

Supplementary Information to:

Arylthio-substituted coronenes as tailored building blocks for molecular electronics

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Analytical data for DFPTC, DPTC, and DMPTC

Dodecakis[p-(trifluoromethyl)phenylthio]coronene (DFPTC):

orange amorphous powder (98 mg, 58% yield); M.p. 170°C (dec); $R_f = 0.68$ (SiO₂, petroleum ether/CH₂Cl₂: 60:40 v/v); ¹H NMR (CDCl₃, 200.13 MHz, δ ppm, TMS): 6.64 (24H, d, ³J= 8.2 Hz), 7.24 (24H, ³J= 8.2 Hz); ¹³C NMR (CDCl₃, 50.32 MHz, δ ppm, TMS): 124.05 (CF₃, q, ¹J= 270.0 Hz), 124.76 (s), 126.07 (d_{app}, ³J= 2.9 Hz), 126.60 (d_{app}, ⁴J < 2 Hz), 126.94 (s), 128.69 (q, ²J= 33.0 Hz), 131.26 (s), 143.67 (s); UV-visible: 271 nm ($\epsilon = 134910 \text{ M}^{-1} \cdot \text{cm}^{-1}$); 429 nm ($\epsilon = 77155 \text{ M}^{-1} \cdot \text{cm}^{-1}$); MALDI-Tof MS (DCTB, THF, positive mode, $\lambda = 337 \text{ nm}$): m/z calcd for C₁₀₈H₄₈S₁₂F₃₆ as [M+H]⁺: 2413.98; found: 2414.0 m/z (maximum isotopic ion).

Dodecakis-(phenylthio)coronene (DPTC):

deep red powder (260 mg; 69% yield.); M.p. 340°C (dec.); $R_f = 0.24$ (SiO₂, petroleum ether/DCM: 60/40); ¹H NMR (200 MHz, CDCl₃, TMS, δ ppm): 6.55 (d_{app}, $J=7.2 \text{ Hz}$, 24H, Ar-H ortho); 6.94-7.03 (m, 36H, Ar-H meta/para); ¹³C NMR (63 MHz, CDCl₃, δ ppm): 128.47 (CH), 126.64 (CH), 125.25 (CH), 120.90 (C-S phenyl); UV-vis (*n*-hexane): $\lambda_{\text{max}} = 262 \text{ nm}$ ($\epsilon = 175500 \text{ M}^{-1} \text{cm}^{-1}$); 434 nm ($\epsilon = 125000 \text{ M}^{-1} \text{cm}^{-1}$); MALDI-Tof MS (DCTB, THF, positive mode, $\lambda = 337 \text{ nm}$); m/z for C₉₆H₆₀S₁₂ [M⁺]: 1596.13; found: 1596.13 m/z (maximum isotopic ion). Cyclic voltammetry: two reversible one-electron reduction waves (vs Fc/Fc⁺): $E_1^0 = -1.42 \text{ V}$; $E_2^0 = -1.83 \text{ V}$.

Dodecakis(*p*-methoxyphenylthio)coronene (DMPTC):

deep red amorphous powder (261 mg, 95% yield); $R_f = 0.55$ (SiO_2 , $\text{CH}_2\text{Cl}_2/\text{acetone} : 98:2$ v/v); ^1H NMR (CDCl_3 , 200.13 MHz, δ ppm, TMS): 6.56 (48H, s_{apparent}), 3.66 (36H, s); ^{13}C NMR (CDCl_3 , 50.32 MHz, δ ppm, TMS): 55.55, 114.44, 123.98, 129.17, 131.10, 133.02, 158.01, 158.71 ; UV-visible (CH_2Cl_2 , 0.02 mM) $\lambda_{\text{max}} = 461$ nm ($\epsilon = 66815 \text{ M}^{-1}\text{cm}^{-1}$); Maldi-Tof MS (DCTB, THF, positive mode, $\lambda = 337$ nm) : m/z calcd for $\text{C}_{108}\text{H}_{84}\text{O}_{12}\text{S}_{12}$ as $[\text{M}+\text{H}]^+$:1957.3; found: 1958.3 m/z (maximum isotopic ion).