Supporting information

Influence of asymmetric modification on coronene and perylene derivative molecule self-assembly on HOPG

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S1 Synthesis procedures

S 1.1 Synthesis of P-DAPPD

A mixture of 2 (0.8 g, 2.3 mmol), N,N'-Dimethyl-1,3-propanediamine (1.0 g, 9.8 mmol), and imidazole (5.5 g) was stirred at 180℃ under Ar gas for 4 h. After purification through silica gel column chromatography, compound P-DAPPD (0.93 g, 95 %) was obtained as a orange solid. 2.3.4.5 compounds were synthesized according to literature methods [1-4].^{1}H-NMR (300 MHz, $CDCl_3$): δ = 1.99 (d, 2H), 2.33 ppm (s, 6H), 2.50 ppm (d, 2H), 3.79 ppm (d, 2H), 7.50 ppm (d, 2H), 7.74 ppm (d, 4H), 8.32 ppm (d, 2H), 8.45 ppm (d, 2H). ESI-MS: m/z =431.2 $[M + H]^+$. ^{13}C NMR (300MHz, $CDCl_3$, δ, ppm): 168.11, 130.12, 128.14, 125.73, 125.62, 124.81, 122.32, 122.02, 121.54, 120.81, 119.74, 55.62, 44.03, 34.55, 25.46. Calcd for $C_{29}H_{22}N_2O_2$ 430.2,

found: 430.2.

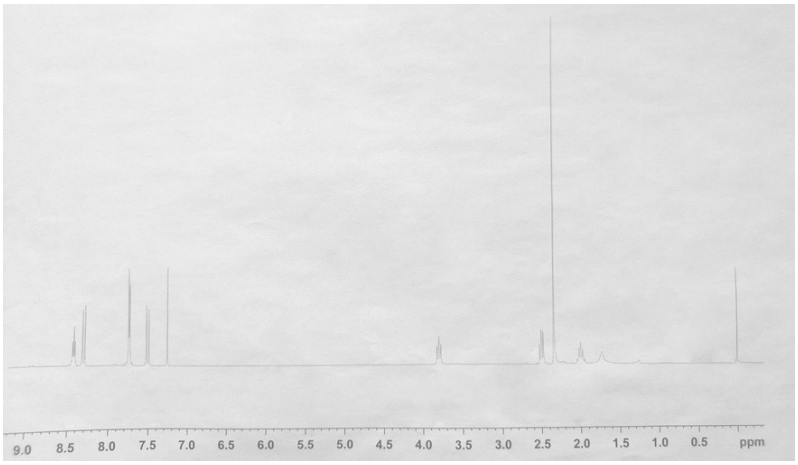


Figure S1.1.1 ^{1}H NMR of P-DAPPD

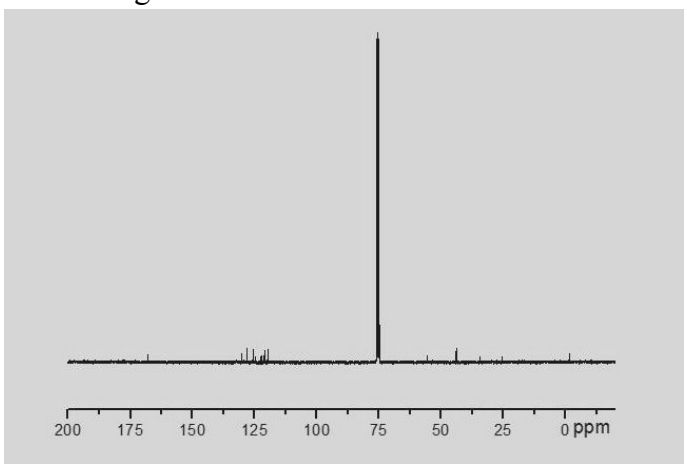


Figure S1.1.2 ^{13}C NMR of P-DAPPD

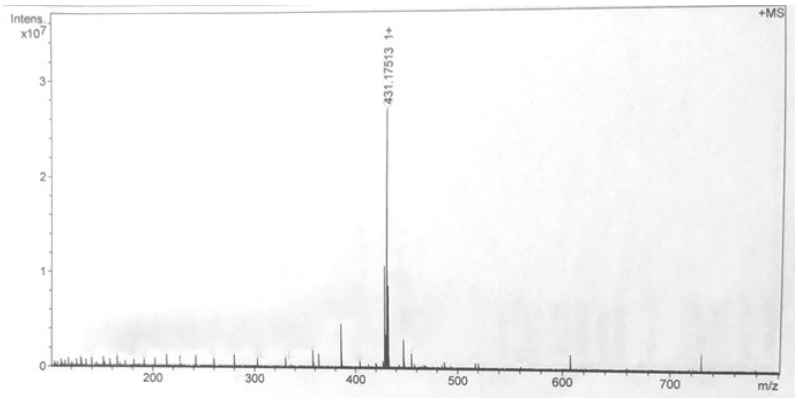


Figure S1.1.3 HR-MS of P-DAPPD

S 1.2 Synthesis of CB-DAP

Compound CB-DAP was synthesized according to the compound P-DAPPD, which

was a orange solid. ESI-MS: m/z =609.5 $[M + H]^+$. ^{1}H-NMR (300 MHz, $CDCl_3$): δ = 2.11 (d, 4H), 2.40 ppm (s, 12H), 2.58 ppm (t, 4H), 3.93 ppm (d, 4H), 7.64 ppm (d, 4H), 8.57 ppm (d, 4H). ^{13}C NMR (300MHz, $CDCl_3$, δ, ppm):169.74, 131.92, 129.63, 127.59, 124.02, 123.58, 122.73, 122.53, 121.14, 56.35, 44.52, 36.02, 26.14. Calcd for $C_{38}H_{32}N_4O_4$, 608.2, found: 608.5.

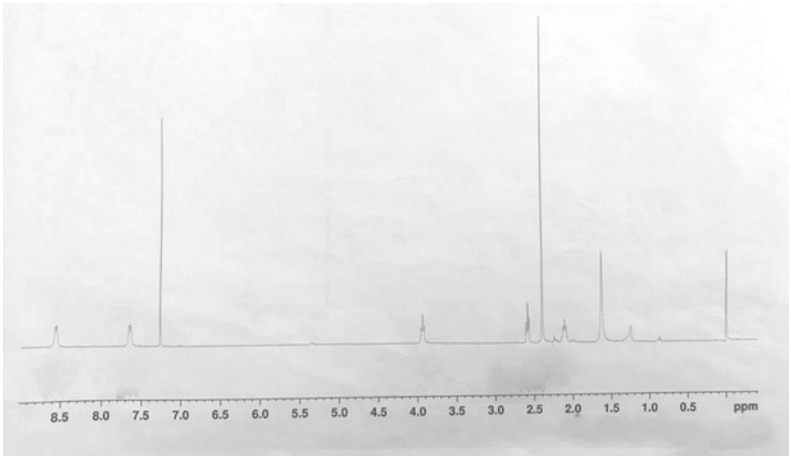


Figure S1.2.1 ^{1}H NMR of CB-DAP

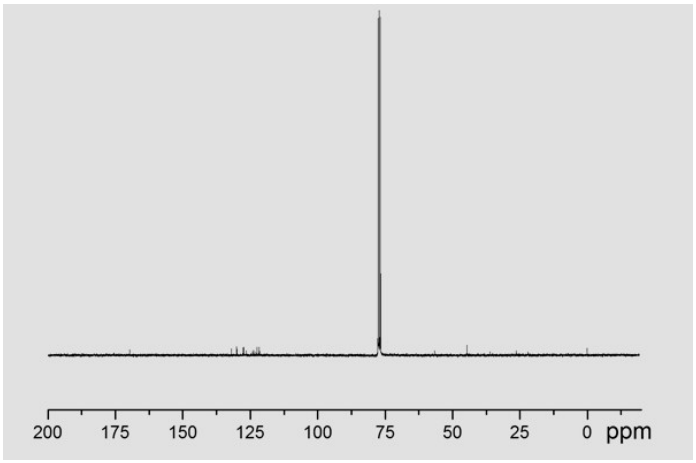


Figure S1.2.2 ^{13}C NMR of CB-DAP

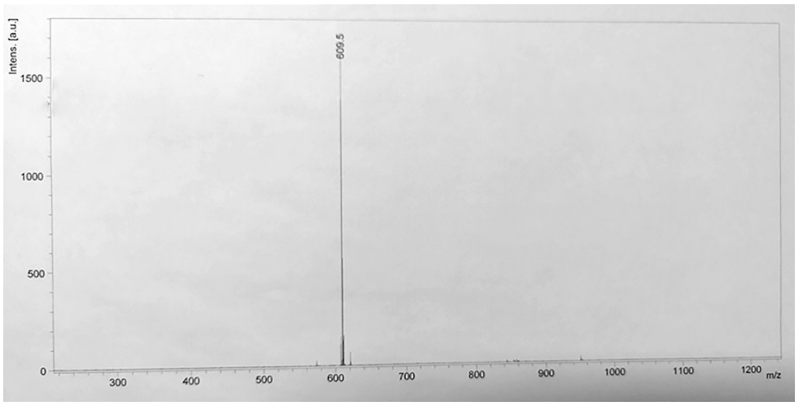
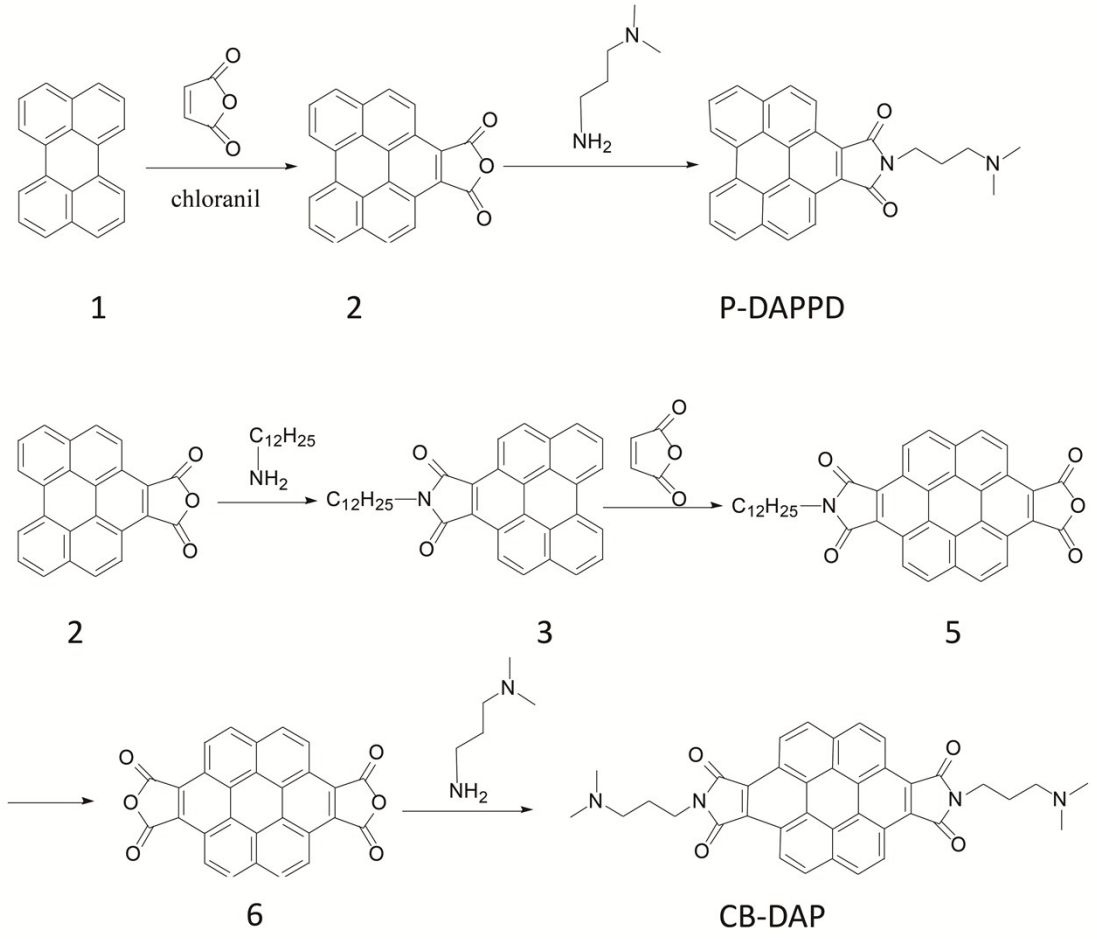


Figure S1.2.3 HR-MS of CB-DAP



Scheme S1. The synthesis procedures of P-DAPPD and CB-DAP.

S2 FT-IR spectra of P-DAPPD and CB-DAP.

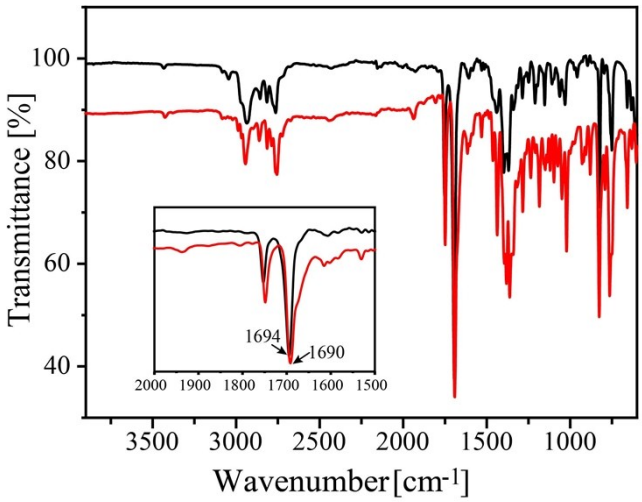


Figure S2.1 FT-IR spectra for P-DAPPD, black line for powder and red line for thin flim.

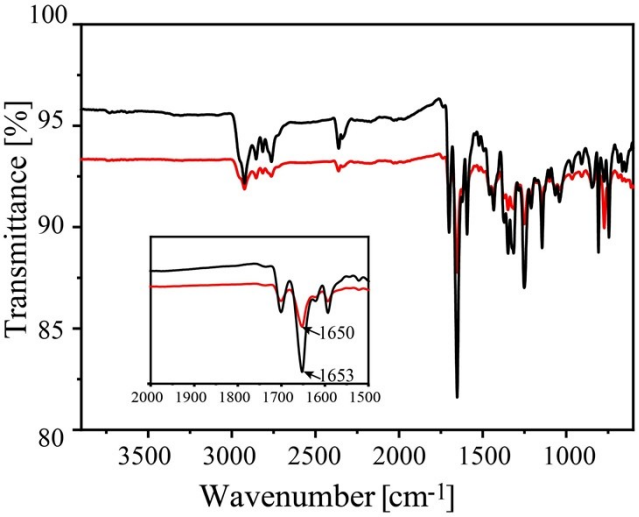


Figure S2.2 FT-IR spectra for CB-DAP: black line for powder and red line for thin flim.

Reference

[1] Z.J. Chen, U. Baumeister, C. Tschierske, F. Wurthner, Chem-Eur J, 2007, 13, 450-465.

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