

Imposing Curvature on a Polyarene by Intramolecular Palladium-Catalyzed Arylation Reactions: A Simple Synthesis of Dibenzo[a,g]corannulene

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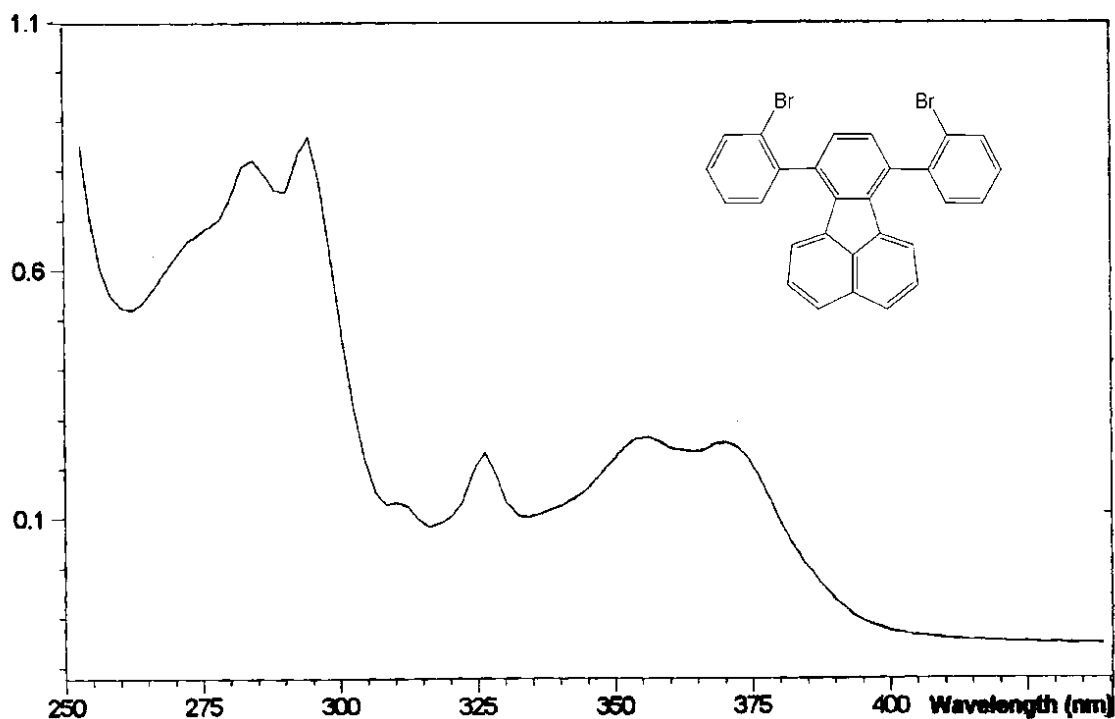
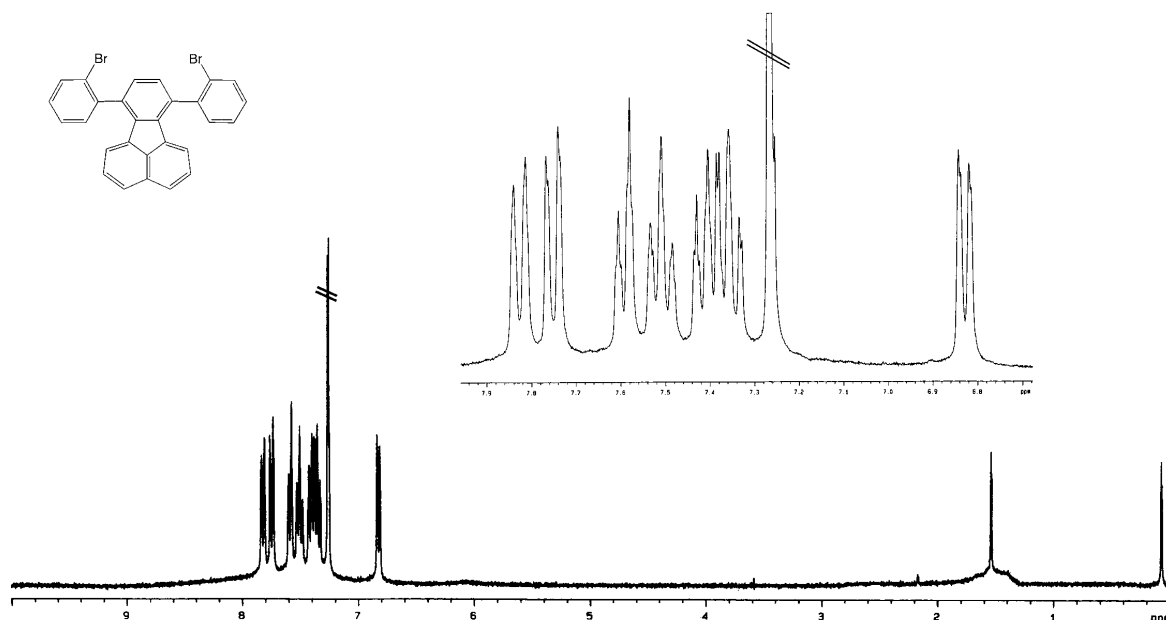
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Received Date (will be automatically inserted after manuscript is accepted)

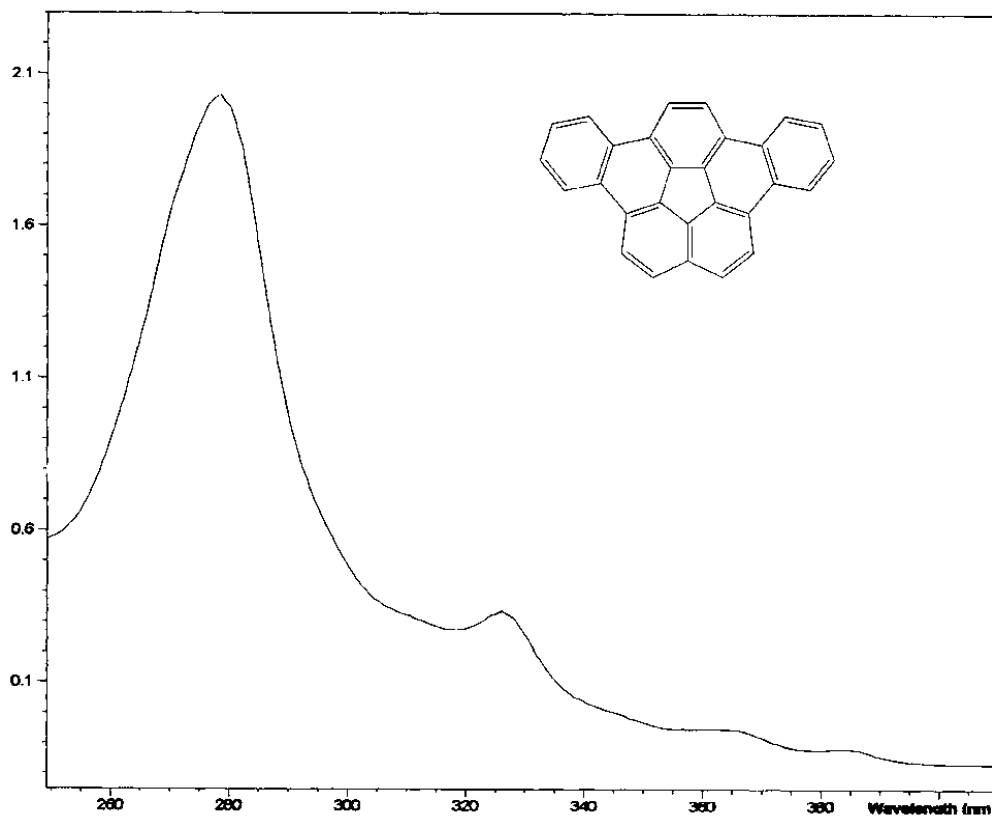
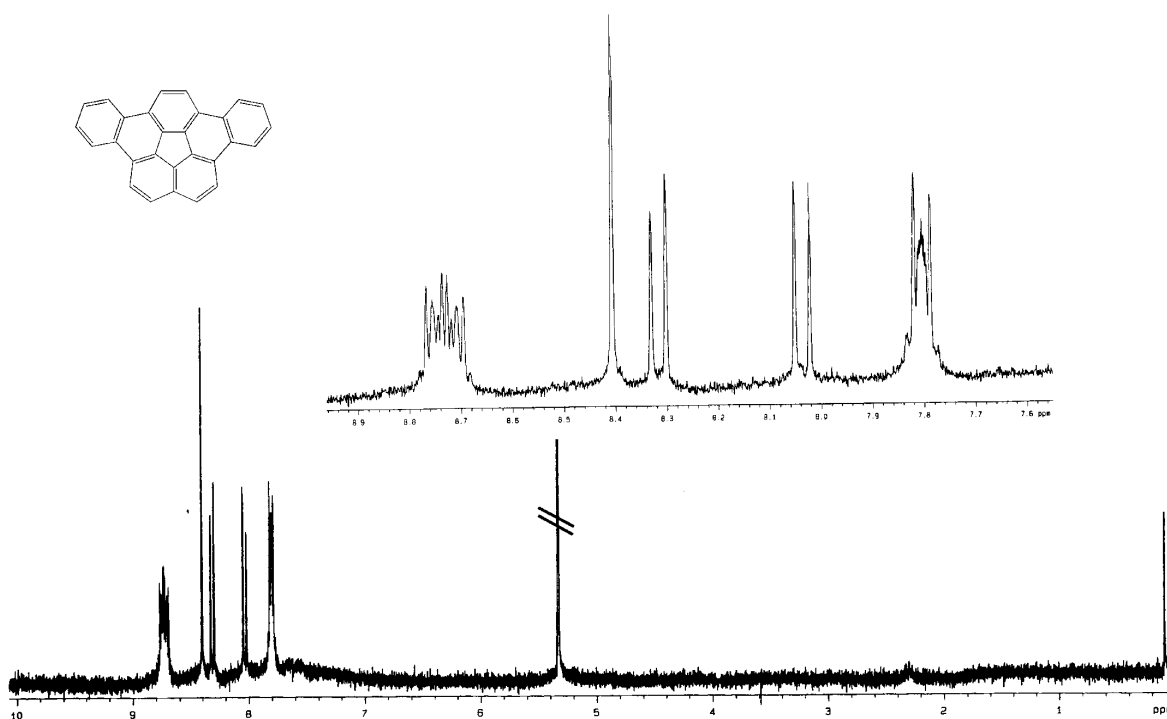
Supporting Information

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7,10-Di(2-bromophenyl)fluoranthene (4) (mixture of two diastereomeric atropisomers): m.p. 174-175 °C; $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ = 7.83 (d, 2H, J = 7.6 Hz), 7.75 (d, 2H, J = 8.4 Hz), 7.59 (d, 2H, J = 7.2 Hz), 7.56-7.49 (m, 2H), 7.40 (dd, 2H, 8.0 and 7.2 Hz), 7.36 (dd, 2H, J = 8.0 and 7.2 Hz), 7.27 (s, 2H), 6.83 (d, 2H, 6.8 Hz). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ = 141.7, 141.6, 137.3, 136.9, 136.3, 133.3, 133.2, 132.9, 131.5, 131.2, 129.9, 129.7, 128.8, 128.0, 127.9, 127.8, 127.0, 123.9, 123.8, 122.8. MS m/z (rel abund): 514 (34), 512 (70), 510 (35), 352 (80), 350 (72). HRMS: Calcd for $\text{C}_{28}\text{H}_{16}\text{Br}_2$: 509.9619, found: 509.9618.



Dibenzo[*a,g*]corannulene (5): m.p. 285-287 °C; $^1\text{H-NMR}$ (400 MHz, CD_2Cl_2): $\delta = 8.77\text{-}8.70$ (m, 4H), 8.40 (s, 2H), 8.32 (d, 2H, $J = 8.7$ Hz), 8.03 (d, 2H, $J = 8.7$ Hz), 7.82-7.79 (m, 4H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): $\delta = 134.6, 133.4, 132.2, 130.7, 129.7, 129.4, 129.2, 129.0, 127.8, 127.6, 127.5, 125.4, 125.3, 124.9, 124.6$. UV-Vis (CH_3CN) λ_{max} : 383, 359, 325, 277, 239, 213. MS m/z (rel abund): 351 (33), 350 (100), 348 (17), 326 (33), 175 (46). HRMS: Calcd for $\text{C}_{28}\text{H}_{14}$: 350.1095, found: 350.1102.



Mono-closed Product (6): mp 176-8 °C. $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ = 8.80-8.77 (m, 1H), 8.72-8.68 (m, 1H), 8.47 (d, 1H, J = 8.0 Hz), 8.44 (d, 1H, J = 8.8 Hz), 8.09 (d, 1H, J = 8.8 Hz), 8.04-7.94 (m, 4H), 7.80-7.75 (m, 4H), 7.66-7.52 (m, 3H). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3): δ = 131.5, 130.3, 129.4, 129.0, 128.9, 128.8, 128.7, 128.6, 128.2, 128.1, 127.2, 127.1, 127.0, 126.7, 126.6, 125.2, 125.1, 124.90, 124.88, 124.81, 123.5, 123.0, 122.4, 122.2, 122.1. MS m/z (rel abund): 353 (32, $\text{M}+1$), 352 (100, M^+), 350 (29), 176 (19), 175 (34). HRMS: Calcd for $\text{C}_{28}\text{H}_{16}$: 352.1252, found: 352.1252.

