Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Synthesis, Photophysics and Reverse Saturable Absorption of Bipyridyl Platinum(II) Bis(arylfluorenylacetylide) Complexes

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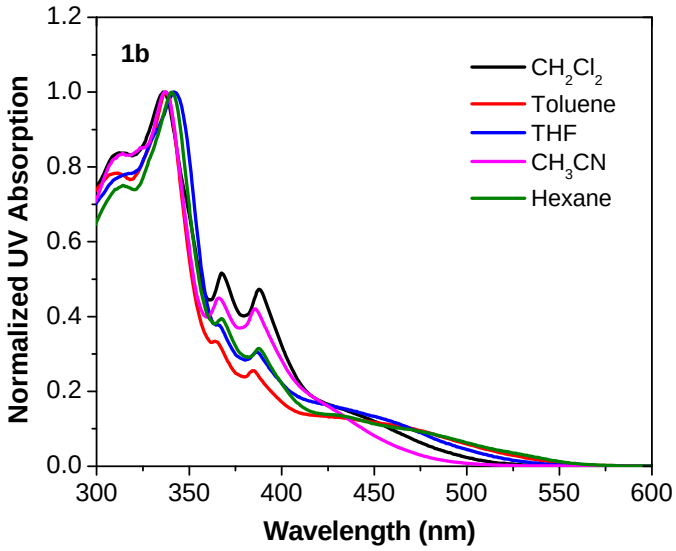


Figure S1. Normalized UV-Vis absorption spectra of **1b** in different solvents. A_{436} = 0.08 in a 1 cm cuvette.

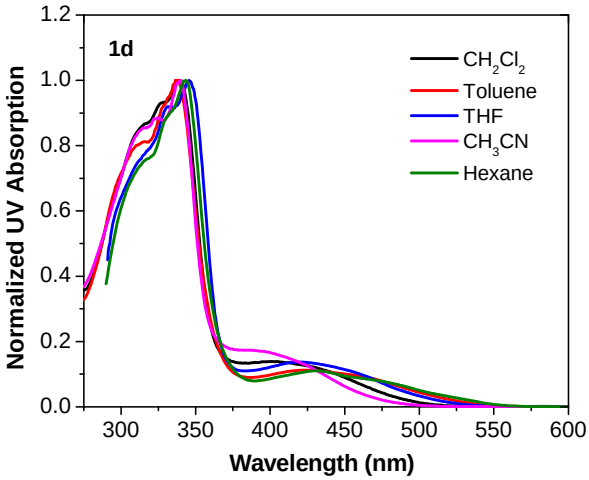


Figure S2. Normalized UV-Vis absorption spectra of **1d** in different solvents. A_{436} = 0.08 in a 1 cm cuvette.

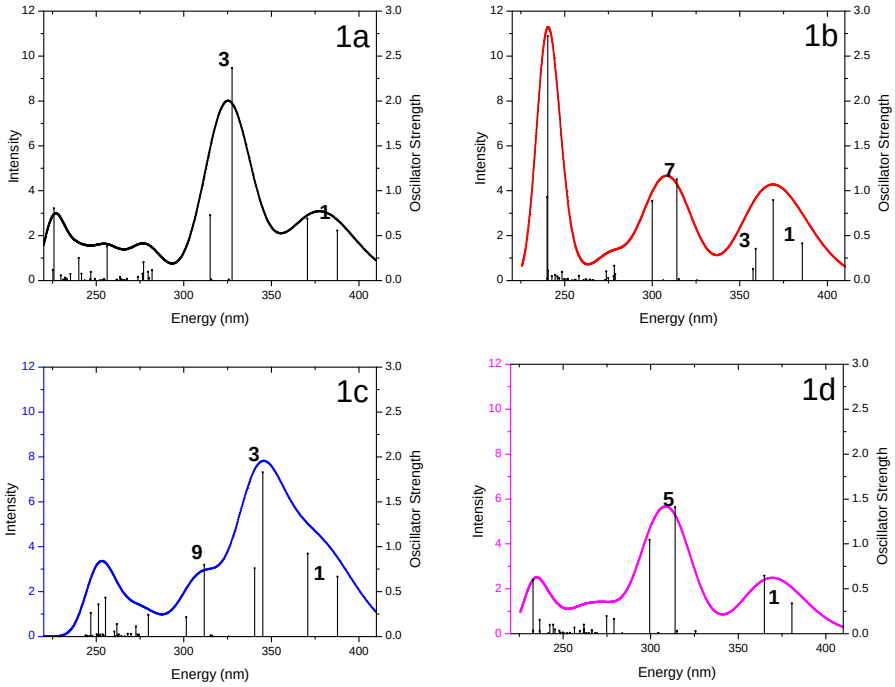


Figure S3. Calculated absorption spectra for complexes **1a** – **1d**; vertical lines represent excited states and the corresponding oscillator strength. Labeled numbers represent the states whose NTO's are shown in Tables 2 and 3.

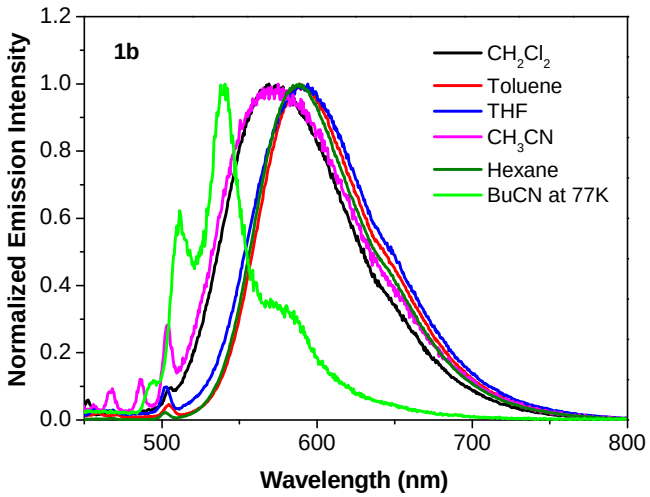


Figure S4. Normalized emission spectra of **1b** in different solvents at room temperature and in BuCN glassy matrix at 77 K, λ_{ex} = 436 nm.

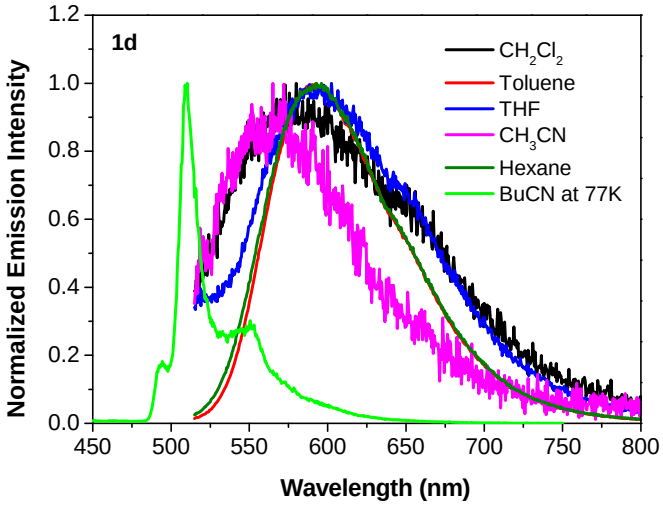


Figure S5. Normalized emission spectra of **1d** in different solvents at room temperature and in BuCN glassy matrix at 77 K, λ_{ex} = 436 nm.

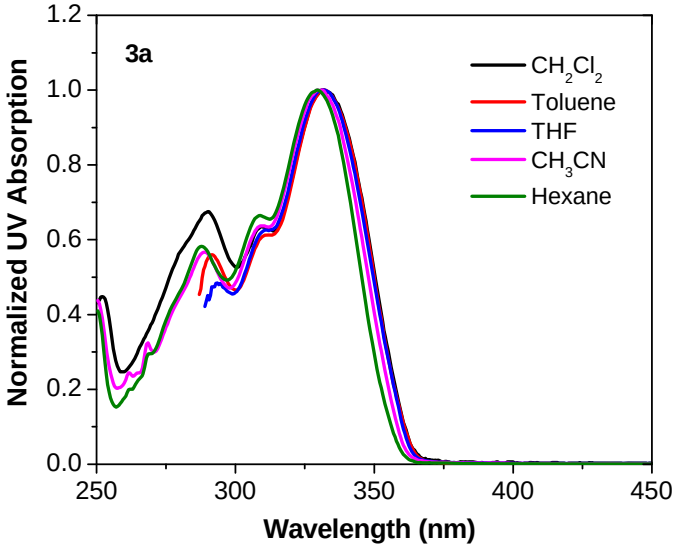


Figure S6. Normalized UV-Vis absorption spectra of **3a** in different solvents. A_{365} = 0.08

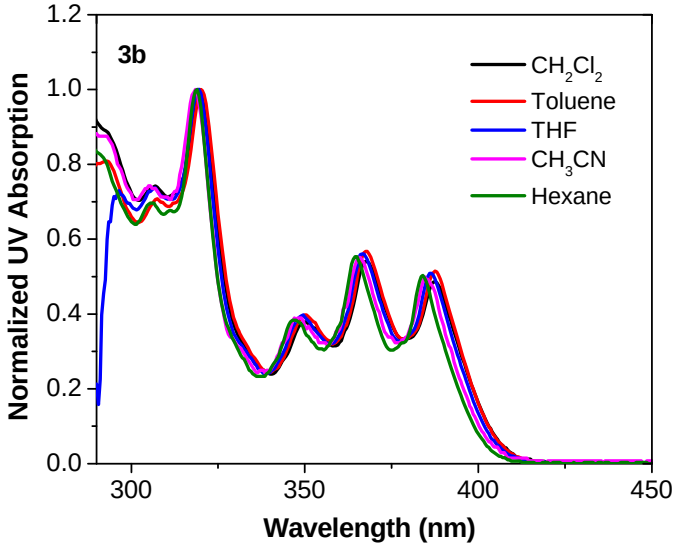


Figure S7. Normalized UV-Vis absorption spectra of **3b** in different solvents. A_{365} = 0.08

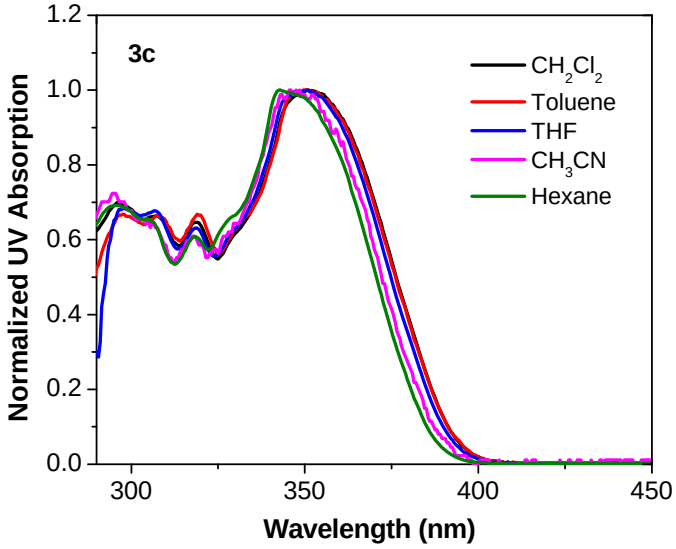


Figure S8. Normalized UV-Vis absorption spectra of **3c** in different solvents. A_{365} = 0.08

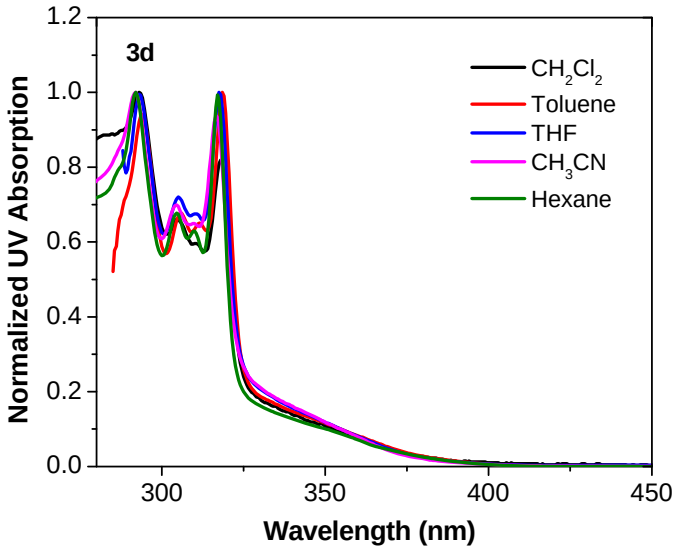


Figure S9. Normalized UV-Vis absorption spectra of **3d** in different solvents. A_{365} = 0.08

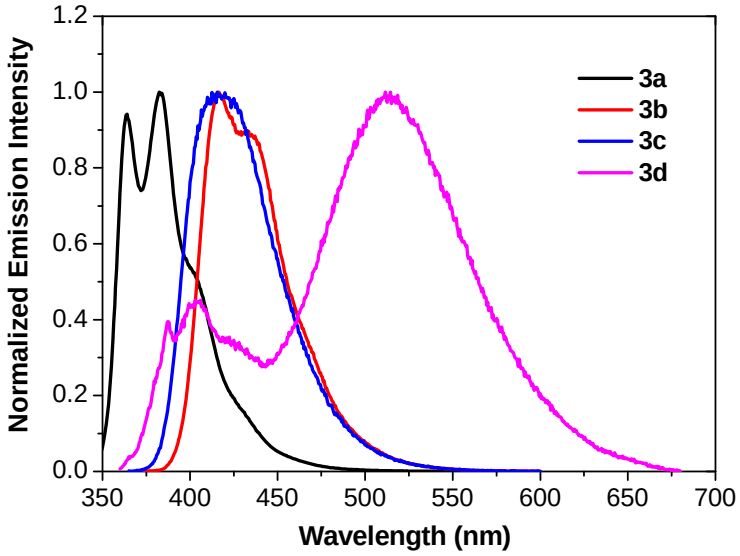


Figure S10. Normalized emission spectra of ligands **3a**, λ_{ex} = 335 nm, **3b**, λ_{ex} = 350 nm, **3c**, λ_{ex} = 355 nm and **3d**, λ_{ex} = 345 nm, in CH_2Cl_2 (1×10^{-5} mol·L^{-1}).

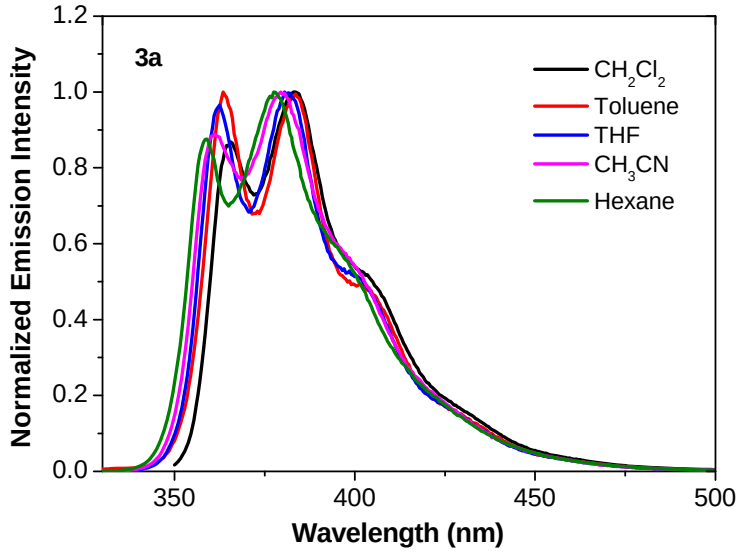


Figure S11. Normalized emission spectra of **3a** in different solvents at room temperature, λ_{ex} = 320 nm.

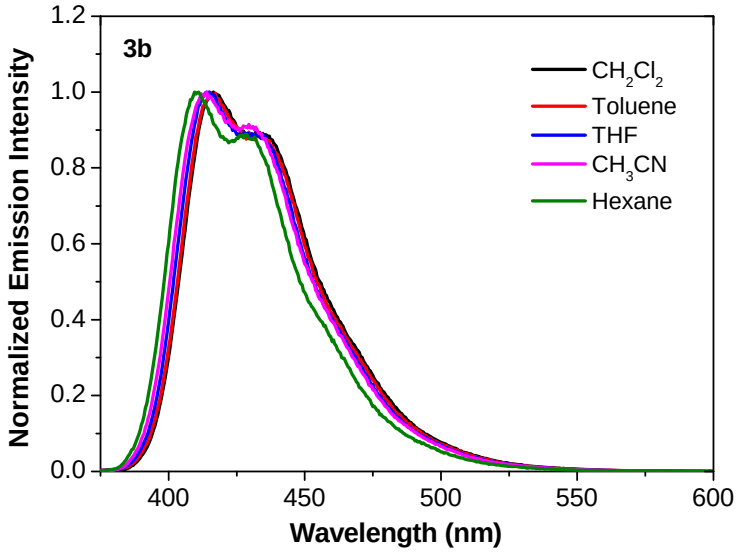


Figure S12. Normalized emission spectra of **3b** in different solvents at room temperature, λ_{ex} = 365 nm.

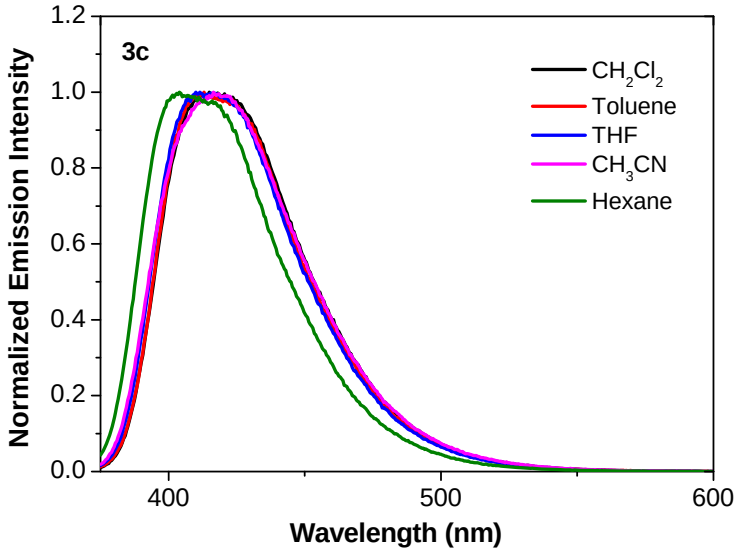


Figure S13. Normalized emission spectra of **3c** in different solvents at room temperature, λ_{ex} = 365 nm.

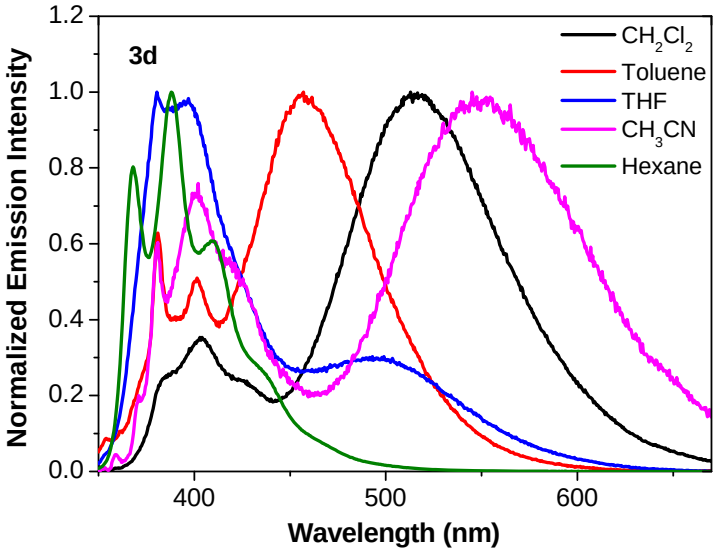


Figure S14. Normalized emission spectra of **3d** in different solvents at room temperature, λ_{ex} = 365 nm.

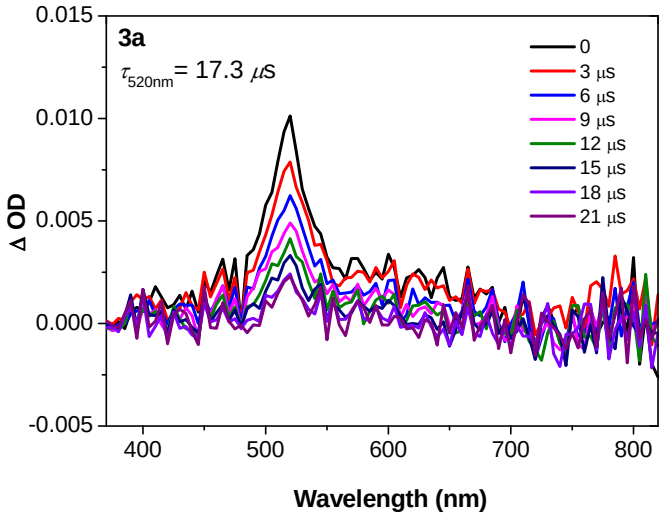


Figure S15. Time-resolved triplet transient difference absorption spectra of **3a** in toluene. λ_{ex} = 355 nm. A = 0.4 at 355 nm in a 1-cm cuvette.

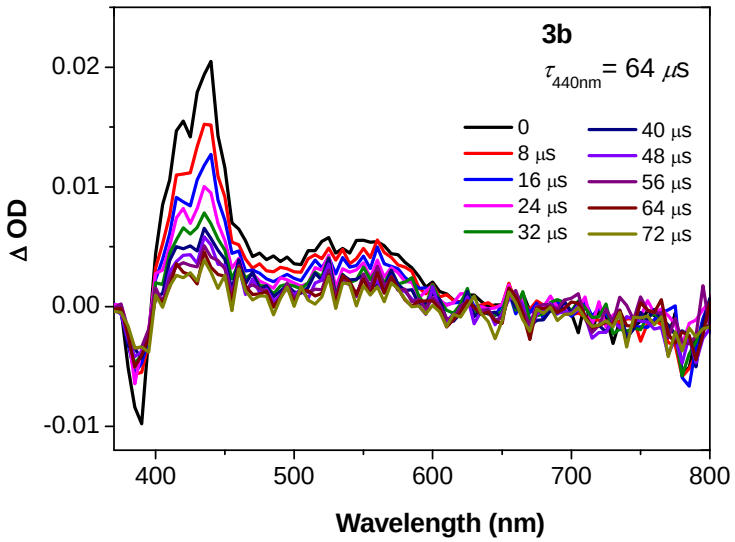


Figure S16. Time-resolved triplet transient difference absorption spectra of **3b** in toluene. λ_{ex} = 355 nm. A = 0.4 at 355 nm in a 1-cm cuvette.

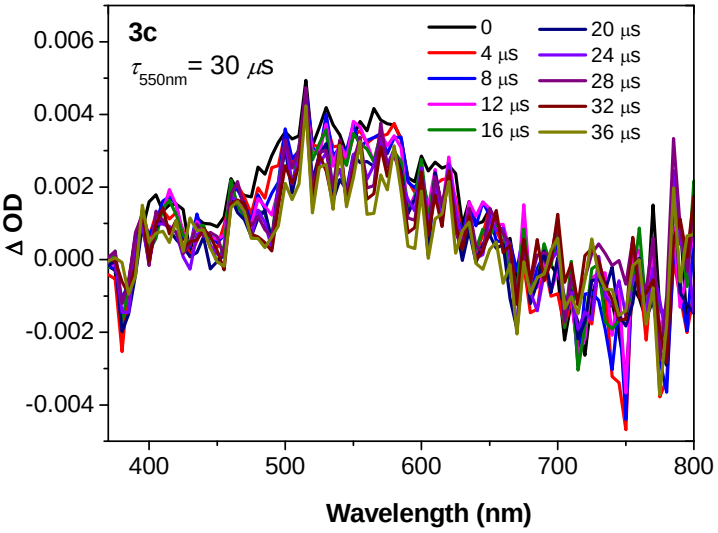


Figure S17. Time-resolved triplet transient difference absorption spectra of **3c** in toluene. λ_{ex} = 355 nm. A = 0.4 at 355 nm in a 1-cm cuvette.

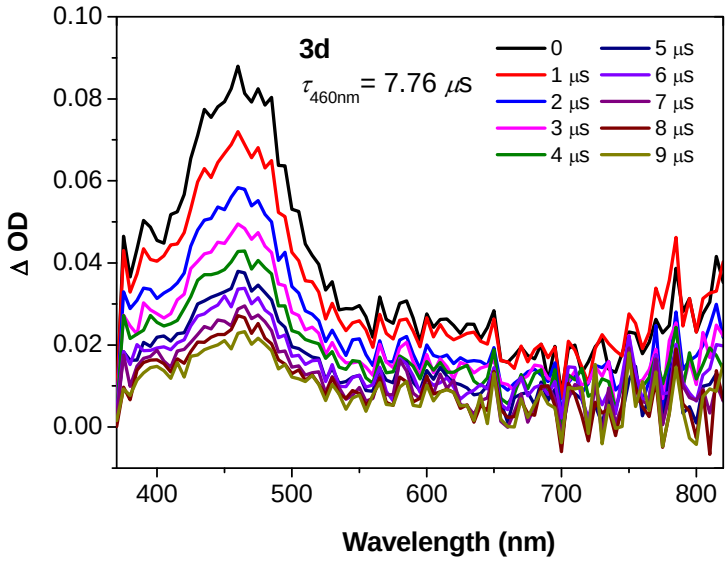


Figure S18. Time-resolved triplet transient difference absorption spectra of **3d** in toluene. λ_{ex} = 355 nm. A = 0.4 at 355 nm in a 1-cm cuvette.

Table S1. Optimized geometries of complexes **1a** – **1d**

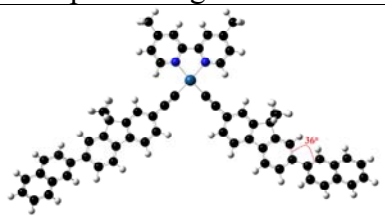
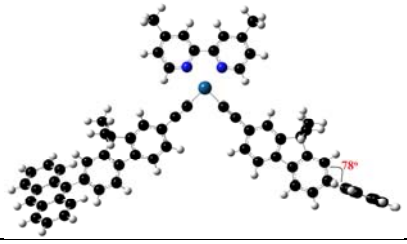
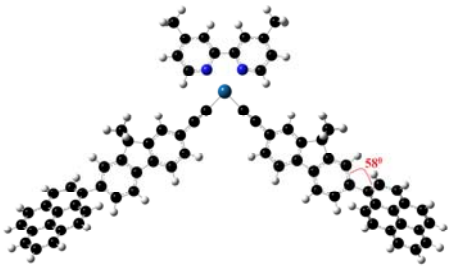
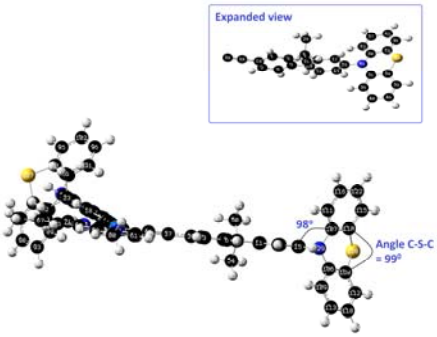
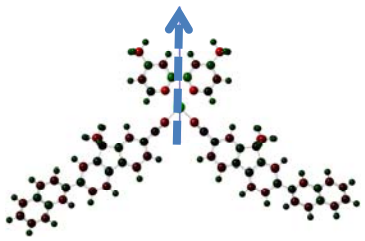
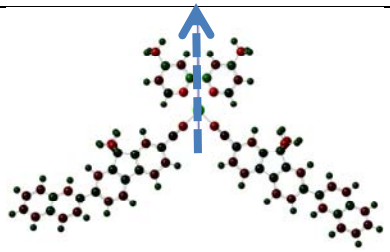
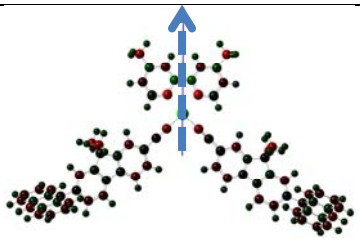
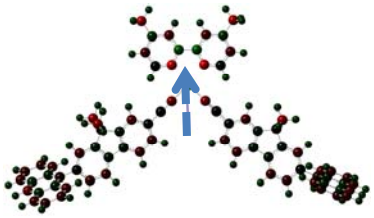
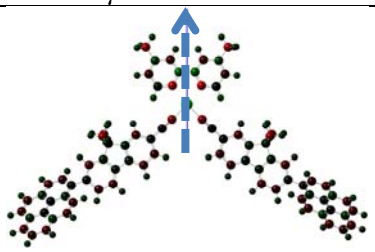
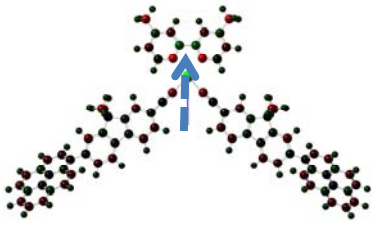
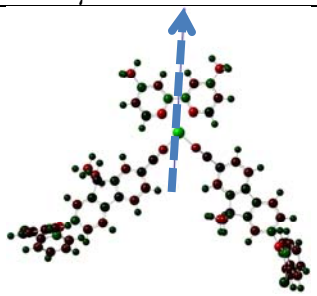
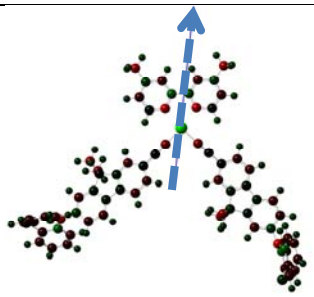
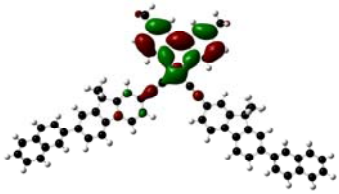
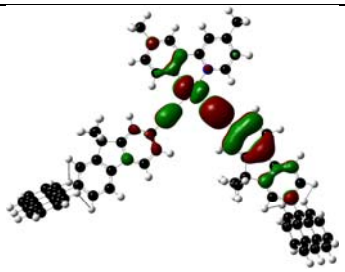
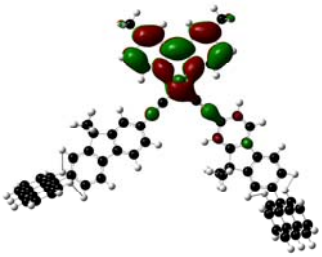
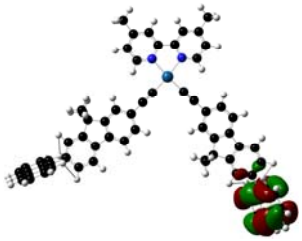
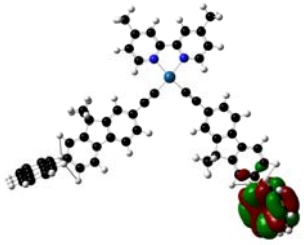
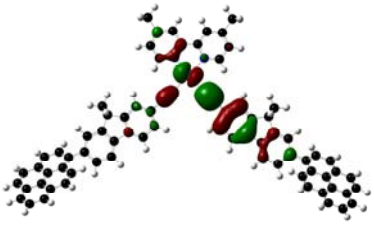
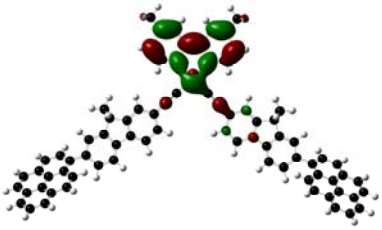
Complex	Optimized geometries
1a	
1b	
1c	
1d	

Table S2. Schematic representation of the magnitude of the static dipole moments and directions of Pt(II) complexes **1a** – **1d** at their ground state and excited state.[a]

Complex	Ground State	Excited State
1a	 μ = 18.21 D	 μ = 17.54 D
1b	 μ = 18.40 D	 μ = 5.89 D
1c	 μ = 18.46 D	 μ = 5.94 D
1d	 μ = 21.72 D	 μ = 21.40 D

[a] The different colors in the structure represent the Milliken charge density distributions, with the green color indicating positive charges and red color representing negative charges.

Table S3 NTOs representing transitions corresponding to singlet emission (S_1) of complexes **1a - 1d** and triplet emission (T_1) of the complex **1b** calculated using CAM-B3LYP functional.

	Excited State and Properties	HOLE	ELECTRON
1a	**S_1 393 nm $f_{o.s.}$ = 0.59**		
1b	**S_1 390 nm $f_{o.s.}$ = 0.44**		
	T_1 820 nm		
1c	**S_1 392 nm $f_{o.s.}$ = 0.68**		
1d	**S_1 385 nm $f_{o.s.}$ = 0.37**