Supplementary Information

A *Meta*-Molecular Tailoring Strategy Towards Efficient Violet-Blue Organic Electroluminescent Material

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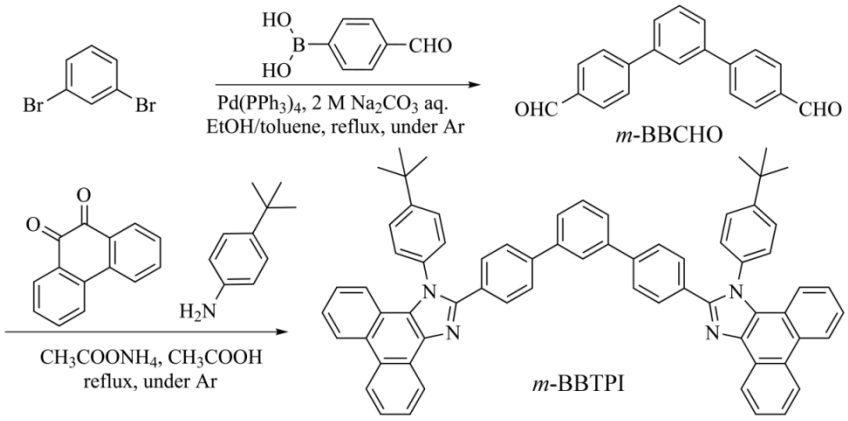
Synthesis:



Scheme S1 Synthetic procedures for ***m*-BBTPI**.

[1,1':3',1''-terphenyl]-4,4''-dicarbaldehyde (*m*-BBCHO): 60 mL toluene, 20 mL ethanol and 30 mL 2 M Na_2CO_3 aqueous were added to a mixture of 1.65 g 1,3-dibromobenzene (7 mmol), 1.6 g (4-formylphenyl)boronic acid (10.68 mmol) and 0.61g $Pd(PPh_3)_4$ (0.56 mmol). Then the mixture was heated at 90 °C with stirring under an argon atmosphere. After 24 h, the mixture was cooled to room temperature and extracted with CH_2Cl_2 and dried over $MgSO_4$, then removed the solvent. At last, the residue was purified by column chromatography on silica gel using CH_2Cl_2 and petroleum ether (2:1) as eluent to give a white solid, with a 91.5 % yield (1.83 g). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.09 (s, 2H), 8.04-7.97 (m, 4H), 7.88 (t, J = 1.6 Hz, 1H), 7.82 (d, J = 8.2 Hz, 4H), 7.72-7.66 (m, 2H), 7.61 (dd, J = 8.4, 6.9 Hz, 1H).

4,4''-bis(1-(4-(*tert*-butyl)phenyl)-1H-phenanthro[9,10-*d*]imidazol-2-yl)-1,1':3',1''-terphenyl (*m*-BBTPI): 9,10-phenanthrenequinone (1.25 g, 6 mmol), *m*-BBCHO (0.72 g, 2.5 mmol), 4-*tert*-butylbenzenamine (0.86 mL, 6 mmol), and

ammonium acetate (3.86 g, 50 mmol) were added into glacial acetic acid (40 mL) and the mixture refluxed for 24 h under an N_2 atmosphere. After cooling to room temperature, a pale-yellow mixture was obtained and poured into methanol under stirring. The precipitate was separated by filtration, washed with methanol, and dried under vacuum. The product was purified by column chromatography on silica gel (CH_2Cl_2 as eluent) to give a white solid, with a 78.2% yield (1.81g). ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.90 (d, J = 8.0 Hz, 2H), 8.78 (d, J = 8.4 Hz, 2H), 8.72 (d, J = 8.5 Hz, 2H), 7.80-7.45 (m, 26H), 7.35-7.28 (m, 2H), 7.21 (d, J = 8.2 Hz, 2H), 1.46 (s, 18H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.33, 153.22, 141.04, 140.98, 137.48, 136.04, 133.54, 129.79, 129.66, 129.28, 129.25, 128.54, 128.41, 128.25, 127.26, 127.23, 127.07, 126.88, 126.31, 126.22, 124.79, 124.05, 123.15, 123.08, 122.74, 120.91, 35.05, 31.44 ppm. MALDI-TOF MS *m/z*: Calcd for $C_{68}H_{54}N_4$: 926.4. Found: 927.5 [M^++H]. Anal. calcd. for $C_{68}H_{54}N_4$: C, 88.09; H, 5.87; N, 6.04. Found: C, 88.15; H, 5.85; N, 5.93.

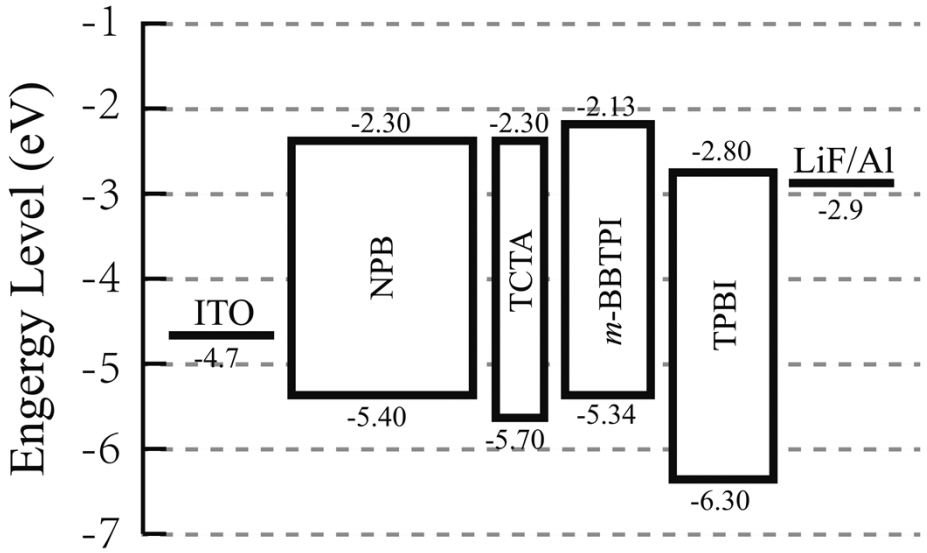


Fig. S1 The configuration and HOMO/LUMO energy alignment of the as-prepared devices.

Table S1 Key performance data for ***m*-BBTPI**-based and some high-efficiency non-doped violet-blue OLEDs.

emitter	V_{on} (V)	λ_{EL} (nm)	CE[a] (cd A^{-1})	PE[b] (lm W^{-1})	EQE[c] (%)	CIE (x, y)	reference[d]
m-BBTPI	3.2	428	1.99	1.81	3.63	0.16, 0.06	This work
XBTPI	3.1	428	2.06	1.60	4.93	0.16, 0.05	13e
TTP-TPI	3.1	424	2.10	1.88	5.02	0.16, 0.05	9d
TCPC-6	-	425	1.35	-	3.72	0.16, 0.05	9b
CzS1	3.5	426	1.89	1.58	4.21	0.157, 0.055	9c
CzS2	2.8	417	0.82	0.84	2.70	0.157, 0.044	9c
SiPIM	4.2	420	1.94	-	6.29	0.163, 0.040	9e
M1	-	420	0.65	0.48	1.94	0.165, 0.050	6b
M2	-	428	1.53	0.86	3.02	0.166, 0.056	6b

[a] Current efficiency, [b] power efficiency, [c] external quantum efficiency at maximum. [d] Parallel to the main text.