

SUPPORTING INFORMATION

¹H- and ¹³C-NMR data for 5-7

¹H-NMR (CDCl₃, 25°C, 400.1 MHz); ¹³C-NMR (CDCl₃, 25°C, 100.6 MHz).

5: ¹H-NMR, δ = 7.07 (td, H₂, H₇), 7.12 (td, H₂, H₇), 7.27 (td, H₃, H₆), 7.36 (td, H₃, H₆), 7.37 (ddd, H₄, H₅), 7.72 (ddd, H₄, H₅), 7.89 (ddd, H₁, H₈), 8.13 (ddd, H₁, H₈) ppm. ¹³C-NMR, δ = 117.63 (C₄, C₅), 119.43 (C₄, C₅), 122.79 (C₂, C₇), 124.27 (C₁, C₈), 124.80 (C_{8a}, C_{9a}), 125.85 (C₂, C₇), 127.44 (C₃, C₆), 129.93 (C₃, C₆), 130.86 (C₉), 130.99 (C₉), 139.34 (C_{8a}, C_{9a}), 140.28 (C_{4a}, C_{4b}), 154.02 (C_{4a}, C_{10a}) ppm.

6: ¹H NMR, δ = 1.23 (d, J = 6.9 Hz, 6H), 2.90 (heptet, J = 6.9 Hz, 1H), 7.04-7.11 (2×td, H₂, H₇), 7.12 (td, J = 8.0 Hz, J = 6.7 Hz, H₇), 7.25-7.32 (m, H₃, H₆, H₃, H₄), 7.36-7.40 (m, H₅, H₆), 7.74 (ddd, J = 7.6 Hz, H₄, H₅), 7.91 (dd, J = 8.0 Hz, H₁, H₈), 8.01 (d, J = 2.1 Hz, H₁), 8.14, (ddd, J = 8.1 Hz, H₈) ppm. ¹³C-NMR, δ = 24.08, 33.76, 117.25 (C₄ or C₅), 117.61 (C₅ or C₄), 119.35 (C₅ or C₄), 119.40 (C₄ or C₅), 122.58 (C₇), 124.29 (C₁ or C₈), 124.38, 124.55 (C₈ or C₁), 124.81, 125.62 (C₃ or C₆), 125.77 (C₆ or C₃), 127.32 (C₇), 127.37 (C₂), 127.64 (C₁), 128.54 (C₃), 129.78 (C₆), 129.97 (C₈), 130.43, 131.27, 139.27, 140.18, 140.21, 143.15, 152.21, 154.20 ppm.

7: ¹H-NMR, δ = 7.10 (td, J = 8.1 Hz, J = 7.3 Hz, H₃), 7.13-7.17 (m, H₂, H₇), 7.33 (td, J = 8.6 Hz, J = 7.6 Hz, H₂), 7.36-7.45 (m, H₇, H₈, H₃, H₆, H₄, H₅), 7.62 (ddd, J = 7.5 Hz, H₆), 7.85-7.91 (m, H₁, H₄, H₉), 8.07 (ddd, J = 7.5 Hz, H₁), 8.10 (s, H₅), 8.23 (ddd, J = 7.5 Hz, H₈), 8.40 (s, H₁₀) ppm. ¹³C-NMR, δ = 117.09 (C₅), 117.64, 117.88, 120.24, 122.61 (C₂ or C₇), 122.70 (C₇ or C₂), 123.48 (C₁₀), 124.62, 125.35, 125.37, 125.37, 125.41, 126.15, 126.49 (C₃), 127.93, 127.98, 128.87, 128.87, 128.99 (C₆), 129.12 (C₈), 129.26 (C₁), 129.58, 129.70, 130.59, 132.43, 133.21, 137.67, 138.53, 140.25, 140.75, 154.59 (C_{4a}, C_{10a}) ppm.

¹³C-DNMR results for 6.

	δ at 295 K ppm	T _c K	Δv_c Hz	ΔG_c^\ddagger kJ/mol
Inversion process (in CDFCl ₂)				
CH ₃	24.08	134±2	57	26.5±0.5
<i>E, Z</i> -Topomerization process (in CDCl ₃)				
	140.21, 140.19	344	1.3	81.6
	139.37, 139.32	357	3.7	81.8
C ₂ , C ₇	127.37, 127.33	357.3	3.4	82.1
C ₄ , C ₅	119.40, 119.35	357.3	3.6	81.8
<i>E, Z</i> -Topomerization process (in toluene-d ₈)				
	141.14, 141.09	363.5	5.1	82.3
	140.15, 140.12	356	2.9	82.2
C ₂ , C ₇	126.12, 125.87	381	23	81.6
C ₄ , C ₅	119.83, 119.80	357	2.6	82.8