Electronic Supplementary Information

Pyridine based meta-linking deep-blue emitter with high conjugation extent and electroluminescent efficiencies

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Scheme S1 Synthetic procedures of 26BTPIPy and 25BTPIPy.
Synthetic procedures

The synthesis of 4,4’-(pyridine-2,6-diyl)dibenzaldehyde (26BCHOPy) and 4,4’-(pyridine-2,5-diyl)dibenzaldehyde (25BCHOPy) was proceeded following reported procedures.¹

**26BTPiPy**: 9,10-phenanthrenequinone (0.92 g, 4.4 mmol), 2,6-BCHOPy (0.57 g, 2 mmol), 4-tert-butylbenzenamine (0.66 g, 4.4 mmol), and ammonium acetate (2.31 g, 30.0 mmol) were added into glacial acetic acid (30 mL). The mixture was refluxed for 24 h under an argon atmosphere. After cooling to room temperature, an orange-yellow mixture was obtained and poured into methanol under stirring. The crude product was separated by filtration, washed with methanol, and dried under vacuum. The product was purified by column chromatography (silica gel) using eluent of petroleum ether/dichloromethane (V/V) 1/4 to give a pale solid, with a 70% yield (1.3 g). ¹H NMR (400 MHz, CD₂Cl₂) δ 8.86 (d, J = 7.9 Hz, 2H), 8.80 (d, J = 8.4 Hz, 2H), 8.75 (d, J = 8.4 Hz, 2H), 8.10 (d, J = 8.2 Hz, 4H), 7.86 (t, J = 7.7 Hz, 1H), 7.76 (t, J = 7.8 Hz, 8H), 7.69 (dd, J = 8.1, 6.2 Hz, 6H), 7.52 (dd, J = 8.3, 6.3 Hz, 6H), 7.30 (t, J = 7.6 Hz, 2H), 7.21 (d, J = 8.3 Hz, 2H), 1.47 (s, 18H). MS (ESI) m/z: [M + H]⁺ calcd for C₆₇H₅₄N₅: 929.17. Found: 929.0. Anal. Calcd for C₆₇H₅₃N₅: C, 86.70; H, 5.76; N, 7.54; found: C, 86.78; H, 5.71; N, 7.49.

**25BTPiPy**: The synthetic procedures were similar to that of 26BTPiPy. Yield: 55.5 %. ¹H NMR (300 MHz, CD₂Cl₂) δ 8.85 (d, J = 1.5 Hz, 1H), 8.81 (d, J = 8.2 Hz, 3H), 8.76 (d, J = 8.3 Hz, 2H), 7.81 – 7.74 (m, 4H), 7.73 – 7.64 (m, 10H), 7.58 (d, J = 2.3 Hz, 1H), 7.55 (t, J = 2.5 Hz, 1H), 7.52 (d, J = 2.2 Hz, 3H), 7.49 (d, J = 2.0 Hz, 2H), 7.37 – 7.25 (m, 8H), 1.47 (s, 18H). MS (ESI) m/z: [M + H]⁺ calcd for C₆₇H₅₄N₅: 929.17. Found: 928.9. Anal. Calcd for C₆₇H₅₃N₅: C, 86.70; H, 5.76; N, 7.54; found: C, 86.75; H, 5.77; N, 7.46.
Fig. S1 Positive CV scans of 26BTPIPy and 25BTPIPy (inset: ferrocene) against saturated calomel electrode (SCE)

Fig. S2 Absorption spectra of m-BBTP, 26BTPIPy and 25BTPIPy in DCM.
Fig. S3 Calculated LUMO distributions of 26BTPIPy with arbitrary fixed twisting angle between the pyridine ring and two connected benzene rings.

Fig. S4 Calculated HOMO distributions of \textit{m}-BBTPI with arbitrary fixed twisting angle between the central benzene ring and two connected benzene rings.
Fig. S5 EL spectra at different voltages (inset is luminescence-current density plot) of a) 26BTPIPy and b) 25BTPIPy-based bilayer devices

References: