Supporting Information

for ***Physical Chemistry Chemical Physics***

Dimeric Phenanthroimidazole for Blue Electroluminescent Materials: The Effect of Substituted Position Attaching to Biphenyl Center

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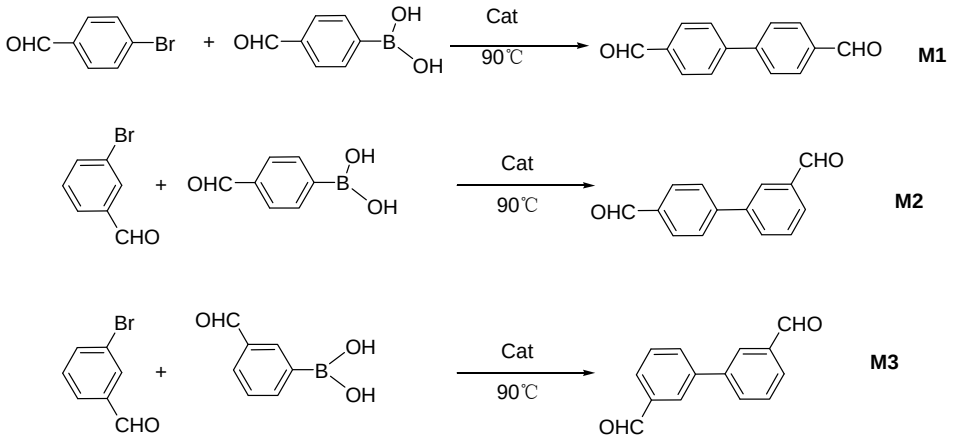
Synthesis and Characterization



Scheme S1 The synthetic routes of the corresponding biphenyl dicarboxaldehyde

Biphenyldicarboxaldehyde (M)

A mixture of 4-bromobenzaldehyde (or 3-bromobenzaldehyde, 2.1 g, 11.2 mmol), 4-formylphenylboronic acid (3-formylphenylboronic acid, 1.65 g, 11.0 mmol), $Pd(PPh_3)_4$ (128.0 mg, 0.11 mmol, 1 %), sodium carbonate (5.3 g, 50 mmol), THF (150 mL) and distilled water (25 mL) was refluxed for 2 days under nitrogen. The crude product was purified by column chromatography on silica gel using $CH_2Cl_2/CH_3COOC_2H_5$ as eluent to afford a yellow solid.

4,4'-Biphenyldicarboxaldehyde (M1)

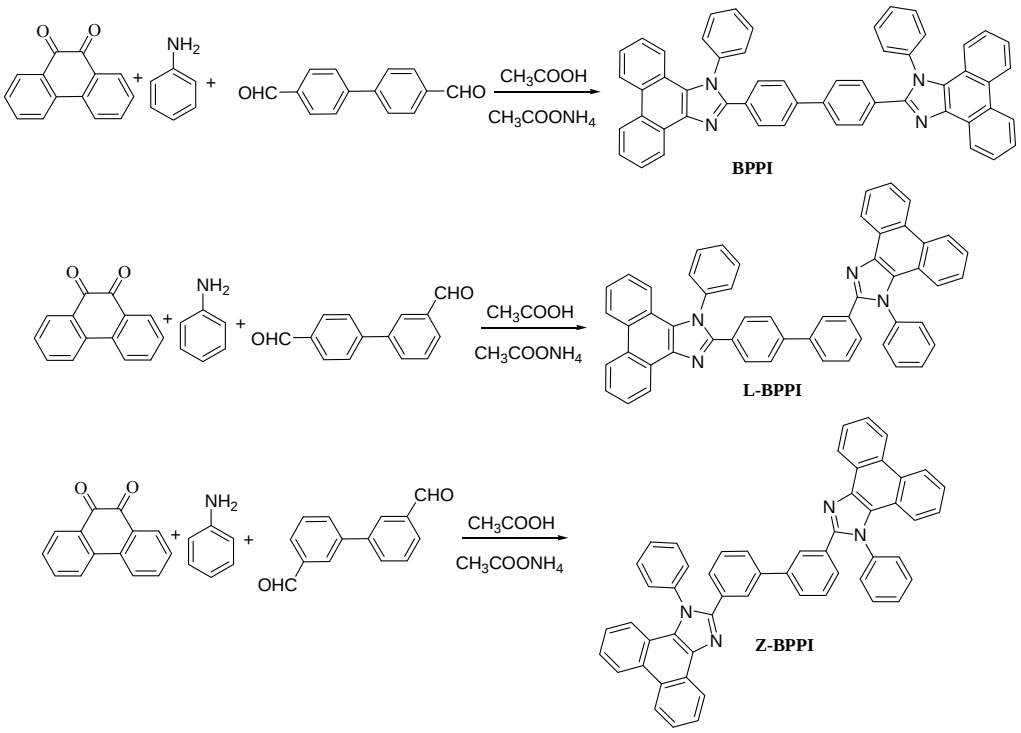
The raw materials are 4-bromobenzaldehyde and 4-formylphenylboronic acid. (1.89 g, Yield: 80.5%) MALDI-TOF (*m*/*z*): [M+] calcd. $C_{14}H_{10}O_2$, 210.07; found, 211.9.

3,4'-Biphenyldicarboxaldehyde (M2)

The raw materials are 3-bromobenzaldehyde and 4-formylphenylboronic acid. (2.10 g, Yield: 84.3%) MALDI-TOF (*m*/*z*): [M+] calcd. $C_{14}H_{10}O_2$, 210.07; found, 211.0.

3,3'-Biphenyldicarboxaldehyde (M3)

The raw materials are 3-bromobenzaldehyde and 3-formylphenylboronic acid. (2.15 g, Yield: 85.0%) MALDI-TOF (*m*/*z*): [M+] calcd. $C_{14}H_{10}O_2$, 210.07; found, 211.7.



Scheme S2 The synthetic routes of **BPPI**, **L-BPPI** and **Z-BPPI**

Bis(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)biphenyl

A mixture of phenanthrene-9,10-dione (1.04 g, 5 mmol), aniline (3.57 g, 30 mmol), ammonium acetate (3.05 g, 50 mmol) and M1 (or M2, or M3, 0.55g, 2.4 mmol) were refluxed in acetate acid for 2 hours, then poured into a methanol solution with stirring. After filtering, the crude product was purified by chromatography.

4,4'-bis(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)biphenyl (BPPI)

(3.16g, Yield:83.3%) ^{1}H NMR (500 MHz, DMSO, ppm): 8.94 (d, 2H), 8.89 (d, 2H), 8.72 (d, 2H), 7.80–7.65 (m, 22H), 7.57 (t, 2H), 7.35 (t, 2H) , 7.09 (d, 2H). MALDI-TOF (*m*/*z*): [M+] calcd. $C_{54}H_{34}N_4$, 738.28; found, 739.0. Anal Calc. for $C_{54}H_{34}N_4$: C, 87.78; H, 4.64; N, 7.58. Found: C, 87.80; H, 4.62; N, 7.57.

3,4'-bis(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)biphenyl (L-BPPI)

(2.84g, Yield:73.6%) ^{1}H NMR (500 MHz, DMSO, ppm): 8.97 (d, 2H), 8.91 (d, 2H), 8.74 (d, 2H), 7.82–7.70 (m, 17H), 7.67 (d, 2H), 7.58 (t, 2H) ,7.51 (t, 1H) , 7.45(d, 2H), 7.37 (t, 2H), 7.16-7.12(m, 2H). MALDI-TOF (*m*/*z*): [M+] calcd. $C_{54}H_{34}N_4$, 738.28;

found, 739.9. Anal Calc. for $C_{54}H_{34}N_4$: C, 87.78; H, 4.64; N, 7.58. Found: C, 87.67; H, 4.61; N, 7.55.

3,3'-bis(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)biphenyl (Z-BPPI)

(2.76g, Yield:75.4%) ^{1}H NMR (500 MHz, DMSO, ppm): 8.97 (d, 2H), 8.92 (d, 2H), 8.78 (d, 2H), 7.83-7.79 (m, 6H), 7.75-7.71 (m, 6H), 7.67-7.64 (m, 6H), 7.61 (t, 2H), 7.48 (m, 4H) ,7.38 (t, 2H), 7.15 (d, 2H). MALDI-TOF (*m*/*z*): [M+] calcd. $C_{54}H_{34}N_4$, 738.28; found, 741.0. Anal Calc. for $C_{54}H_{34}N_4$: C, 87.78; H, 4.64; N, 7.58. Found: C, 87.76; H, 4.64; N, 7.57.