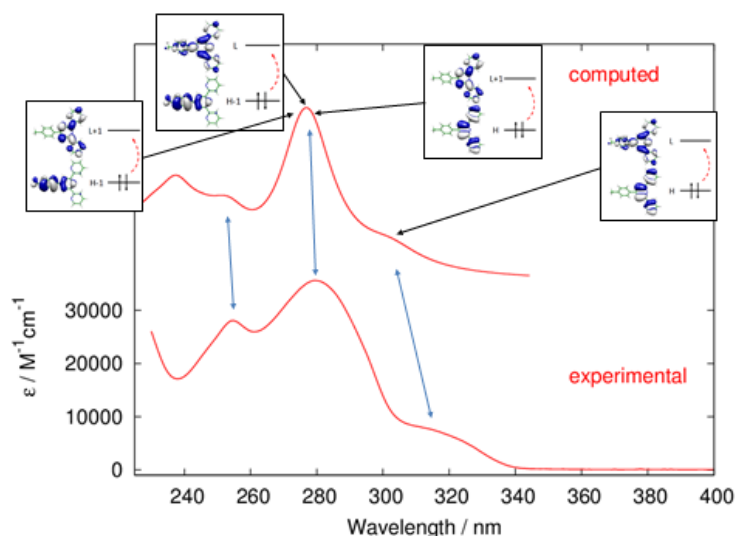


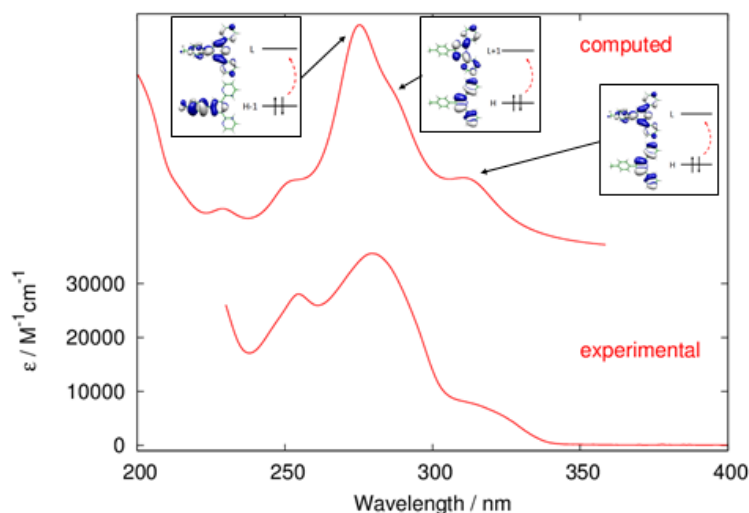
Supporting Information

Luminescent multi-terpyridine ligands: towards 2D polymer formation in solution

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Paola Ceroni^{a*}



A)



B)

Figure S1. A) Comparison between experimental (bottom) and TD-B3LYP/6-31G* computed absorption spectrum of tol-tpy (top). B) Similar comparison but with TD-CAM-B3LYP/6-31G* computed absorption spectrum of tol-tpy. In this case computed excitation energies were rescaled to the observed values for an easier comparison. The orbital nature of the lowest energy transitions is also indicated.

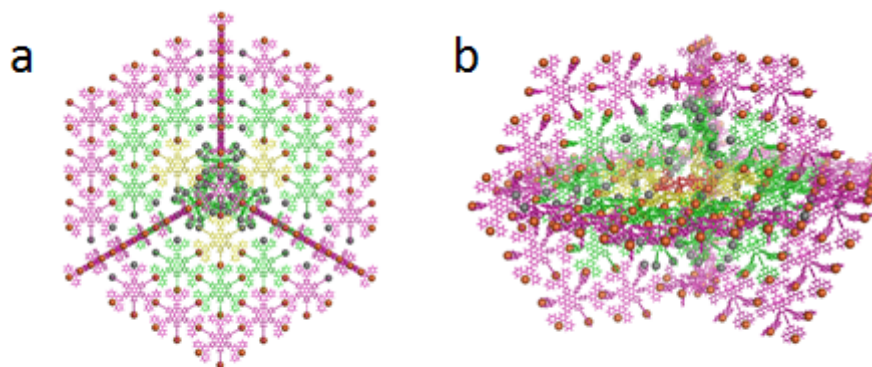


Figure S2. Model of a 3D structure similar to that of Figure 6, but built using **M6-90** less stable conformers. The core monomer is shown in red, the first generation row in yellow, the second generation row in green and the third generation in magenta; Fe^{2+} are shown as brown spheres when involved in 2:1 ligand to metal binding and grey for Fe^{2+} bound to only one tpy unit.

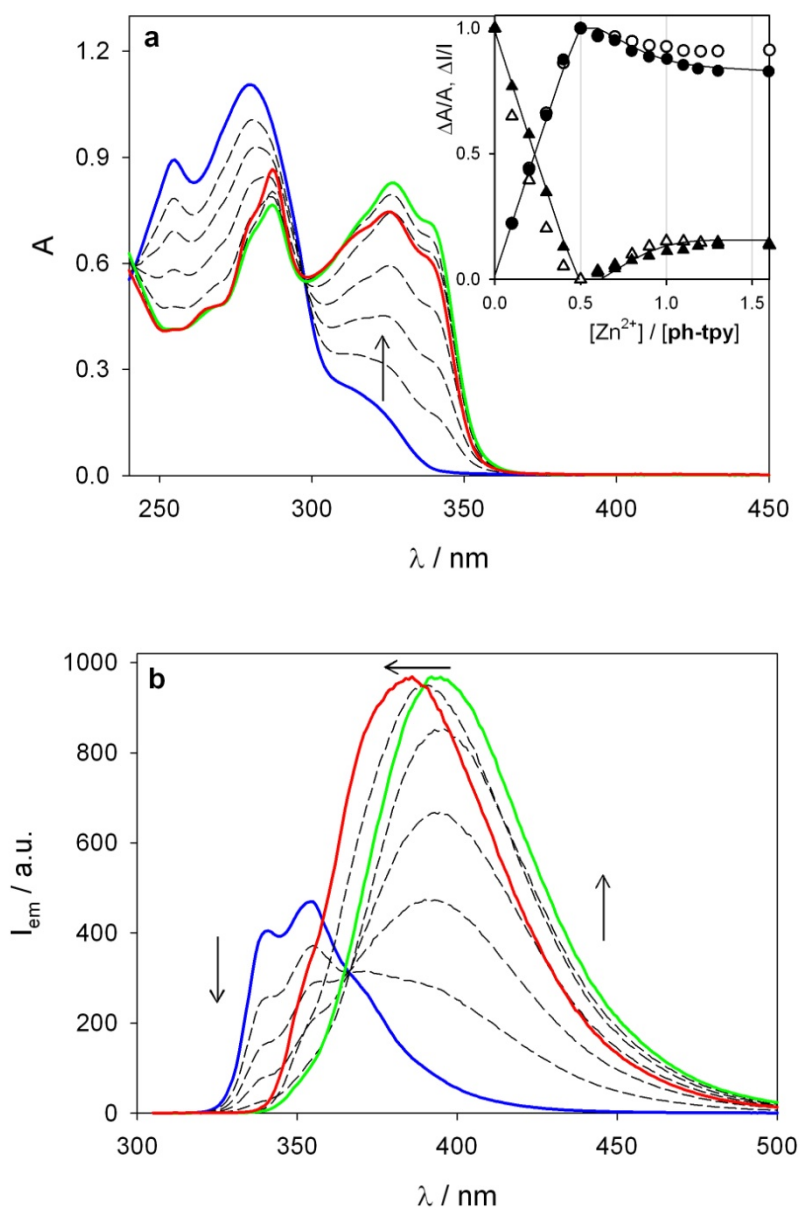


Figure S3. Absorption (a) and emission spectra (b) of a 3.1×10^{-5} M solution of **tol-tpy** in CH_2Cl_2 upon titration with $\text{Zn}(\text{CF}_3\text{SO}_3)_2$: 0 eq. (solid blue line), 0.5 eq. (solid green line), 1.0 eq. (solid red line). $\lambda_{\text{ex}} = 297$ nm. Inset shows normalized absorption changes at 287 (solid triangles) and 326 nm (solid circles), and normalized emission changes at 344 (empty triangles) and 392 nm (empty circles).

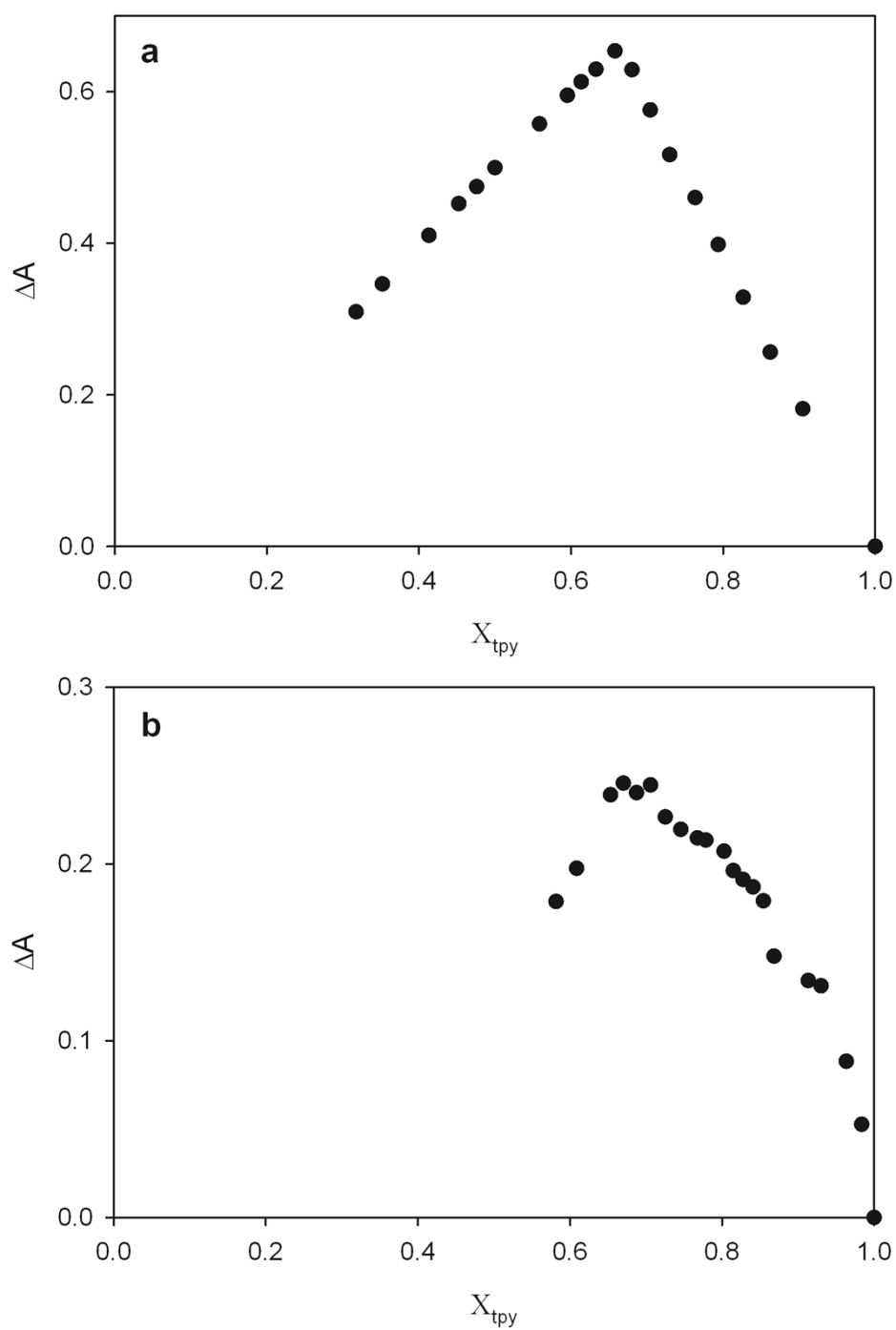


Figure S4. Job's plot corresponding to the titration of **tol-tpy** and **M6** in CH_2Cl_2 upon addition of $\text{Zn}(\text{CF}_3\text{SO}_3)_2$. The absorbance changes are plotted at 570 nm (a) and 286 nm (b) as a function of the molar fraction of terpyridine ligands. Slightly different plots are obtained for **M6** at different wavelength.