

Electronic supporting information

Dual Phosphorescent Emission of Dinuclear Platinum (II) Complexes Incorporating Cyclometallating Pyrenyl- Dipyrdine-Based Ligands and Materials Application in Near- Infrared Solution-Processed Polymer Light-Emitting Diodes

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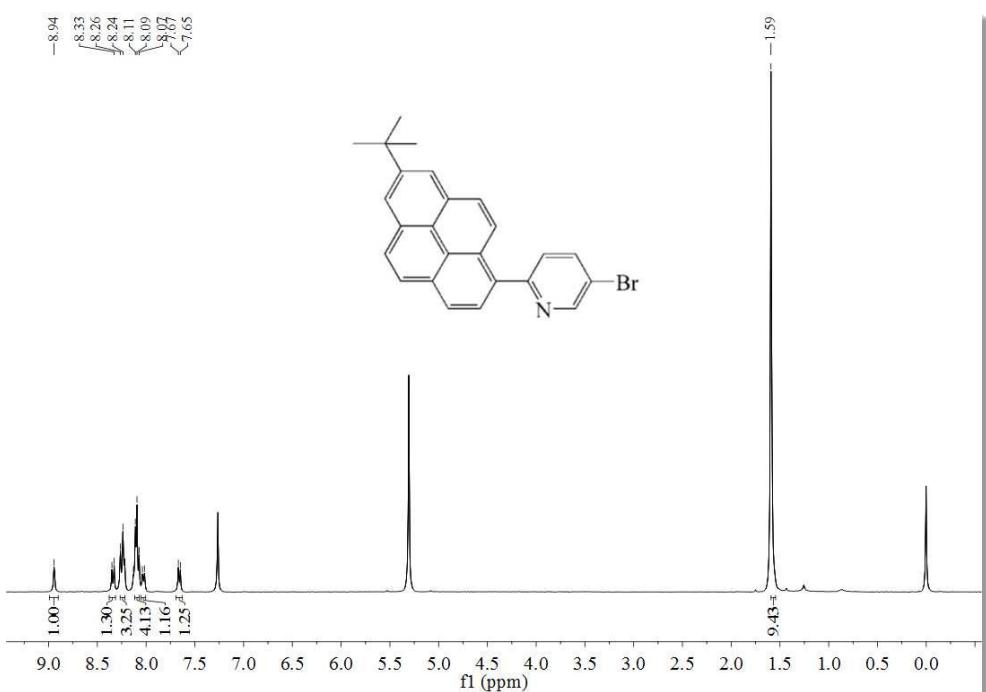
Figure S2. TGA curves of the platinum (II) complexes.

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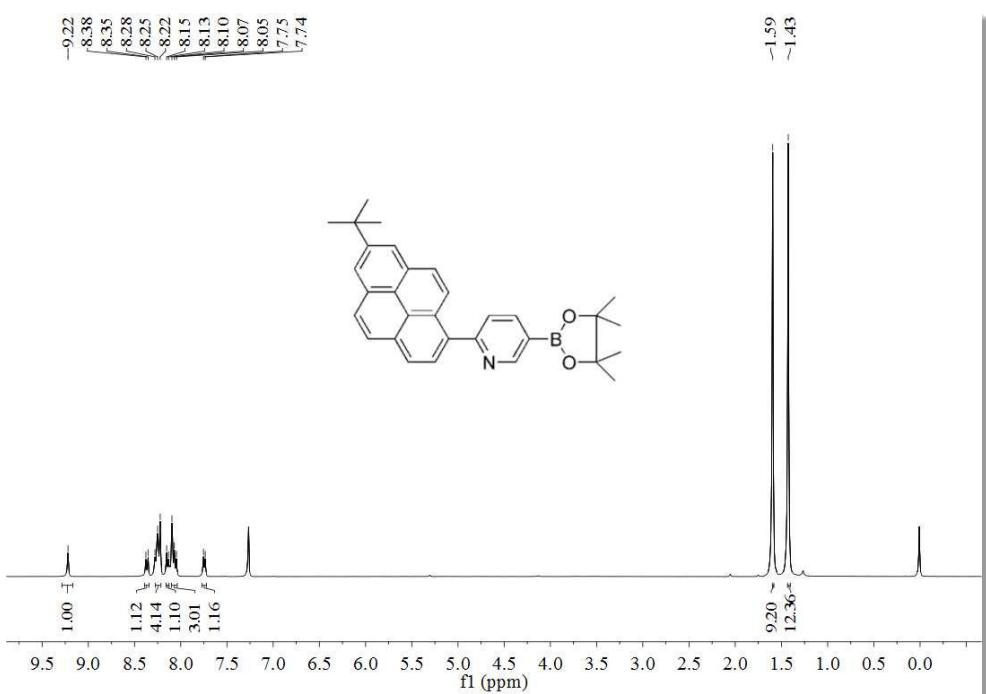
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Table S1. Selected Bond Lengths (\AA) and Angles ($^\circ$)

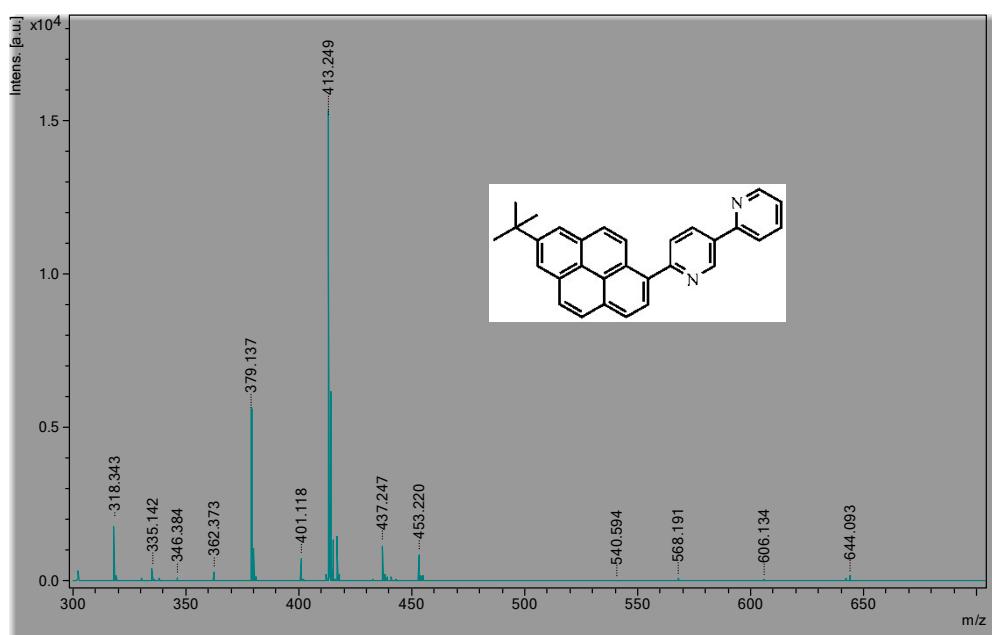
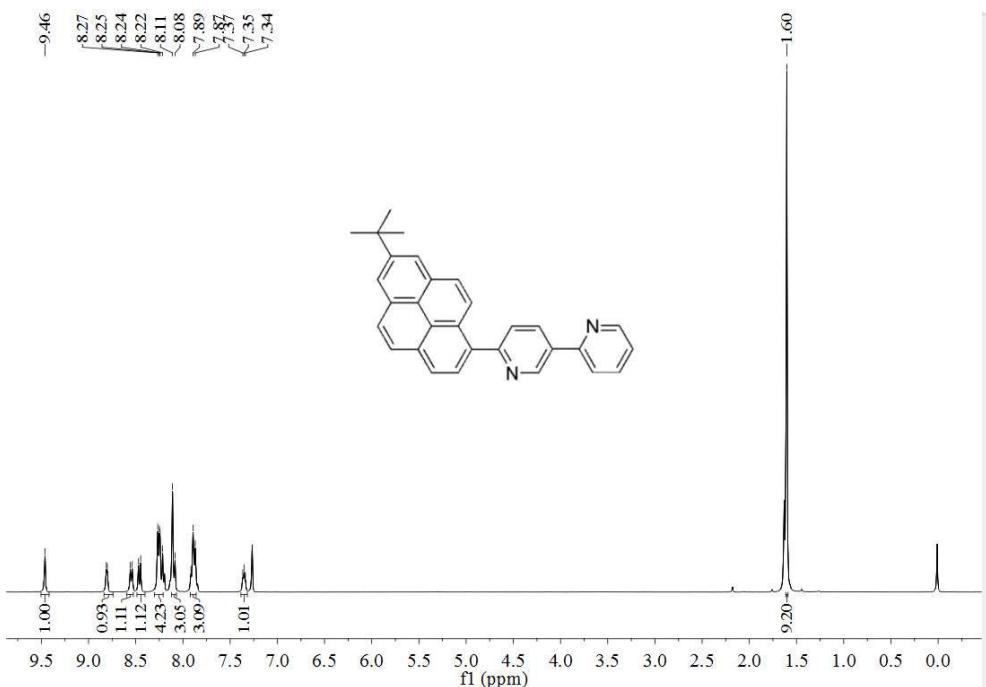
Figure S1. NMR and MS spectra of the intermediates and the platinum complexes.



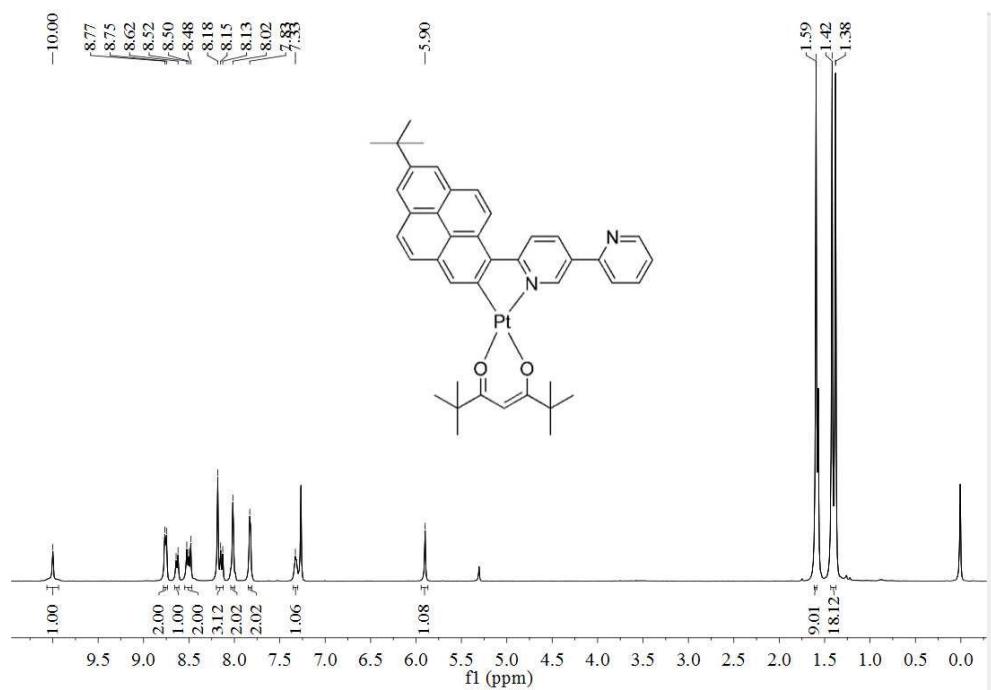
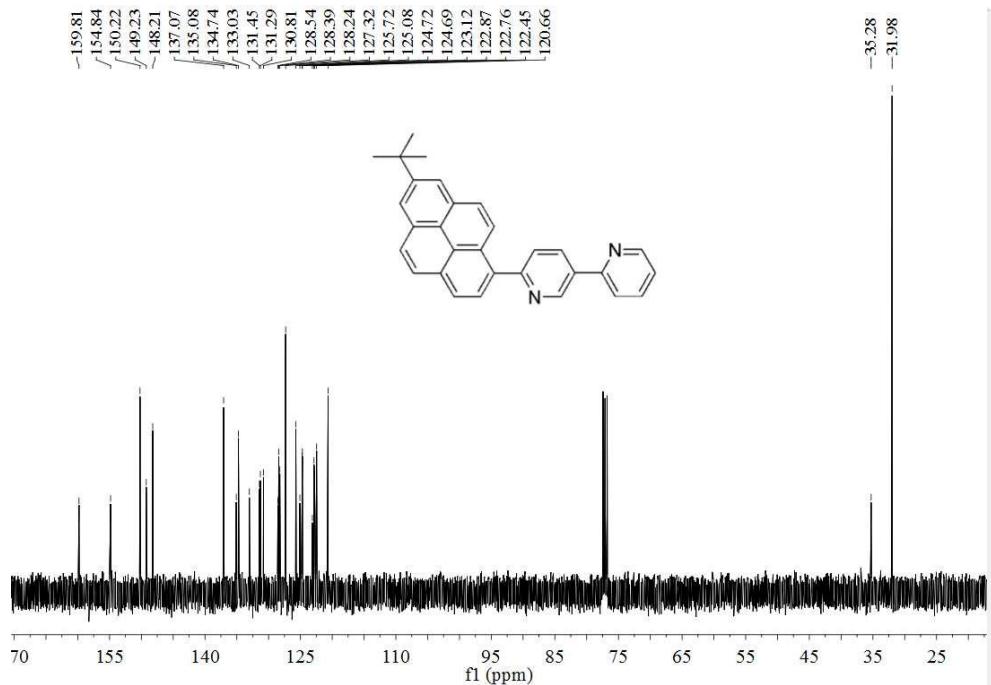
¹H NMR (400MHz) spectrum of compound 2 in CDCl₃.

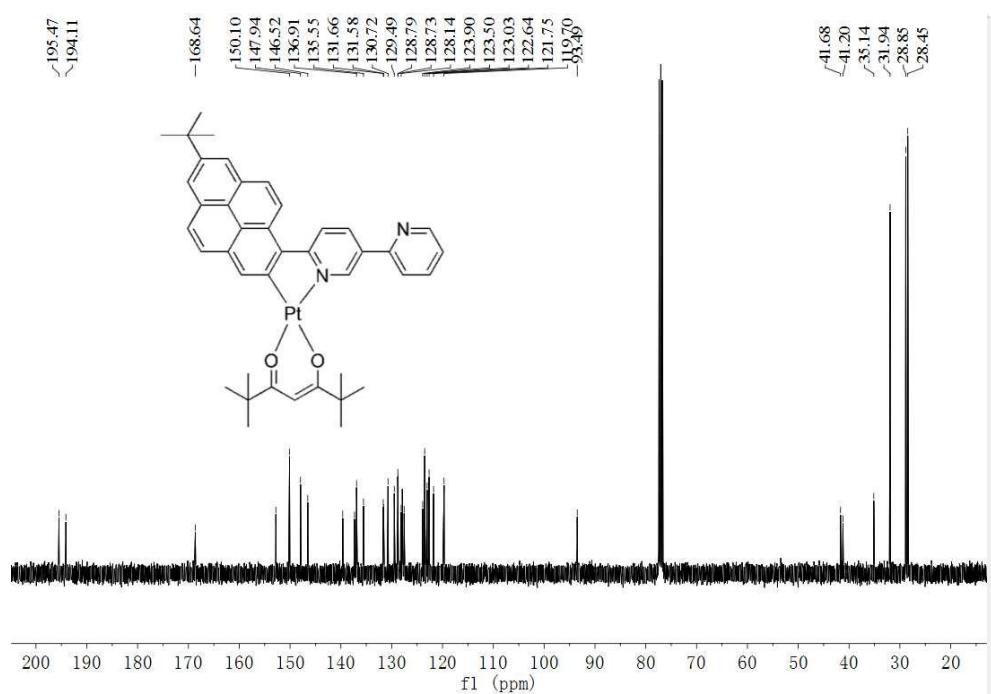
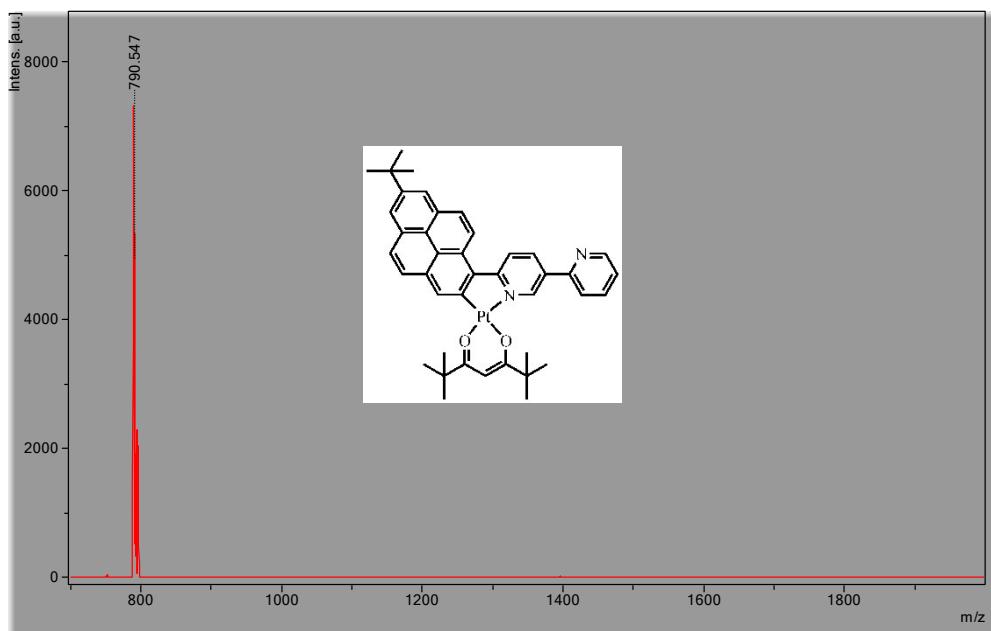


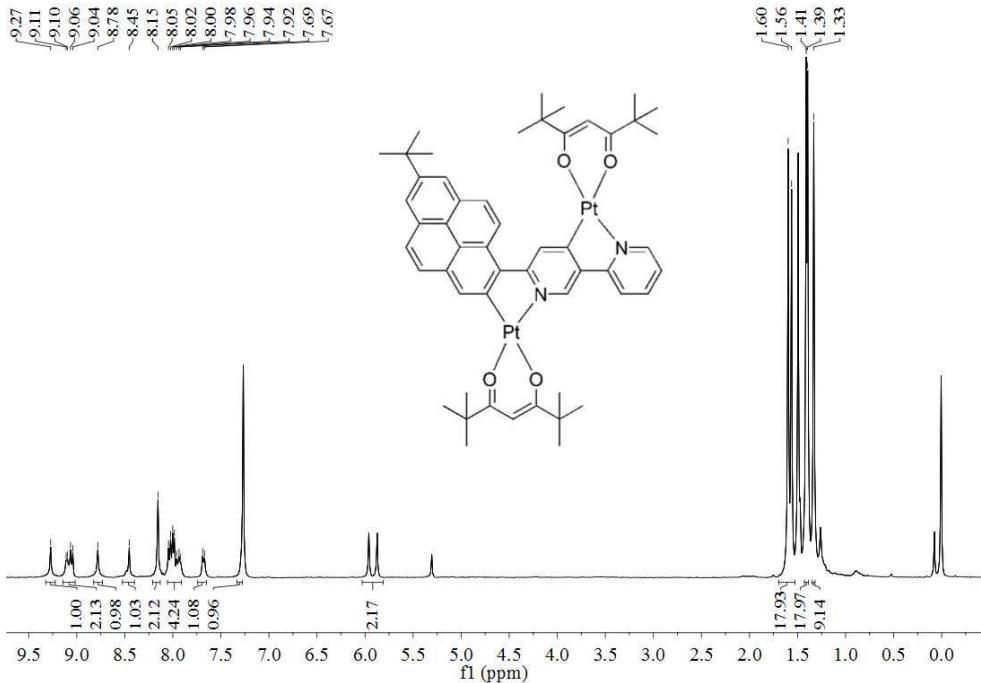
¹H NMR (400MHz) spectrum of compound 3 in CDCl₃.



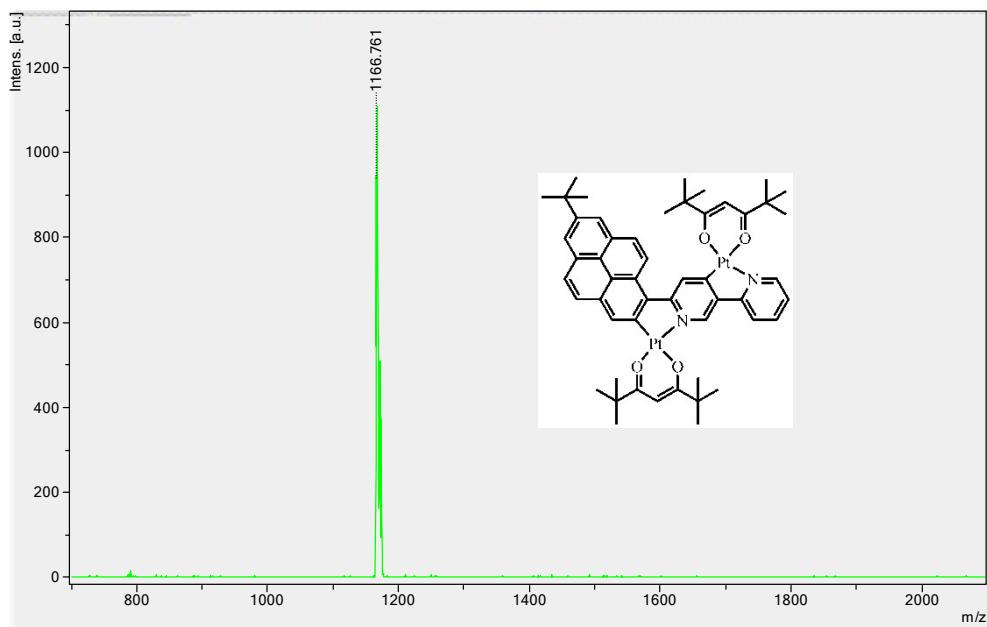
MS spectrum of BuPyrDPy in DCM.



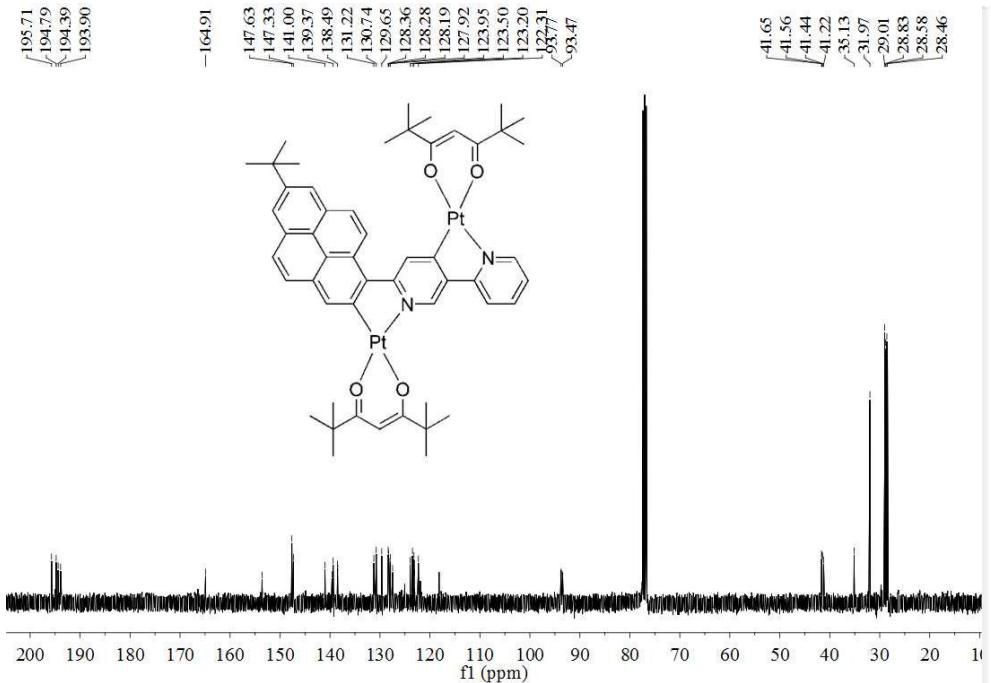




^1H NMR (400MHz) spectrum of (BuPyrDPy)[Pt(dpm)]₂ in CDCl_3 .



MS spectrum of (BuPyrDPy)[Pt(dpm)]₂ in DCM.



^{13}C NMR (400MHz) spectrum of (BuPyrDPy)[Pt(dpm)]₂ in CDCl_3 .

Figure S2. TGA curves of the platinum (II) complexes.

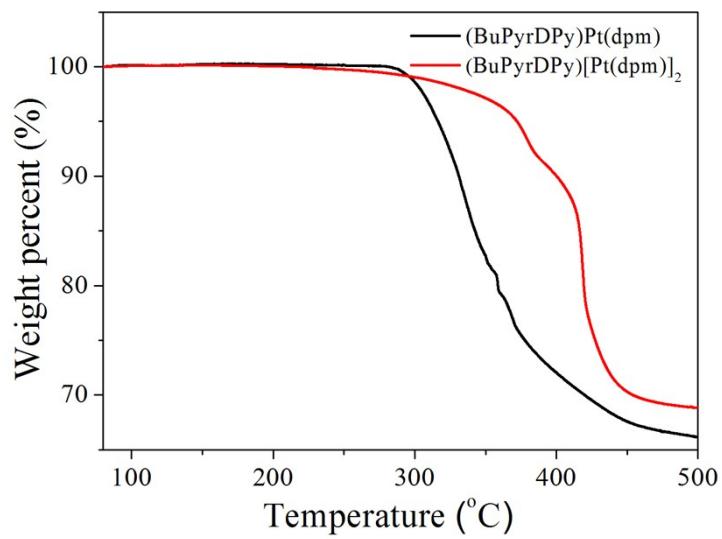


Figure S3. Photophysical properties.

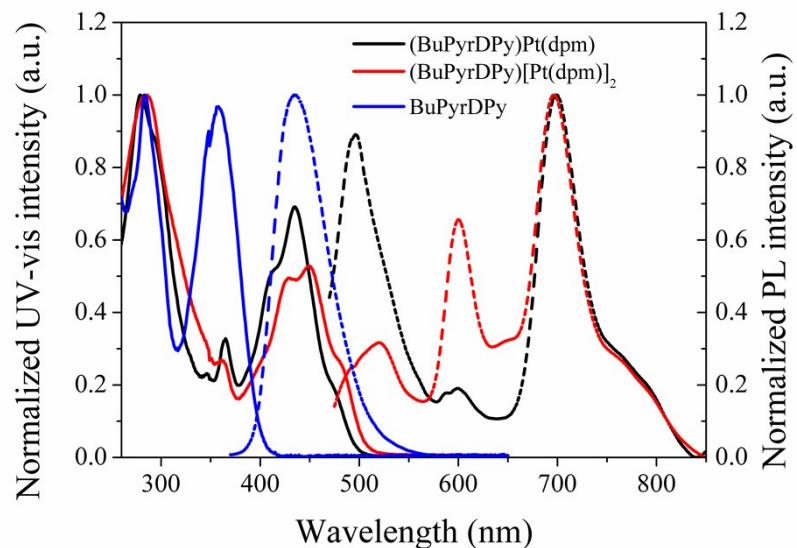


Figure S3-1. Absorption (solid line)/emission (dash line) spectra of the ligand and complexes in dilute DCM solutions at room temperature.

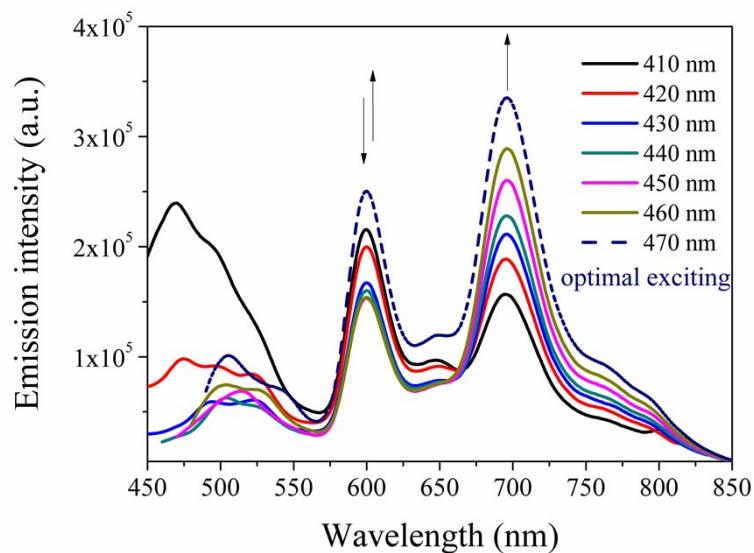


Figure S3-2. PL spectra of (BuPyrDPy)[Pt(dpm)]₂ under varied excitation wavelengths.

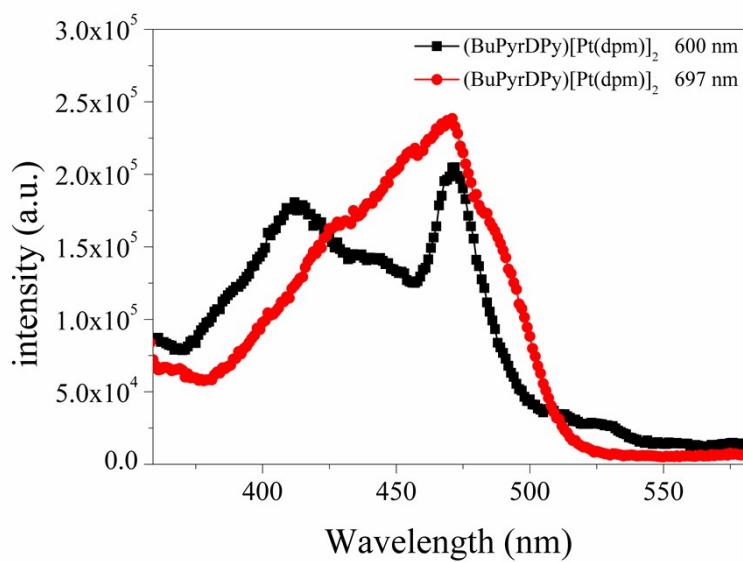


Figure S3-3. Excitation spectra of (BuPyrDPy)₂[Pt(dpm)]₂ were independent of λ_{em} (black line: $\lambda_{\text{em}} = 697 \text{ nm}$, red line: $\lambda_{\text{em}} = 600 \text{ nm}$).

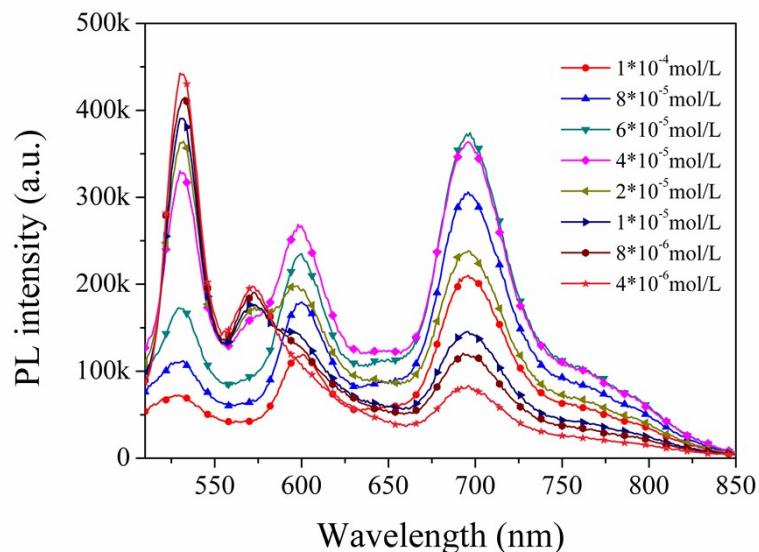
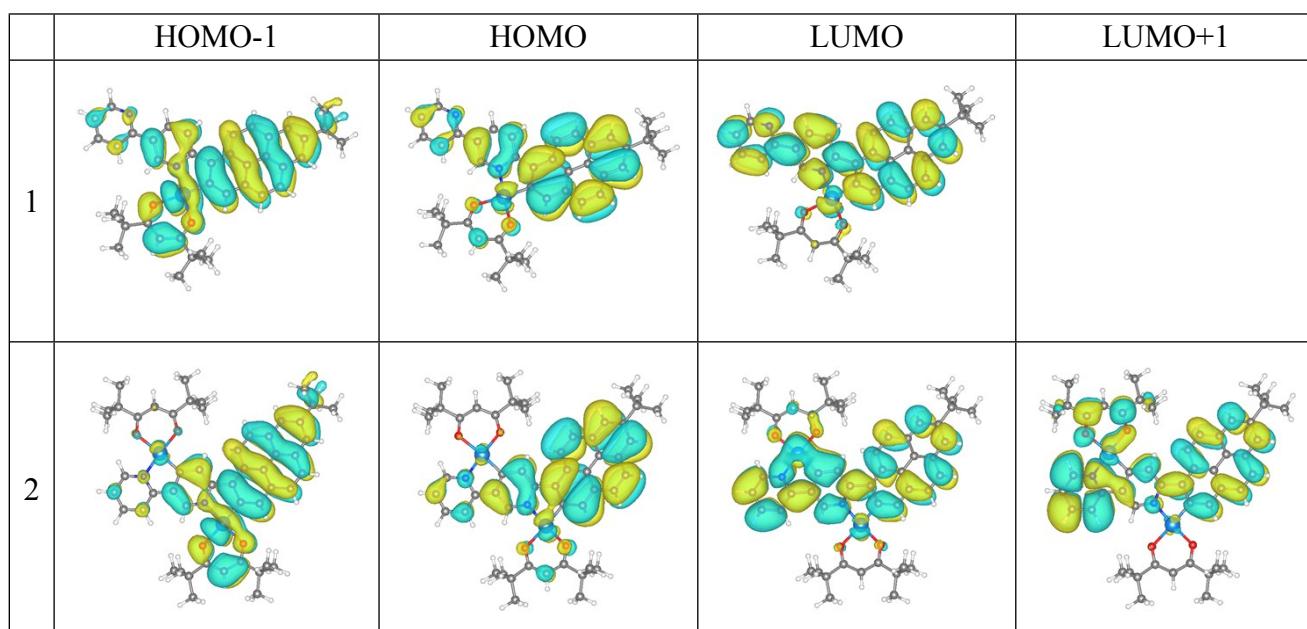


Figure S3-4. PL spectra of (BuPyrDPy)₂[Pt(dpm)]₂ under varied concentration in DCM solutions.

Figure S4. DFT calculations



Molecular orbital energy diagrams of (BuPyrDPy)Pt(dpm) (1) and (BuPyrDPy)[Pt(dpm)]₂ (2) obtained at the UB3LYP theory level on the optimized triplet state geometry.

Table S1. Selected Bond Lengths (Å) and Angles (°)

Main bond distances (Å) and selected angles (°) for complexes from X-ray data and TD-DFT.

	Bond	Experimental/Calculated bond distances (Å)	Torsional Angles	Experimental/Calculated torsional Angles (°)
1	Pt1-N1	1.9800 (0.0037)/2.01728	C13-C12-C9-N1	10.05/10.46
	Pt1-C13	1.9645 (0.0045)/1.98210	C29-C12-C9-C10	16.37/14.91
	Pt1-O1	2.0100 (0.0034)/2.04081	C8-C7-C6-N2	0.80/10.85
	Pt1-O2	2.0782 (0.0034)/2.14787	C11-C7-C6-C5	4.66/13.89
	C6-C7	1.4846 (0.0060)/1.48313		
	C9-C12	1.4717 (0.0057)/1.46220		
2	Pt1-N1	1.9932 (0.0044)/2.03131	C23-C22-C20-N2	8.21/11.48
	Pt1-C18	1.9563 (0.0055)/1.97894	C31-C22-C20-C19	11.61/16.09
	Pt1-O1	2.0852 (0.0039)/2.12787	C18-C17-C16-N1	0.77/1.00
	Pt1-O2	1.9898 (0.0038)/2.03337	C21-C17-C16-C1	1.06/3.73
	C16-C17	1.4624 (0.0073)/1.45561		
	C20-C22	1.4947 (0.0072)/1.46427		
	Pt2-N2	1.9731 (0.0045)/2.01665		
	Pt2-C23	1.9412 (0.0055)/1.98146		
	Pt2-O3	2.0870 (0.0039)/2.14951		
	Pt2-O4	2.0115 (0.0039)/2.04380		