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

Platinum(II) complexes with cyclometallated 5-π-delocalized-donor-1,3-di(2-pyridyl)benzene ligands as efficient phosphors for NIR-OLEDs

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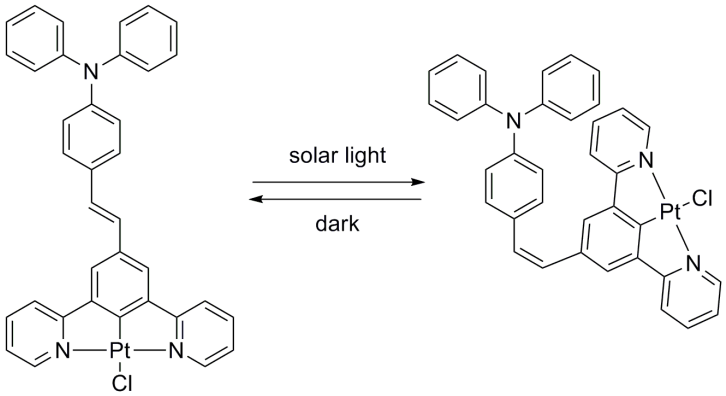
Supporting Information

(1) ^{1}H NMR data for *trans-cis* isomerisation of PtL^{2}Cl in solution



The ^{1}H NMR spectrum in CD_2Cl_2 of freshly prepared PtL^{2}Cl is shown in Figure 1(a), putting in evidence the presence of the *trans* isomer only. After 2 h under solar light exposure at room temperature in CD_2Cl_2, a mixture of *cis* and *trans* isomers is obtained {Figure 4(b)}. Simply leaving the solution in the dark for 18 h restores the *trans* isomer. No isomerisation is detectable in the solid state.

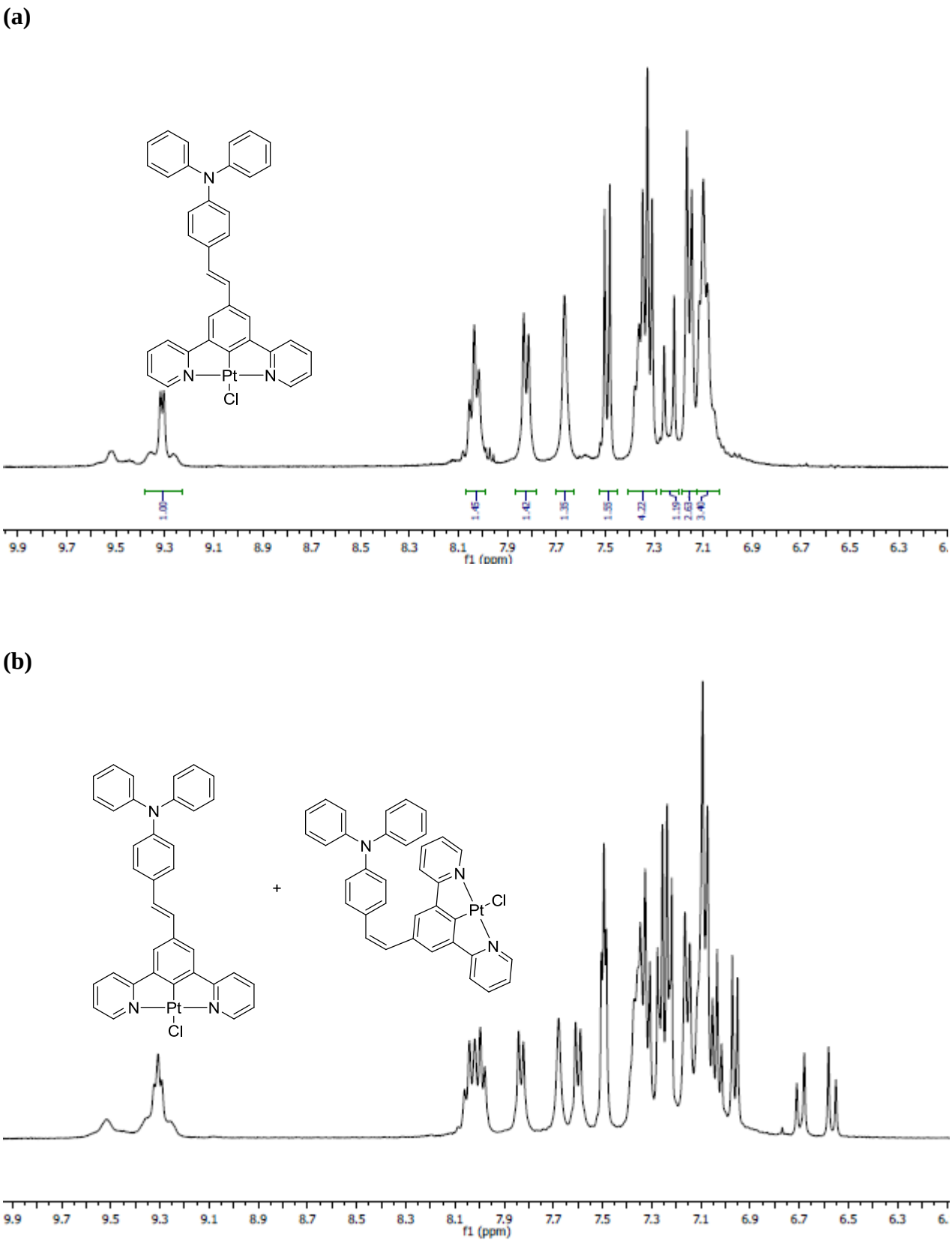


Figure S1 ^{1}H NMR spectra (400 MHz) for PtL^{2}Cl in CD_2Cl_2: (a) freshly prepared sample, (b) after exposure of the solution to solar light for 2 h.

(2) Absorption and photoluminescence of PtL[1]NCS

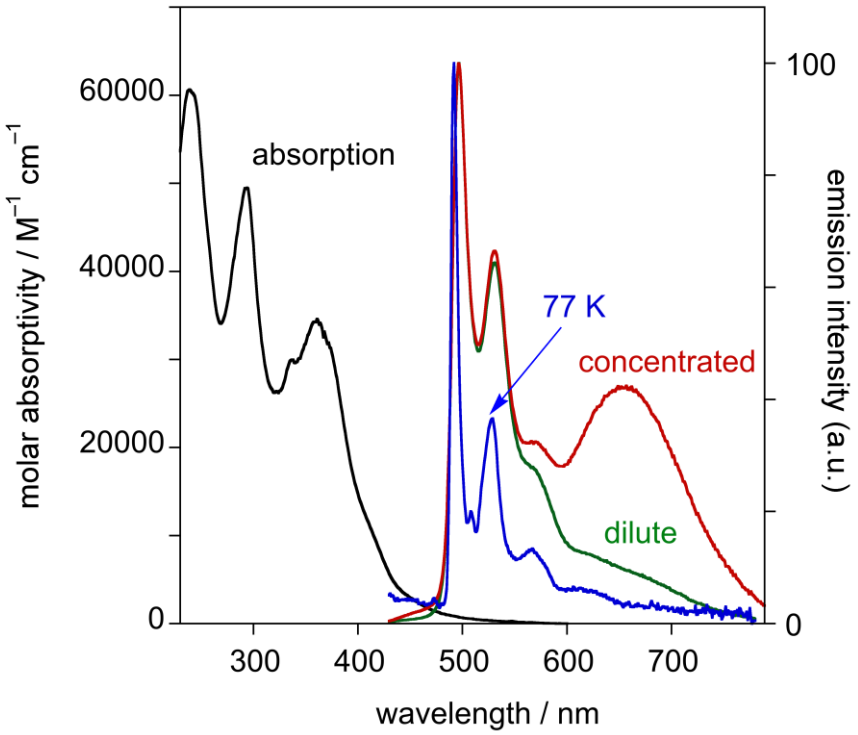


Figure S2 Absorption spectrum of PtL[1]NCS in CH_2Cl_2 at 298 K (black line); emission spectra under the same conditions for solutions of concentration 1.24×10^{-5} and 1.03×10^{-4} M (green and red lines respectively), and the emission spectrum at 77 K in a glass of diethyl ether / isopentane / ethanol (2:2:1 v/v) (blue line).

(3) Additional TD-DFT data for PtL^2Cl

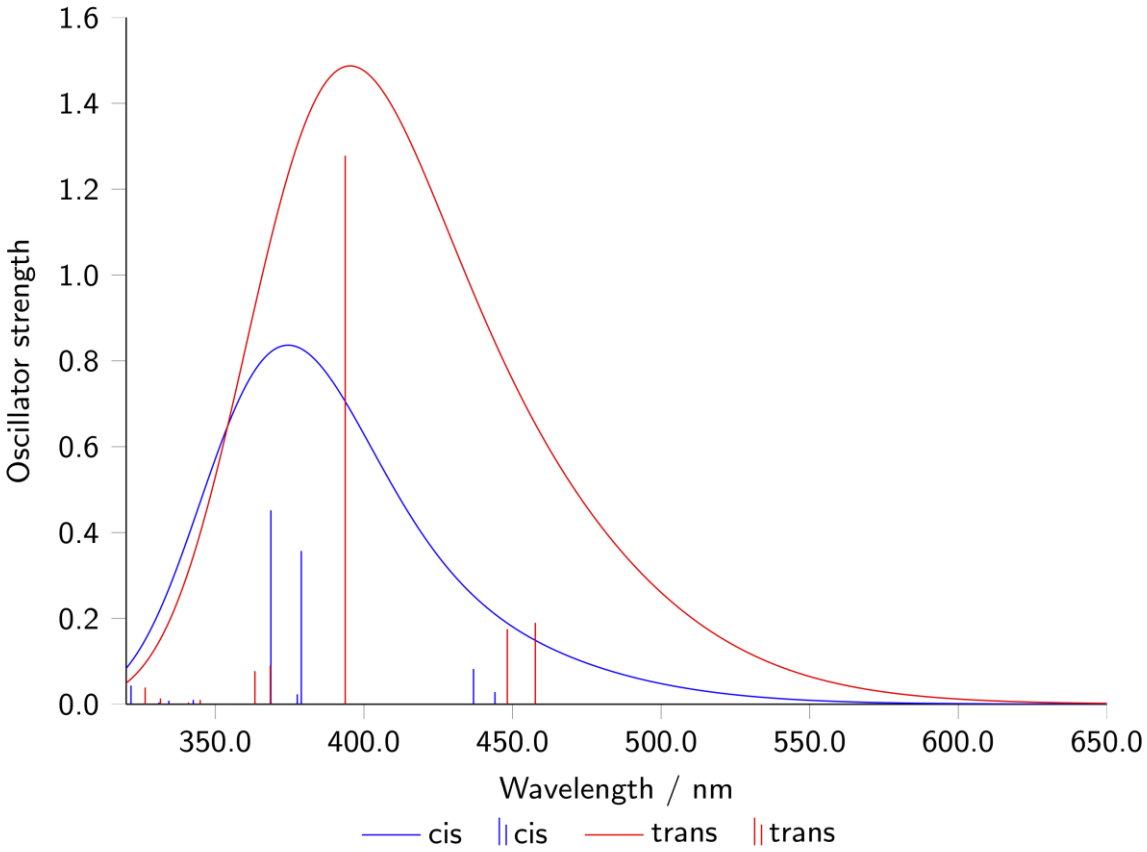


Figure S3 Simulated absorption spectra in the near-UV region for the *trans* (red) and *cis* (blue) forms of PtL^2Cl, convoluted from the individual calculated excitations represented by the vertical lines.

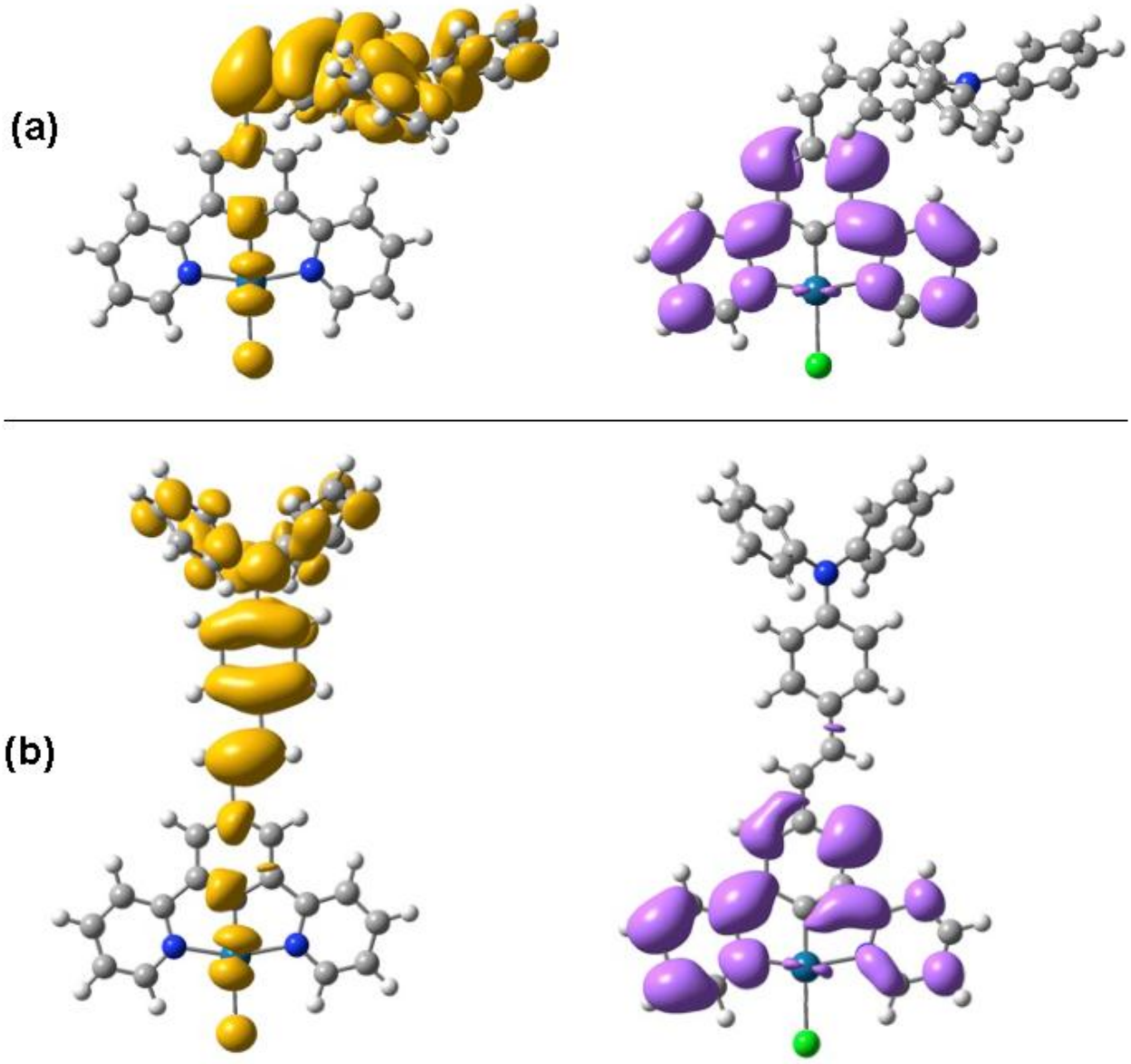


Figure S4 Density difference plots for the lowest singlet excitations of the *cis* (a) and *trans* (b) forms of PtL^2Cl calculated at the ground state geometry, using PBE0 with the PCM model for CH_2Cl_2. Yellow and purple respresent zones of depletion and augmentation of electron density in the first singlet excitation versus the S_0 ground state.

(4) Additional OLED data

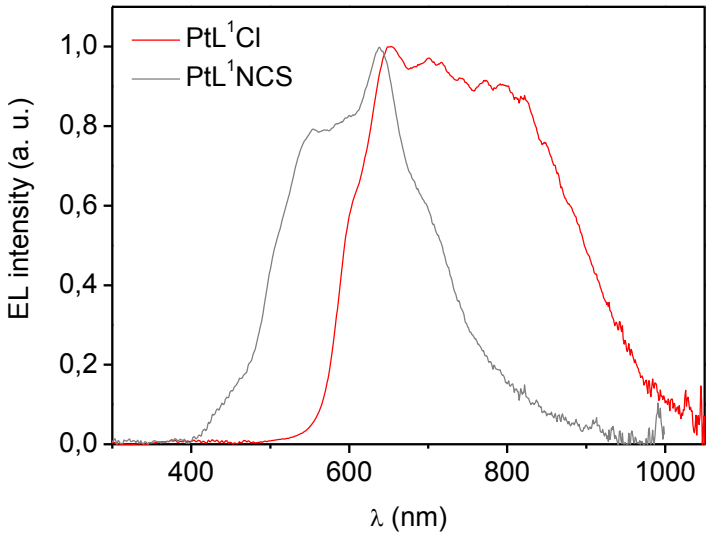


Figure S5 Electroluminescence spectra of OLEDs based on PtL^1Cl or PtL^1NCS neat film as the emitting layer.

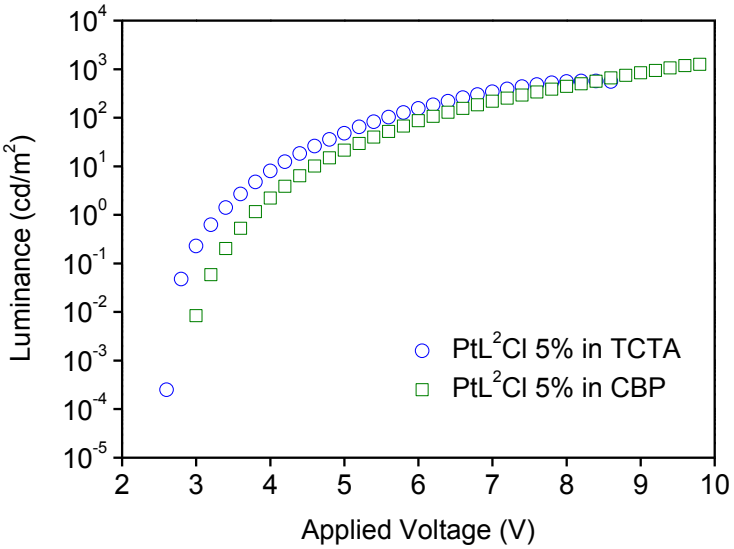


Figure S6 Luminance versus applied voltage for OLEDs based on PtL^2Cl diluted in TCTA or CBP as the emitting layer.

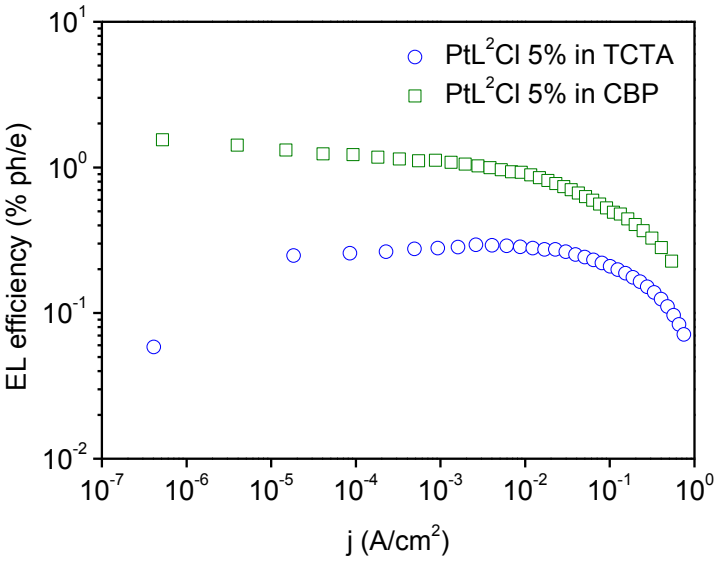


Figure S7 External quantum efficiencies versus electric current density for the OLEDs based on PtL^2Cl diluted in TCTA or CBP as emitting layer.