Electronic Supplementary Information

Mono-, di- and tri-nuclear Pt^{II}(C^N)(N-donor ligand)Cl complexes showing aggregation-induced phosphorescent emission (AIPE) behavior for efficient solution-processed organic light-emitting devices †

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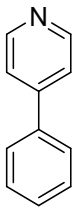
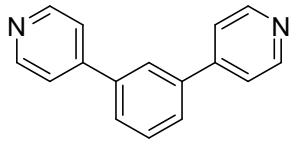
Ph-N1



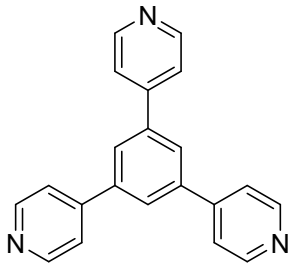
Under a nitrogen atmosphere, bromobenzene (5.00 g, 0.03 mol), pyridyl-4-boronic acid (4.70 g, 0.04 mol) and $Pd(PPh_3)_4$ (1.84 g, 1.59 mmol) were heated to 110 ^oC for 16 h in the mixture of 1,4-dioxane (20 mL) and Na_2CO_3 (2 M, 10 mL) under vigorous stirring. After the reaction, the mixture was extracted with CH_2Cl_2 and then purified by column chromatography, using CH_2Cl_2 and ethyl acetate as the eluent. The products were obtained as white solid (4.29 g, 87%). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.66 (d, J = 6.0 Hz, 2H), 7.66-7.63 (m, 2H), 7.52-7.44 (m, 5H); FAB-MS (m/z): 155 $[M]^+$; Anal. Calcd for $C_{11}H_9N$: C 85.13, H 5.85, N 9.03; found, C 85.04, H 5.76, N 8.96.

Ph-N2



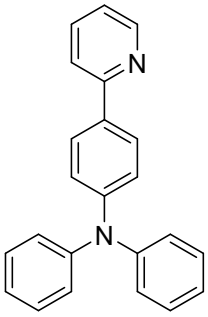
Under a nitrogen atmosphere, 1,3-dibromobenzene (5.00g, 0.02 mol), pyridyl-4-boronic acid (6.26 g, 0.05 mol) and $Pd(PPh_3)_4$ (1.22 g, 1.06 mmol) were heated to 110 ^oC for 16 h in the mixture of 1,4-dioxane (20 mL) and Na_2CO_3 (2 M, 10 mL) under vigorous stirring. After the reaction, the mixture was extracted with CH_2Cl_2 and then purified by column chromatography, using CH_2Cl_2 and ethyl acetate as the eluent. The products were obtained as white solid (3.69 g, 75%). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.70 (d, J = 4.0 Hz, 4H), 7.86 (s, 1H), 7.71-7.69 (m, 2H), 7.63-7.59 (m, 2H), 7.50 (d, J = 6.0 Hz, 4H); FAB-MS (m/z): 232 $[M]^+$; Anal. Calcd for $C_{16}H_{12}N_2$: C 82.73, H 5.21, N 12.06; found, C 82.65, H 5.16, N 11.98.

Ph-N3



Under a nitrogen atmosphere, 1,3,5-tribromobenzene (5.00 g, 0.02 mol), pyridyl-4-boronic acid (7.03 g, 0.06 mol) and $Pd(PPh_3)_4$ (0.92 g, 0.79 mmol) were heated to 110 °C for 16 h in the mixture of 1,4-dioxane (20 mL) and Na_2CO_3 (2 M, 10 mL) under vigorous stirring. After the reaction, the mixture was extracted with CH_2Cl_2 and then purified by column chromatography, using CH_2Cl_2 and ethyl acetate as the eluent. The products were obtained as white solid (3.14 g, 64%). ^1H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.75 (d, J = 5.2 Hz, 6H), 7.92 (s, 3H), 7.61 (d, J = 6.0 Hz, 6H); FAB-MS (m/z): 309 $[M]^+$; Anal. Calcd for $C_{21}H_{15}N_3$: C 81.53, H 4.89, N 13.58; found, C 81.45, H 4.80, N 13.46.

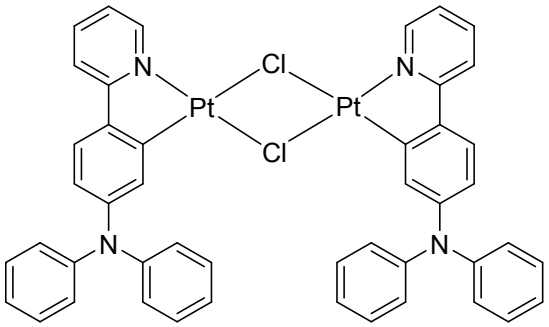
L-N



Under a nitrogen atmosphere, 4-(diphenylamino)phenylboronic acid (5.00 g, 0.02 mol), 2-bromopyridine (3.28 g, 0.02 mol) and $Pd(PPh_3)_4$ (1.00g, 0.86 mmol) were heated to 100 °C for 16 h in a mixed solvent of 2 M Na_2CO_3 and THF. After the reaction, the mixture was extracted with CH_2Cl_2 three times. The organic phase was dried over by anhydrous Na_2SO_4 and then purified by column chromatography, using petroleum ether as the eluent. The final product was white solid (4.40

g, 79%).^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 8.65 (d, J = 4.4 Hz, 1H), 7.86 (d, J = 8.8 Hz, 2H), 7.74–7.65 (m, 2H), 7.30–7.25 (m, 4H), 7.19–7.13 (m, 7 H), 7.05 (t, J = 7.2 Hz, 2H).

[(PAY)Pt(II)]μ-Cl_2[(PAY)Pt(II)]



Under a nitrogen atmosphere, K_2PtCl_4 (5.00 g, 0.01 mol) and L-N (4.27 g, 0.01 mol) were heated to 90 ^{o}C for 16 h in a mixed solvent of 2-ethoxyethanol (22.5 mL) and water (7.5 mL). After cooling to the room temperature, saturated NaCl solution was added and the coarse dimer was collected by filtration and dried under vacuum.

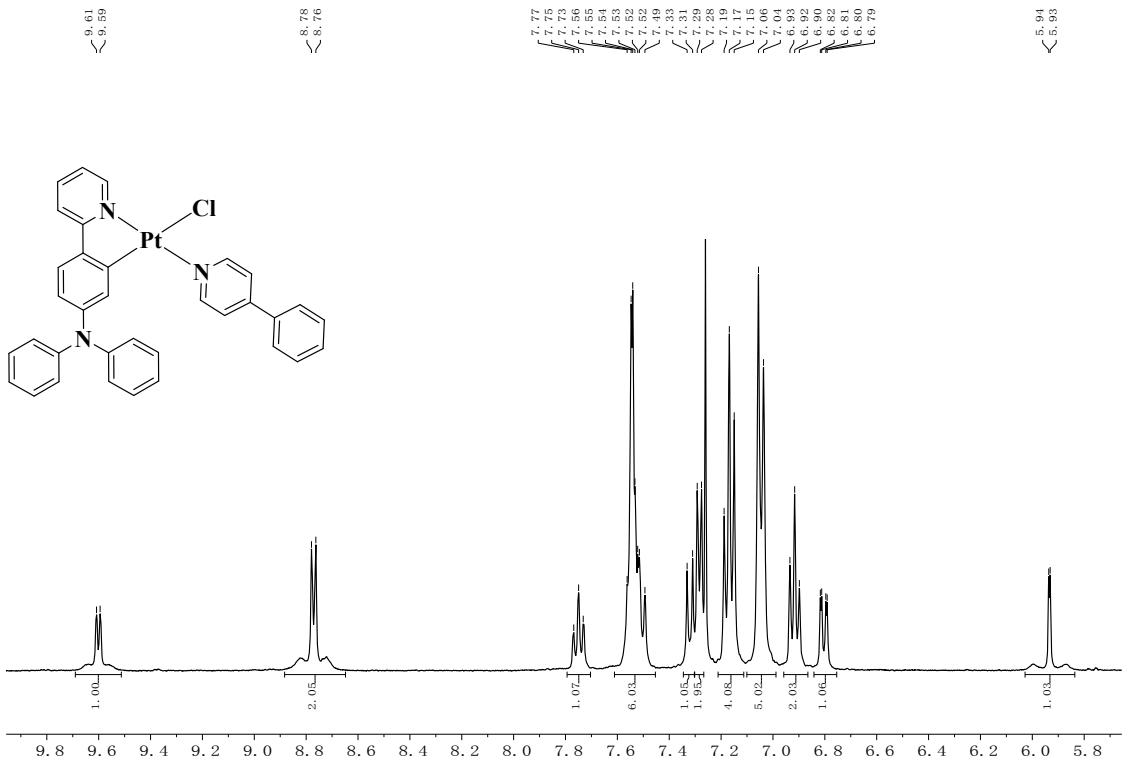


Figure F.1 ^{1}H NMR spectrum of **Pt-Ph-1**

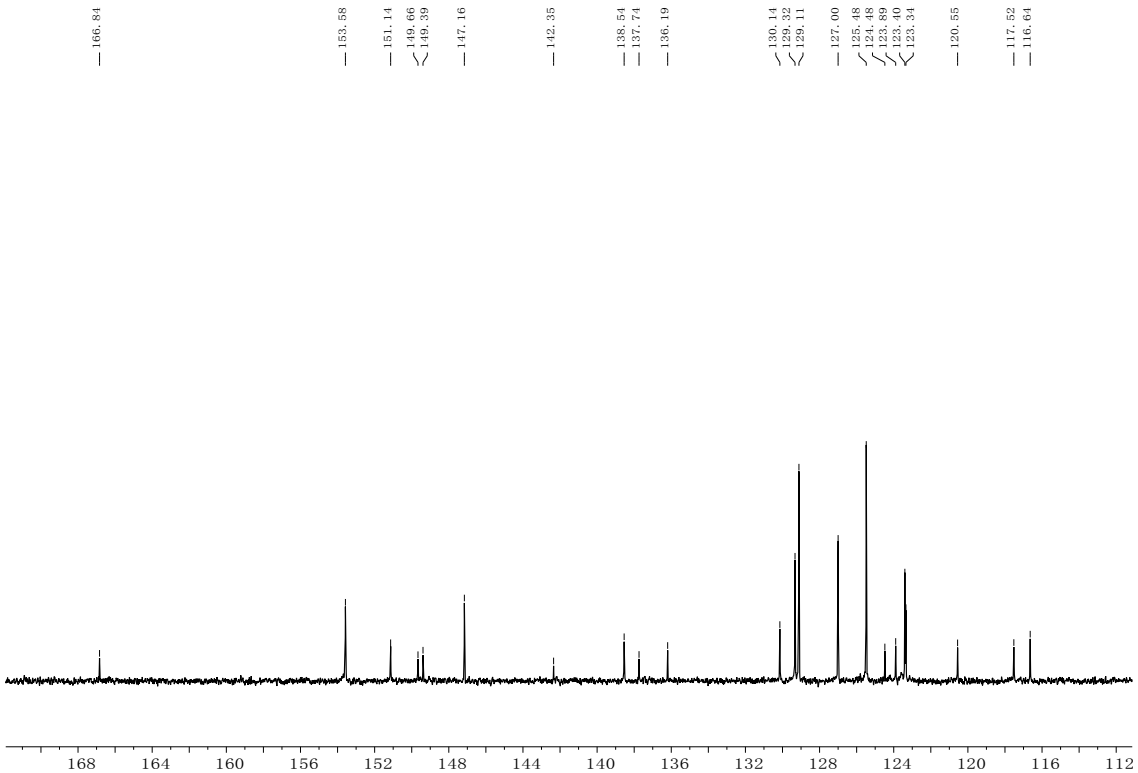


Fig. S1 ^{1}H NMR spectrum and ^{13}C NMR spectrum of **Ph-PAYPt1**

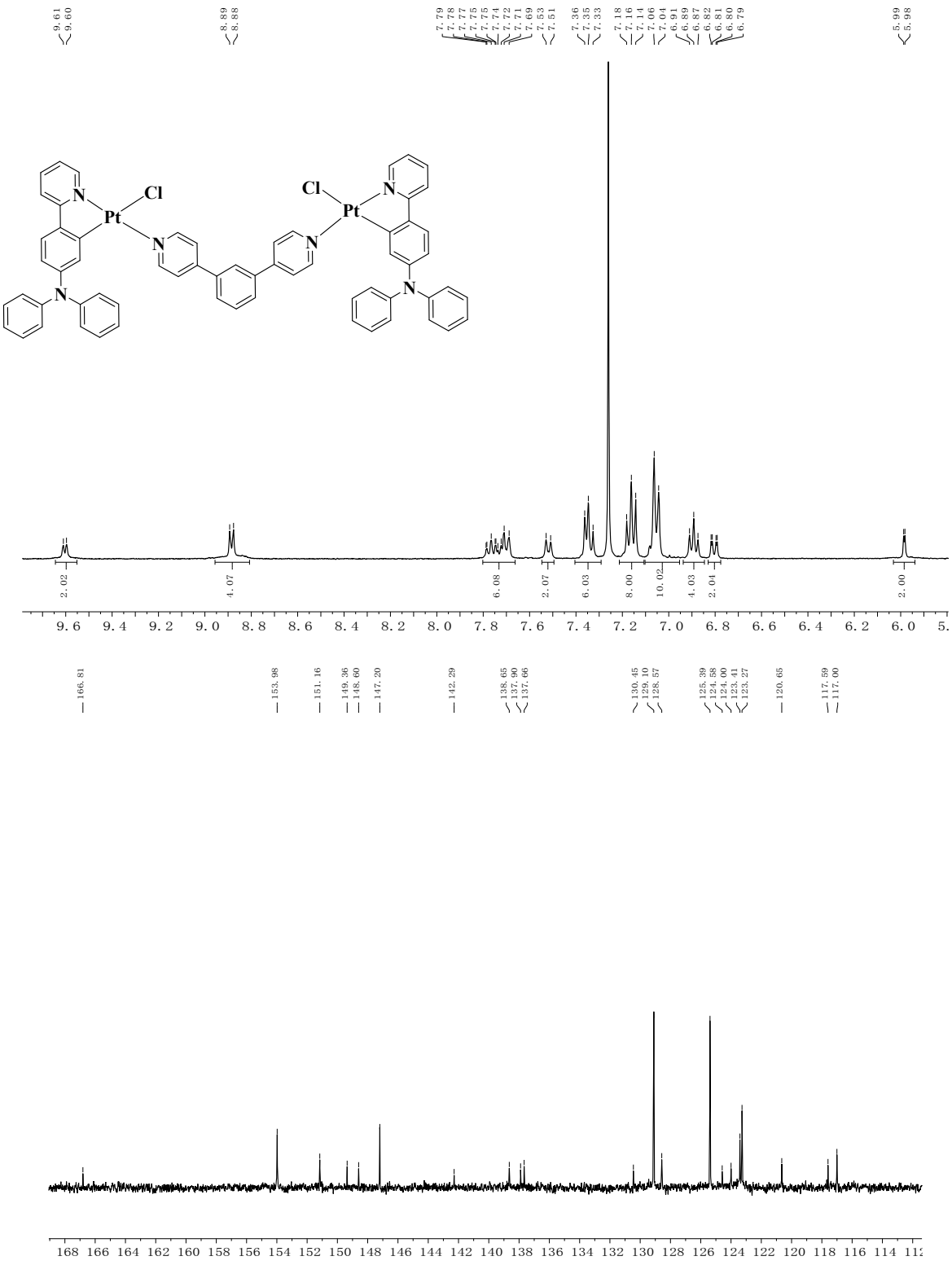


Fig. S2 ^{1}H NMR spectrum and ^{13}C NMR spectrum of **Ph-PAYPt2**

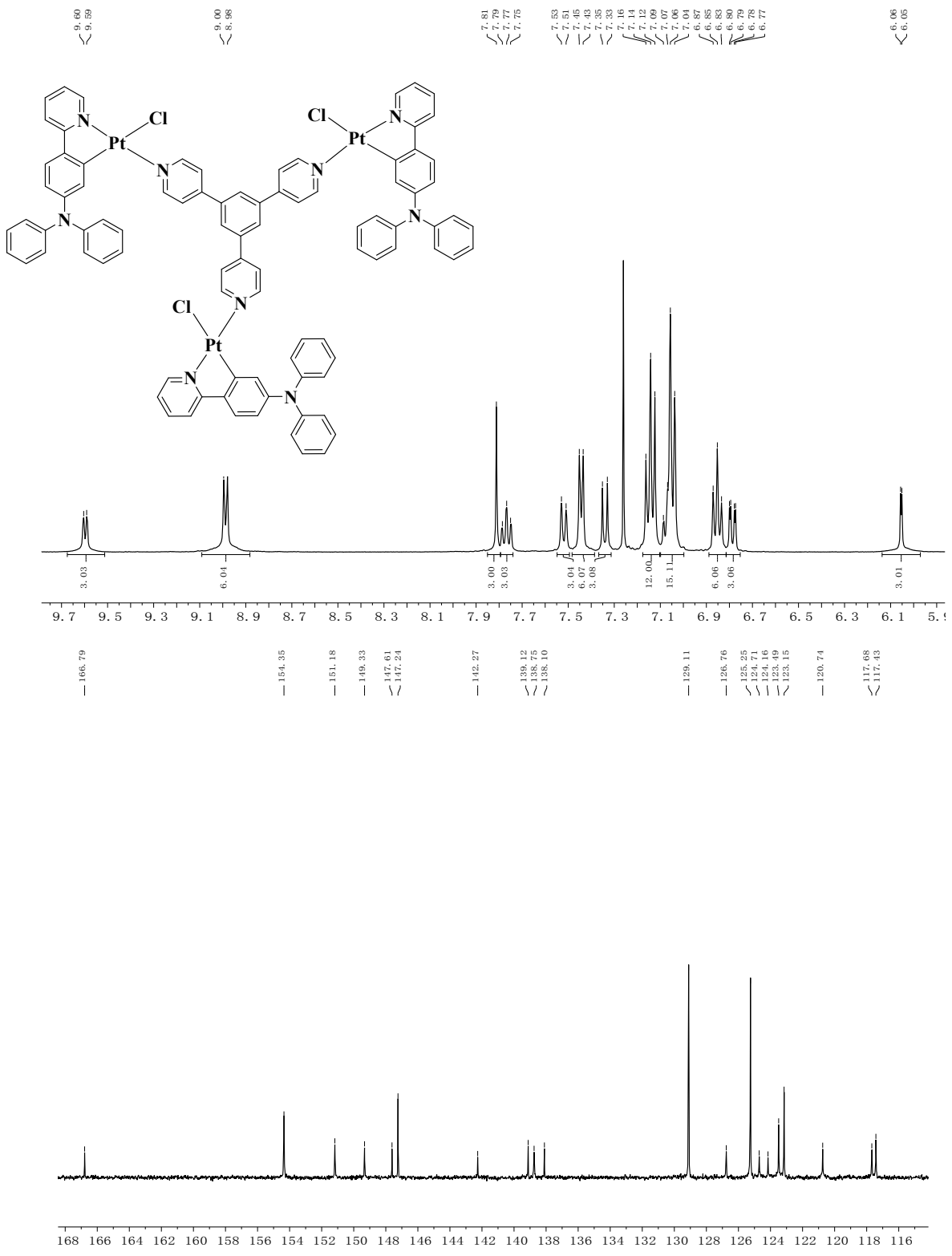


Fig. S3 ^{1}H NMR spectrum and ^{13}C NMR spectrum of **Ph-PAYPt3**

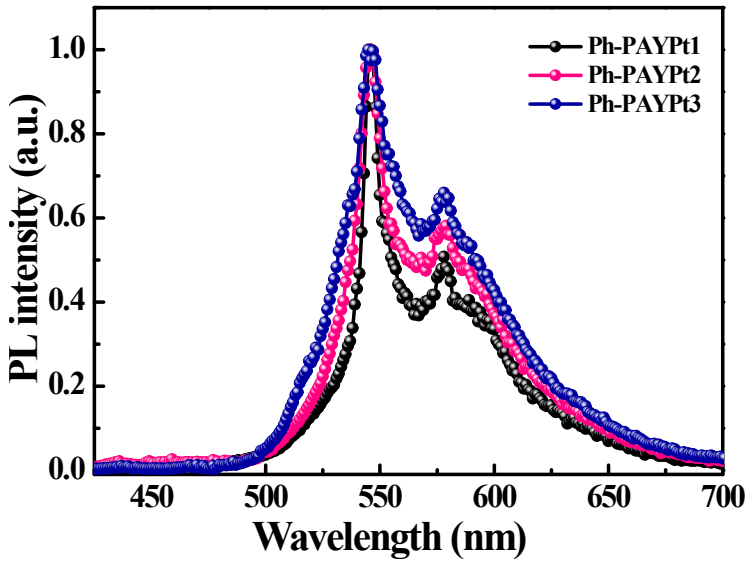


Fig. S4 PL spectra of these mono-, di- and tri-nuclear Pt^{II}(C^N)(N-donor ligand)Cl complexes in CH_2Cl_2 at 77 K.

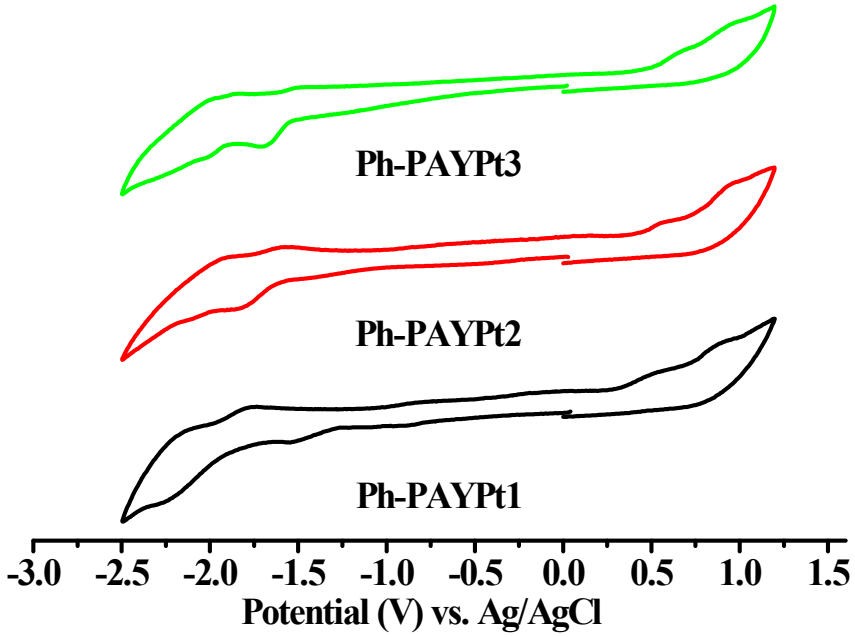


Fig. S5 CV curves for **Ph-PAYPt1**, **PhPAYPt2** and **PhPAYPt3**

OLED fabrication and measurements

The ITO glass substrates were cleaned in advance and exposed to ultraviolet-ozone for *ca.* 7 min. The PEDOT:PSS, which plays the role of a hole injection layer, was spin-coated on the ITO glass substrates and then annealed at 120 °C for 20 min in the air. Then, the chlorobenzene solution containing the host materials and emitters with a certain doping ratio was spin-coated on surface of PEDOT:PSS layer to form the emission layer. The obtained ITO chip was dried at 80 °C for 20 min before it was transferred to the deposition system to deposit other active layers, i.e., electron-transporting layer, electron-injection layer and Al cathode. The orange phosphorescent Ir-Tz-1 was synthesized by our laboratory. The EL spectra and CIE coordinates were measured with a PR655 spectra colorimeter. The driving voltages and efficiencies of the devices were measured with the Keithley 2400/2000 source meter. The efficiency and spectral measurements were carried out under ambient conditions.

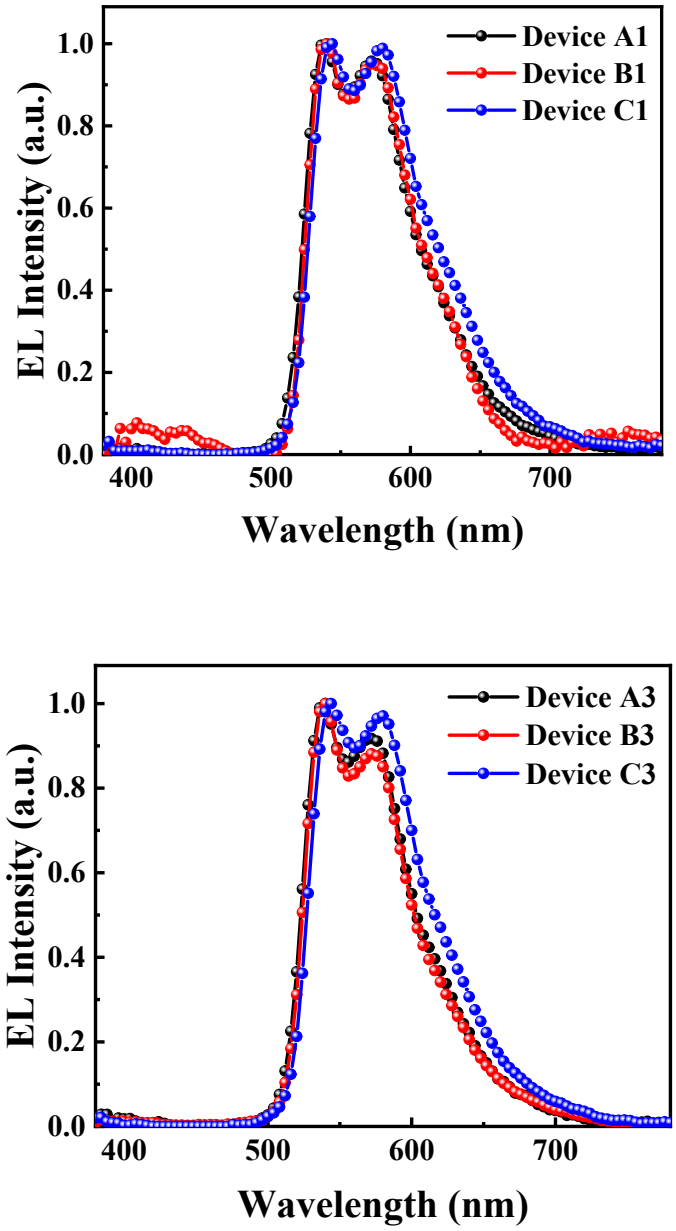


Fig. S6 EL spectrum for the devices except the optimized ones.

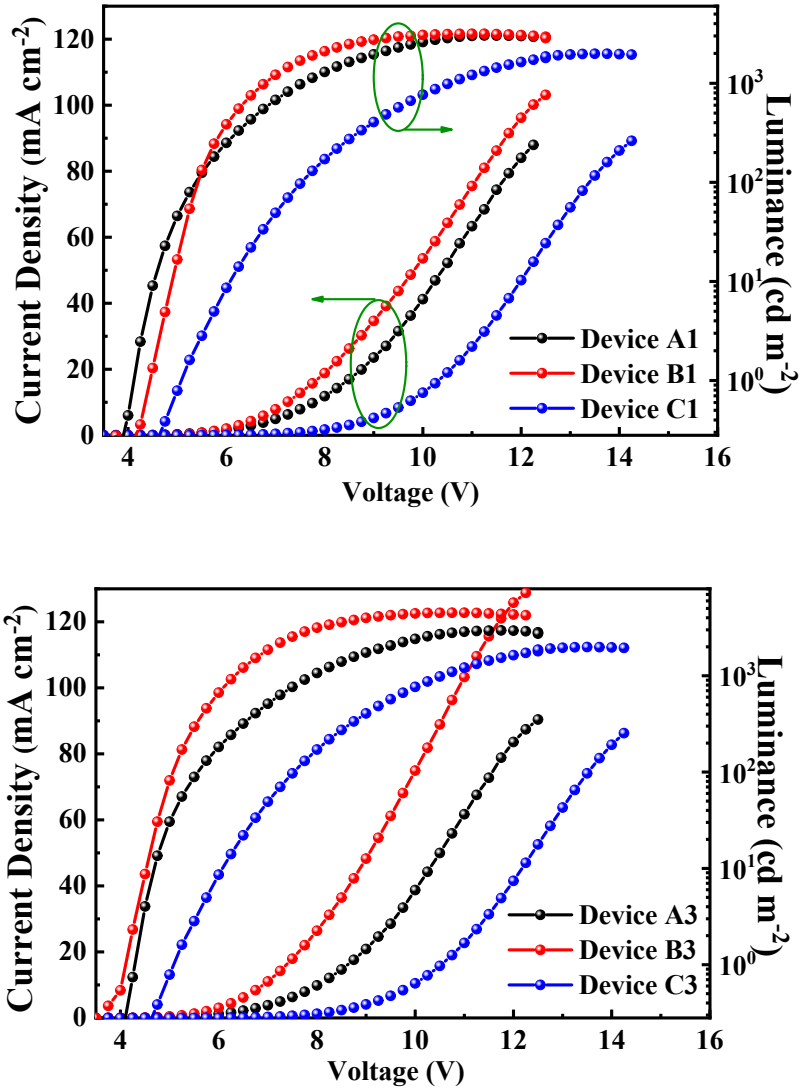


Fig. S7. Current density–voltage–luminance (*J*–*V*–*L*) curves for the devices except the optimized ones.

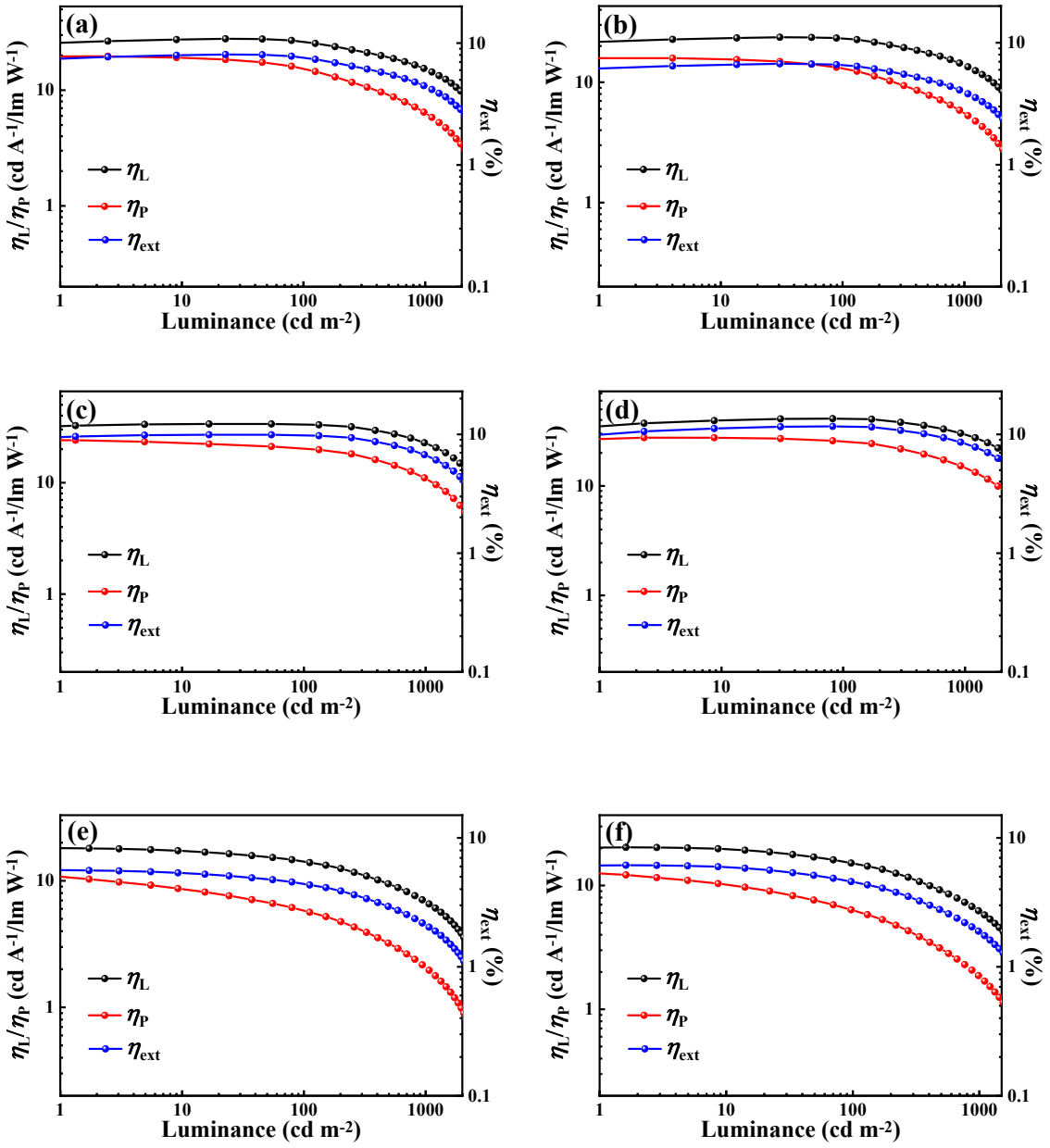


Fig. S8. Relationship between EL efficiencies and luminance for the devices except the optimized ones. (a) Device **A1**, (b) Device **A3**, (c) Device **B1**, (d) Device **B3**, (e) Device **C1** and (f) Device **C3.**