Supplementary information

A charge neutral iron (II) complex with above room temperature spin crossover (SCO) and hysteresis loop

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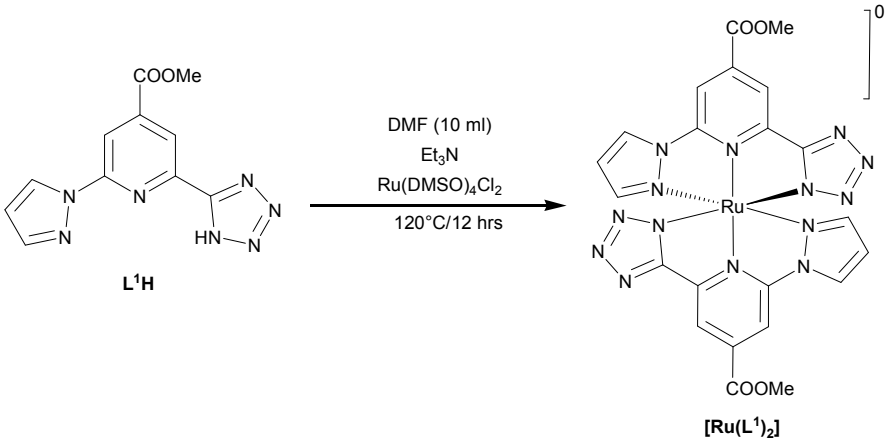
Synthesis of $[Ru(L^1)_2]$



Scheme S1 Synthesis of **$[Ru(L^1)_2]$**

Synthesis of $[Ru(L^1)_2]$

L^1H (0.108g, 0.4 mmol) was added to 10 ml of dry DMF under Ar. To this 55 µL (0.4 mmol) of Et_3N was added and stirred for 15 mins. To this $Ru(DMSO)_4Cl_2$ (0.097g, 0.2 mmol) was added and the mixture stirred at 120°C for 12 hrs and cooled. A precipitate was obtained which was filtered and washed with 2x10ml each of H_2O and MeOH and dried under vacuum to yield 32 mg (25%) of dark yellow-orange powder. ESI-MS in CH_2Cl_2/CH_3OH (Da): m/z, (assigned structure) = 665.04 ($C_{22}H_{16}N_{14}O_4RuNa$, calc. = 665.04). Elemental Analysis of the powder: Calc. for: **$[Ru(L^1)_2]$**. $1H_2O$ ($C_{22}H_{18}N_{14}O_5Ru$) C, 40.06; H, 2.75; N, 29.73; Found: C, 40.28; H, 2.7; N, 29.9. UV-vis in 7:3 CH_2Cl_2/CH_3OH; λ_{max}/nm ($\varepsilon/10^{-4}$ cm^{-1} M^{-1}): 428 (0.78), 308 (1.07), 299 (1.13, 265 (1.8) and 255 (1.9).

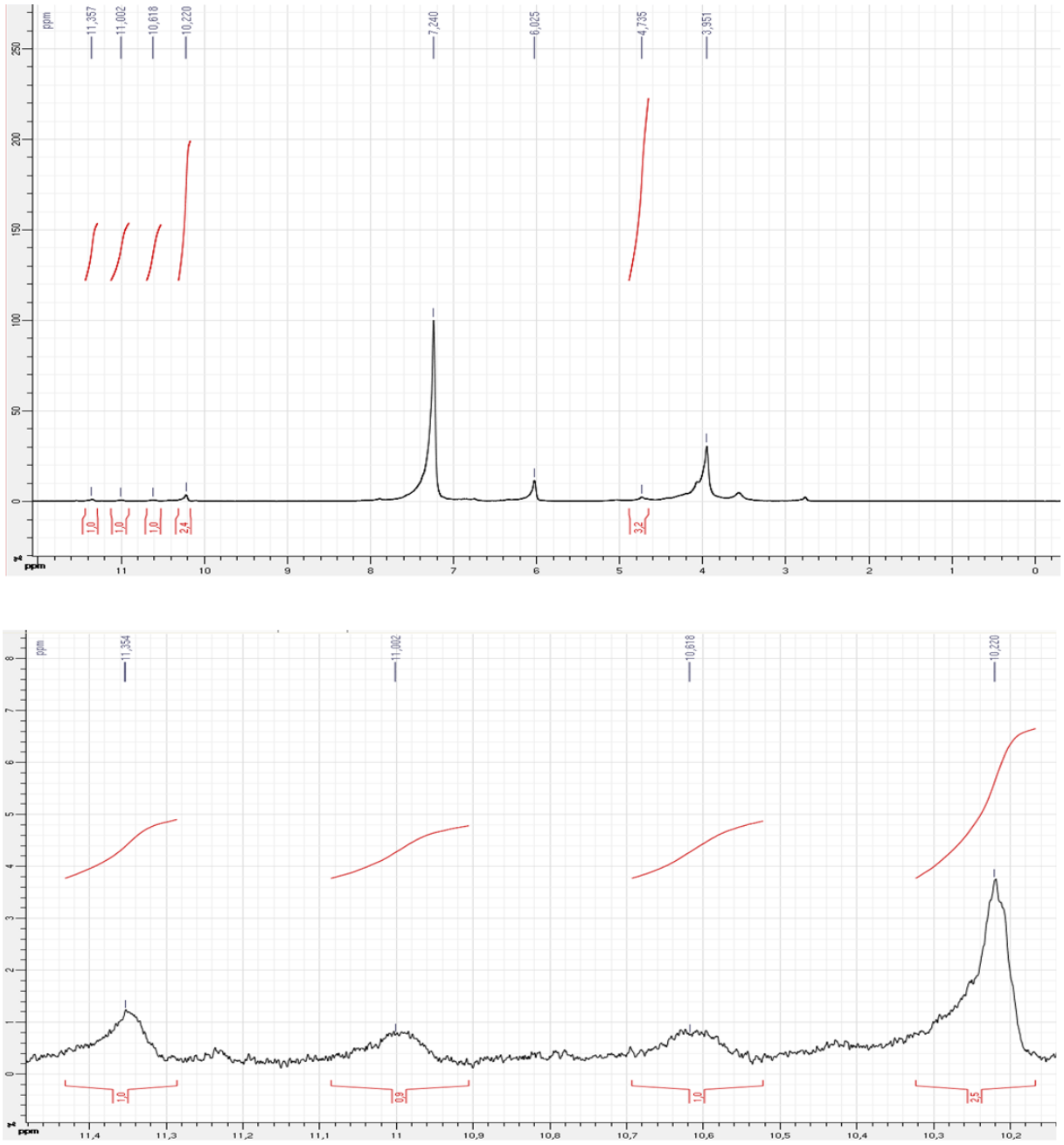


Figure S1 ^{1}H NMR spectrum of **[Fe(L)$_2$]** in $CHCl_3$/ CH_3OH solvent mixture (top). Expanded version of the top spectrum in the 10 -11.5 ppm spectral range (bottom).

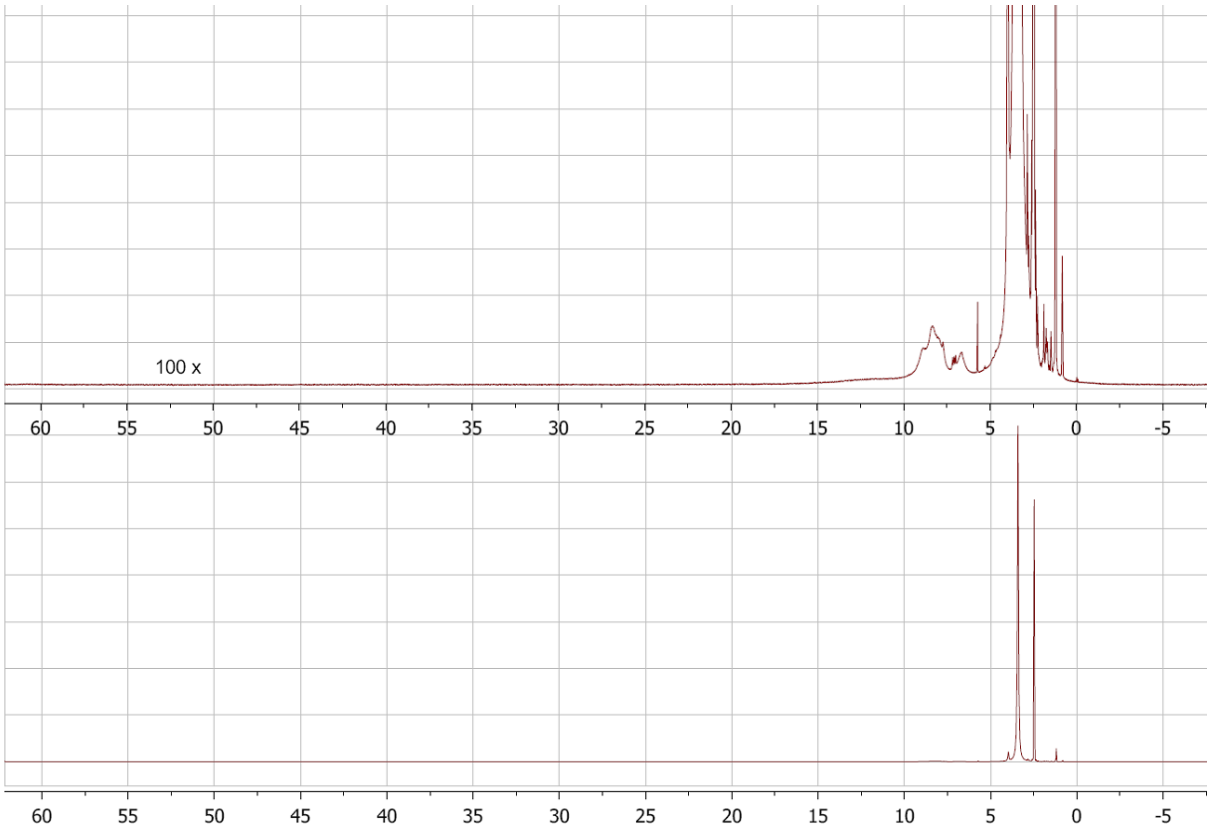


Figure S2 ^{1}H NMR spectrum of **[Fe(L)$_2$]** in DMSO solvent. The spectrum at the top is 100 times magnified version of the below spectrum.

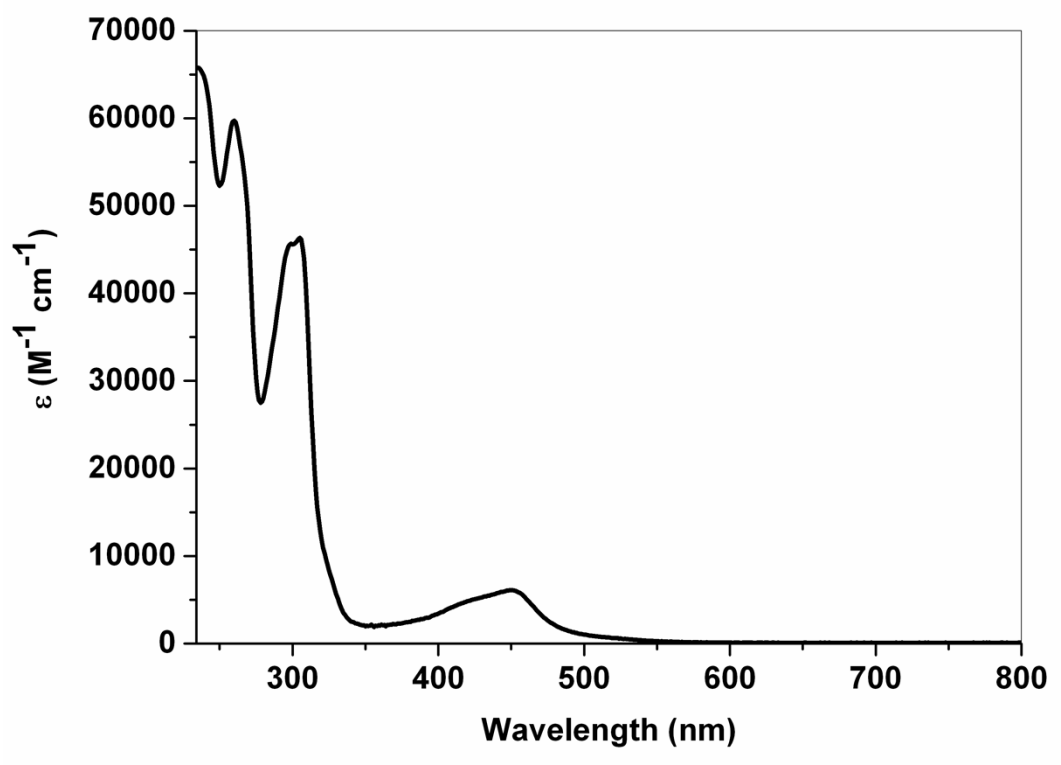


Figure S3 UV-vis absorption spectrum of **[Fe(L)$_2$]** in DCM/MeOH solvent mixture.

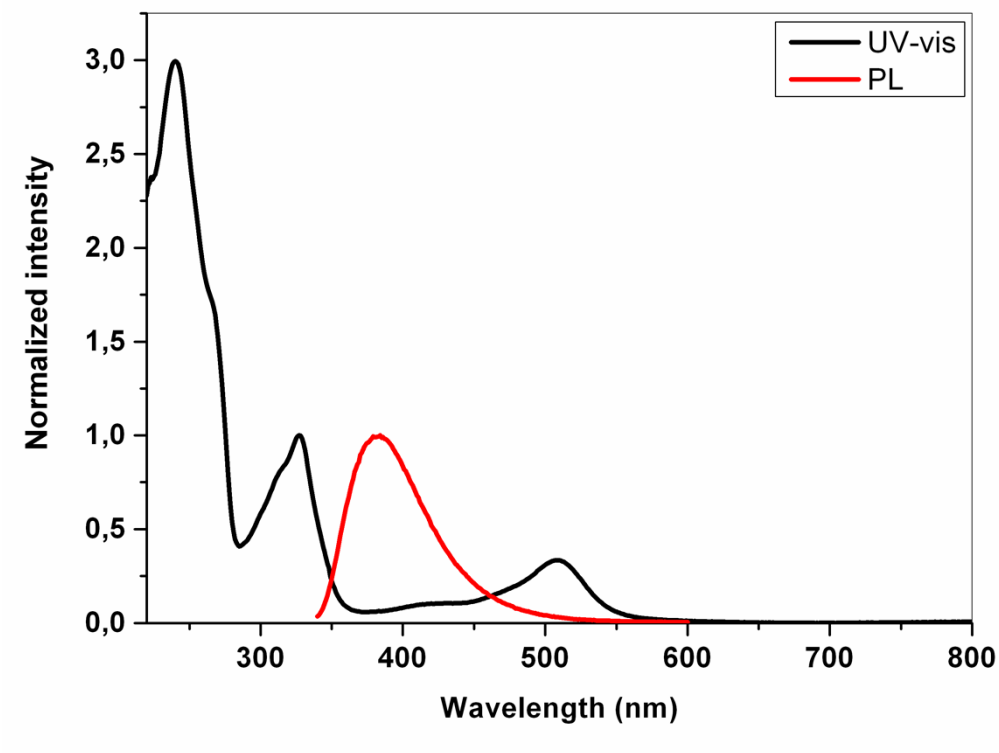


Figure S4 UV-vis absorption and PL spectra of **[Fe(L^1)$_2$]** in DCM/MeOH solvent mixture.

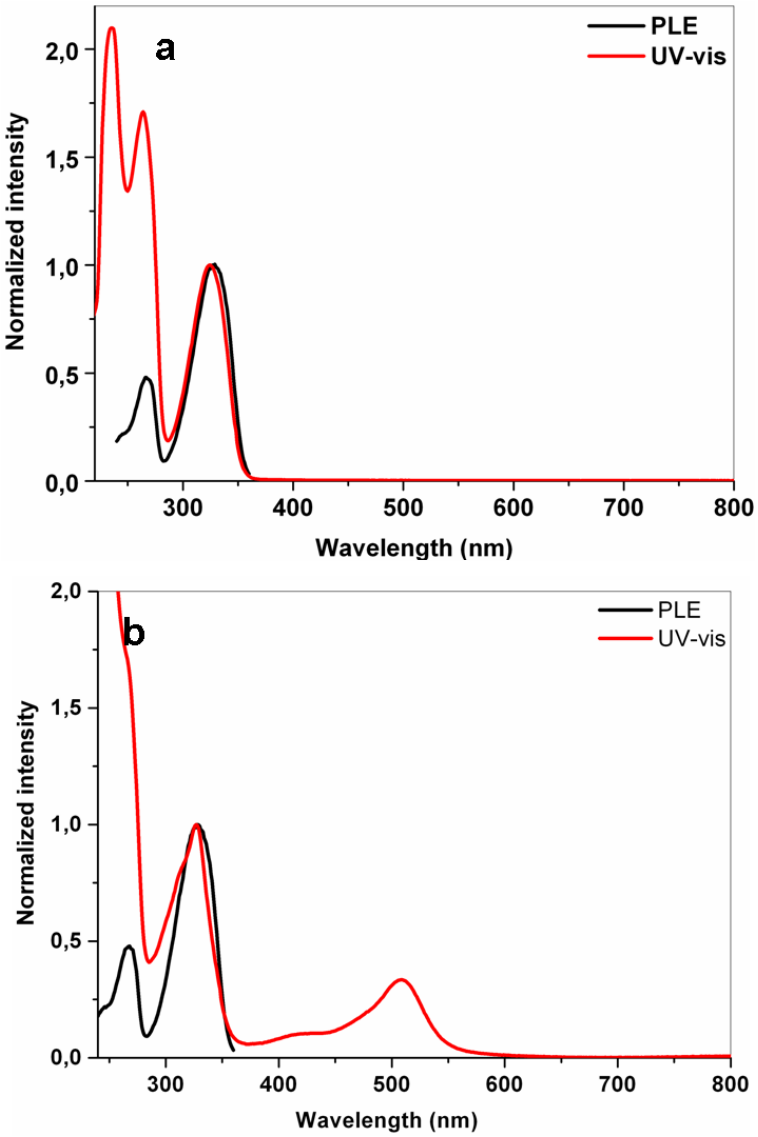


Figure S5 UV-vis absorption and PLE spectra of (a) **L^1H** and (b) **$[Fe(L^1)_2]$** in DCM/MeOH solvent mixture.

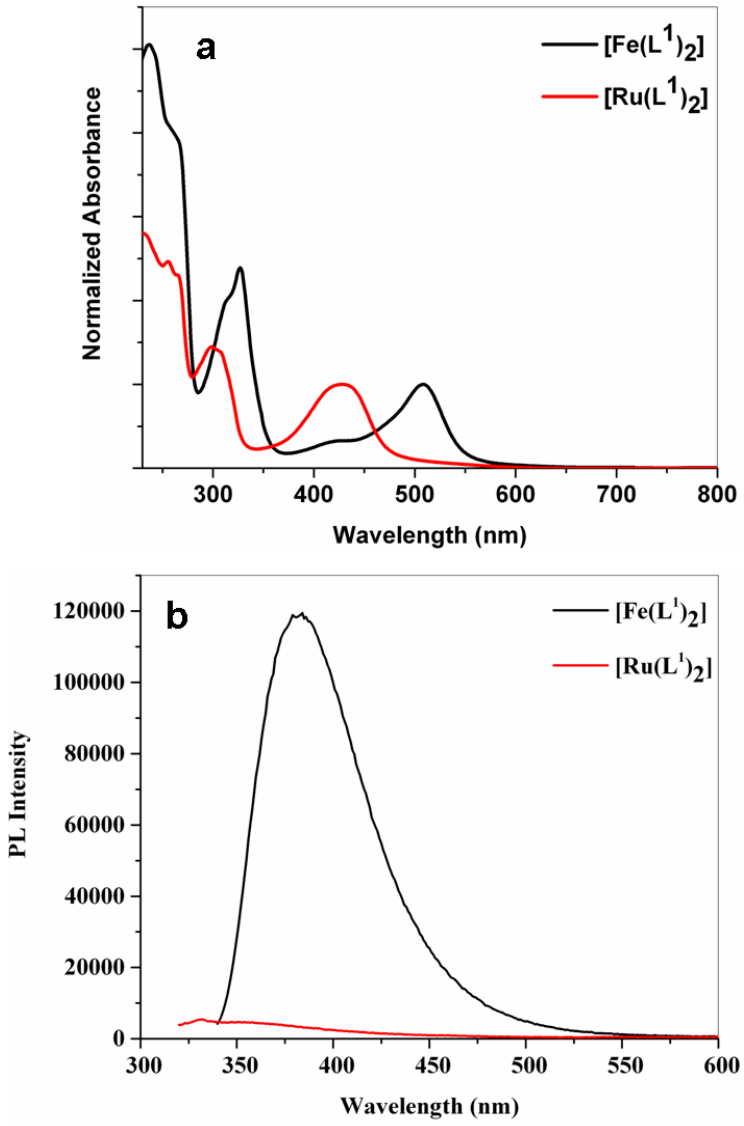


Figure S6 (a) UV-vis absorption and (b) PL spectra of **[Fe(L^1)$_2$]** and **[Ru(L^1)$_2$]** in DCM/MeOH solvent mixture. The UV-vis spectra are normalized at MLCT maxima for comparison purpose and the optical densities of the complex solutions were fixed at ca. 0.09 for PL measurements.

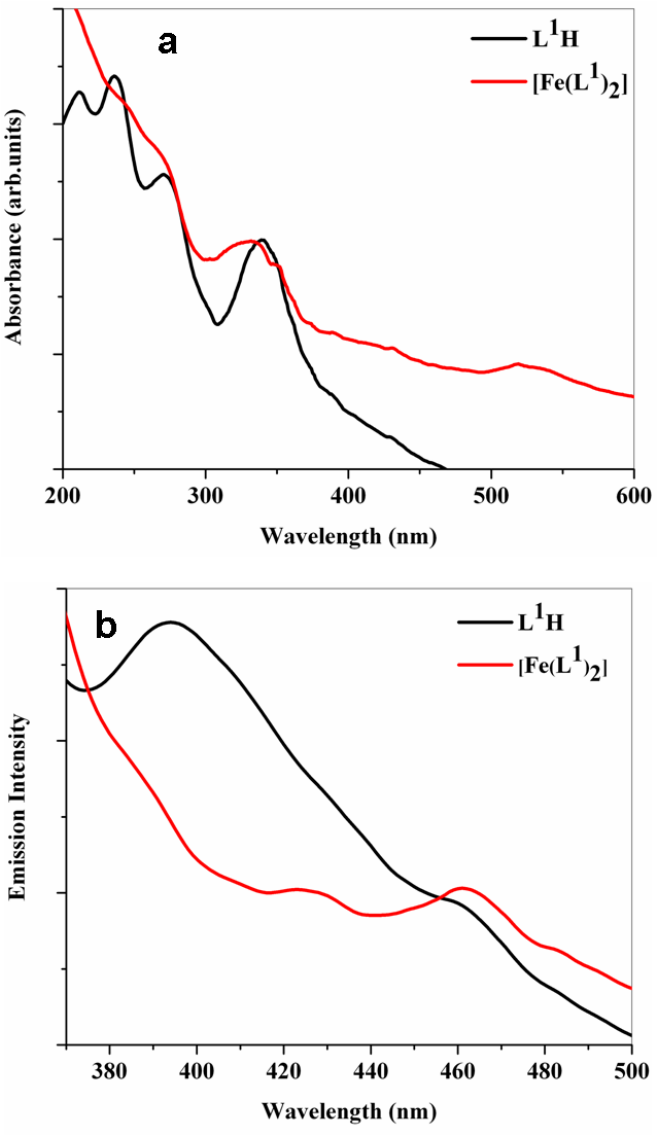


Figure S7 UV-vis absorption and PL spectra of (a) **L^1H** and (b) **$[Fe(L^1)_2]$** in solid state. The small peaks around 430 and 470 nm are originated from the light source. The excitation wavelengths are 338 and 334 nm for **L^1H** and **$[Fe(L^1)_2]$** respectively.

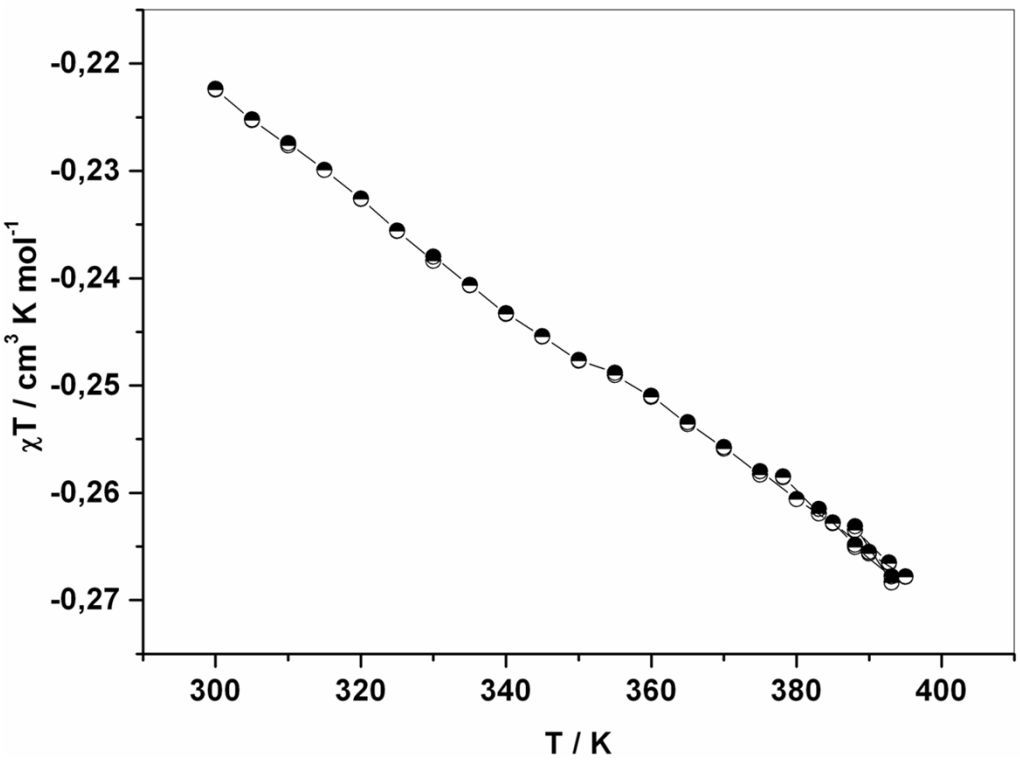


Figure S8 χT vs. T plot of crystalline form of [**Fe(L^1)$_2$**] under standard measurement conditions, this form of the complex is photomagnetically inactive upon either red or green light irradiation (λ = 637 nm or 532 nm, 10 mW cm^{-2}).