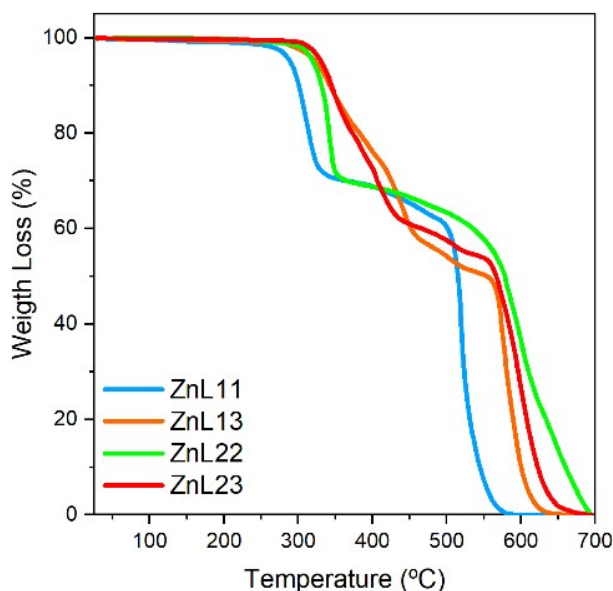


Figure S14. TGA thermograms of all complexes.

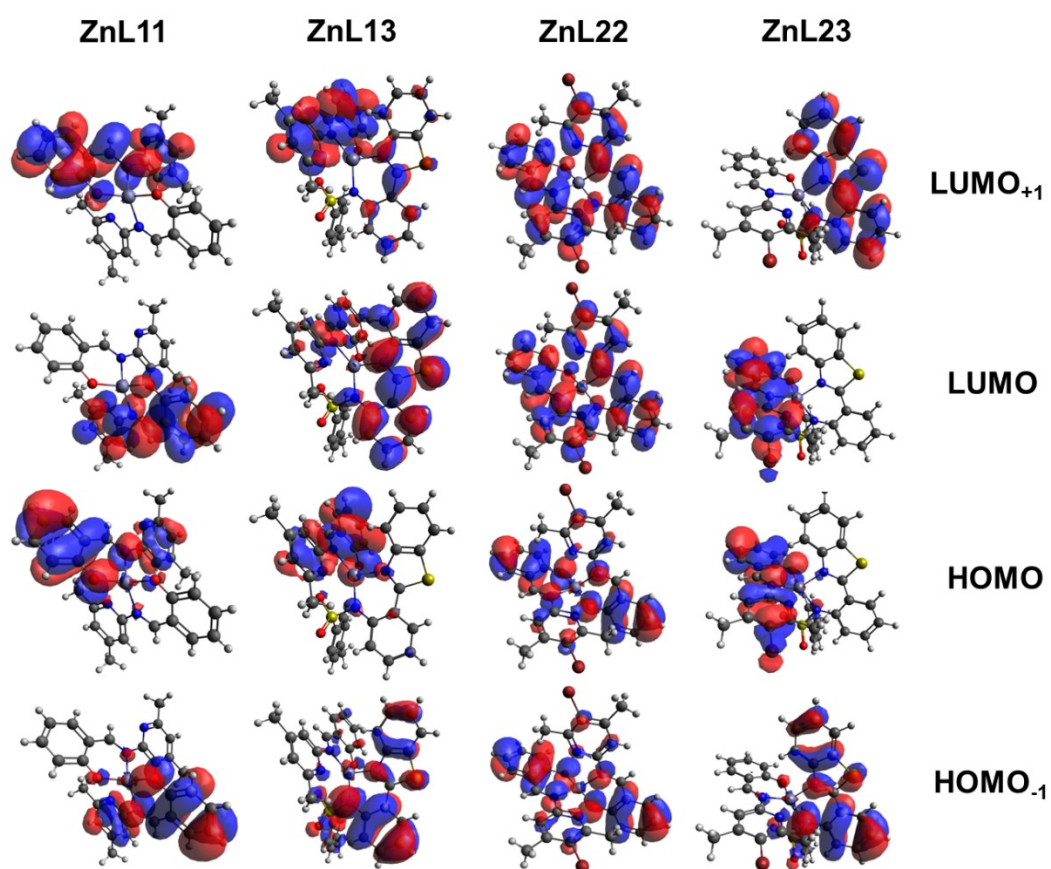


Figure S15. Zn(II)-homo and heteroligands HOMO and LUMO frontier molecular orbitals.

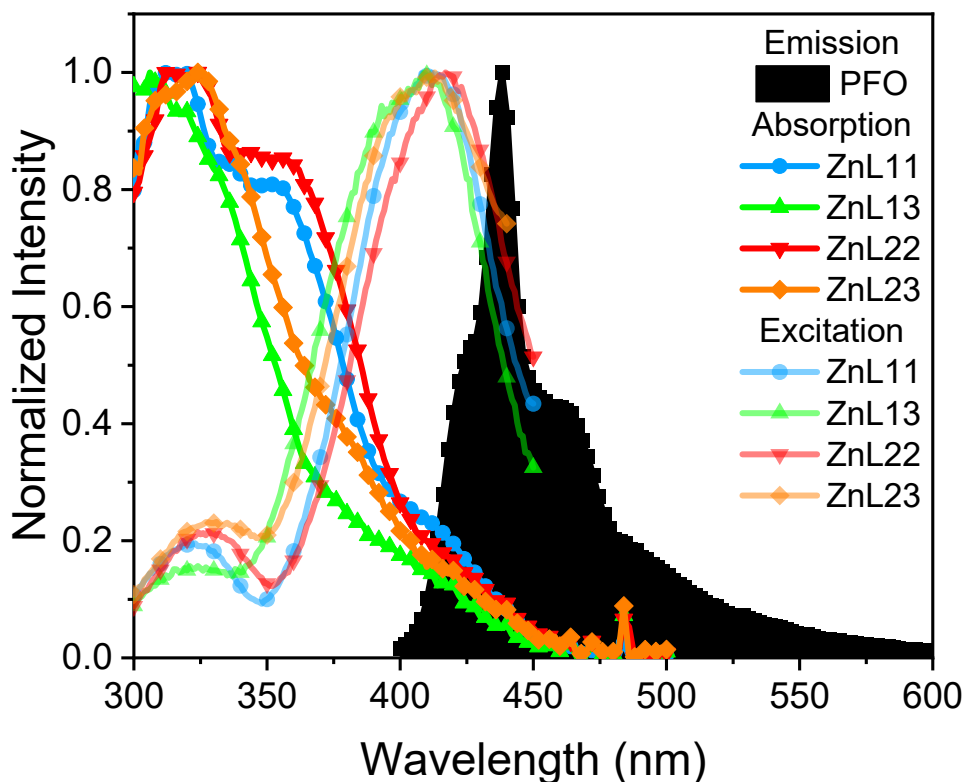


Figure S16. Spectral overlap between Zn(II) coordination compounds absorption/excitation and PFO photoluminescence spectra at solid-state and thin-film, respectively.

Table S2. Summary of time-resolved photoluminescence data used for FRET's efficiencies calculations.

Film	Conc. (%)	τ_1 (ns)	FRET (%)
PFO		0.278	
ZnL11	0.1	0.250	10
	0.5	0.184	34
	1.0	0.127	54
	2.5	0.089	68
ZnL13	0.1	0.231	17
	0.5	0.166	40
	1.0	0.143	49
	2.5	0.117	58
ZnL22	0.1	0.247	11

	0.5	0.167	40
	1.0	0.132	53
	2.5	0.088	68
ZnL23	0.1	0.180	35
	0.5	0.135	51
	1.0	0.123	56
	2.5	0.115	59

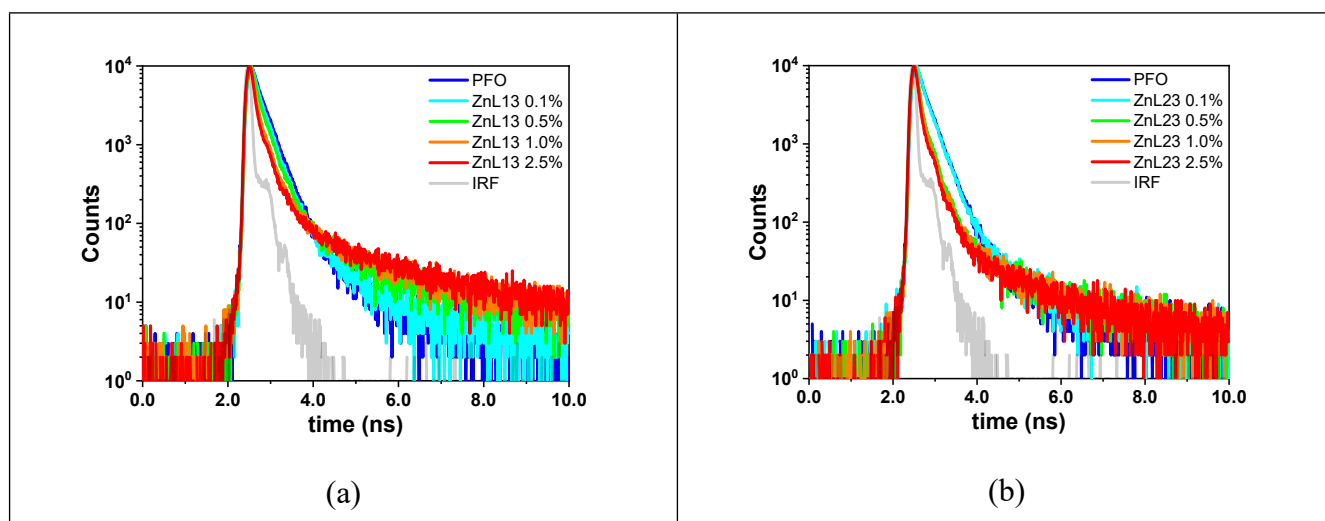


Figure S17. Photoluminescence decay curves of (a) **ZnL13** and (b) **ZnL23** at different concentrations in PFO matrix.

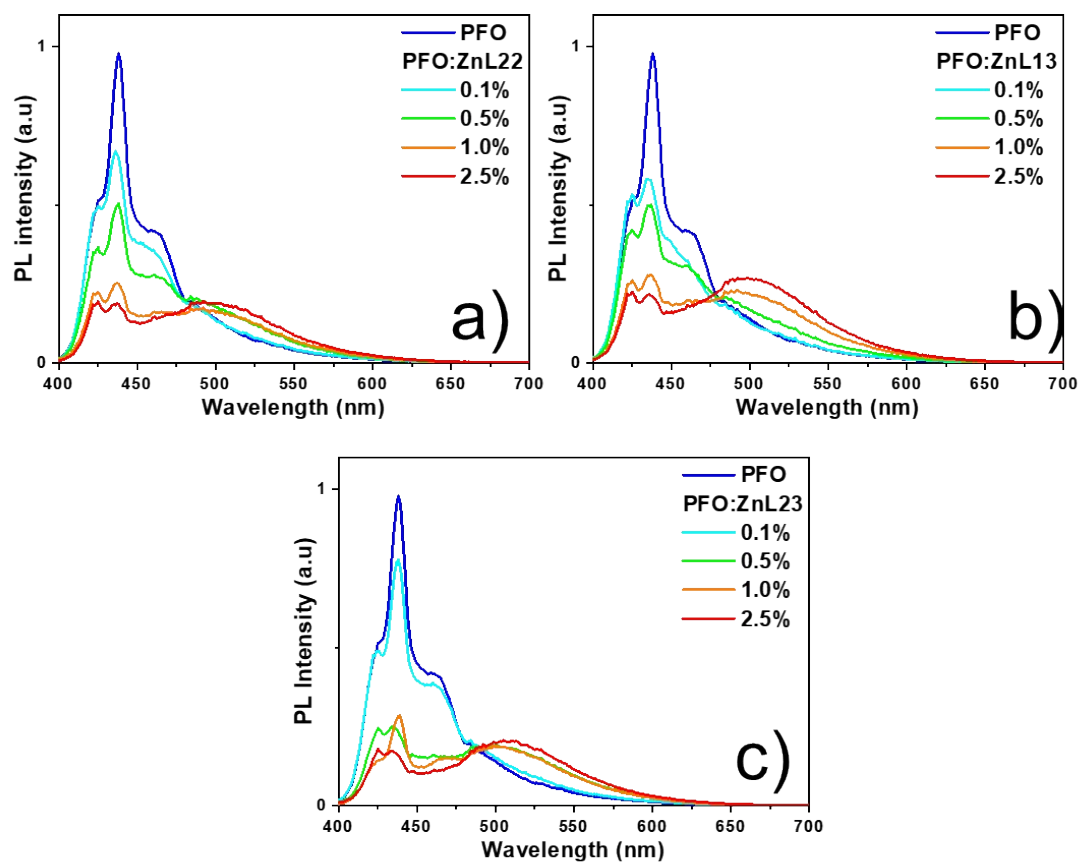


Figure S18. Thin film photoluminescence spectra of the Zn(II) coordination compounds excited into PFO matrix ($\lambda_{\text{exc}}=375$ nm), where: (a) **ZnL22**; (b) **ZnL23**; and (c) **ZnL13**.

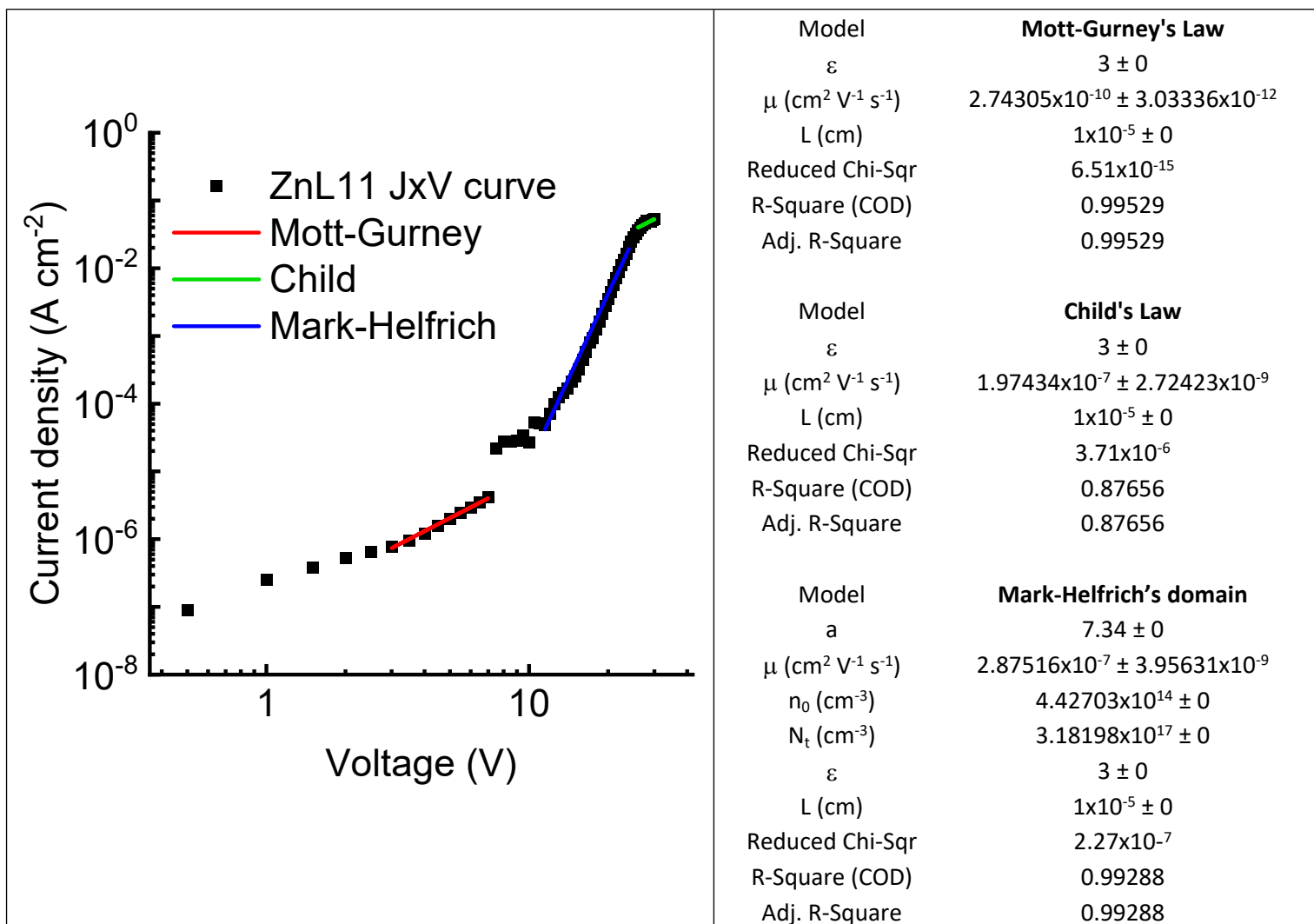


Figure S19. Mott-Gurney's, Child's and Mark-Helfrich's space-charge electrical transport models adjusted applied to PFO:ZnL11 (1 % mol/mol) OLED current density versus voltage curve and their fit parameters.

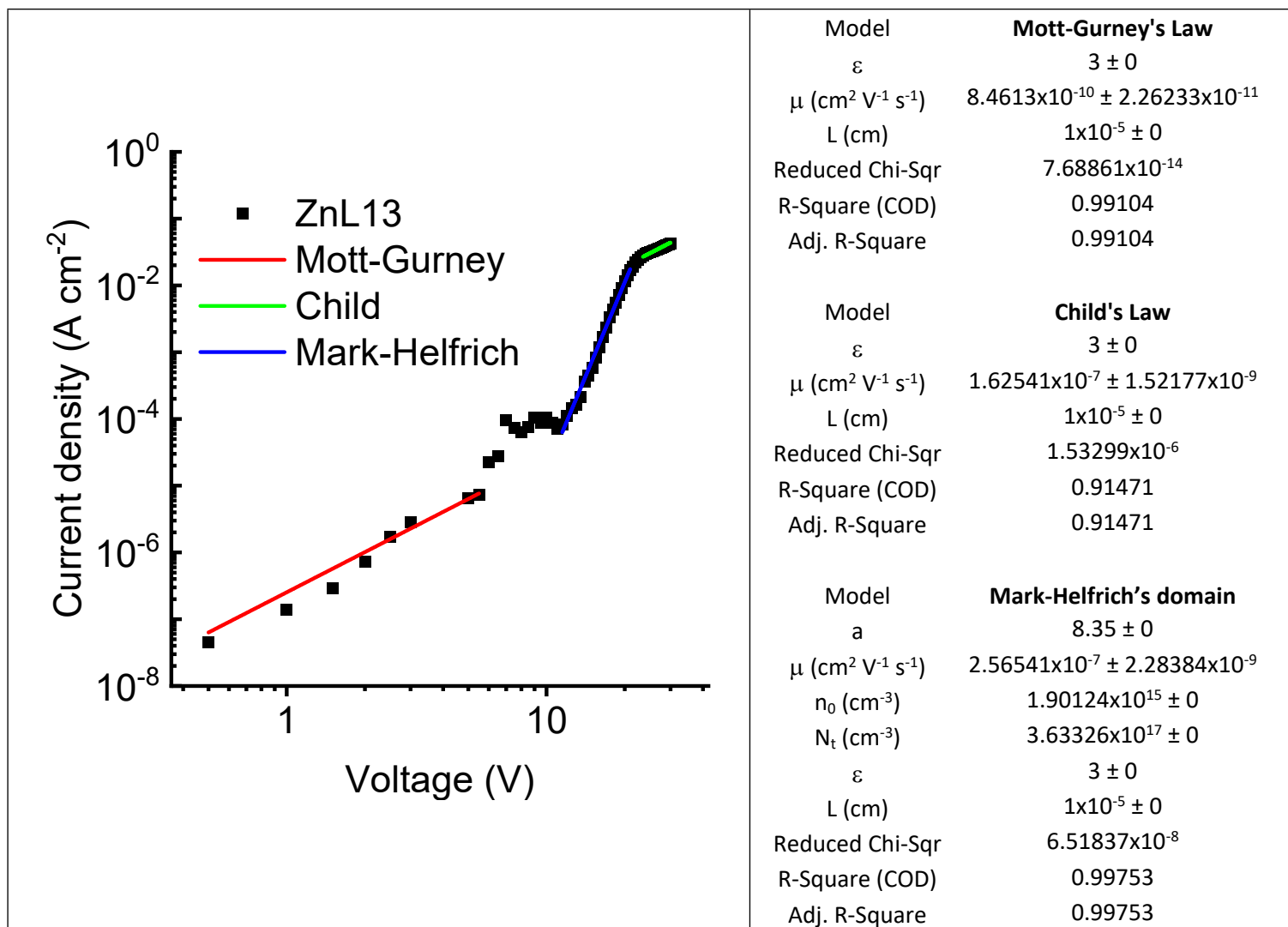


Figure S20. Mott-Gurney's, Child's and Mark-Helfrich's space-charge electrical transport models adjusted applied to PFO:ZnL13 (1 % mol/mol) OLED current density versus voltage curve and their fit parameters.

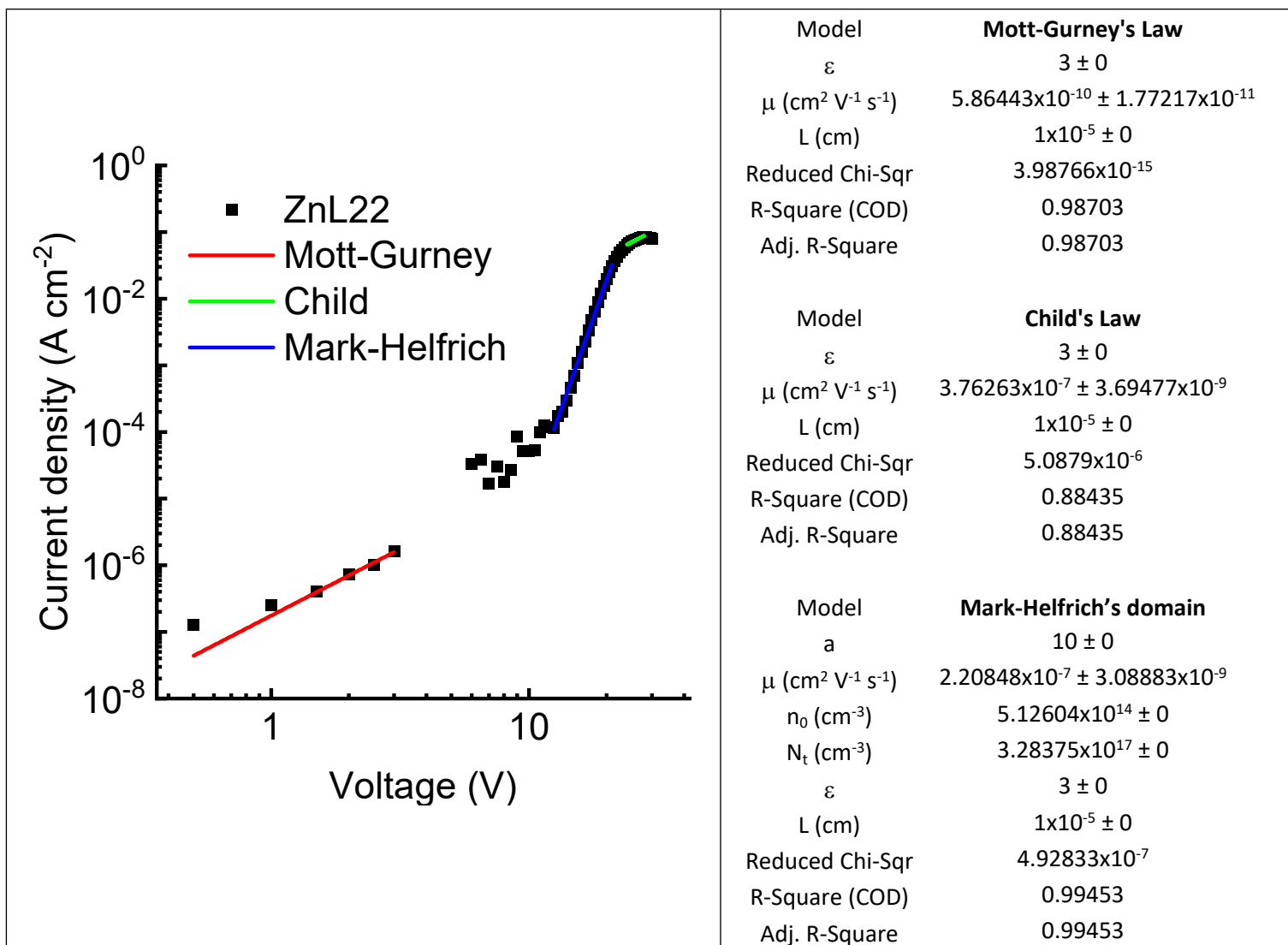


Figure S21. Mott-Gurney's, Child's and Mark-Helfrich's space-charge electrical transport models adjusted applied to PFO:ZnL22 (1 % mol/mol) OLED current density versus voltage curve and their fit parameters.

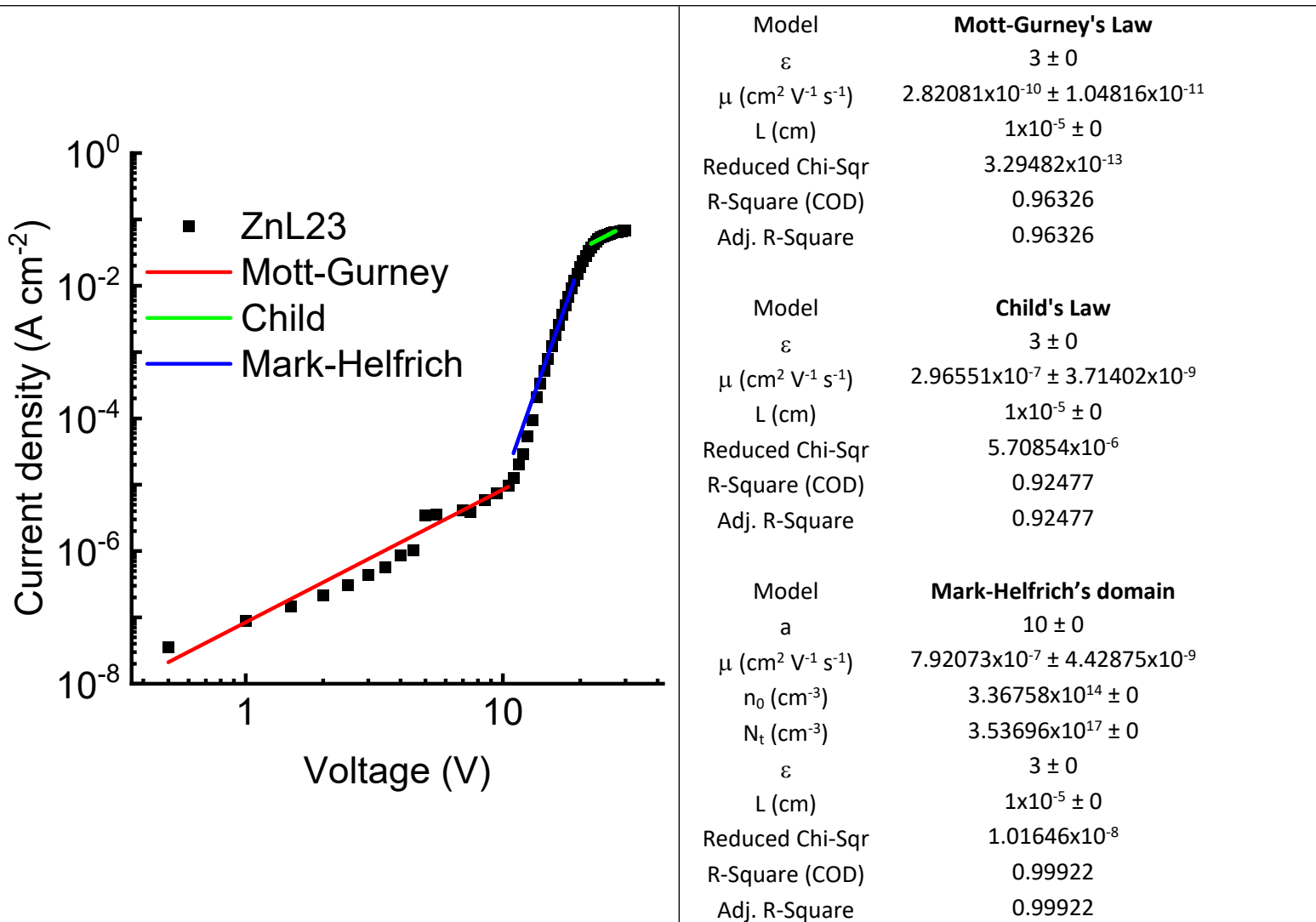


Figure S22. Mott-Gurney's, Child's and Mark-Helfrich's space-charge electrical transport models adjusted applied to PFO:ZnL2 (1 % mol/mol) OLED current density versus voltage curve and their fit parameters.

References

- 1 A. Zianna, S. Vecchio, M. Gdaniec, A. Czapik, A. Hatzidimitriou and M. Lalia-Kantouri, in *Journal of Thermal Analysis and Calorimetry*, 2013, vol. 112, pp. 455–464.