

Conjugated metallo-supramolecular polymers containing a phosphole unit.

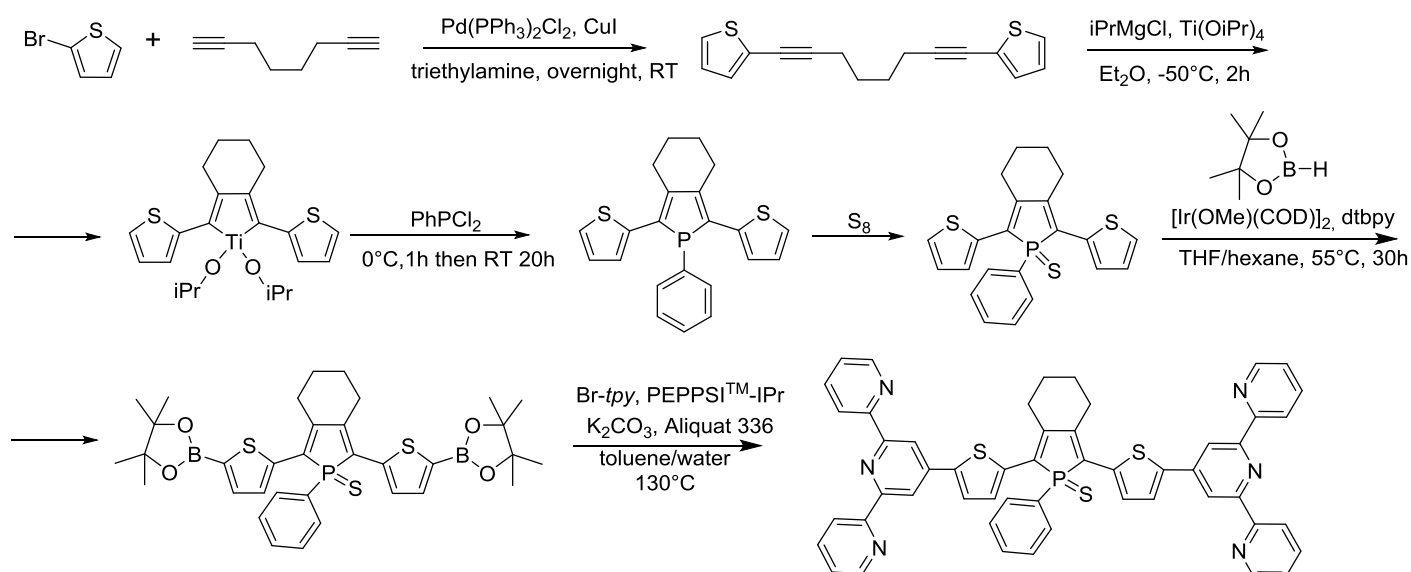
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Supporting Information Placeholder

Supporting Information



Scheme S1: Synthesis of unimer **TPT** starting from commercially available materials

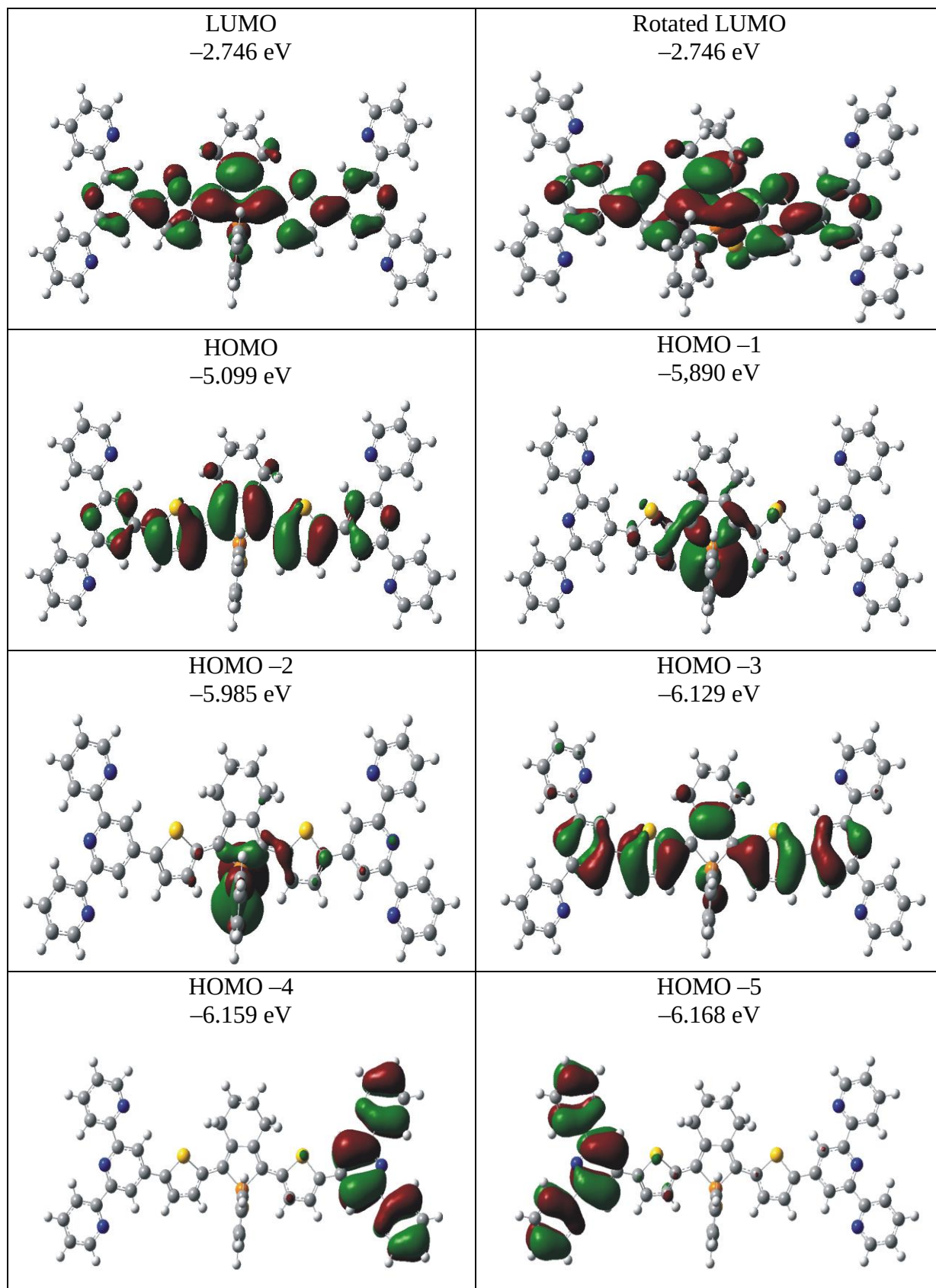


Figure S1a): Electronic density contours and energy values for LUMO and HOMOs of **TPT** obtained using DFT calculations.

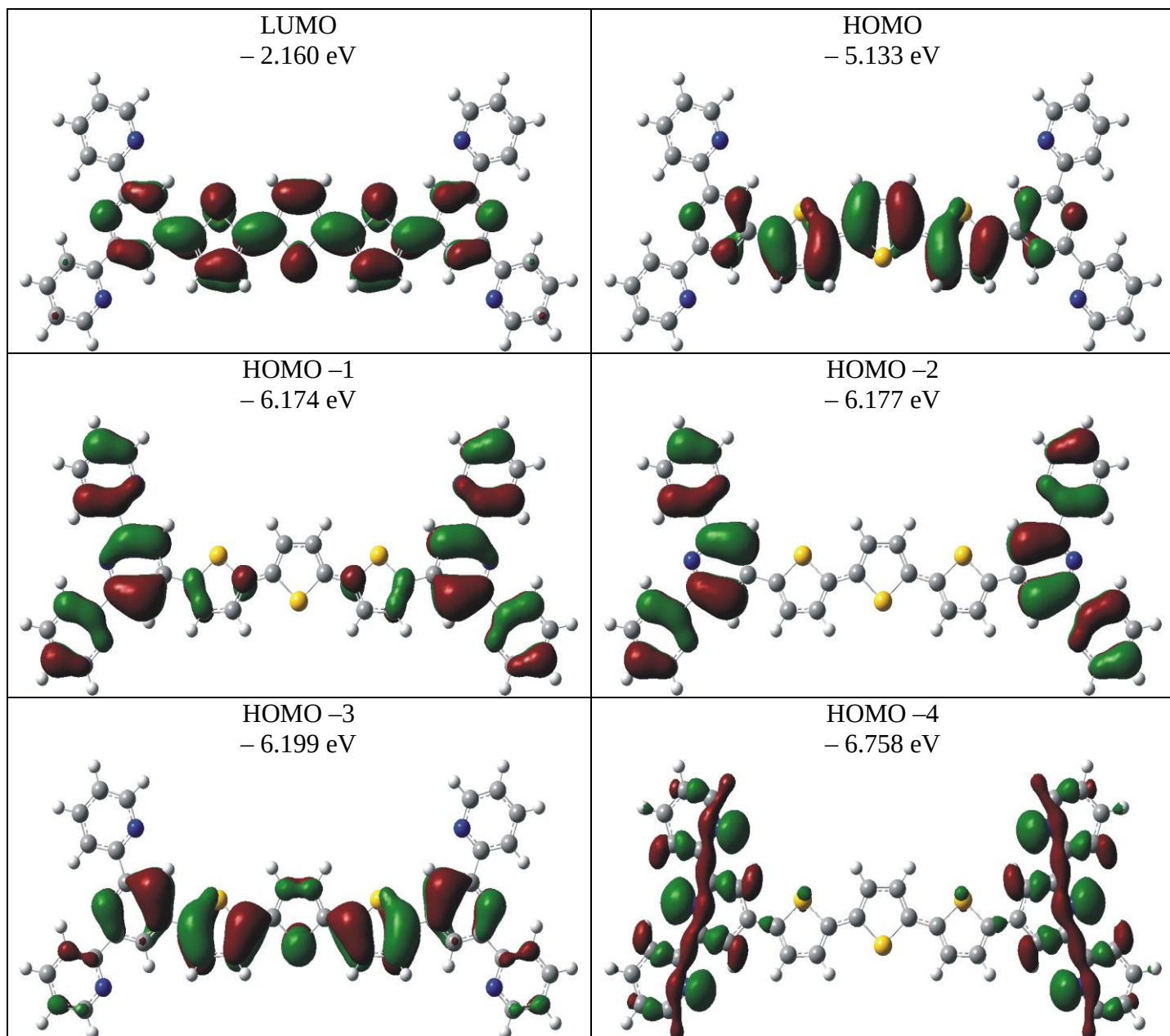


Figure S1b): Electronic density contours and energy values for LUMO and HOMOs of **T** obtained using DFT calculations.

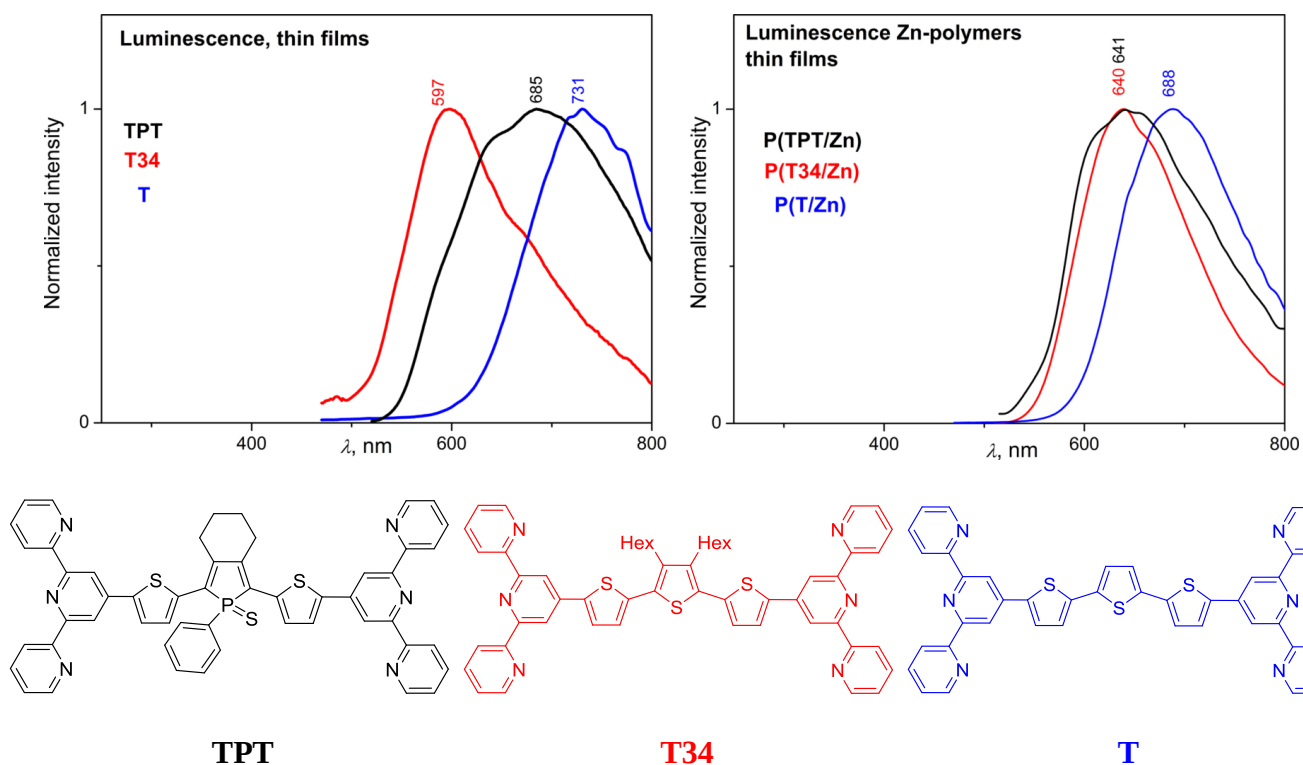
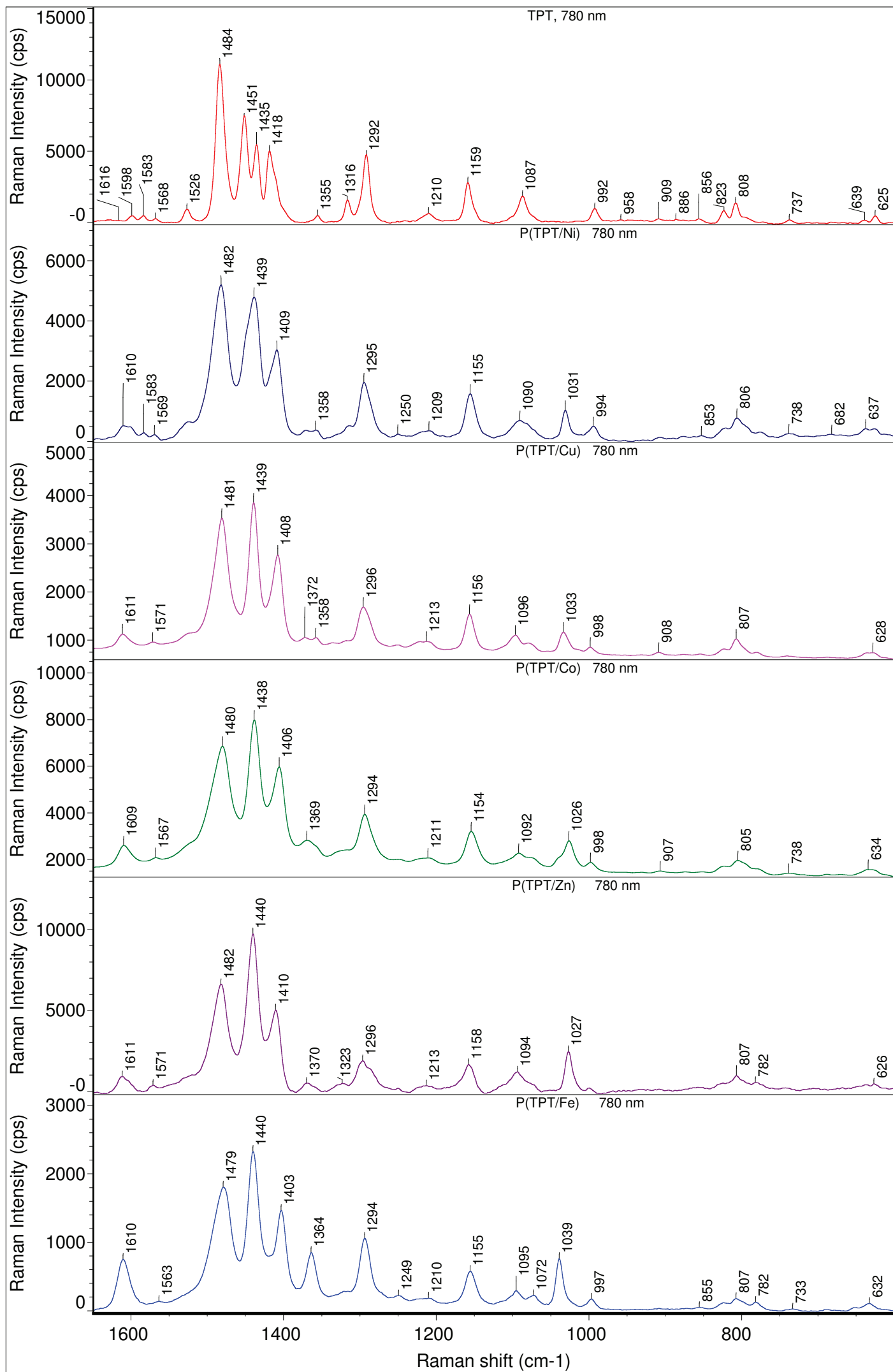


Figure S2: The solid-state luminescence spectra of unimers **T**, **T34** and **TPT** and related Zn-polymers.

Next page contains the following figure

Figure S3: Off-resonance ($\lambda_{\text{exc}} = 780$ nm) Raman spectra of the **TPT** and related MSPs with various ion-couplers



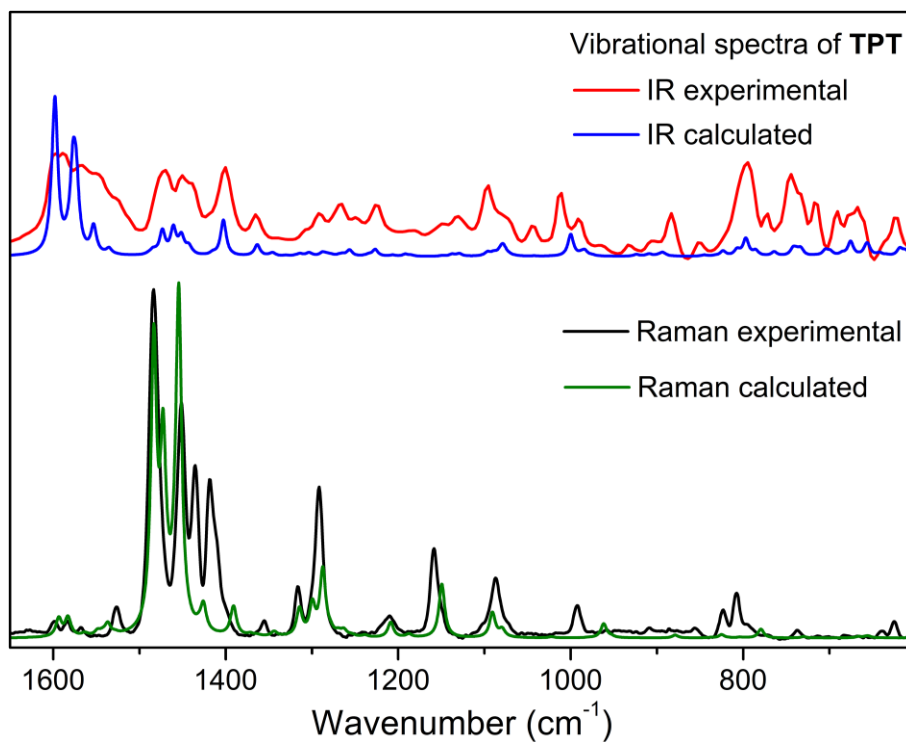
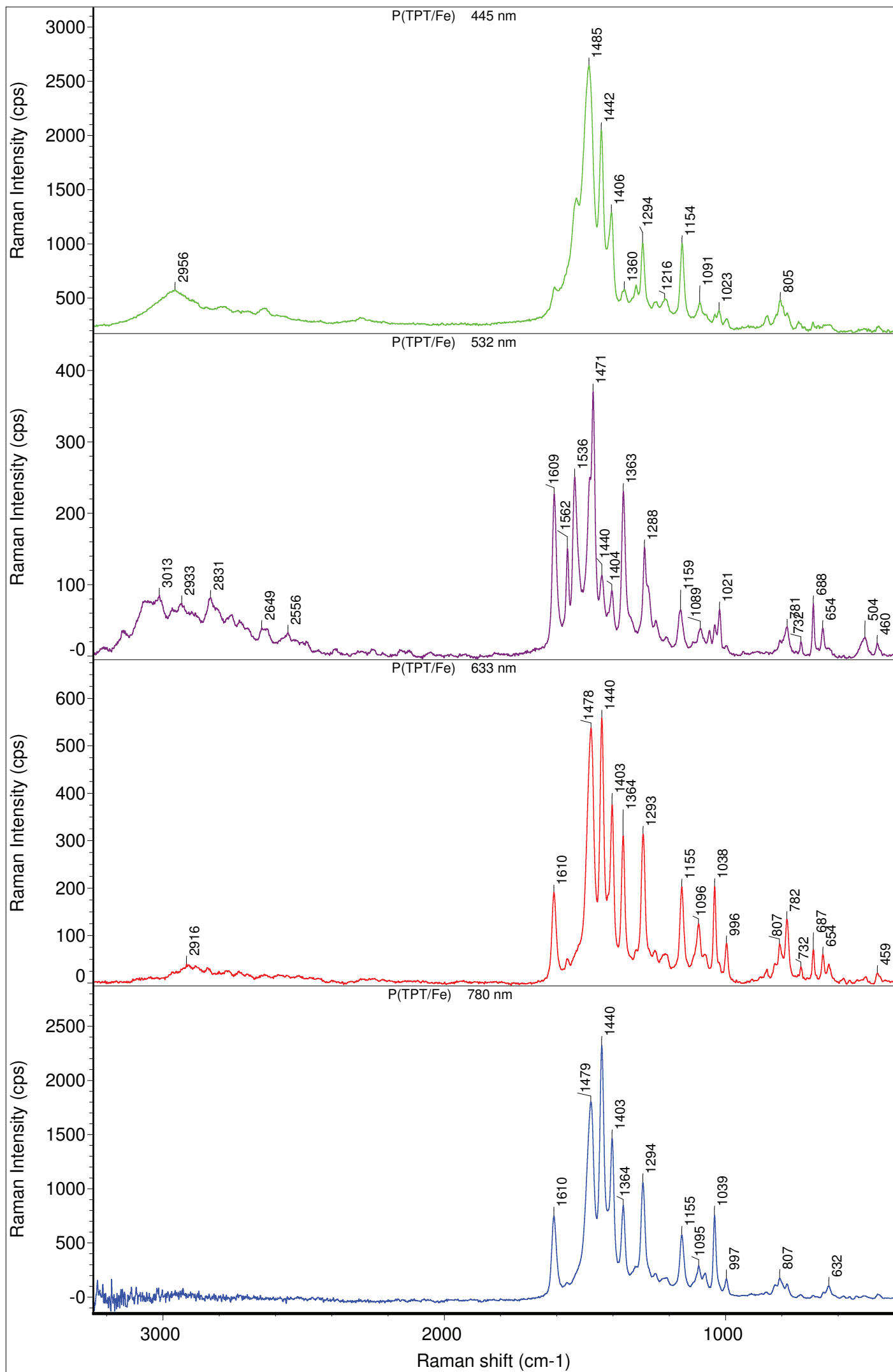


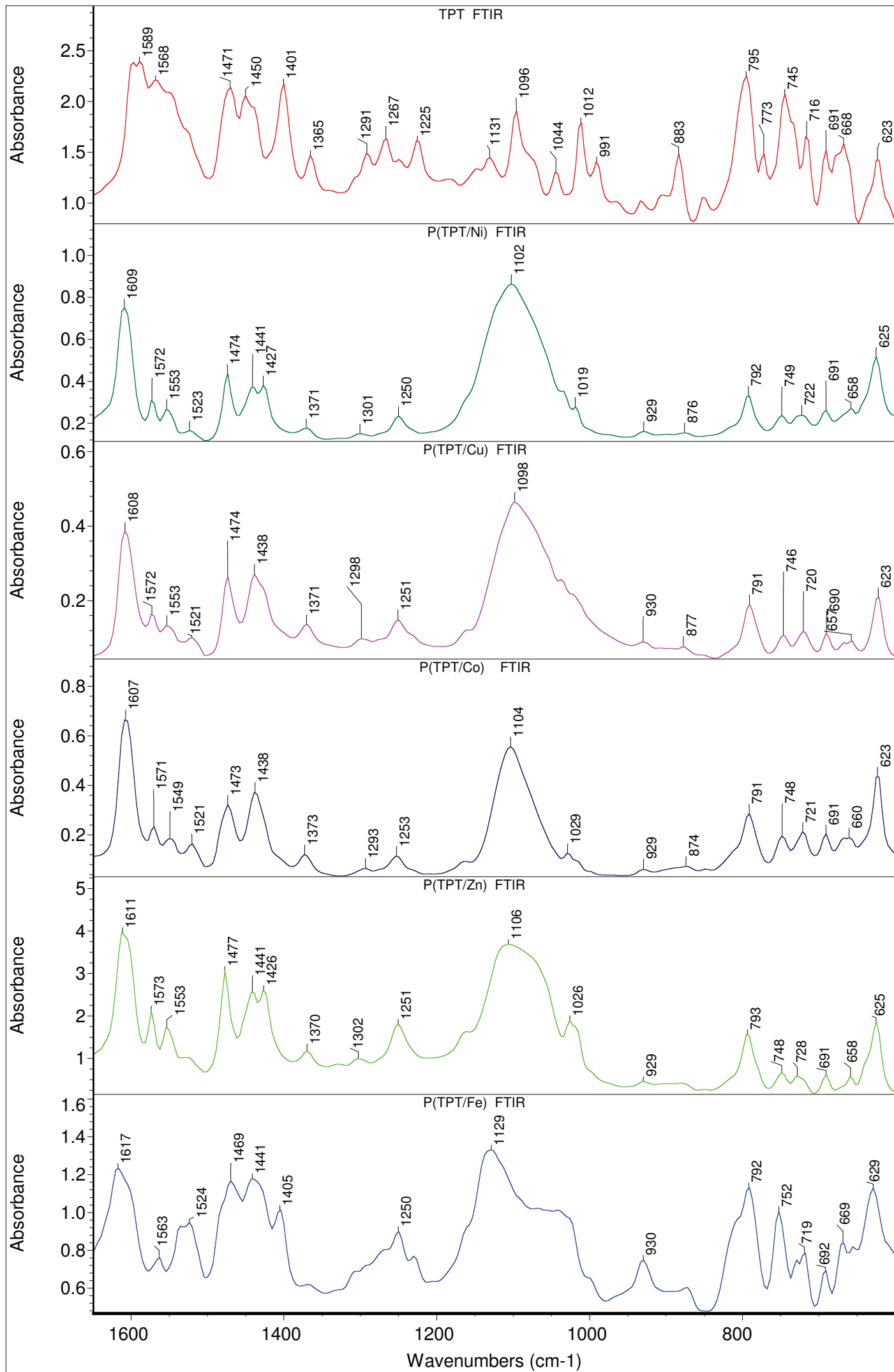
Figure S4: Comparison of the calculated and measured IR and Raman spectra of **TPT**.

Next two pages show the following spectra

Figure S5: Raman spectra of P(**TPT**/Fe) taken with different excitation wavelengths

Figure S6: Infrared spectra of the **TPT** MSPs with various ion-couplers.





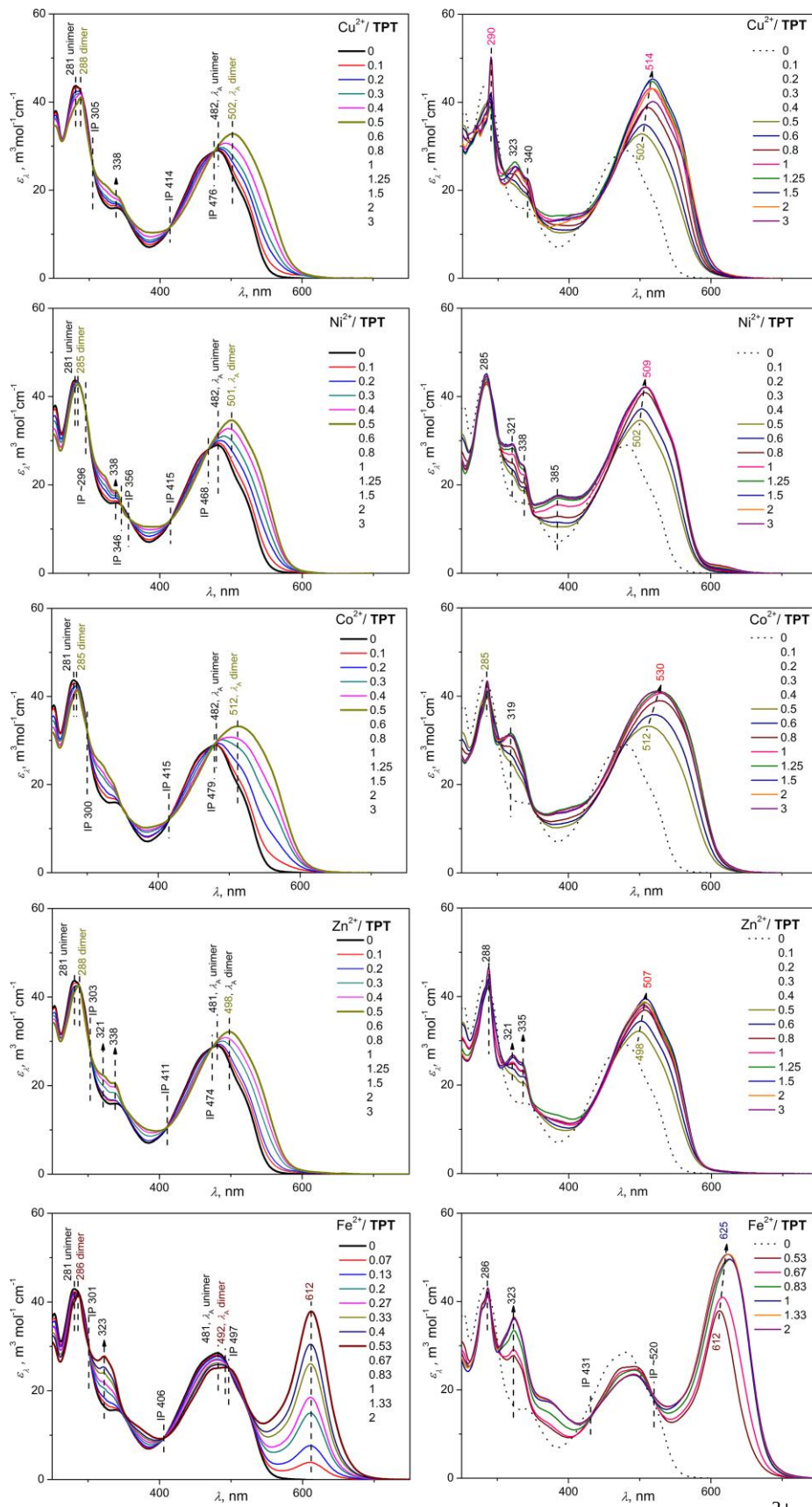


Figure S7. The UV-vis spectral changes at assembling of **TPT** with M^{2+} ions.

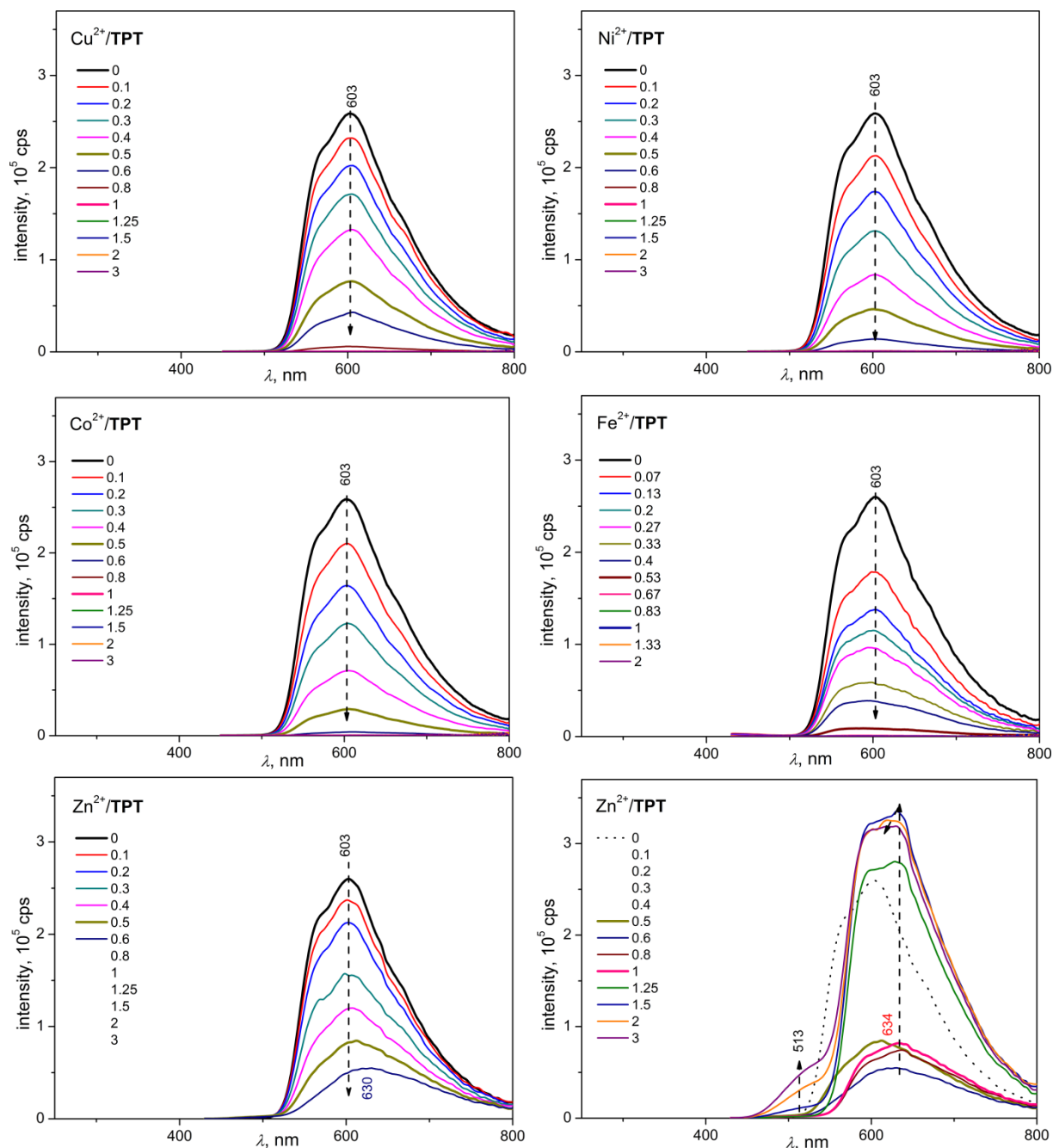


Figure S8. Luminescence spectral changes at assembling of **TPT** with M^{2+} ions.

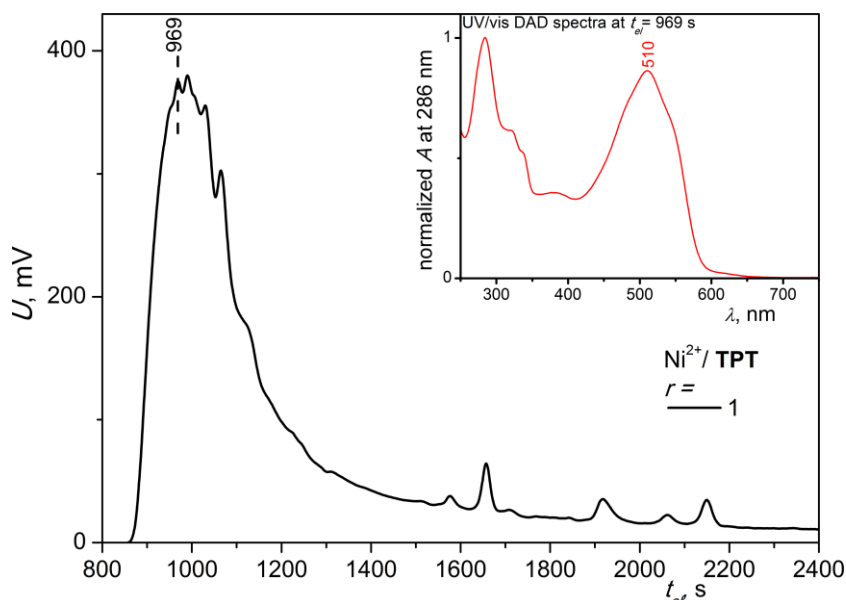


Figure S9. SEC record of the $\text{Ni}^{2+}/\text{TPT}$ system ($r = 1$); inset: the UV/vis DAD spectrum of the apex fraction.

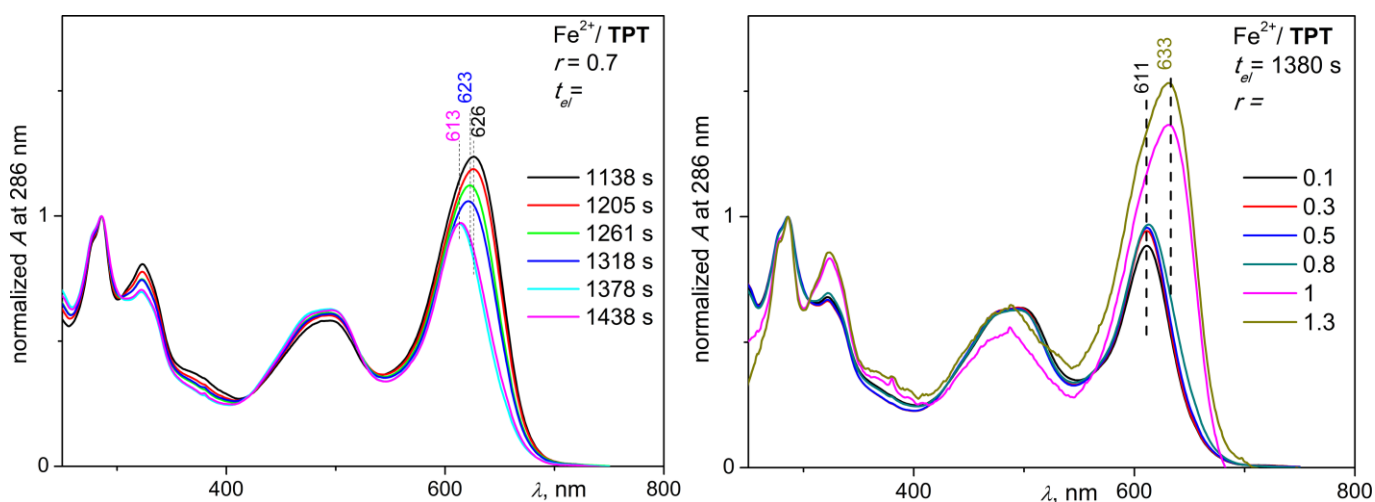


Figure S10. The UV/vis DAD spectra of SEC fractions of the $\text{Fe}^{2+}/\text{TPT}$ system: *Left*: composition $r = 0.7$, different elution times, t_{el} . *Right*: fractions of dimers ($t_{el} = 1380 \text{ s}$) present in the $\text{Fe}^{2+}/\text{TPT}$ systems of different composition r .

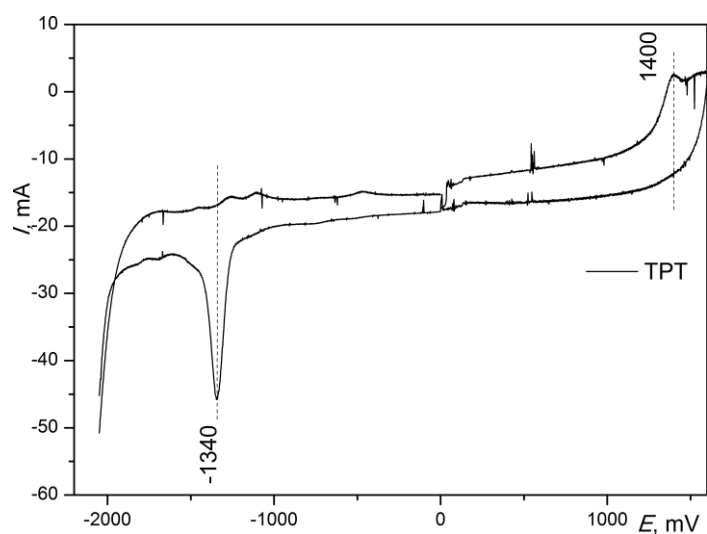


Figure S11. Cyclic voltammetry of unimer TPT

Next 4 pages show the following spectra

Figure S12: ^1H NMR of 1-phenyl-2,5-bis[5-(4,4,5,5-tetramethyl-1,3,2-dioxaboralene-2-yl)thiophen-2-yl]thioxophosphole (**2**).

Figure S13: ^{13}C NMR of 1-phenyl-2,5-bis[5-(4,4,5,5-tetramethyl-1,3,2-dioxaboralene-2-yl)thiophen-2-yl]thioxophosphole (**2**)

Figure S14: ^1H NMR of 1-phenyl-2,5-bis(5-*tpy*-thiophen-2-yl)thioxophosphole (**TPT**)

Figure S15: ^{13}C NMR of 1-phenyl-2,5-bis(5-*tpy*-thiophen-2-yl)thioxophosphole (**TPT**)

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