Electronic Supporting Information

Achieving pure yellow, high-efficiency (EQE > 20%) electroluminescence from ultrathin emitting-layer (0.6~2.0 nm) OLEDs having a rare aggregation-free heteroleptic platinum complex

Hagos Tesfay Kidanu,[†,‡, §] and Chin-Ti Chen[*,†]*

[†] Institute of Chemistry, Academia Sinica, Taipei 11529, Taiwan, Republic of China.

[‡]Sustainable Chemical Science and Technology, Taiwan International Graduate Program (TIGP), Academia Sinica, Taipei 11529, Taiwan, Republic of China.

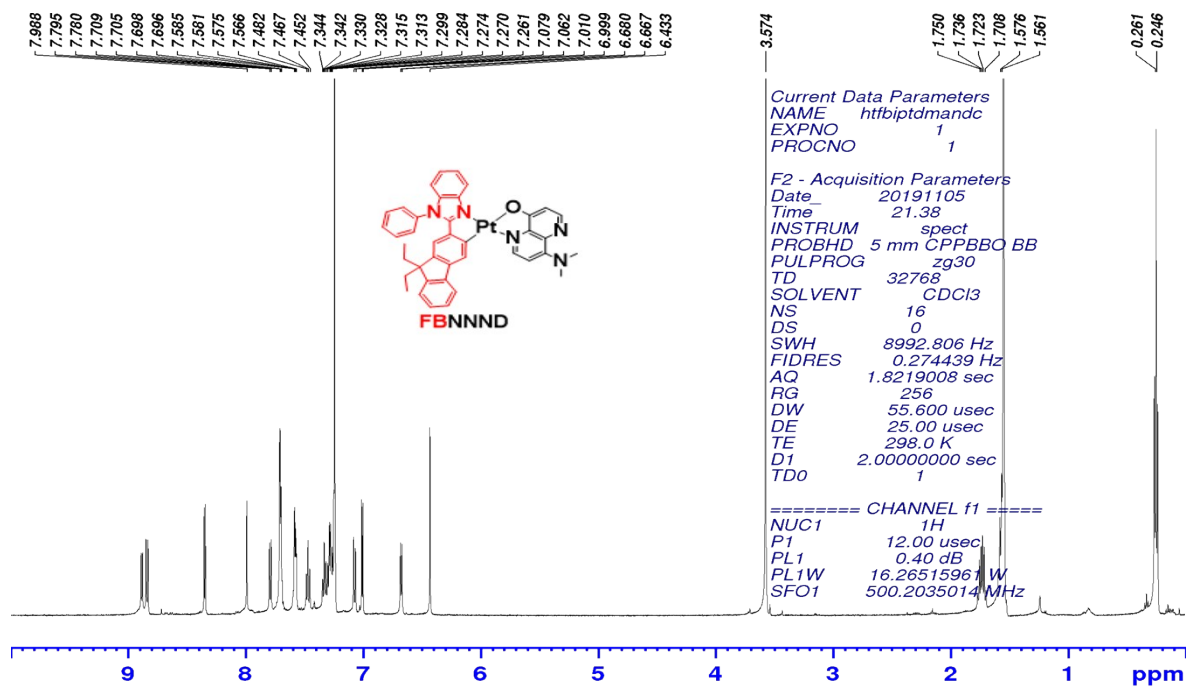[§]Department of Applied Chemistry, National Chiao Tung University, Hsinchu 30050, Taiwan, Republic of China.

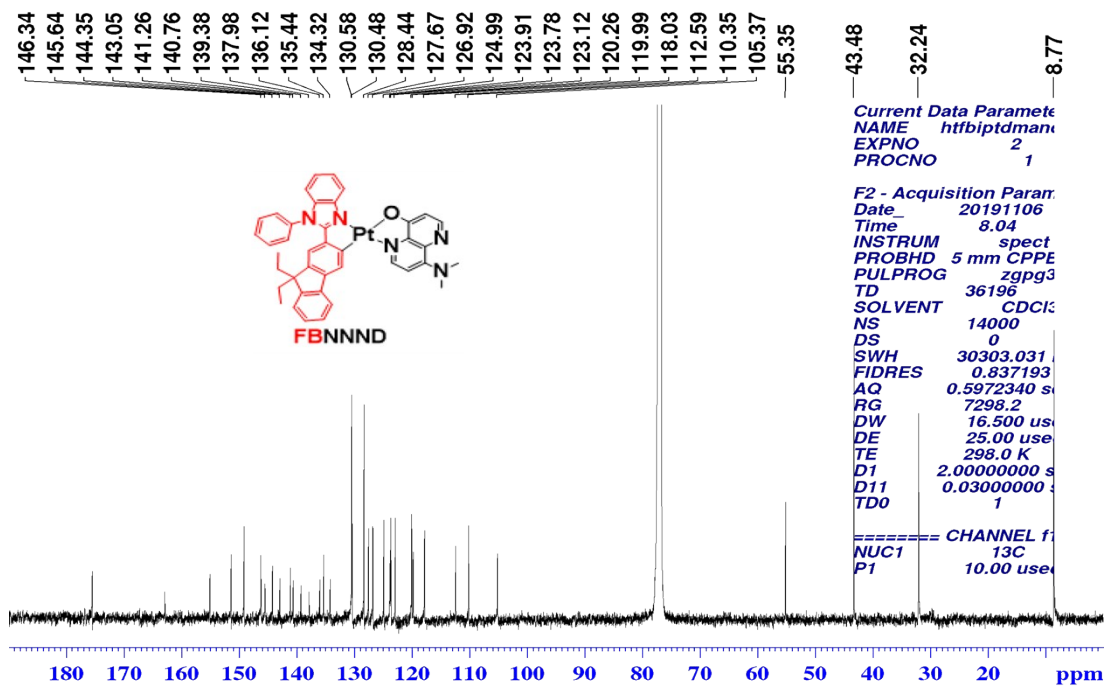Figure S1. ^{1}H NMR spectrum of **FBNNND** (400 MHz, CDCl$_3$).

Figure S2. ^{13}C NMR spectrum of **FBNNND** (125 MHz, CDCl$_3$).

[Mass Spectrum]
Data : 20190214_htFBIPtdmaND-HR-002   Date : 14-Feb-2019 14:55
Sample : htFBIPtdmaND
Note : NBA
Ion Mode : FAB+
RT : 0.17 min   Scan# : 4
Elements : C 1000/0, H 1000/0, N 5/5, O 1/1, Pt 1/1
Mass Tolerance   : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

Observed m/z   Int%   Err[ppm / mmu]   U.S.   Composition
1   797.2567   100.00   -0.1 / -0.1   25.5   C40 H36 N5 O Pt = 797.2568
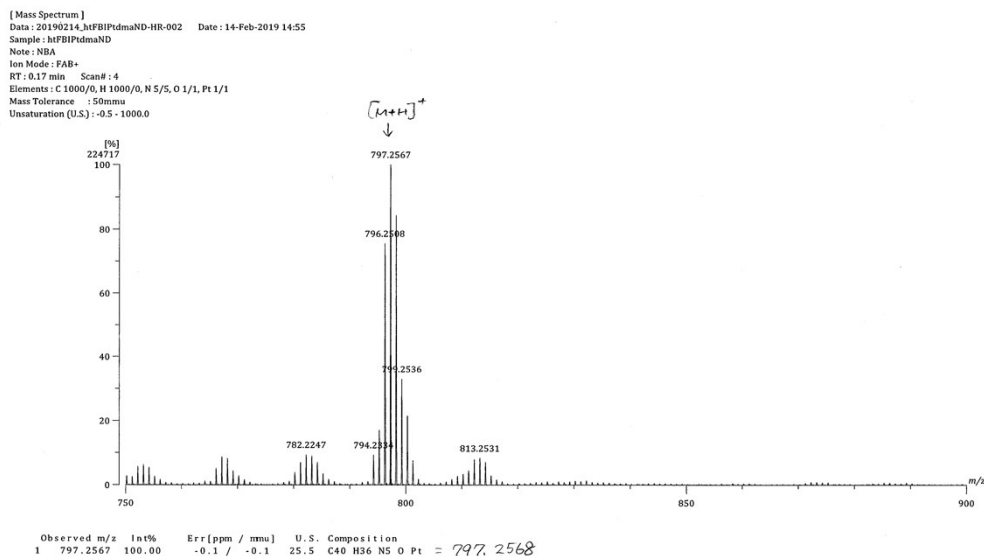
Figure S3. HR-MS spectrum of **FBNNND**.

Table S1. Comparison of selected geometric parameters of **FBNNND** theoretically and experimentally.

FBNNND	Selected bond lengths (Å)			
	Pt-N(1)	Pt-C	Pt-O	Pt-N(qn)
DFT[a]	2.028	2.025	2.141	2.068
X-ray[b]	2.001	2.020	2.081	2.047

FBNNND	Selected bond angles (°)					
	O-Pt-N(1)	N(1)-Pt-C	C-Pt-N(qn)	N(qn)-Pt-O	N1-Pt-Nqn	O-Pt-C
DFT[a]	96.83	79.48	105.28	78.92	172.95	173.38
X-ray[b]	94.45	79.95	104.96	80.78	174.26	173.77

[a] Results obtained by DFT calculation using b3lyp method. [b] Results obtained experimentally from the single crystal X-ray structure.

Table S2. Calculated wavelengths, and molecular orbitals character of the optical transitions for the studied **FBNNND** complex in dichloromethane solvent.

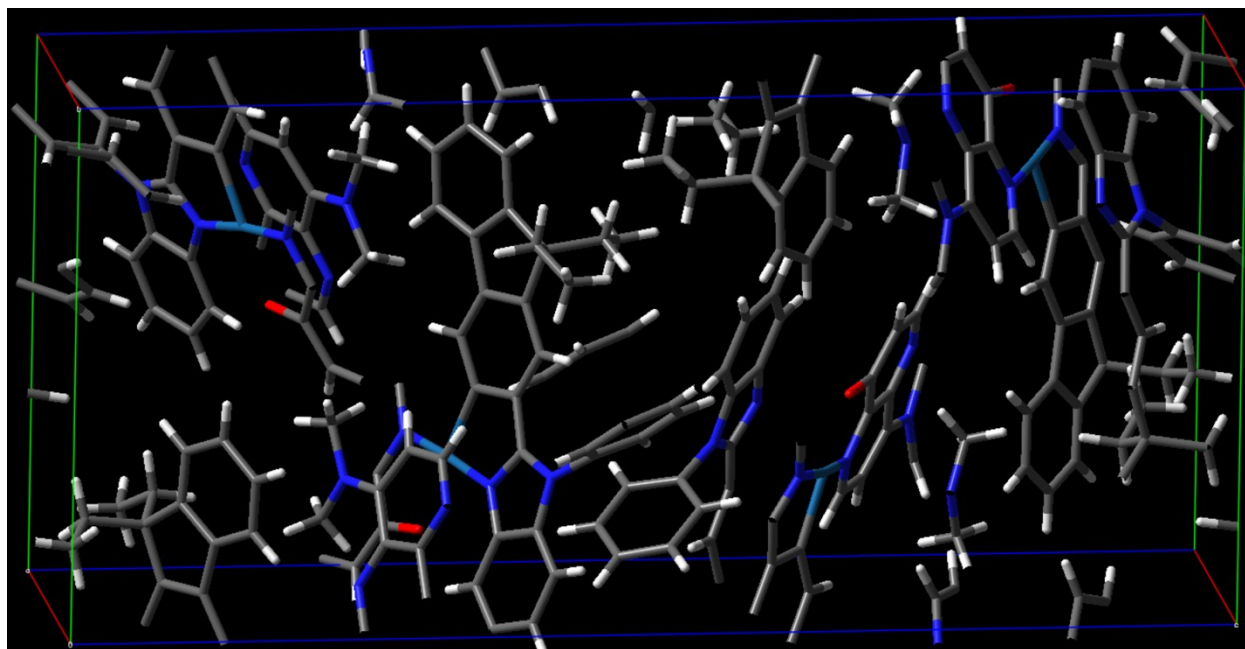| States	λ (nm)	MO transition contributions
S_1	414.6	HOMO → LUMO (64%) HOMO-1 → LUMO (26%) HOMO-2 → LUMO (10%)
S_2	397.0	HOMO-1 → LUMO (64%) HOMO → LUMO (28%)
T_1	516.0	HOMO-1 → LUMO (59%) HOMO → LUMO (27%)
T_2	502.0	HOMO → LUMO+1 (53%) HOMO → LUMO (32%)

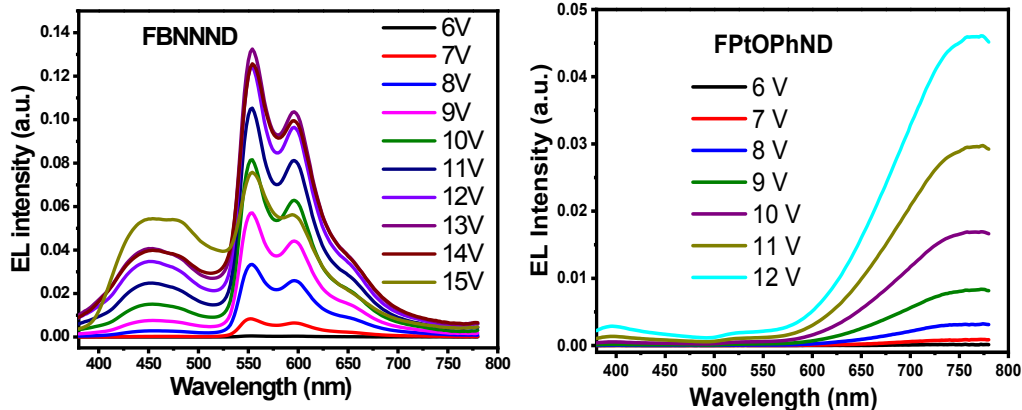Figure S4 Molecular packing of **FBNNND** inside a unit cell.

Figure S5 Voltage-dependent EL spectra of **FBNNND** OLED (1.0 nm ultrathin film) and **FPtOPhND** OLED (0.6 nm ultrathin film).
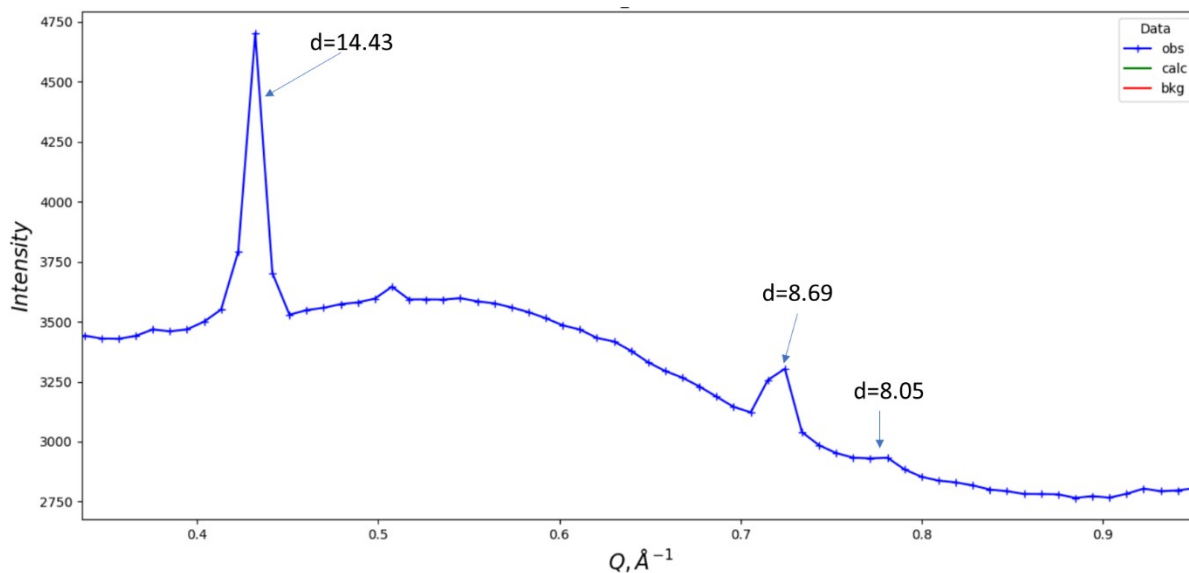

Figure S6 1D GIWAXS spectrum of **FBNNND** along the direction of Q_z (out-of-plane direction to the substrate) extracted from the corresponding 2D GIWAXS patterns (Figure 11). The corresponding d-spacing, $d = 2\pi/Q_z$.