Supporting information for

Approaching a Stable, Green Twisted Heteroacene Through “Clean reaction” Strategy

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1. General methods

1.1 Measurements. The NMR spectra were taken on a Bruker ARX 400 and 500 spectrometer. Electrochemistry was carried out with a BAS 100B/W potentiostat, employing a platinum button (diameter: 1.6 mm; area 0.02 cm$^2$), a platinum wire and a 0.01 M Ag/AgNO$_3$ (Ag/Ag$^+$) as working, counter and reference electrode, respectively. 0.1 M of tetrabutylammonium perchlorate (TBAP) in ODCB was used as the electrolyte. Since compound 3 was not very soluble in ODCB at room temperature, CV measurements were conducted at higher temperatures (ca. 150 °C).

Single-crystal data set of precursor 6 was collected at 103 K on a Bruker SMART APEX II CCD fitted with graphite monochromatized Mo K$_\alpha$ radiation ($\lambda$ = 0.71073 Å). Data processing (APEXII and SMART) and absorption correction (SADABS) were accomplished by standard methods. The structure was solved by direct-methods using SHELXS-97 and refinement (anisotropic displacement parameters, hydrogen atoms in the riding model approximation and a weighting scheme of the form $w = 1/[\sigma^2(F_0^2) + (0.064P)^2 + 0.376P]$ for $P = (F_0^2 + 2F_c^2)/3$) was on $F^2$ by means of SHELXL-97. CCDC number for compound 6 is 858853.

Materials. Meso-ionic pyrimidines (5)$^1$ and 3-amino-5,12-diphenyl-6:7,10:11-bisbenzotetracene-2-carboxylic acid (4)$^2$ were prepared from reported procedures. All solvents were used without further purification.

2. Synthesis

2.1 Lactam cycloadduct 6. To mesoion 5 (114 mg, 0.39 mmol) and isoamyl nitrite (0.060 mL, 0.40 mmol) in 20 mL DCE was added a suspension of 3-amino-5,12-diphenyl-6:7,10:11-
bisbenzotetracene-2-carboxylic acid (4) (100 mg, 0.20 mmol) in 10 mL DCE over a span of 1h. After refluxing for an additional hour, DCE was removed. The resulting brown residue was purified by silica-gel column chromatography using dichloromethane : diethyl ether (9:1) as eluent to yield the lactam 6 (88 mg, 60%) as a tan powder; $^1$H-NMR (500 MHz, CDCl$_3$) $\delta$ 8.12 (d, 2H), 8.05 (s, 1H), 7.88-7.85 (m, 6H), 7.79 (bs, 2H), 7.54-7.24 (bm, 19H), 2.71 (d, 6H); $^{13}$C-NMR (400 MHz, CDCl$_3$) $\delta$ 171.90, 142.13, 141.21, 137.06, 136.81, 134.73, 131.92, 131.72, 131.62, 131.42, 131.10, 130.81, 130.55, 130.22, 130.1, 130.01, 129.93, 129.82, 129.26, 129.07, 128.80, 128.60, 127.68, 127.61, 127.46, 126.96, 126.86, 126.13, 125.86, 125.78, 125.28, 124.79, 124.73, 119.99, 81.06, 65.99, 33.93; IR (DRIFT) 3053, 2921, 1715, 1675, 1490, 1367, 1206, 1072, 831, 751, 694, 544 cm$^{-1}$. MS (ESI): 745.01 (M$^+$ + H), calcd 745.28 (M$^+$ + H); Elemental analysis, found C, 86.86; H, 4.95; N, 3.55; calcd C, 87.07; H, 4.87; N, 3.76.

2.2 2-Methyl-1,4,6,13-tetraphenyl-7:8,11:12-bisbenzo-anthro[g]isoquinolin-3(2H)-one 3.

A neat sample of the lactam cycloadduct 6 (117 mg, 0.16 mmol) was purged 3x using nitrogen gas before heating at 220 °C under vacuum for 4h to give a green powder as 3 (105 mg, 100%). An alternate method is as follows: the lactam cycloadduct 6 was dispersed in tetrahydronaphthalene solvent. The solution was heated up to 220 °C for 4 hours and slow cooled to room temperature will give dark green crystals (98%). $^1$H-NMR (400 MHz, CDCl$_3$) $\delta$ 7.89 (s, 1H), 7.81-7.44 (m, 11H), 7.44-7.21 (m, 18H), 3.81 (s, 3H); $^{13}$C-NMR (400 MHz, CDCl$_3$) $\delta$ 158.24, 153.97, 141.18, 141.10, 136.82, 135.76, 135.65, 133.26, 132.17, 131.92, 131.78, 131.01, 130.79, 130.72, 130.43, 130.37, 130.17, 129.72, 129.60, 129.22, 129.07, 128.83, 128.76, 128.14, 127.48, 127.31, 126.80, 126.71, 126.19, 125.06, 125.00, 119.99, 117.40, 115.82, 37.18; IR (DRIFT): 3053, 2923, 1703, 1630, 1447, 1382, 1350, 1012, 829, 750, 701; MS (ESI): 688.47 (M$^+$ + H), calcd 688.26 (M$^+$ + H); MS (HiResMALDI-TOF): 688.2637 (M$^+$ + H), calcd 688.2640 (M$^+$ + H). Elemental analysis, found C, 90.56; H, 4.65; N, 2.11; calcd C, 90.80; H, 4.84; N, 2.04.
Figure S1. The IR spectrum of compound 6.
Figure S2. The MS (ESI) spectrum of compound 6.
Figure S3. The $^1$H-NMR spectrum of compound 6.
**Figure S4.** The $^{13}$C-NMR spectrum of compound 6.
Figure S5. (a) The $^1$H-NMR spectrum of compound 3. (b) The magnified part of $^1$H-NMR spectrum.
Figure S6. The $^{13}$C-NMR spectrum of compound 3.
Figure S7. The FT-IR spectrum of compound 3.
Figure S8. The MS-ESI spectrum of compound 3.
Figure S9. The MS-HiResMALDI-TOF plot of compound 3.

Figure S10. The TGA analysis of compound 3.
3. X-ray crystallographic data of compound 6

Table S1. Cell data parameters of Compound 6

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**Table S2.** Bond lengths (Å) and angles (deg.).

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4. References
