Supplementary Information

Substituent-induced modulation of proaromaticity in benzo-fused fluorenophenalene exhibiting low-lying LUMO

Sakshi Sahewal,[a] Suman Sharma,[a] Dibyendu Mallick [b] and Soumyajit Das*[a]

[a]*Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar 140001, Punjab, India.*

[b]*Department of Chemistry, Presidency University, Kolkata 700073, West Bengal, India.*

Email: chmsdas@iitrpr.ac.in

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1. Experimental section

1.1 General information: Chemicals and reagents were purchased from local and international commercial suppliers (Merck, GLR innovations, BLD pharm, Spectrochem) and used without further purification. Compound **4** was synthesized according to a known method.[1] Thin layer chromatography (TLC) was performed using pre-coated silica plates purchased from Merck (silica gel 60 PF254, 0.25 mm). Column chromatography was performed using silica gel 100-200 mesh. NMR spectra were recorded in $CDCl_3$ (Eurisotop) at room temperature on a JEOL JNM-ECS400 spectrometer, operating at frequencies of 400 MHz (^1H) or 100 MHz (^{13}C), as indicated in the individual spectra. Chemical shifts (δ) are given in ppm relative to residual solvent (chloroform δ = 7.26 for ^1H, and δ = 77.16 for proton-decoupled ^{13}C NMR), and coupling constants (*J*) are expressed in Hertz (Hz). Multiplicity is tabulated as s (singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quartet), and m (multiplet). High-resolution mass spectra (HRMS) were recorded using electrospray ionization (ESI) methods on a Waters (XEVO G2-XS QTOF) mass spectrometer. UV-vis-NIR spectra were recorded in the JASCO V-770 spectrophotometer. Cyclic voltammetry was performed using an Electrochemical Analyzer potentiostat model CHI-1115C from CH Instruments with a conventional three-electrode cell at room temperature under a nitrogen atmosphere at a scan rate of 50 mV s^{-1}. This electrochemical cell contains a glassy carbon (disc-shaped with 3-mm diameter) as a working electrode, a Pt wire as a counter electrode, and an Ag wire as a pseudo-reference electrode. The glassy carbon working electrode was polished with 1.0-micron α-alumina polishing powder using a figure-eight motion. Electrolyte solution (0.1 M) was prepared from dichloromethane (DCM) and tetra-*n*-butylammonium hexafluorophosphate (nBu$_4$NPF$_6$). The DCM was degassed by nitrogen gas sparging for 10 minutes before measurements. The potential was externally calibrated against the ferrocene/ferrocenium couple. Melting points were determined using a Cole-Parmer MP 250D-P melting point analyzer.

1.2 Syntheses and characterization data

Compound 5: An oven-dried glass tube was charged with **4** (282 mg, 936.31 μmol), bis(pinacolatodiboron) (285 mg, 1.12 mmol), KOAc (460 mg, 4.68 mmol), and dry 1,4-dioxane (8 mL). The suspension was purged with N_2 for 30 mins before adding $PdCl_2$(dppf)·DCM (38 mg, 5 mol%), and the glass tube was sealed. The reaction mixture was stirred at 85 °C for 12 h. After being cooled to room temperature, volatile organics were removed under reduced pressure, and water was added. The mixture was extracted with EtOAc (5 x 60 mL), dried over anhydrous Na_2SO_4, and filtered. The organic layer was removed under reduced pressure, and the crude obtained was quickly column chromatographed on a short silica gel pad (hexanes:

EtOAc, 90:10) to afford the compound **5** as a white solid (214 mg, 65% yield). R_f = 0.36 (hexanes:EtOAc = 9:1). mp: 124 °C. ^{1}H NMR (400 MHz, $CDCl_3$):δ 8.67 (d, *J* = 9.0 Hz, 1H), 8.57 (d, *J* = 8.3 Hz, 1H), 7.83 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.76 (d, *J* = 9.0 Hz, 1H), 7.68 (d, *J* = 9.1 Hz, 1H), 7.60 (ddd, *J* = 8.4, 7.1, 1.4 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.27-7.25 (d, 1H), 4.18 (q, *J* = 7.0 Hz, 2H), 1.50 (s, 12H), 1.47 (t, *J* = 6.9 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 161.4 , 136.2, 130.8, 128.5, 127.6, 126.4, 125.9, 125.5, 124.5, 122.2, 112.2, 84.1, 64.4, 25.0, 15.1. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{22}H_{26}BO_3$ 349.1975, found 349.1959 (error: –1.6 ppm).

Compound 7: An oven-dried thick-walled glass tube was charged with 5-bromo-2-iodobenzaldehyde **6** (200 mg, 643.26 µmol), 2-(2-ethoxyphenanthren-1-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane **5** (142 mg, 643.26 µmol), anhydrous K_3PO_4 (682 mg, 3.22 mmol), toluene (5 mL), water (0.5 mL), and the mixture was purged with nitrogen for 40 mins. Catalyst $PdCl_2$(dppf)·DCM (26 mg, 5 mol%) was subsequently added under nitrogen, and the glass vial was sealed before being warmed to 110 °C using an oil bath. After 12 h, the flask was cooled to room temperature, and the solvent was evaporated under reduced pressure. Water was added, and the mixture was extracted with EtOAc (3 x 30 mL). The organic layer was dried over sodium sulfate and then evaporated to dryness. The residue was purified by silica gel column chromatography (hexanes:EtOAc, 95:5) to afford the product **7** as a light yellow solid (115 mg, 44% yield). R_f = 0.44 (hexanes:EtOAc = 9:1). mp: 155 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.57 (s, 1H), 8.79 (d, *J* = 9.2 Hz, 1H), 8.66 (d, *J* = 8.3 Hz, 1H), 8.25 (d, *J* = 2.2 Hz, 1H), 7.84 (dd, *J* = 8.1, 2.0 Hz, 2H), 7.71 – 7.65 (m, 1H), 7.63 (d, *J* = 9.2 Hz, 1H), 7.60 – 7.55 (m, 1H), 7.41 (d, *J* = 9.2 Hz, 1H), 7.28 (d, *J* = 1.4 Hz, 1H), 7.26 (s, 1H), 4.14 (q, *J* = 7.0 Hz, 2H), 1.25 (t, *J* = 6.9 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 191.3, 154.4, 139.4, 136.6, 136.5, 134.4, 132.2, 130.6, 130.3, 130.0, 128.7, 128.5, 127.2, 126.2, 125.0, 124.9, 123.5, 122.4, 122.3, 120.6, 112.4, 64.5, 14.8. HRMS (ESI) *m/z*: $[M + H]^+$ Calcd for $C_{23}H_{18}BrO_2$ 405.0490, found 405.0507 (error: 4.2 ppm).

Compound 9: 2-Mesitylmagnesium bromide (1 M solution in THF, 3.21 mL, 3.21 mmol) was added dropwise to the 10 mL dry THF solution of compound **7** (650 mg, 1.60 mmol) under nitrogen, and the mixture was stirred at room temperature for 12 h. The reaction mixture was quenched with a saturated solution of ammonium chloride (50 mL), and the volatile organics were evaporated in vacuo. The residue was extracted with DCM (3 x 50 mL), washed with water, and dried over sodium sulfate. The organic layer was filtered, and the filtrate was removed under reduced pressure to afford crude **8**. To the solution of crude **8** in anhydrous

DCM (10 mL) at room temperature, $BF_3 \cdot Et_2O$ (0.1 mL) was added dropwise under nitrogen, and the reaction mixture was stirred for 15 min at room temperature to perform an intramolecular ring-closure reaction. After 15 min, a saturated aqueous NH_4Cl solution was added to the reaction mixture and extracted with DCM (3 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure to afford a residue which was purified by silica gel column chromatography (hexanes) to give **9** as a yellow solid (300 mg, 37% yield over two steps). R_f = 0.48 (hexanes). mp: 140 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.8 Hz, 1H), 8.64 (d, *J* = 9.2 Hz, 1H), 8.55 (d, *J* = 8.3 Hz, 1H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.56 –7.52 (m, 1H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.39 (ddd, *J* = 8.7, 2.3, 0.9 Hz, 1H), 7.06 (s, 1H), 7.04 (d, *J* = 2.5 Hz, 1H), 6.95 (dd, *J* = 2.2, 1.5 Hz, 1H), 6.92 (s, 1H), 5.99 (s, 1H), 4.41 (dq, *J* = 9.1, 7.0 Hz, 1H), 4.29 (dq, *J* = 9.2, 7.0 Hz, 1H), 2.41 (d, *J* = 6.4 Hz, 6H), 1.63 (s, 3H), 1.59 (t, *J* = 7.0 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 155.2, 141.1, 137.9, 136.7, 134.1, 131.7, 131.1, 130.6, 130.3, 129.6, 129.3 – 128.8, 128.7, 128.1, 126.0, 125.0, 124.1, 123.7, 122.1, 121.5, 118.1, 115.2, 65.4, 44.2, 21.9, 21.0, 15.3. HRMS (ESI) *m/z*: $[M]^+$ Calcd for $C_{32}H_{27}BrO$ 506.1245, found 506.1230 (error: –2.96 ppm).

Compound 11: An oven-dried thick-walled glass tube was charged with 6-bromo-3-ethoxy-8-mesityl-8H-benzo[*fg*]tetracene **9** (300 mg, 591.17 µmol), (2-formylphenyl)boronic acid **10** (133 mg, 886.75 µmol), anhydrous K_2CO_3 (408 mg, 2.96 mmol), toluene (10 mL), water (1 mL), ethanol (1 ml) and the mixture was purged with nitrogen for 40 mins. Catalyst Pd_2dba_3 (27 mg, 5 mol%), SPhos (48 mg, 20 mol%) was subsequently added under nitrogen, and the glass vial was sealed before being warmed to 110 °C using an oil bath. After 12 h, the flask was cooled to room temperature, and the solvent was evaporated under reduced pressure. Water was added, and the mixture was extracted with EtOAc (3 x 30 mL). The organic layer was dried over sodium sulfate and then evaporated to dryness. The residue was purified by washing with methanol to afford the product **11** as a light green solid (200 mg, 63% yield). R_f = 0.44 (hexanes:DCM = 8:2). mp: 220 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.91 (s, 1H), 9.02 (d, *J* = 8.4 Hz, 1H), 8.67 (d, *J* = 9.2 Hz, 1H), 8.57 (d, *J* = 8.3 Hz, 1H), 7.99 – 7.93 (m, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.59 – 7.52 (m, 3H), 7.46 (d, *J* = 7.1 Hz, 1H), 7.43 (d, *J* = 7.3 Hz, 1H), 7.36 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 7.09 (d, *J* = 2.4 Hz, 1H), 7.01 (s, 1H), 6.94 (s, 1H), 6.85 (s, 1H), 6.09 (s, 1H), 4.46 (dq, *J* = 14.0, 7.0 Hz, 1H), 4.34 (dq, *J* = 14.0, 7.0 Hz, 1H), 2.40 (s, 3H), 2.36 (s, 3H), 1.68 (s, 3H), 1.64 (t, *J* = 7.0 Hz, 3H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 192.3, 155.5, 145.9, 139.1, 137.8, 137.2, 136.5, 136.3, 134.4, 133.8, 133.5, 131.6, 131.2, 130.7, 129.8, 129.1, 128.7, 128.6, 128.2, 128.1, 127.9, 127.6, 127.5, 126.0, 125.9, 125.0, 124.2,

123.8, 122.1, 118.2, 115.0, 65.4, 44.3, 22.0, 21.0, 15.3. HRMS (ESI) *m/z*: $[M+H]^+$ Calcd for $C_{39}H_{33}O_2$ 533.2481, found 533.2459 (error: –4.1 ppm).

Compound 1: 2-Mesitylmagnesium bromide (1 M solution in THF, 0.4 mL, 375.46 µmol) was added dropwise to the 10 mL dry THF solution of compound **11** (100 mg, 187.73 µmol) under nitrogen, and the mixture was stirred at room temperature for 12 h. The reaction mixture was quenched with a saturated solution of ammonium chloride (50 mL), and the volatile organics were evaporated in vacuo. The residue was extracted with DCM (3 x 50 mL), washed with water, and dried over sodium sulfate. The organic layer was filtered, and the filtrate was removed under reduced pressure to afford the precursor alcohol as a yellow solid. To the solution of crude alcohol in anhydrous DCM (10 mL) at room temperature, $BF_3{\cdot}Et_2O$ (0.1 mL) was added dropwise under nitrogen, and the reaction mixture was stirred for 15 min at room temperature to perform an intramolecular ring-closure reaction. After 15 min, a saturated aqueous NH_4Cl solution was added to the reaction mixture and it was extracted with DCM (3 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure to afford a residue which was purified by silica gel column chromatography (hexanes) to give dihydro derivative **12** (50 mg, crude). DDQ (48 mg, 75.61 µmol) was added to the solution of **12** (17 mg, 75.61 µmol) in dry toluene (5 mL) under nitrogen, and the reaction mixture was stirred at 110 ˚C for 5 h. Once the starting material was consumed (as monitored by TLC), the toluene was removed in vacuo, and the crude was purified by silica gel column chromatography (hexanes:DCM, 95:5) to afford target compound **1** as a dark-green solid (30 mg, 62% yield): R_f = 0.3 (10% DCM/hexanes). mp: 321 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (s, 1H), 8.58 (d, *J* = 9.2 Hz, 1H), 8.50 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.60 (m, 2H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.42 – 7.40 (m, 2H), 7.28 (s, 1H), 7.22 (s, 1H), 7.18 (t, *J* = 7.4 Hz, 1H), 7.13 – 7.09 (m, 3H), 7.01 – 6.98 (m, 3H), 4.22 (q, *J* = 6.9 Hz, 2H), 2.51 (s, 3H), 2.38 (s, 3H), 2.16 (s, 6H), 2.04 (s, 6H), 1.16 (t, *J* = 6.9 Hz, 3H).^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.2, 144.4, 141.7, 138.3, 137.6, 137.4, 137.3, 136.8, 136.5, 134.9, 134.6, 134.4, 131.6, 131.4, 130.9, 130.4, 129.3, 128.4, 128.0, 127.9, 127.4, 127.3, 126.2, 126.1, 124.4, 124.3, 122.9, 122.8, 122.2, 121.8, 120.7, 120.5, 118.9, 113.0, 64.9, 21.4, 21.2, 20.5, 20.1, 14.1. HRMS (ESI) *m/z*: $[M]^+$ Calcd for $C_{48}H_{40}O$ 632.3079, found 632.3084 (error: 0.72 ppm).

Compound 2: (2,4,6-Trifluorophenyl)magnesium bromide (1 M solution in THF, 0.56 mL, 563.19 µmol) was added dropwise to the 10 mL dry THF solution of compound **11** (150 mg, 281.59 µmol) under nitrogen, and the mixture was stirred at room temperature for 12 h. The reaction mixture was quenched with a saturated solution of ammonium chloride (50 mL), and the volatile organics were evaporated in vacuo. The residue was extracted with DCM (3 x 50

mL), washed with water, and dried over sodium sulfate. The organic layer was filtered, and the filtrate was removed under reduced pressure to afford the alcohol intermediate. To the solution of crude alcohol in anhydrous DCM (10 mL) at room temperature, $BF_3 \cdot Et_2O$ (0.1 mL) was added dropwise under nitrogen, and the reaction mixture was stirred for 15 min at room temperature to perform an intramolecular ring-closure reaction. After 10 min, a saturated aqueous NH_4Cl solution was added to the reaction mixture and it was extracted with DCM (3 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure to afford a residue which was purified by silica gel column chromatography (hexanes) to give as dihydro precursor **13** as a white-green solid (118 mg). *p*-Chloranil (84 mg, 340.16 μmol) was added to the solution of **13** (55 mg, 85.04 μmol) in dry toluene (5 mL) under nitrogen, and the reaction mixture was stirred at 110 ˚C for 6 h. Once the starting material was consumed (as monitored by TLC), the toluene was removed in vacuo, and the crude was purified by silica gel column chromatography (hexanes:DCM, 95:5) to afford target compound **2** as a dark-green solid (30 mg, 85% yield): R_f = 0.4 (10% DCM/hexanes). mp: 330 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (s, 1H), 8.65 (d, *J* = 9.2 Hz, 1H), 8.54 (d, *J* = 8.2 Hz, 1H), 7.64 (dd, *J* = 7.5, 3.8 Hz, 2H), 7.59 – 7.55 (m, 1H), 7.50 (d, *J* = 9.2 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.39 (s, 1H), 7.35 (s, 1H), 7.28 – 7.24 (m, 1H), 7.15 (d, *J* = 7.3 Hz, 2H), 7.11 (s, 2H), 6.90 – 6.86 (m, 2H), 4.36 (q, *J* = 6.9 Hz, 2H), 2.51 (s, 3H), 2.01 (s, 6H), 1.45 (t, *J* = 7.0 Hz, 3H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 169.6, 157.6, 144.0, 143.2, 140.8, 138.1, 137.5, 137.4, 134.3, 134.1, 131.29, 130.0, 129.5, 128.5, 128.4, 127.9, 127.7, 126.2, 124.5, 123.4, 122.8, 122.3, 121.0, 120.8, 120.3, 118.7, 113.3, 100.7, 65.0, 21.4, 20.1, 14.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.2, -108.9. HRMS (ESI) *m/z*: $[M]^+$ Calcd for $C_{45}H_{31}F_3O$ 644.2327, found 644.2314 (error: –0.51 ppm).

Compound 3: To a 10 mL dry THF solution of **11** (200 mg, 375.46 μmol) under a nitrogen atmosphere, dropwise addition of pentafluorophenylmagnesium bromide (0.5 M in THF, 0.7 mL, 750.92 μmol) was done, and the mixture was stirred at room temperature for 24 h. The reaction mixture was quenched with NH_4Cl (20mL) and extracted with DCM (3 × 40mL) after evaporation of THF. After drying the solvent mixture over sodium sulfate, the solvents were removed to isolate the crude alcohol. To the solution of crude alcohol in anhydrous DCM (10 mL) at room temperature, $BF_3 \cdot Et_2O$ (0.1 mL) was added dropwise under nitrogen, and the reaction mixture was stirred for 10 min at room temperature to perform an intramolecular ring-closure reaction. After 10 min, a saturated aqueous NH_4Cl solution was added to the reaction mixture, and was extracted with DCM (3 x 50 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure to afford a residue which was purified

by silica gel column chromatography (hexanes) to give dihydro precursor **14** (170 mg, crude). *p*-Chloranil (110 mg, 451.13µmol) was added to the solution of **14** (77 mg, 112.78 µmol) in dry toluene (10 mL) under nitrogen, and the reaction mixture was stirred at 110 ˚C for 24 h. Once the starting material was consumed (as monitored by TLC), the toluene was removed in vacuo, and the crude was purified by silica gel column chromatography (hexanes:DCM, 95:5) to afford target compound **3** as a dark-green solid (70 mg, 91% yield): R_f = 0.3 (10% DCM/hexanes). mp: 253 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (s, 1H), 8.69 (d, *J* = 9.2 Hz, 1H), 8.56 (d, *J* = 8.2 Hz, 1H), 7.67 (dd, *J* = 7.4, 3.5 Hz, 2H), 7.62 – 7.58 (m, 1H), 7.54 (d, *J* = 9.1 Hz, 1H), 7.48 – 7.44 (m, 2H), 7.41 (s, 1H), 7.30 – 7.27 (m, 1H), 7.18 – 7.11 (m, 4H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.52 (s, 3H), 2.01 (s, 6H), 1.53 (t, *J* = 6.9 Hz, 3H). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.9, 145.5, 142.5, 140.8, 137.8, 137.7, 137.3, 136.9, 134.1, 134.0, 131.4, 131.1, 130.9, 129.7, 129.7, 129.1, 129.0, 128.8, 128.5, 128.2, 128.1, 127.5, 126.3, 124.6, 124.3, 123.8, 123.4, 122.4, 121.5, 120.9, 120.1, 118.4, 117.7, 113.3, 65.1, 21.4, 20.1, 14.5. ^{19}F NMR (376 MHz, $CDCl_3$) δ -135.46 (d, *J* = 19.1 Hz), -155.64 (t, *J* = 19.7 Hz), - 161.73 (t, *J* = 19.1 Hz). HRMS (ESI) *m/z*: $[M]^+$ Calcd for $C_{45}H_{29}F_5O$ 680.2139, found 680.2124 (error: –2.2 ppm).

1.3 NMR spectra

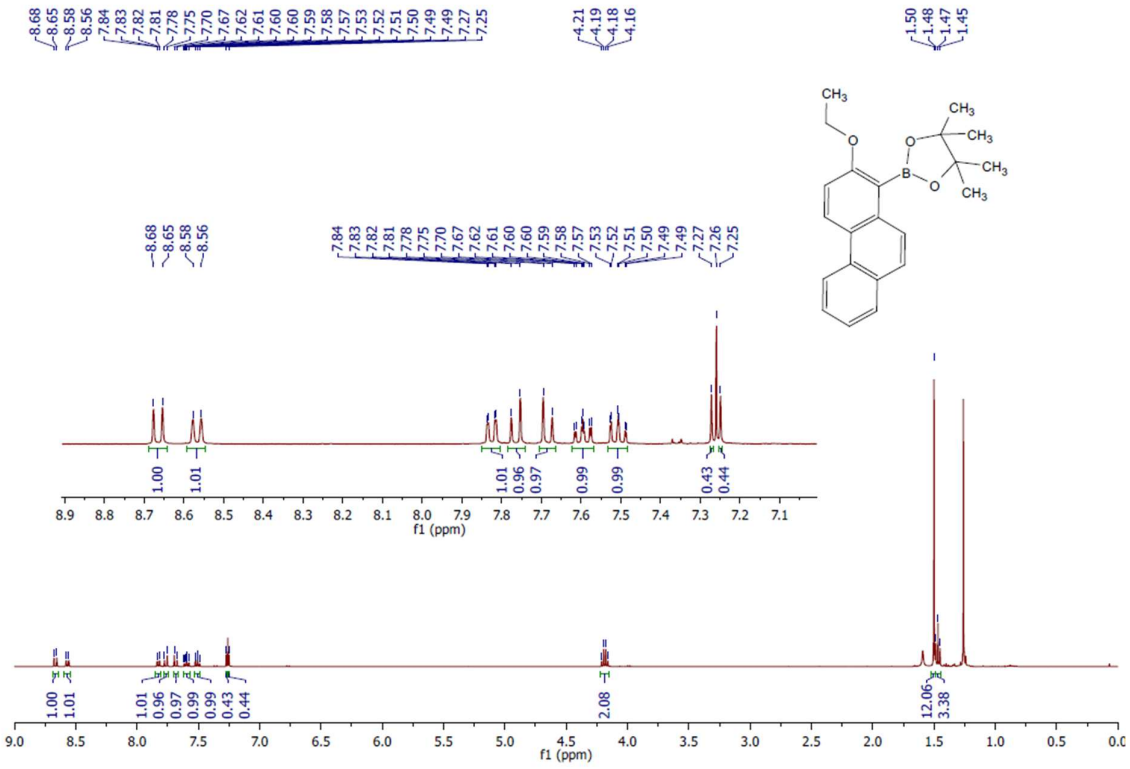

Fig. S1. ^{1}H NMR spectrum of **5** (in $CDCl_3$, 400 MHz, 298 K).

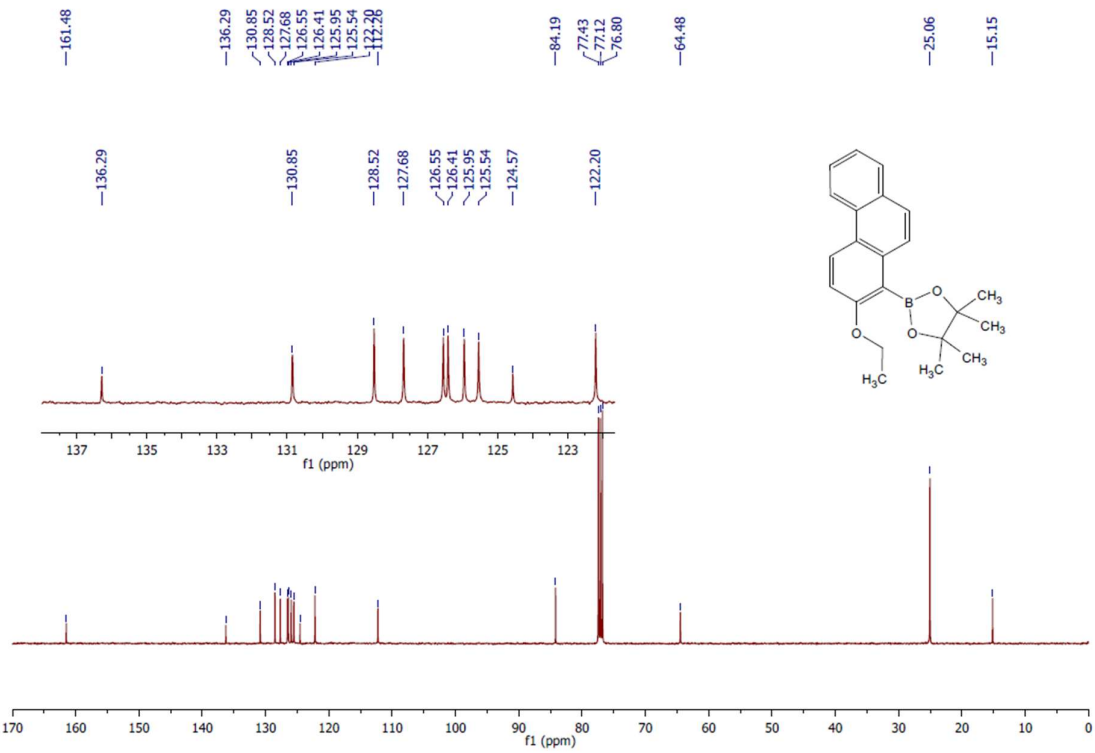

Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum of **5** (in $CDCl_3$, 400 MHz, 298 K).

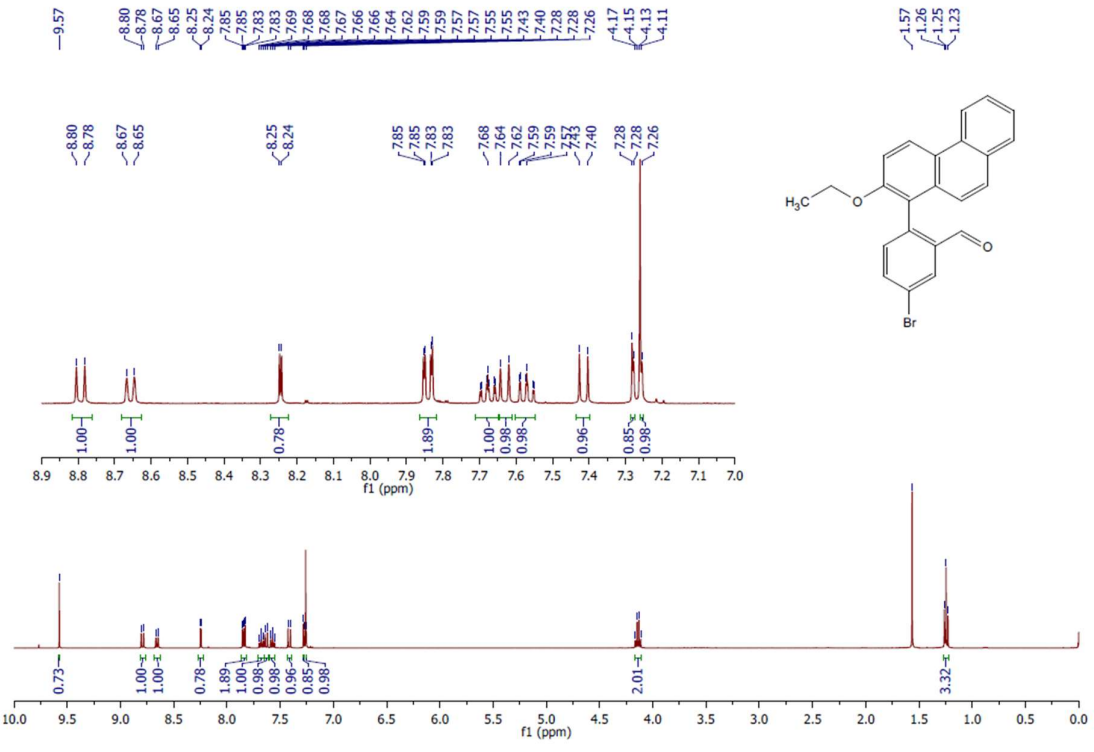

Fig. S3. ^{1}H NMR spectrum of **7** (in $CDCl_3$, 400 MHz, 298 K).

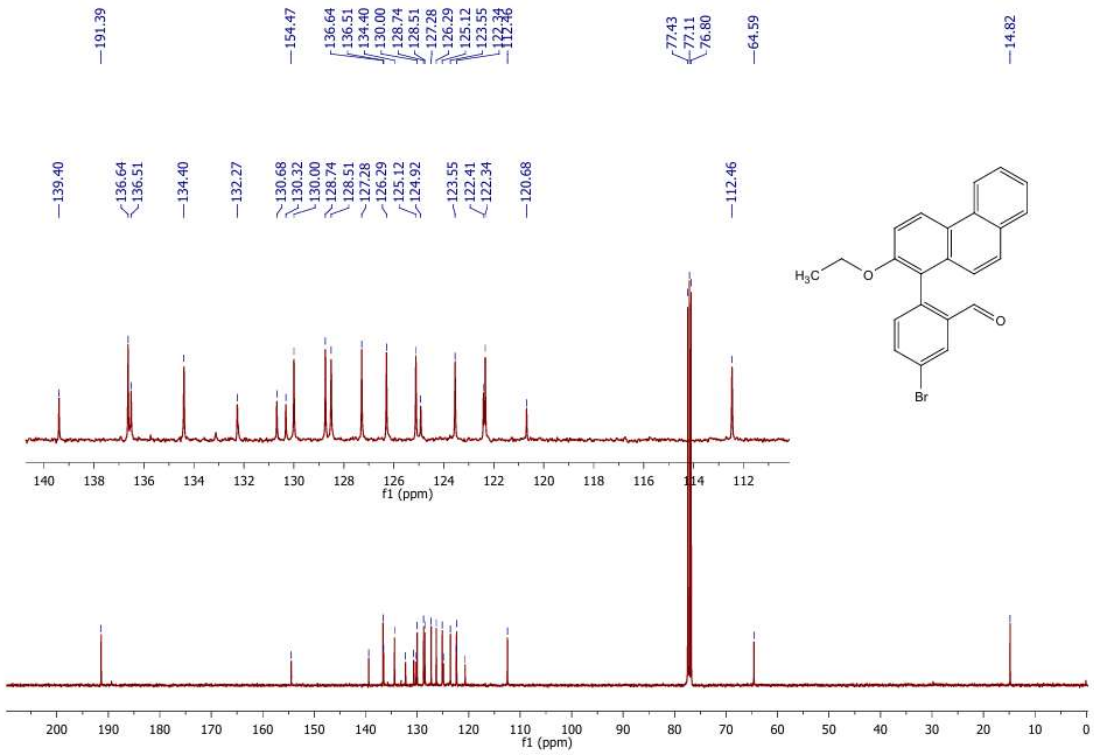

Fig. S4. $^{13}C\{^{1}H\}$ NMR spectrum of **7** (in $CDCl_3$, 400 MHz, 298 K).

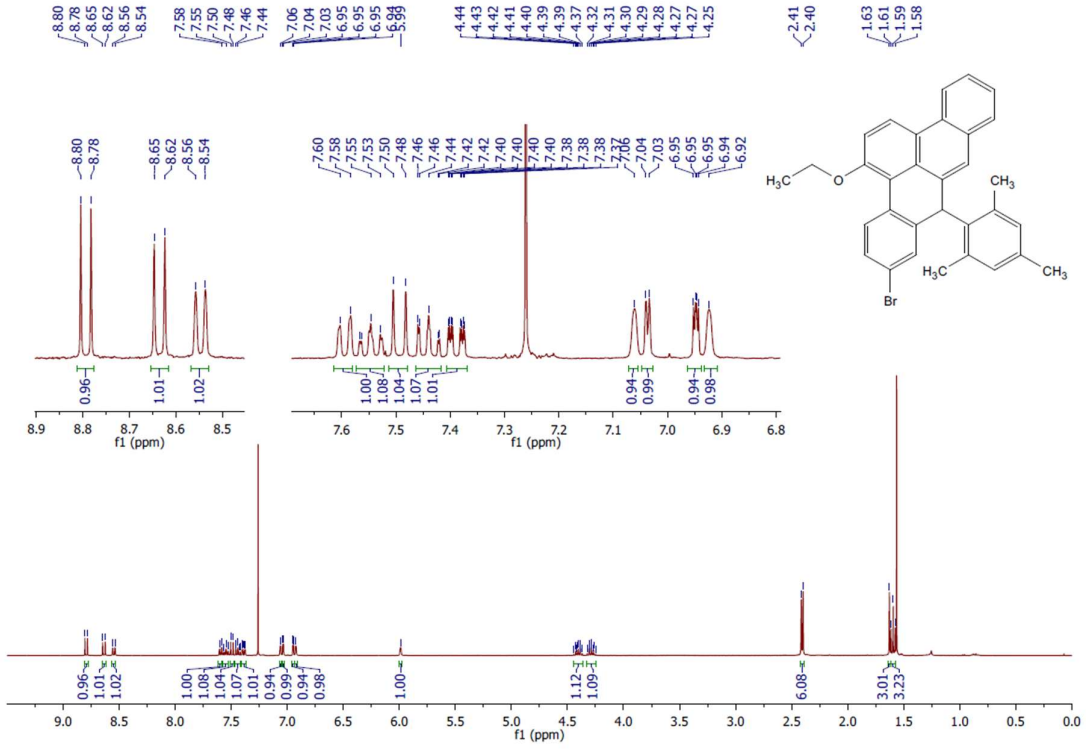

Fig. S5. ^{1}H NMR spectrum of **9** (in $CDCl_3$, 400 MHz, 298 K).

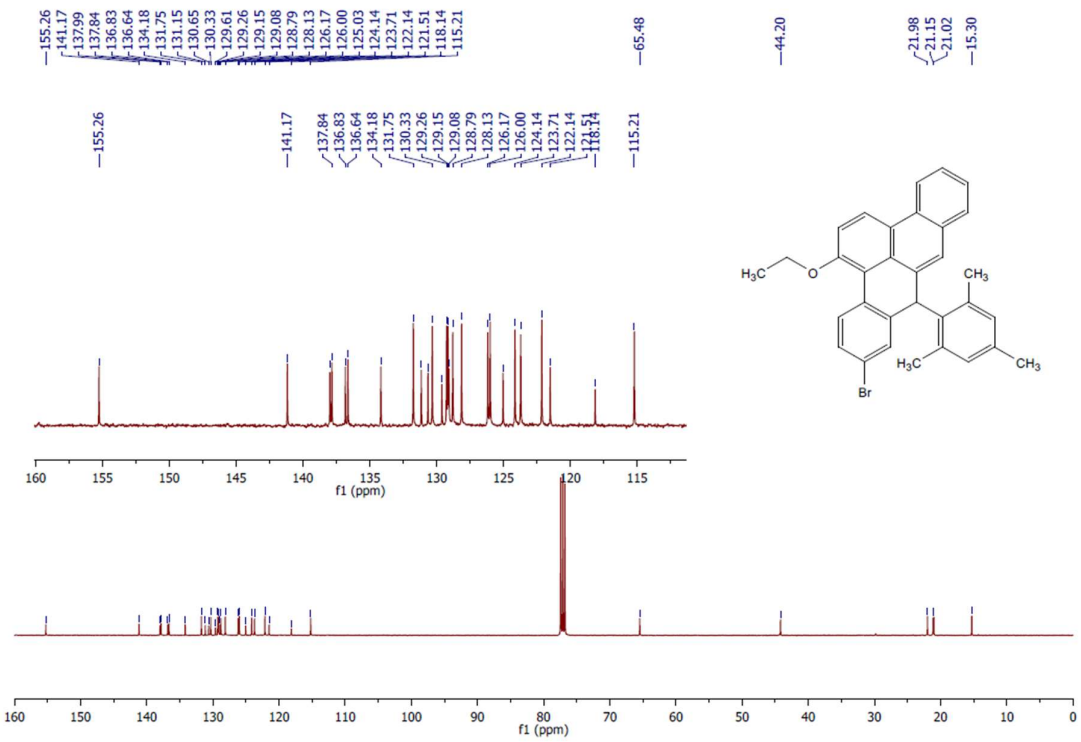

Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of **9** (in $CDCl_3$, 400 MHz, 298 K).

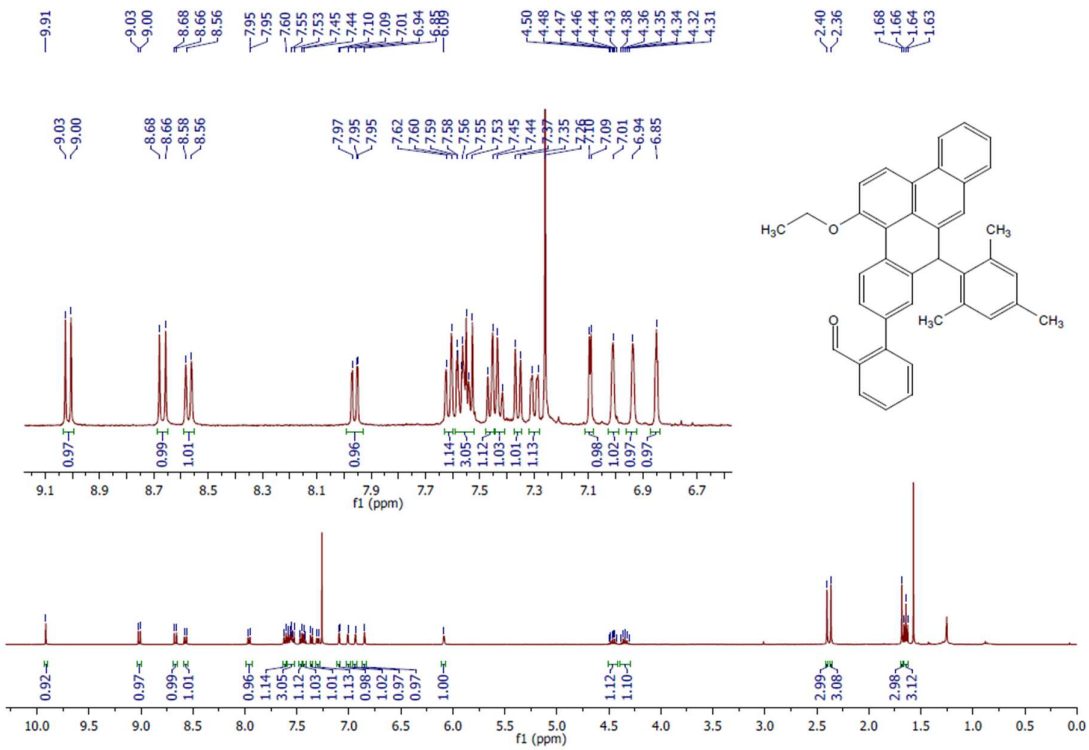

Fig. S7. ^{1}H NMR spectrum of **11** (in $CDCl_3$, 400 MHz, 298 K).

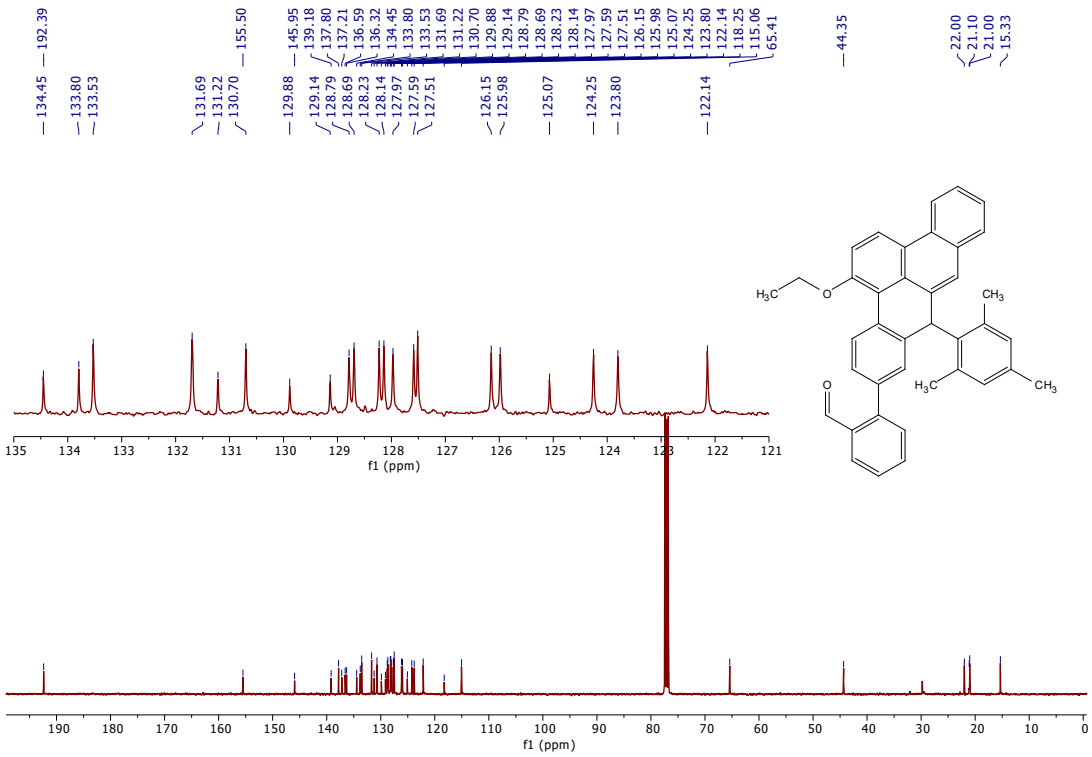

Fig. S8. $^{13}C\{^{1}H\}$ NMR spectrum of **11** (in $CDCl_3$, 400 MHz, 298 K).

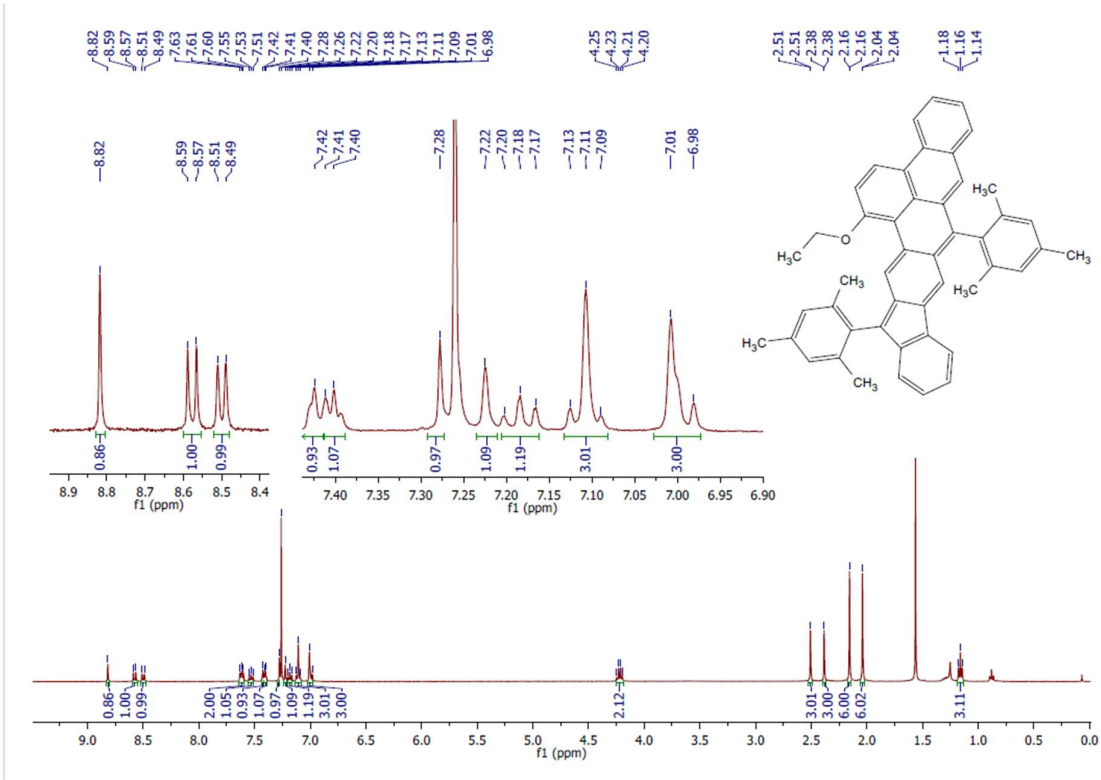

Fig. S9. ^{1}H NMR spectrum of **1** (in $CDCl_3$, 400 MHz, 298 K).

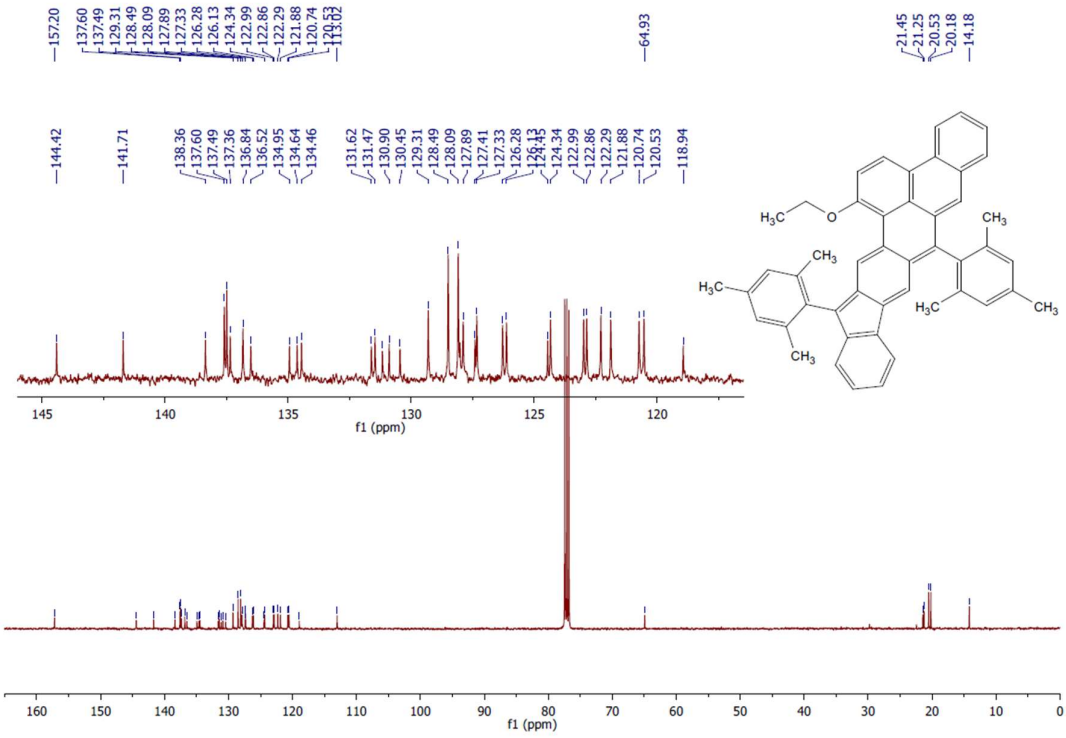

Fig. S10. $^{13}C\{^{1}H\}$ NMR spectrum of **1** (in $CDCl_3$, 400 MHz, 298 K).

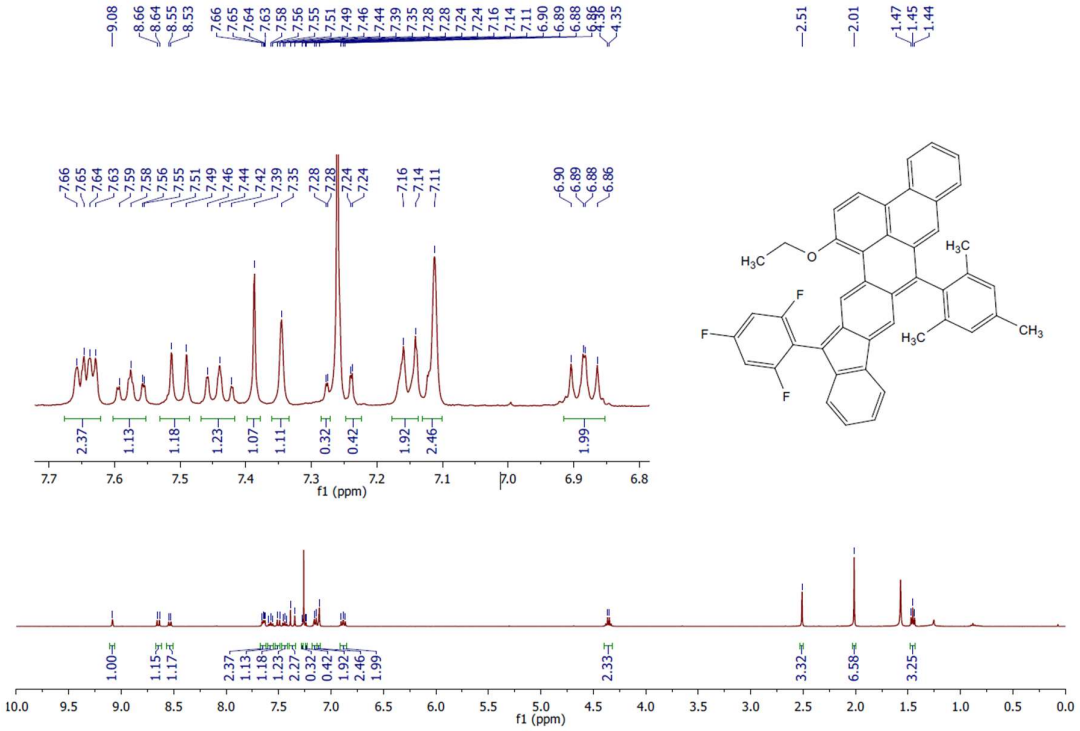

Fig. S11. ^{1}H NMR spectrum of **2** (in $CDCl_3$, 400 MHz, 298 K).

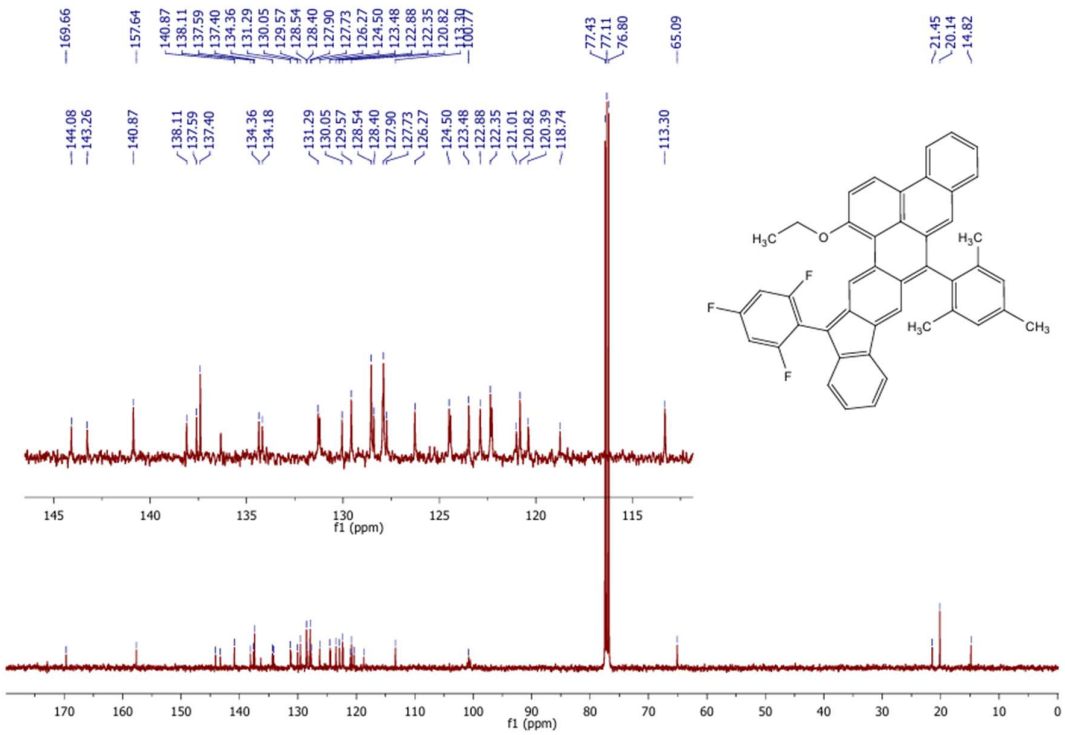

Fig. S12. $^{13}C\{^{1}H\}$ NMR spectrum of **2** (in $CDCl_3$, 400 MHz, 298 K).

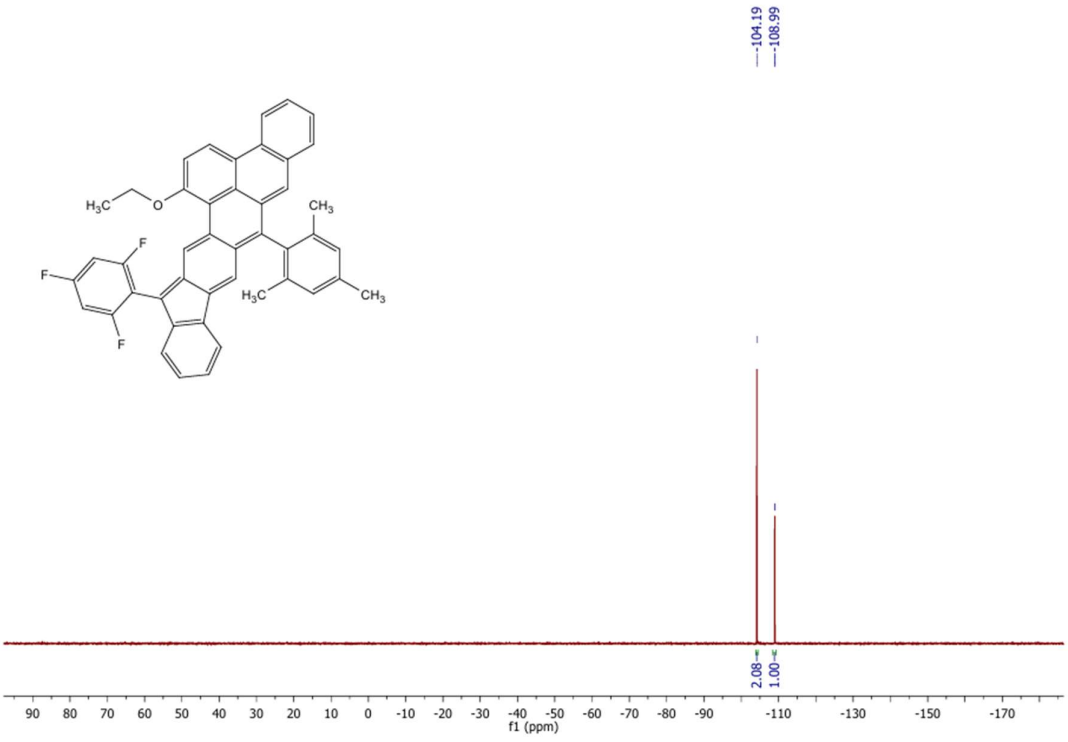

Fig. S13. ^{19}F NMR spectrum of **2** (in $CDCl_3$, 400 MHz, 298 K).

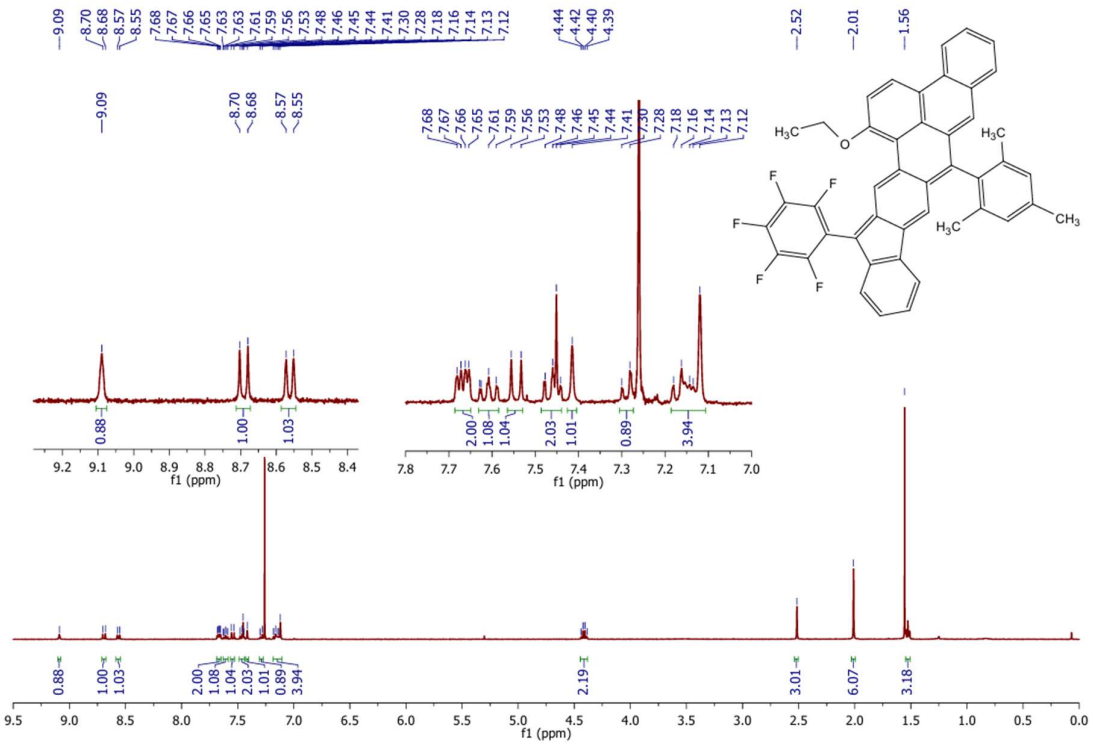

Fig. S14. ^{1}H NMR spectrum of **3** (in $CDCl_3$, 400 MHz, 298 K).

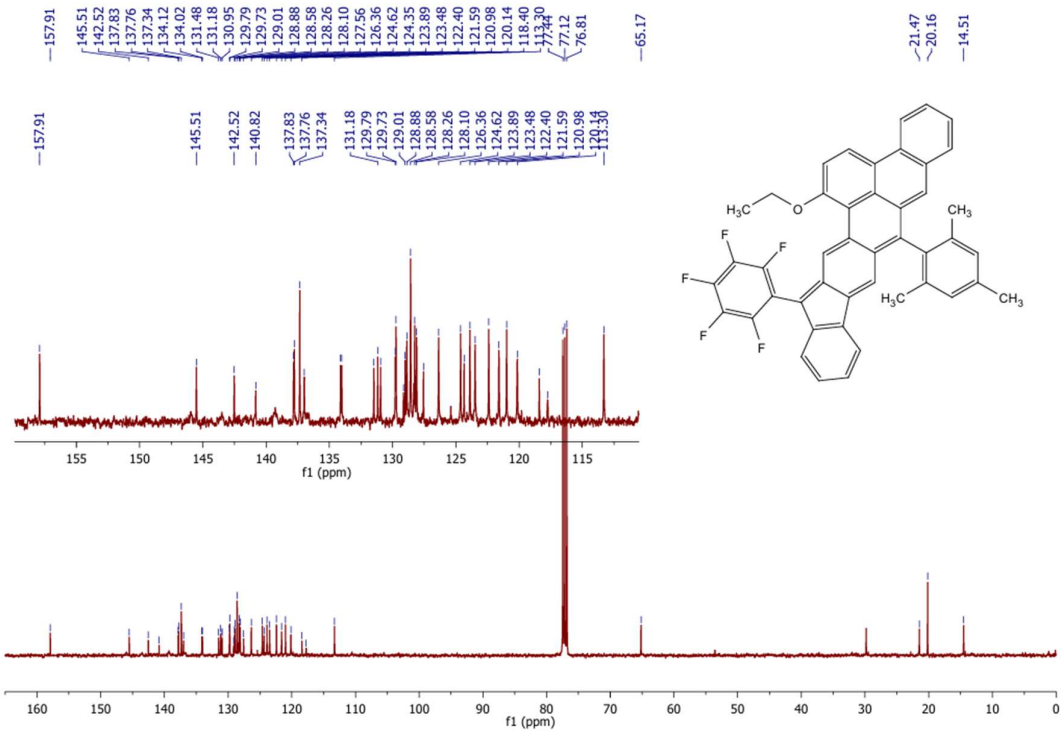

Fig. S15. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (in $CDCl_3$, 400 MHz, 298 K)

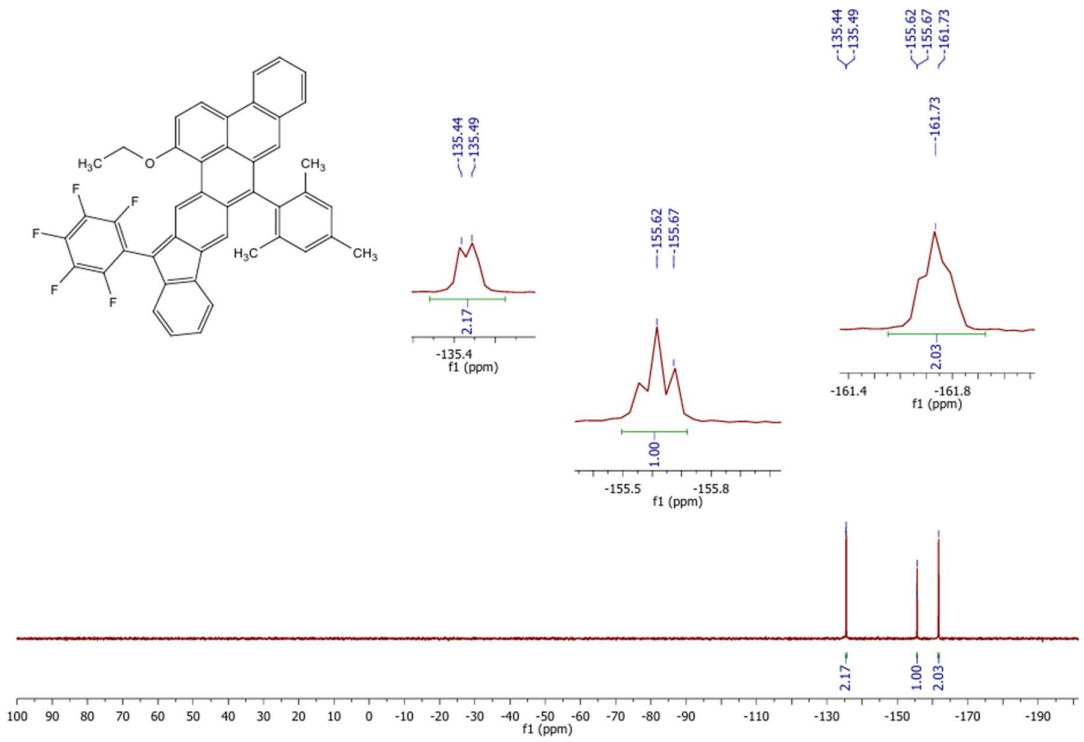

Fig. S16. ^{19}F NMR spectrum of **3** (in $CDCl_3$, 400 MHz, 298 K)

2. X-ray crystallographic analysis

A suitable single crystal of **1** was selected using paratone oil and mounted on glass fiber with the help of gum. The intensity data and geometric parameters of these crystals were garnered with the help of Bruker D8 Venture X-ray diffractometer having a micro-focus sealed X-ray tube Mo-Kα (λ = 0.71073 Å) source of X-rays along with a PHOTON 100 detector with inclining Phi and Omega (width of 0.5 for one frame) working at a scan speed of 10 s per frame. The crystal was kept at 298 K during data collection. Data acquisition and extraction were accomplished by utilizing Bruker Apex-3 and Bruker SAINT software packages using a narrow-frame algorithm.[2] By utilizing OLex2,[3] the crystal structure was solved with the help of olex2.solve[4] structure solution program by employing intrinsic Phasing methods and crystal structure refinement was done with the SHELXL[5] refinement package by putting into use Least Squares minimization. Refinement of all non-hydrogen atoms was completed with the help of anisotropic thermal parameters.

Table S1. X-ray crystallographic information of **1.**

CCDC number	2538833
Empirical formula	$C_{48}H_{40}O$
Formula weight	632.80
Temperature [K]	298
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	9.0236(14)
b [Å]	16.688(3)
c [Å]	26.510(5)
α [°]	96.376(8)
β [°]	93.001(5)
γ [°]	98.414(5)
Volume [Å^3]	3915.1(12)
Z	4
ρ_{calc} [gcm^{-3}]	1.074
μ [mm^{-1}]	0.062
F(000)	1344.0
Crystal size [mm^3]	0.056×0.123×0.325
Crystal colour	metallic brownish brown
Crystal shape	plate
Radiation	MoK_α (λ=0.71073 Å)
2θ range [°]	3.73 to 51.75 (0.81 Å)
Index ranges	$-10 \le h \le 11$, $-20 \le k \le 20$, $-32 \le l \le 32$
Reflections collected	23803
Independent reflections	15178, R_{int} = 0.0538, R_{sigma} = 0.1075
Data/Restraints/Parameters	14461 / 0 / 897
Absorption correction T_{min}/T_{max} (method)	0.9910 / 0.9970 (multi-scan)
Goodness-of-fit on F^2	1.026
Final *R* indexes [$I \ge 2\sigma(I)$]	R_1 = 0.0905 wR_2 = 0.2061
Final *R* indexes [all data]	R_1 = 0.1624 wR_2 = 0.2396
Largest peak/hole [eÅ^{-3}]	0.29/−0.25

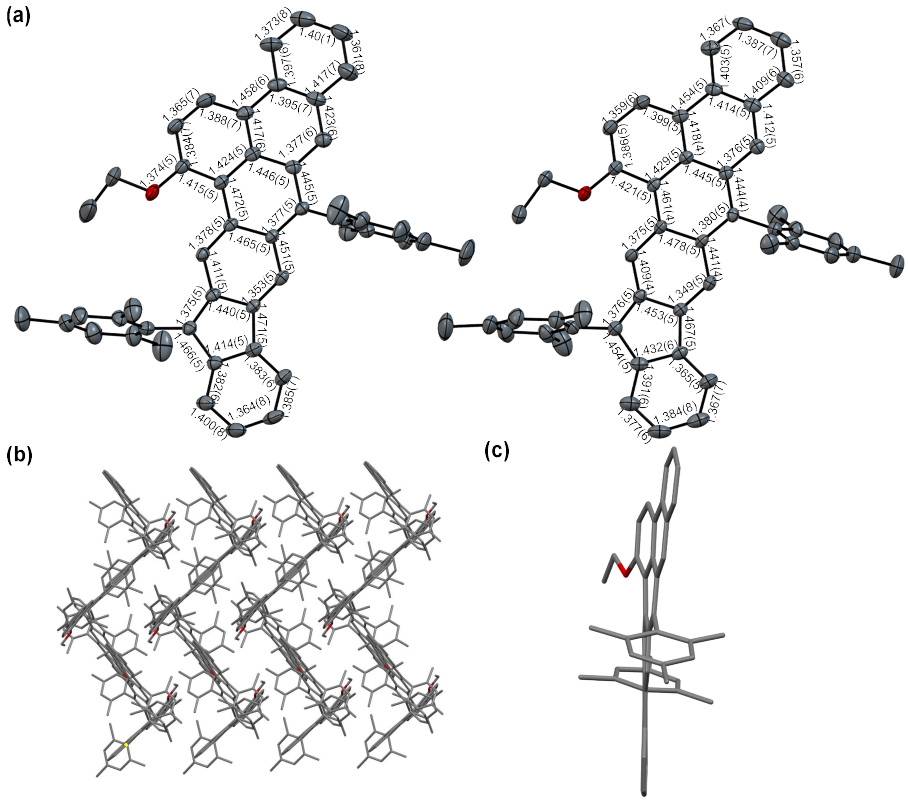

Fig. S17. (a) ORTEP drawing with thermal ellipsoids at 30% probability level, showing the core bond lengths with e.s.d values for **1**; (b) Packing of **1**; (c) Side view of **1.**

3. DFT calculations:

Density functional theory (DFT) calculations, in the gas phase, were performed with Gaussian 09 package using a high-performance computing cluster facility of IIT Ropar at the B3LYP level of theory with basis set 6-31G(d,p).[6] Optimization of the molecular geometries for **1**, taken from x-ray crystallographic data, and **1** was done by restricted B3LYP, and unrestricted B3LYP wavefunctions using broken symmetry formalism.[7] $NICS(1)_{zz}$[8] (standard GIAO method), and Natural Population Analysis (NPA) were calculated for the optimized closed-shell structure of **1**, **2** and **3** using the more reliable BHandHLYP[9] functional and 6-31G(d,p) basis set in a SMD solvation model. The reported $NICS(1)_{zz}$ indices are the average of two positions (1 Å above and below the plane) for **1**, **2** and **3**. The excitation energies of **1**, **2**, and **3** were computed using time-dependent density functional theory (TDDFT) for the closed-shell optimized structure in the gas phase. Molecular orbital contributions of **1, 2,** and **3** were determined using GaussSum 3.0 package.[10] Anisotropy of the induced current density (ACID) plots were generated at BHandHLYP/6-31G(d,p) in the SMD solvation model (in DMF) following Herges's protocol.[11]

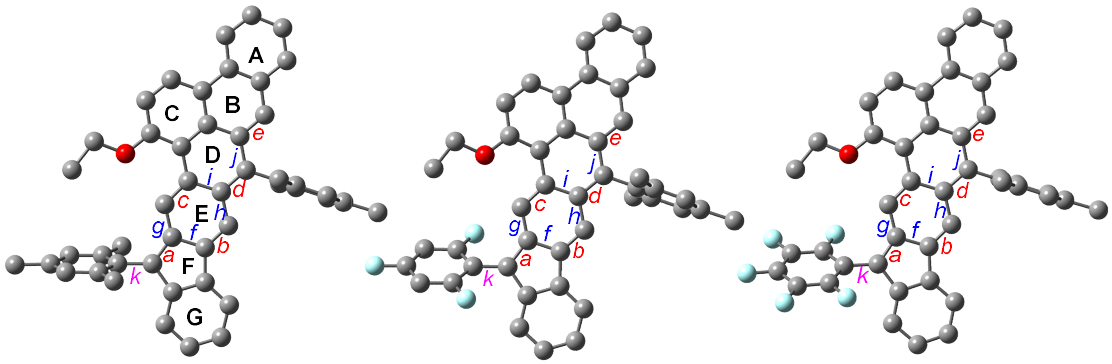

Table S2. Comparison of C-C bond lengths (Å) for the quinoidal core of **1**, **2** & **3** using DFT optimised files at the BHandHLYP level of theory with 6-31G(d,p) basis set in a SMD solvation model in DMF.

Bonds	*a*	*b*	*c*	*d*	*e*	*f*	*g*	*h*	*i*	*j*	*k*
1	1.368	1.340	1.365	1.362	1.366	1.451	1.425	1.449	1.470	1.447	1.480
2	1.372	1.341	1.365	1.364	1.367	1.450	1.423	1.445	1.467	1.446	1.465
3	1.375	1.341	1.369	1.365	1.368	1.449	1.424	1.443	1.468	1.443	1.464

Table S3. Comparison of NICS(1)$_{zz}$ (ppm) for **1** in different solvents.

1	A	B	C	D	E	F	G
Gas phase	−27.40	−15.56	−24.63	5.53	0.05	0.43	−24.41
n-Hexane	−27.43	−15.66	−24.52	5.43	−0.25	−0.33	−24.65
DCM	−27.48	−15.83	−24.32	5.12	−0.95	−1.76	−25.05
DMF	−27.49	−15.85	−24.22	4.96	−1.25	−2.29	−25.17

Table S4. Comparison of NICS(1)$_{zz}$ (ppm) for **2** in different solvents.

2	A	B	C	D	E	F	G
Gas phase	−27.24	−15.35	−24.16	5.15	−0.76	0.65	−24.41
n-Hexane	−27.32	−15.53	−24.05	4.89	−1.27	−0.23	−24.73
DCM	−27.37	−15.74	−23.80	4.39	−2.28	−2.15	−25.19
DMF	−27.36	−15.75	−23.70	4.19	−2.67	−2.75	−25.32

Table S5. Comparison of NICS(1)$_{zz}$ (ppm) for **3** in different solvents.

3	A	B	C	D	E	F	G
Gas phase	−27.40	−15.86	−24.26	4.69	−1.54	−0.36	−24.77
n-Hexane	−27.50	−16.10	−24.21	4.34	−2.22	−1.38	−25.09
DCM	−27.52	−16.28	−23.93	3.75	−3.31	−3.18	−25.55
DMF	−27.46	−16.22	−23.77	3.58	-3.66	−3.79	−25.69

Table S6. Relative energies of **1** in closed- and open-shell states.

Compound **1**	**Electronic energy (Hartree)**	**Electronic energy (kcal mol^{-1})**
Singlet closed-shell	−1928.561632	−1210172.424
Singlet open-shell	−1928.561632	−1210172.424
Triplet open-shell	−1928.540278	−1210159.024

Compound 1: $\Delta E_{\text{Singlet- Triplet}} = -13.39$ kcal/mol

Table S7. Relative energies of **2** in closed- and open-shell states.

Compound **2**	**Electronic energy (Hartree)**	**Electronic energy (kcal mol^{-1})**
Singlet closed-shell	−2108.296224	−1322956.881
Singlet open-shell	−2108.296224	−1322955.881
Triplet open-shell	−2108.274834	−1322942.458

Compound 2: $\Delta E_{\text{Singlet- Triplet}} = -13.42$ kcal/mol

Table S8. Relative energies of **3** in closed- and open-shell states.

Compound **3**	**Electronic energy (Hartree)**	**Electronic energy (kcal mol^{-1})**
Singlet closed-shell	−2306.730124	−1447473.153
Singlet open-shell	−2306.730124	−1447473.153
Triplet open-shell	−2306.707754	−1447459.116

Compound 3: $\Delta E_{\text{Singlet- Triplet}} = -14.03$ kcal/mol

3.1 NPA Charges:

Compound 1.

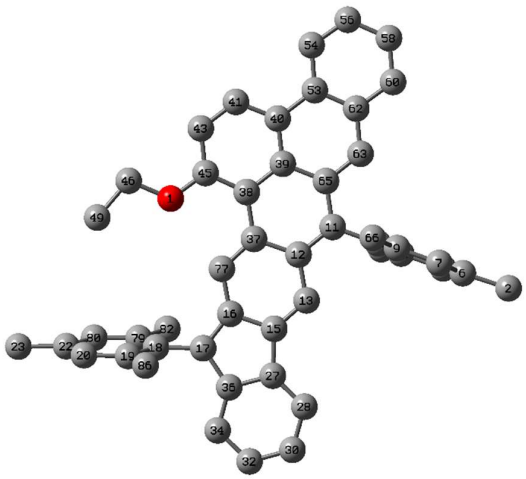

Table S9. Natural Population of **1** in DMF solvent.

Atom		Natural No Charge	Core	Valence	Rydberg	Total
O	1	-0.57294	1.99971	6.55936	0.01387	8.57294
C	2	-0.69985	1.99940	4.69184	0.00860	6.69985
H	3	0.25118	0.00000	0.74742	0.00140	0.74882
H	4	0.24612	0.00000	0.75258	0.00131	0.75388
H	5	0.24662	0.00000	0.75206	0.00132	0.75338
C	6	-0.01579	1.99902	4.00039	0.01637	6.01579
C	7	-0.25716	1.99896	4.24438	0.01381	6.25716
H	8	0.24704	0.00000	0.75142	0.00154	0.75296
C	9	0.00456	1.99895	3.98057	0.01591	5.99544
C	10	-0.09152	1.99891	4.07478	0.01783	6.09152
C	11	0.04818	1.99898	3.93295	0.01989	5.95182
C	12	-0.05474	1.99891	4.03987	0.01596	6.05474
C	13	-0.15900	1.99898	4.14621	0.01381	6.15900
H	14	0.26182	0.00000	0.73648	0.00170	0.73818
C	15	-0.04485	1.99902	4.02819	0.01764	6.04485
C	16	-0.04885	1.99895	4.03315	0.01675	6.04885
C	17	-0.03482	1.99896	4.01547	0.02039	6.03482
C	18	-0.07991	1.99890	4.06433	0.01668	6.07991
C	19	0.00370	1.99898	3.98165	0.01567	5.99630
C	20	-0.26148	1.99896	4.24875	0.01376	6.26148
H	21	0.24562	0.00000	0.75283	0.00155	0.75438
C	22	-0.01783	1.99902	4.00233	0.01648	6.01783
C	23	-0.69962	1.99940	4.69163	0.00859	6.69962
H	24	0.25062	0.00000	0.74796	0.00141	0.74938
H	25	0.24561	0.00000	0.75308	0.00131	0.75439
H	26	0.24622	0.00000	0.75245	0.00133	0.75378
C	27	-0.06233	1.99899	4.04683	0.01652	6.06233
C	28	-0.21886	1.99903	4.20519	0.01463	6.21886
H	29	0.25502	0.00000	0.74359	0.00139	0.74498
C	30	-0.26777	1.99913	4.25243	0.01622	6.26777
H	31	0.25240	0.00000	0.74634	0.00126	0.74760
C	32	-0.24597	1.99912	4.23077	0.01607	6.24597
H	33	0.25273	0.00000	0.74601	0.00127	0.74727
C	34	-0.24853	1.99903	4.23444	0.01506	6.24853
H	35	0.25488	0.00000	0.74363	0.00150	0.74512
C	36	-0.04090	1.99899	4.02537	0.01654	6.04090
C	37	-0.04102	1.99903	4.02453	0.01746	6.04102
C	38	-0.09381	1.99897	4.07866	0.01619	6.09381
C	39	-0.00463	1.99902	3.99076	0.01485	6.00463
C	40	-0.06698	1.99902	4.05229	0.01566	6.06698
C	41	-0.18557	1.99908	4.17138	0.01511	6.18557
H	42	0.25622	0.00000	0.74226	0.00153	0.74378
C	43	-0.31792	1.99905	4.30447	0.01441	6.31792
H	44	0.26577	0.00000	0.73269	0.00154	0.73423

C	45	0.38739	1.99882	3.59077	0.02302	5.61261
C	46	-0.09668	1.99927	4.08115	0.01627	6.09668
H	47	0.22322	0.00000	0.77430	0.00248	0.77678
H	48	0.22342	0.00000	0.77407	0.00250	0.77658
C	49	-0.70579	1.99946	4.69727	0.00906	6.70579
H	50	0.24004	0.00000	0.75809	0.00187	0.75996
H	51	0.23919	0.00000	0.75886	0.00194	0.76081
H	52	0.24854	0.00000	0.75032	0.00115	0.75146
C	53	-0.02410	1.99901	4.00956	0.01553	6.02410
C	54	-0.23153	1.99908	4.21805	0.01440	6.23153
H	55	0.25277	0.00000	0.74572	0.00150	0.74723
C	56	-0.23307	1.99911	4.21770	0.01625	6.23307
H	57	0.25683	0.00000	0.74190	0.00127	0.74317
C	58	-0.25293	1.99910	4.23768	0.01615	6.25293
H	59	0.25723	0.00000	0.74151	0.00126	0.74277
C	60	-0.21156	1.99907	4.19726	0.01523	6.21156
H	61	0.25609	0.00000	0.74245	0.00147	0.74391
C	62	-0.07712	1.99902	4.06200	0.01610	6.07712
C	63	-0.16615	1.99905	4.15308	0.01401	6.16615
H	64	0.26094	0.00000	0.73728	0.00178	0.73906
C	65	-0.06207	1.99898	4.04680	0.01630	6.06207
C	66	-0.70167	1.99940	4.69398	0.00829	6.70167
H	67	0.25125	0.00000	0.74729	0.00147	0.74875
H	68	0.25009	0.00000	0.74841	0.00150	0.74991
H	69	0.24655	0.00000	0.75221	0.00124	0.75345
C	70	-0.25734	1.99896	4.24456	0.01382	6.25734
H	71	0.24713	0.00000	0.75133	0.00154	0.75287
C	72	0.00415	1.99895	3.98098	0.01592	5.99585
C	73	-0.70146	1.99940	4.69375	0.00831	6.70146
H	74	0.24656	0.00000	0.75220	0.00124	0.75344
H	75	0.24985	0.00000	0.74863	0.00152	0.75015
H	76	0.25124	0.00000	0.74728	0.00148	0.74876
C	77	-0.21660	1.99905	4.20276	0.01479	6.21660
H	78	0.27073	0.00000	0.72684	0.00243	0.72927
C	79	0.00328	1.99898	3.98200	0.01573	5.99672
C	80	-0.26292	1.99896	4.25019	0.01377	6.26292
H	81	0.24595	0.00000	0.75251	0.00155	0.75405
C	82	-0.69947	1.99940	4.69177	0.00830	6.69947
H	83	0.24913	0.00000	0.74946	0.00142	0.75087
H	84	0.25004	0.00000	0.74841	0.00156	0.74996
H	85	0.24393	0.00000	0.75480	0.00127	0.75607
C	86	-0.70066	1.99940	4.69302	0.00824	6.70066
H	87	0.24442	0.00000	0.75432	0.00126	0.75558
H	88	0.24999	0.00000	0.74858	0.00143	0.75001
H	89	0.24951	0.00000	0.74890	0.00158	0.75049
* Total *		0.00000	97.95495	237.25376	0.79129	336.00000

Compound 2.

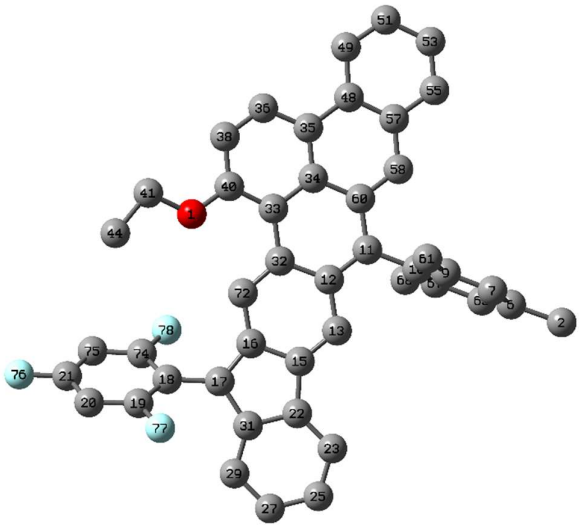

Table S10. Natural Population of **2** in DMF solvent

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
O	1	-0.57247	1.99971	6.55889	0.01387	8.57247
C	2	-0.69996	1.99940	4.69195	0.00861	6.69996
H	3	0.25137	0.00000	0.74724	0.00139	0.74863
H	4	0.24600	0.00000	0.75271	0.00130	0.75400
H	5	0.24714	0.00000	0.75154	0.00132	0.75286
C	6	-0.01485	1.99903	3.99945	0.01637	6.01485
C	7	-0.25668	1.99896	4.24391	0.01382	6.25668
H	8	0.24743	0.00000	0.75103	0.00154	0.75257
C	9	0.00533	1.99896	3.97982	0.01590	5.99467
C	10	-0.09410	1.99891	4.07745	0.01774	6.09410
C	11	0.06448	1.99898	3.91668	0.01986	5.93552
C	12	-0.06095	1.99891	4.04610	0.01594	6.06095
C	13	-0.15146	1.99899	4.13865	0.01383	6.15146
H	14	0.26345	0.00000	0.73487	0.00168	0.73655
C	15	-0.04884	1.99902	4.03231	0.01751	6.04884
C	16	-0.02658	1.99898	4.01082	0.01679	6.02658
C	17	-0.07033	1.99894	4.04969	0.02170	6.07033
C	18	-0.19942	1.99881	4.18383	0.01678	6.19942
C	19	0.48951	1.99842	3.48456	0.02752	5.51049
C	20	-0.39705	1.99887	4.38155	0.01662	6.39705
C	21	0.47047	1.99844	3.50281	0.02828	5.52953
C	22	-0.06347	1.99899	4.04803	0.01645	6.06347
C	23	-0.21886	1.99903	4.20518	0.01465	6.21886
H	24	0.25528	0.00000	0.74334	0.00139	0.74472
C	25	-0.26784	1.99912	4.25248	0.01623	6.26784
H	26	0.25258	0.00000	0.74617	0.00126	0.74742
C	27	-0.24562	1.99912	4.23048	0.01602	6.24562
H	28	0.25285	0.00000	0.74589	0.00127	0.74715

C	29	-0.24614	1.99903	4.23148	0.01562	6.24614
H	30	0.25349	0.00000	0.74486	0.00165	0.74651
C	31	-0.03636	1.99901	4.02079	0.01656	6.03636
C	32	-0.02977	1.99903	4.01335	0.01739	6.02977
C	33	-0.09491	1.99897	4.07974	0.01620	6.09491
C	34	-0.00340	1.99902	3.98951	0.01486	6.00340
C	35	-0.06763	1.99902	4.05294	0.01567	6.06763
C	36	-0.18206	1.99908	4.16789	0.01508	6.18206
H	37	0.25700	0.00000	0.74148	0.00152	0.74300
C	38	-0.31826	1.99905	4.30478	0.01444	6.31826
H	39	0.26648	0.00000	0.73199	0.00153	0.73352
C	40	0.39070	1.99881	3.58743	0.02306	5.60930
C	41	-0.09665	1.99927	4.08113	0.01625	6.09665
H	42	0.22336	0.00000	0.77419	0.00245	0.77664
H	43	0.22396	0.00000	0.77353	0.00250	0.77604
C	44	-0.70493	1.99946	4.69650	0.00897	6.70493
H	45	0.24005	0.00000	0.75814	0.00181	0.75995
H	46	0.23813	0.00000	0.76001	0.00186	0.76187
H	47	0.24864	0.00000	0.75021	0.00115	0.75136
C	48	-0.02017	1.99901	4.00563	0.01554	6.02017
C	49	-0.23215	1.99908	4.21865	0.01442	6.23215
H	50	0.25347	0.00000	0.74503	0.00150	0.74653
C	51	-0.22931	1.99911	4.21396	0.01623	6.22931
H	52	0.25745	0.00000	0.74128	0.00127	0.74255
C	53	-0.25318	1.99910	4.23793	0.01615	6.25318
H	54	0.25786	0.00000	0.74089	0.00126	0.74214
C	55	-0.20873	1.99907	4.19443	0.01523	6.20873
H	56	0.25685	0.00000	0.74169	0.00146	0.74315
C	57	-0.07954	1.99902	4.06444	0.01608	6.07954
C	58	-0.15410	1.99905	4.14106	0.01400	6.15410
H	59	0.26244	0.00000	0.73579	0.00177	0.73756
C	60	-0.06683	1.99897	4.05160	0.01626	6.06683
C	61	-0.70214	1.99940	4.69444	0.00830	6.70214
H	62	0.25156	0.00000	0.74698	0.00146	0.74844
H	63	0.25040	0.00000	0.74811	0.00149	0.74960
H	64	0.24703	0.00000	0.75173	0.00124	0.75297
C	65	-0.25719	1.99896	4.24441	0.01382	6.25719
H	66	0.24761	0.00000	0.75086	0.00153	0.75239
C	67	0.00484	1.99895	3.98029	0.01591	5.99516
C	68	-0.70186	1.99940	4.69414	0.00832	6.70186
H	69	0.24705	0.00000	0.75171	0.00124	0.75295
H	70	0.25003	0.00000	0.74846	0.00151	0.74997
H	71	0.25170	0.00000	0.74682	0.00148	0.74830
C	72	-0.22075	1.99904	4.20630	0.01540	6.22075
H	73	0.26858	0.00000	0.72876	0.00266	0.73142
C	74	0.48955	1.99842	3.48433	0.02770	5.51045
C	75	-0.39978	1.99887	4.38418	0.01672	6.39978
F	76	-0.35706	1.99993	7.35070	0.00643	9.35706
F	77	-0.35699	1.99993	7.35064	0.00642	9.35699
F	78	-0.35649	1.99993	7.35012	0.00644	9.35649

H	79	0.29018	0.00000	0.70817	0.00165	0.70982
H	80	0.29056	0.00000	0.70779	0.00165	0.70944
* Total *		0.00000	97.95460	237.22865	0.81675	336.00000

Compound 3.

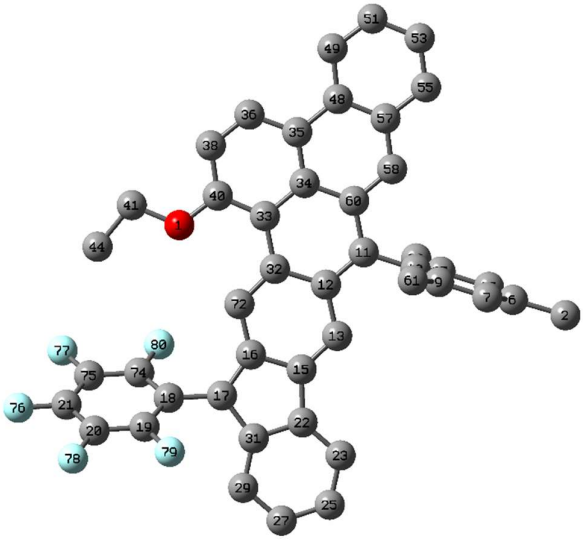

Table S11. Natural Population of **3** in DMF solvent

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
O	1	-0.57101	1.99971	6.55743	0.01388	8.57101
C	2	-0.69999	1.99940	4.69197	0.00862	6.69999
H	3	0.25153	0.00000	0.74708	0.00139	0.74847
H	4	0.24689	0.00000	0.75179	0.00132	0.75311
H	5	0.24640	0.00000	0.75230	0.00131	0.75360
C	6	-0.01447	1.99903	3.99908	0.01637	6.01447
C	7	-0.25666	1.99896	4.24386	0.01383	6.25666
H	8	0.24786	0.00000	0.75061	0.00153	0.75214
C	9	0.00534	1.99895	3.97978	0.01592	5.99466
C	10	-0.09630	1.99891	4.07965	0.01774	6.09630
C	11	0.07585	1.99899	3.90530	0.01986	5.92415
C	12	-0.06557	1.99891	4.05075	0.01590	6.06557
C	13	-0.14629	1.99899	4.13347	0.01384	6.14629
H	14	0.26413	0.00000	0.73416	0.00171	0.73587
C	15	-0.05145	1.99902	4.03494	0.01750	6.05145
C	16	-0.01604	1.99899	4.00017	0.01688	6.01604
C	17	-0.08991	1.99894	4.06944	0.02153	6.08991
C	18	-0.15729	1.99887	4.14168	0.01675	6.15729
C	19	0.40619	1.99837	3.56798	0.02746	5.59381
C	20	0.32215	1.99833	3.65126	0.02826	5.67785
C	21	0.34238	1.99837	3.63098	0.02827	5.65762
C	22	-0.06432	1.99899	4.04885	0.01648	6.06432
C	23	-0.21804	1.99903	4.20437	0.01464	6.21804

H	24	0.25558	0.00000	0.74303	0.00139	0.74442
C	25	-0.26821	1.99912	4.25286	0.01623	6.26821
H	26	0.25285	0.00000	0.74590	0.00125	0.74715
C	27	-0.24465	1.99912	4.22948	0.01605	6.24465
H	28	0.25320	0.00000	0.74553	0.00127	0.74680
C	29	-0.24782	1.99903	4.23319	0.01560	6.24782
H	30	0.25346	0.00000	0.74491	0.00163	0.74654
C	31	-0.03539	1.99901	4.01989	0.01650	6.03539
C	32	-0.02384	1.99904	4.00738	0.01741	6.02384
C	33	-0.09753	1.99897	4.08241	0.01616	6.09753
C	34	-0.00233	1.99902	3.98842	0.01488	6.00233
C	35	-0.06821	1.99902	4.05355	0.01564	6.06821
C	36	-0.17824	1.99908	4.16402	0.01513	6.17824
H	37	0.25748	0.00000	0.74099	0.00153	0.74252
C	38	-0.31924	1.99905	4.30580	0.01440	6.31924
H	39	0.26700	0.00000	0.73144	0.00156	0.73300
C	40	0.39490	1.99882	3.58319	0.02310	5.60510
C	41	-0.09707	1.99926	4.08146	0.01635	6.09707
H	42	0.22448	0.00000	0.77303	0.00249	0.77552
H	43	0.22397	0.00000	0.77357	0.00246	0.77603
C	44	-0.70578	1.99945	4.69628	0.01004	6.70578
H	45	0.23755	0.00000	0.76066	0.00178	0.76245
H	46	0.23820	0.00000	0.75852	0.00328	0.76180
H	47	0.24904	0.00000	0.74979	0.00117	0.75096
C	48	-0.01723	1.99901	4.00268	0.01554	6.01723
C	49	-0.23255	1.99908	4.21905	0.01442	6.23255
H	50	0.25386	0.00000	0.74464	0.00150	0.74614
C	51	-0.22665	1.99912	4.21131	0.01622	6.22665
H	52	0.25796	0.00000	0.74077	0.00127	0.74204
C	53	-0.25308	1.99909	4.23783	0.01616	6.25308
H	54	0.25834	0.00000	0.74041	0.00125	0.74166
C	55	-0.20659	1.99907	4.19228	0.01523	6.20659
H	56	0.25744	0.00000	0.74110	0.00146	0.74256
C	57	-0.08128	1.99902	4.06619	0.01608	6.08128
C	58	-0.14559	1.99905	4.13255	0.01399	6.14559
H	59	0.26355	0.00000	0.73466	0.00179	0.73645
C	60	-0.07050	1.99897	4.05530	0.01623	6.07050
C	61	-0.70213	1.99940	4.69440	0.00833	6.70213
H	62	0.25171	0.00000	0.74682	0.00147	0.74829
H	63	0.25030	0.00000	0.74820	0.00150	0.74970
H	64	0.24741	0.00000	0.75136	0.00123	0.75259
C	65	-0.25635	1.99896	4.24357	0.01382	6.25635
H	66	0.24777	0.00000	0.75069	0.00153	0.75223
C	67	0.00567	1.99895	3.97946	0.01591	5.99433
C	68	-0.70236	1.99940	4.69465	0.00831	6.70236
H	69	0.24743	0.00000	0.75134	0.00124	0.75257
H	70	0.25045	0.00000	0.74805	0.00149	0.74955
H	71	0.25180	0.00000	0.74674	0.00146	0.74820
C	72	-0.22934	1.99905	4.21498	0.01531	6.22934
H	73	0.27066	0.00000	0.72668	0.00266	0.72934

C	74	0.40856	1.99835	3.56575	0.02734	5.59144
C	75	0.32074	1.99833	3.65256	0.02838	5.67926
F	76	-0.33502	1.99993	7.32730	0.00778	9.33502
F	77	-0.33886	1.99993	7.33121	0.00772	9.33886
F	78	-0.33909	1.99993	7.33147	0.00768	9.33909
F	79	-0.34445	1.99993	7.33740	0.00712	9.34445
F	80	-0.34336	1.99993	7.33628	0.00714	9.34336
* Total *		0.00000	101.95326	249.18990	0.85684	352.00000

3.2 TDDFT calculations *in vacuo*.

Optimized closed-shell structure of 1

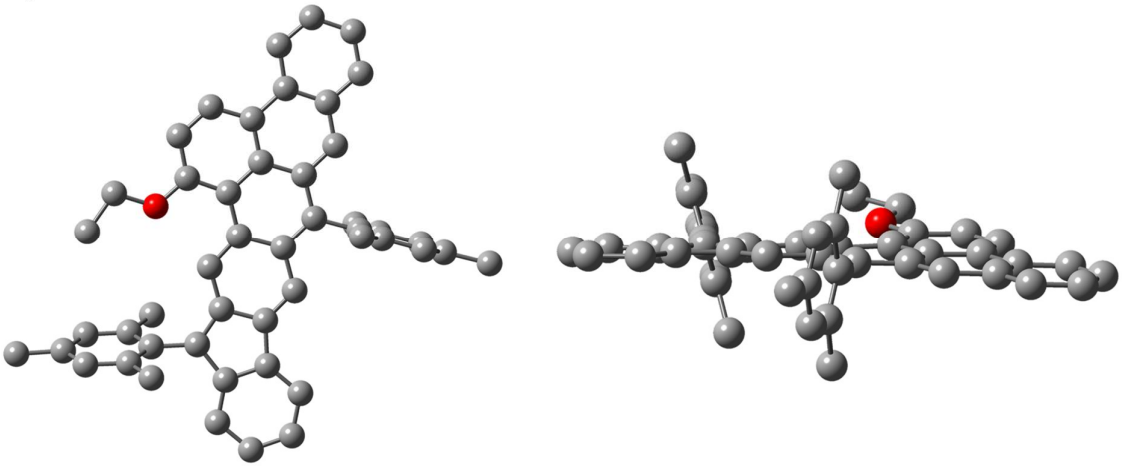

Fig. S18. Optimized structure of **1** top-view (left) and side-view (right).

Table S12. Summary of TTDFT calculation for **1**

Wavelength (nm)	**Oscillator Strength (*f*)**	**Major contribution**
651	0.4517	HOMO->LUMO (89%)
462	0.3058	H-1->LUMO (76%)
435	0.083	H-2->LUMO (47%), HOMO->L+1 (38%)
423	0.1568	H-2->LUMO (35%), HOMO->L+1 (44%), HOMO->L+2 (13%)
401	0.0385	H-3->LUMO (83%)
390	0.0074	H-6->LUMO (35%), H-4->LUMO (38%), HOMO->L+2 (15%)
388	0.0013	H-6->LUMO (62%), H-4->LUMO (26%)
377	0.0167	H-5->LUMO (82%)
370	0.1831	H-5->LUMO (14%), H-4->LUMO (14%), HOMO->L+2 (44%)
368	0.0099	H-7->LUMO (95%)
330	0.0092	HOMO->L+3 (74%)
320	0.001	HOMO->L+4 (98%)

317	0.0044	H-8->LUMO (74%), HOMO->L+5 (13%)
313	0.0313	HOMO->L+5 (19%), HOMO->L+6 (73%)
312	0.004	H-8->LUMO (12%), HOMO->L+5 (57%), HOMO->L+6 (13%)
302	0.1323	H-9->LUMO (53%), H-1->L+1 (22%)
301	0.0202	HOMO->L+7 (87%)
295	0.0214	HOMO->L+8 (92%)
293	0.1516	H-9->LUMO (18%), H-2->L+1 (14%), H-1->L+1 (32%), H-1->L+2 (10%)
291	0.0016	H-10->LUMO (68%), H-1->L+2 (21%)

Optimized closed-shell structure of 2

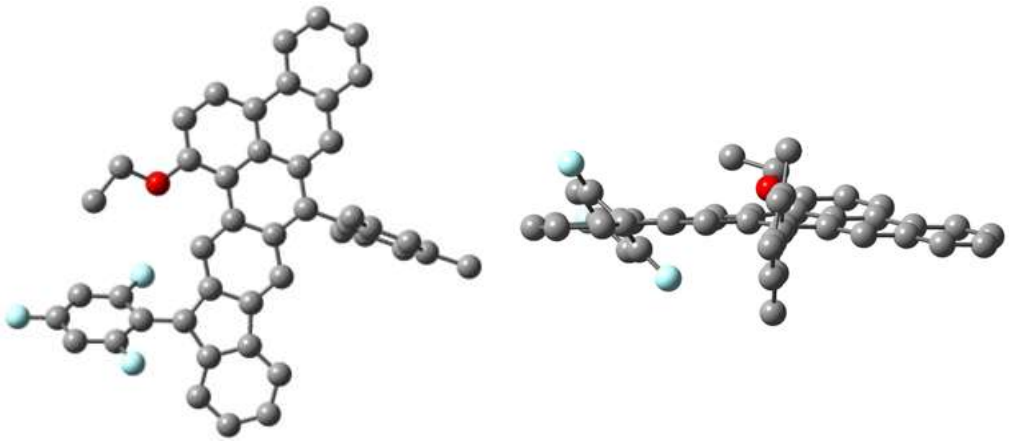

Fig. S19. Optimized structure of **2** top-view (left) and side-view (right).

Table S13. Summary of TTDFT calculation for **2**

Wavelength (nm)	**Oscillator Strength (*f*)**	**Major contribution**
671	0.4437	H-1->LUMO (10%), HOMO->LUMO (89%)
475	0.3835	H-1->LUMO (80%)
442	0.0286	H-2->LUMO (76%), HOMO->L+1 (13%)
421	0.1253	H-2->LUMO (10%), HOMO->L+1 (66%), HOMO->L+2 (13%)
401	0.0038	H-4->LUMO (85%), H-3->LUMO (10%)
398	0.0378	H-4->LUMO (14%), H-3->LUMO (56%), HOMO->L+1 (12%), HOMO->L+2 (13%)
378	0.0008	H-5->LUMO (99%)
372	0.207	H-3->LUMO (18%), HOMO->L+2 (63%)
348	0.0033	H-6->LUMO (66%), HOMO->L+3 (27%)
337	0.0837	H-8->LUMO (15%), H-6->LUMO (22%), HOMO->L+3 (49%)
334	0.0144	HOMO->L+4 (86%)
320	0.0735	H-8->LUMO (15%), HOMO->L+5 (67%)

318	0.0137	H-8->LUMO (16%), H-7->LUMO (63%)
317	0.018	H-8->LUMO (39%), H-7->LUMO (29%), HOMO->L+6 (11%)
315	0.0099	HOMO->L+6 (79%)
310	0.0095	HOMO->L+7 (86%)
302	0.1409	H-9->LUMO (59%), H-1->L+1 (28%)
297	0.0037	HOMO->L+8 (95%)
294	0.022	H-10->LUMO (73%), H-1->L+2 (16%)
291	0.1193	H-9->LUMO (19%), H-2->L+1 (17%), H-1->L+1 (23%), H-1->L+2 (13%)

Optimized closed-shell structure of 3

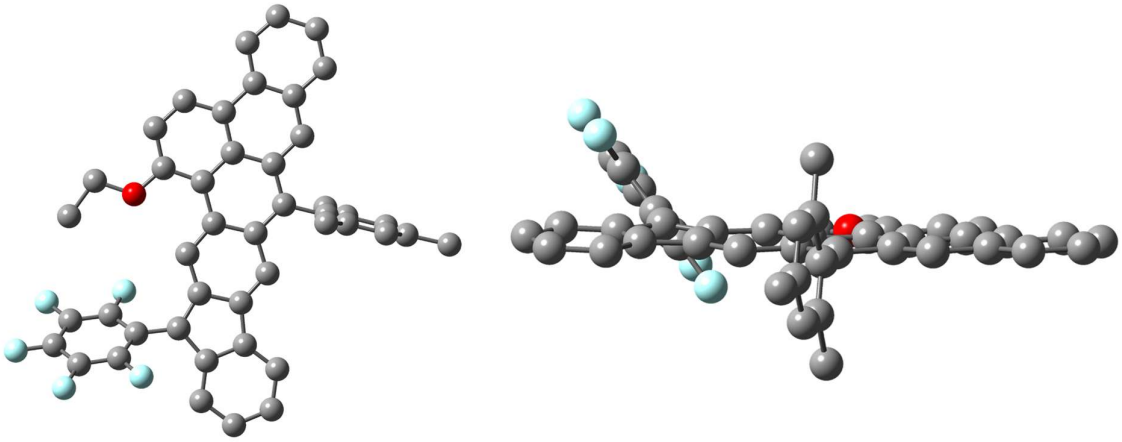

Fig. S20. Optimized structure of **3** top-view (left) and side-view (right).

Table S14. Summary of TTDFT calculation for **3**

Wavelength (nm)	**Oscillator Strength (*f*)**	**Major contribution**
671	0.4426	H-1->LUMO (10%), HOMO->LUMO (89%)
479	0.4059	H-1->LUMO (80%)
445	0.0235	H-2->LUMO (82%)
417	0.1026	H-3->LUMO (11%), HOMO->L+1 (69%), HOMO->L+2 (11%)
408	0.0001	H-4->LUMO (99%)
398	0.0693	H-3->LUMO (67%), HOMO->L+1 (17%)
385	0.0003	H-5->LUMO (100%)
369	0.1941	H-3->LUMO (12%), HOMO->L+2 (70%)
352	0.026	H-7->LUMO (15%), HOMO->L+3 (74%)
342	0.0041	H-6->LUMO (91%)
337	0.0862	H-8->LUMO (14%), H-7->LUMO (69%), HOMO->L+3 (11%)
323	0.0178	HOMO->L+4 (59%), HOMO->L+5 (25%)
322	0.0415	H-8->LUMO (26%), HOMO->L+5 (53%)

316	0.041	H-8->LUMO (47%), HOMO->L+4 (16%), HOMO->L+5 (12%)
312	0.0006	HOMO->L+6 (99%)
307	0.0051	H-10->LUMO (11%), HOMO->L+7 (82%)
302	0.1406	H-9->LUMO (58%), H-1->L+1 (30%)
296	0.0262	H-10->LUMO (72%)
293	0.0067	HOMO->L+8 (93%)
292	0.1176	H-9->LUMO (19%), H-2->L+1 (17%), H-1->L+1 (21%), H-1->L+2 (19%)

Cartesian coordinates (in Angstroms) for the optimized structures:

Singlet closed-shell structure of 1: Electronic energy = −1928.561632 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.733808 (Hartree/Particle)
Thermal correction to Energy = 0.777130
Thermal correction to Enthalpy = 0.778074
Thermal correction to Gibbs Free Energy = 0.654587
Sum of electronic and zero-point Energies = -1927.827824
Sum of electronic and thermal Energies = -1927.784502
Sum of electronic and thermal Enthalpies = -1927.783558
Sum of electronic and thermal Free Energies = -1927.907045

Atom	x	y	z
O	-1.17214000	-3.21235700	-0.37506100
C	5.17142000	5.68818900	-0.07641700
H	6.24997100	5.48813400	-0.04789000
H	4.93448800	6.31151700	0.79089900
H	4.97531800	6.27429000	-0.97937300
C	4.37662600	4.40365300	-0.06765900
C	4.06498100	3.74252500	-1.25887600
H	4.37909200	4.17623700	-2.20582700
C	3.35666300	2.53655500	-1.27308700
C	2.93890600	1.97152500	-0.04901600
C	2.17600200	0.67751800	-0.04215700
C	0.79489800	0.66686800	-0.07799800
C	0.08004800	1.93034700	-0.09603800
H	0.66702600	2.84148400	-0.13421800
C	-1.27316200	1.97077200	-0.04623500
C	-2.02957600	0.72887500	0.02152400
C	-3.38680000	1.01381000	0.07921700
C	-4.50195900	0.03741800	0.15813000
C	-5.29792000	-0.22347100	-0.98073800
C	-6.34051600	-1.15071800	-0.88905100
H	-6.94328400	-1.35068900	-1.77260300
C	-6.62614800	-1.82783000	0.29977800
C	-7.78392800	-2.79449600	0.38535300
H	-8.70904000	-2.28159600	0.67754700

H	-7.60031600	-3.57681800	1.12820000
H	-7.97384600	-3.27881900	-0.57742000
C	-2.24269000	3.06743700	-0.02913800
C	-2.10149800	4.44960200	-0.06474300
H	-1.11772500	4.90793200	-0.12342100
C	-3.25104000	5.24933400	-0.02183400
H	-3.15583000	6.33074000	-0.04970000
C	-4.52100000	4.66613500	0.06032000
H	-5.40044000	5.30300800	0.09706300
C	-4.67467100	3.27667100	0.09917500
H	-5.66271600	2.83085600	0.17133000
C	-3.53460500	2.46980500	0.04890700
C	0.03552100	-0.59456400	-0.06842700
C	0.79113000	-1.86495300	-0.11234400
C	2.22150700	-1.83464400	-0.03322000
C	3.00142200	-3.03433900	-0.01584800
C	2.32555300	-4.26092400	-0.10903000
H	2.87533600	-5.19383400	-0.09920100
C	0.95362700	-4.31447200	-0.22824700
H	0.47305300	-5.28003900	-0.31107100
C	0.18156500	-3.14376900	-0.23811300
C	-1.81951200	-4.47142900	-0.58239200
H	-1.64677600	-5.12584600	0.28267700
H	-1.39797400	-4.96227200	-1.46966800
C	-3.30169800	-4.19762300	-0.76627100
H	-3.47180300	-3.54401000	-1.62560000
H	-3.72669000	-3.71509200	0.11768100
H	-3.83284400	-5.13938900	-0.93595700
C	4.45395100	-2.98498300	0.09252200
C	5.27329800	-4.13600400	0.14144900
H	4.83025800	-5.12436100	0.10163700
C	6.64987500	-4.03762700	0.24520200
H	7.25033100	-4.94182800	0.28205500
C	7.27586800	-2.77735700	0.30394300
H	8.35645800	-2.70854800	0.38484900
C	6.50459800	-1.63542300	0.25856100
H	6.96752800	-0.65319500	0.30310300
C	5.09286000	-1.71413000	0.15377800
C	4.30009000	-0.53888900	0.10363000
H	4.80700600	0.41923000	0.13675700
C	2.91973400	-0.56254300	0.01513700
C	3.03872700	1.86591400	-2.59019800
H	1.95805600	1.79481700	-2.75407700
H	3.43193000	0.84440700	-2.62479600
H	3.47054000	2.42319200	-3.42554000
C	3.95262200	3.82729200	1.13253000
H	4.17864000	4.32758900	2.07171300
C	3.24075700	2.62332900	1.16559600
C	2.79670800	2.04813600	2.49139300
H	3.17221200	2.65064000	3.32255600
H	3.15733100	1.02289400	2.62552800

H	1.70451500	2.01251700	2.56714600
C	-1.34378500	-0.51710200	-0.00202800
H	-1.93792700	-1.41321800	0.02848300
C	-4.77395100	-0.63970600	1.36841900
C	-5.82735900	-1.55953800	1.41480900
H	-6.03440800	-2.07171800	2.35229300
C	-3.95537600	-0.37750500	2.61267700
H	-3.88101200	0.69425700	2.82256200
H	-2.93017300	-0.74903200	2.50968200
H	-4.40370500	-0.86571700	3.48240800
C	-5.01763200	0.46307200	-2.29819000
H	-5.67771900	0.08518000	-3.08368400
H	-3.98157400	0.30498300	-2.61587000
H	-5.16096400	1.54651300	-2.22829600

Singlet open-shell structure of 1: Electronic energy = −1928.561632 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.733808 (Hartree/Particle)
Thermal correction to Energy = 0.777130
Thermal correction to Enthalpy = 0.778074
Thermal correction to Gibbs Free Energy = 0.654587
Sum of electronic and zero-point Energies = -1927.827824
Sum of electronic and thermal Energies = -1927.784502
Sum of electronic and thermal Enthalpies = -1927.783558
Sum of electronic and thermal Free Energies = -1927.907045

Atom	x	y	z
O	-1.17214000	-3.21235700	-0.37506100
C	5.17142000	5.68818900	-0.07641700
H	6.24997100	5.48813400	-0.04789000
H	4.93448800	6.31151700	0.79089900
H	4.97531800	6.27429000	-0.97937300
C	4.37662600	4.40365300	-0.06765900
C	4.06498100	3.74252500	-1.25887600
H	4.37909200	4.17623700	-2.20582700
C	3.35666300	2.53655500	-1.27308700
C	2.93890600	1.97152500	-0.04901600
C	2.17600200	0.67751800	-0.04215700
C	0.79489800	0.66686800	-0.07799800
C	0.08004800	1.93034700	-0.09603800
H	0.66702600	2.84148400	-0.13421800
C	-1.27316200	1.97077200	-0.04623500
C	-2.02957600	0.72887500	0.02152400
C	-3.38680000	1.01381000	0.07921700
C	-4.50195900	0.03741800	0.15813000
C	-5.29792000	-0.22347100	-0.98073800
C	-6.34051600	-1.15071800	-0.88905100
H	-6.94328400	-1.35068900	-1.77260300
C	-6.62614800	-1.82783000	0.29977800

C	-7.78392800	-2.79449600	0.38535300
H	-8.70904000	-2.28159600	0.67754700
H	-7.60031600	-3.57681800	1.12820000
H	-7.97384600	-3.27881900	-0.57742000
C	-2.24269000	3.06743700	-0.02913800
C	-2.10149800	4.44960200	-0.06474300
H	-1.11772500	4.90793200	-0.12342100
C	-3.25104000	5.24933400	-0.02183400
H	-3.15583000	6.33074000	-0.04970000
C	-4.52100000	4.66613500	0.06032000
H	-5.40044000	5.30300800	0.09706300
C	-4.67467100	3.27667100	0.09917500
H	-5.66271600	2.83085600	0.17133000
C	-3.53460500	2.46980500	0.04890700
C	0.03552100	-0.59456400	-0.06842700
C	0.79113000	-1.86495300	-0.11234400
C	2.22150700	-1.83464400	-0.03322000
C	3.00142200	-3.03433900	-0.01584800
C	2.32555300	-4.26092400	-0.10903000
H	2.87533600	-5.19383400	-0.09920100
C	0.95362700	-4.31447200	-0.22824700
H	0.47305300	-5.28003900	-0.31107100
C	0.18156500	-3.14376900	-0.23811300
C	-1.81951200	-4.47142900	-0.58239200
H	-1.64677600	-5.12584600	0.28267700
H	-1.39797400	-4.96227200	-1.46966800
C	-3.30169800	-4.19762300	-0.76627100
H	-3.47180300	-3.54401000	-1.62560000
H	-3.72669000	-3.71509200	0.11768100
H	-3.83284400	-5.13938900	-0.93595700
C	4.45395100	-2.98498300	0.09252200
C	5.27329800	-4.13600400	0.14144900
H	4.83025800	-5.12436100	0.10163700
C	6.64987500	-4.03762700	0.24520200
H	7.25033100	-4.94182800	0.28205500
C	7.27586800	-2.77735700	0.30394300
H	8.35645800	-2.70854800	0.38484900
C	6.50459800	-1.63542300	0.25856100
H	6.96752800	-0.65319500	0.30310300
C	5.09286000	-1.71413000	0.15377800
C	4.30009000	-0.53888900	0.10363000
H	4.80700600	0.41923000	0.13675700
C	2.91973400	-0.56254300	0.01513700
C	3.03872700	1.86591400	-2.59019800
H	1.95805600	1.79481700	-2.75407700
H	3.43193000	0.84440700	-2.62479600
H	3.47054000	2.42319200	-3.42554000
C	3.95262200	3.82729200	1.13253000
H	4.17864000	4.32758900	2.07171300
C	3.24075700	2.62332900	1.16559600
C	2.79670800	2.04813600	2.49139300

H	3.17221200	2.65064000	3.32255600
H	3.15733100	1.02289400	2.62552800
H	1.70451500	2.01251700	2.56714600
C	-1.34378500	-0.51710200	-0.00202800
H	-1.93792700	-1.41321800	0.02848300
C	-4.77395100	-0.63970600	1.36841900
C	-5.82735900	-1.55953800	1.41480900
H	-6.03440800	-2.07171800	2.35229300
C	-3.95537600	-0.37750500	2.61267700
H	-3.88101200	0.69425700	2.82256200
H	-2.93017300	-0.74903200	2.50968200
H	-4.40370500	-0.86571700	3.48240800
C	-5.01763200	0.46307200	-2.29819000
H	-5.67771900	0.08518000	-3.08368400
H	-3.98157400	0.30498300	-2.61587000
H	-5.16096400	1.54651300	-2.22829600

Triplet open-shell structure of 1: Electronic energy = −1928.540278 Hartree
No. of Imaginary Frequency = Zero

Zero-point correction = 0.731713 (Hartree/Particle)

Thermal correction to Energy = 0.775182
Thermal correction to Enthalpy = 0.776127
Thermal correction to Gibbs Free Energy = 0.651510
Sum of electronic and zero-point Energies = -1927.808564
Sum of electronic and thermal Energies = -1927.765096
Sum of electronic and thermal Enthalpies = -1927.764151
Sum of electronic and thermal Free Energies = -1927.888768

Atom	x	y	z
O	-1.17574900	-3.17355600	-0.43247300
C	5.12679400	5.73303600	-0.12577100
H	6.20954300	5.55586500	-0.10358600
H	4.88320800	6.35567800	0.74037500
H	4.91250700	6.31086600	-1.02998800
C	4.35888000	4.43228300	-0.10537500
C	4.03477900	3.76920700	-1.29208900
H	4.31928900	4.21268700	-2.24399800
C	3.35112200	2.54886600	-1.29476800
C	2.97288100	1.96844700	-0.06509300
C	2.22744400	0.66709600	-0.04827300
C	0.79548700	0.66869900	-0.06733000
C	0.09781700	1.91349300	-0.06494500
H	0.67882700	2.82849800	-0.09287800
C	-1.27526100	1.95151400	-0.01294500
C	-2.00840200	0.72641200	0.04979900
C	-3.43287700	1.02993200	0.11236500
C	-4.53400800	0.04272700	0.17625900
C	-5.32920800	-0.21047100	-0.96518400
C	-6.35514100	-1.15727000	-0.88535000

H	-6.95703400	-1.35279000	-1.77034000
C	-6.62429100	-1.86062400	0.29187800
C	-7.76421000	-2.84905400	0.36416700
H	-8.69312400	-2.36034100	0.68422100
H	-7.55727800	-3.64948200	1.08107500
H	-7.95944800	-3.30776200	-0.60986100
C	-2.24573100	3.04364700	0.00783300
C	-2.09941000	4.42604900	-0.02492100
H	-1.11354700	4.87947900	-0.08074300
C	-3.24340400	5.23229500	0.01612300
H	-3.13866000	6.31296200	-0.01000900
C	-4.52716200	4.66300300	0.09475900
H	-5.39729700	5.31203200	0.13041200
C	-4.69375000	3.28268600	0.13132200
H	-5.68479700	2.84347700	0.20171900
C	-3.55447400	2.45511300	0.08213100
C	0.06329200	-0.56985300	-0.06284900
C	0.79848300	-1.83733200	-0.10998000
C	2.23095100	-1.81859600	-0.02575300
C	2.99766500	-3.02782800	0.00650500
C	2.30924700	-4.24304200	-0.07516100
H	2.84859400	-5.18184200	-0.05106700
C	0.93256200	-4.28934600	-0.21232800
H	0.44947800	-5.25336900	-0.29714700
C	0.17385900	-3.11931000	-0.24759900
C	-1.82510400	-4.42972400	-0.64827300
H	-1.68465700	-5.07728700	0.22780800
H	-1.37759700	-4.93160500	-1.51647200
C	-3.29860100	-4.14855500	-0.88341400
H	-3.43534000	-3.49912600	-1.75191600
H	-3.75128500	-3.65955800	-0.01685000
H	-3.82884700	-5.08833200	-1.06649300
C	4.45574100	-2.99831000	0.11479300
C	5.25424300	-4.15838600	0.18346600
H	4.79476400	-5.14008300	0.16423500
C	6.63569100	-4.08473500	0.28123400
H	7.21956200	-4.99881800	0.33351800
C	7.28214300	-2.83371800	0.31357500
H	8.36424100	-2.78152300	0.38937000
C	6.53197300	-1.67936200	0.25007600
H	7.01288700	-0.70514800	0.27563900
C	5.11425300	-1.73113100	0.15172400
C	4.34791900	-0.55068400	0.09011200
H	4.86457700	0.40224600	0.11078500
C	2.93675400	-0.54924100	0.00982300
C	3.02357900	1.87083300	-2.60554600
H	1.94477300	1.72035600	-2.72058500
H	3.48983600	0.88184900	-2.67075200
H	3.37466300	2.46682600	-3.45216900
C	3.97335300	3.84285600	1.10162900
H	4.20943400	4.34452700	2.03775600

C	3.28788000	2.62408900	1.14452000
C	2.89167200	2.02856500	2.47622400
H	3.20205800	2.67538800	3.30114600
H	3.34942500	1.04479600	2.62650600
H	1.80771300	1.88748600	2.54518100
C	-1.35696700	-0.49407400	0.01942400
H	-1.94097300	-1.39656800	0.06157100
C	-4.78827200	-0.66195600	1.37560600
C	-5.82573100	-1.59917800	1.40919800
H	-6.02054700	-2.13111500	2.33814900
C	-3.97605300	-0.39600200	2.62289600
H	-3.99247600	0.66652000	2.88798700
H	-2.92445900	-0.66996200	2.48937900
H	-4.36782400	-0.96315800	3.47148100
C	-5.06767000	0.50316300	-2.27246000
H	-5.69899000	0.09995600	-3.06881400
H	-4.02205900	0.40031200	-2.58105500
H	-5.26757300	1.57712700	-2.19601200

Singlet closed-shell structure of 2: Electronic energy = −2108.296224 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.626697 (Hartree/Particle)
Thermal correction to Energy = 0.667144
Thermal correction to Enthalpy = 0.668088
Thermal correction to Gibbs Free Energy = 0.552054
Sum of electronic and zero-point Energies = -2107.669527
Sum of electronic and thermal Energies = -2107.629080
Sum of electronic and thermal Enthalpies = -2107.628136
Sum of electronic and thermal Free Energies = -2107.744171

Atom	x	y	z
O	-1.09637100	-3.20019600	-0.66039400
C	5.07761600	5.76557700	-0.07954800
H	6.15737700	5.58296500	-0.00978100
H	4.80094000	6.39974900	0.76790600
H	4.90452100	6.33294600	-0.99897800
C	4.30271400	4.46900100	-0.07597500
C	4.03930000	3.78529400	-1.26608300
H	4.37653700	4.20963400	-2.20927000
C	3.35090300	2.56795000	-1.28393400
C	2.90292600	2.01553700	-0.06479800
C	2.16209800	0.70929400	-0.06313100
C	0.78159200	0.67486400	-0.13030800
C	0.04033500	1.91918600	-0.16533900
H	0.60349000	2.84383500	-0.22899700
C	-1.31326100	1.92823500	-0.08973800
C	-2.04367600	0.67537100	0.03146400
C	-3.40608900	0.95058100	0.11469100
C	-4.49068100	-0.02778900	0.26807200
C	-5.63263500	-0.03377700	-0.55151400

C	-6.68103100	-0.93657800	-0.42725100
C	-6.58377000	-1.89680800	0.57151800
C	-2.29632700	3.00994500	-0.08019500
C	-2.16142800	4.39219400	-0.14896100
H	-1.18059600	4.85107600	-0.24134900
C	-3.31114300	5.18772100	-0.09337400
H	-3.22304600	6.26872000	-0.14665000
C	-4.57409100	4.59807500	0.03517200
H	-5.45696900	5.22941000	0.08126900
C	-4.71990700	3.20999200	0.10518000
H	-5.70747600	2.77251200	0.20451200
C	-3.57909300	2.40477500	0.04249300
C	0.04660500	-0.59779500	-0.11653800
C	0.82432700	-1.85071400	-0.19235700
C	2.24807700	-1.80093000	-0.05455300
C	3.04338700	-2.98927800	-0.02774300
C	2.39066700	-4.22158200	-0.19078700
H	2.95226000	-5.14743900	-0.17404600
C	1.02927000	-4.28858700	-0.39884900
H	0.56848200	-5.25680800	-0.54309100
C	0.24247800	-3.12742300	-0.41616900
C	-1.68802500	-4.44065700	-1.05884700
H	-1.61876600	-5.16847000	-0.23908300
H	-1.14574700	-4.84785100	-1.92225000
C	-3.13816000	-4.16303500	-1.41264100
H	-3.20400000	-3.43437200	-2.22482900
H	-3.68403700	-3.77006000	-0.55068600
H	-3.62440100	-5.08870800	-1.73544200
C	4.48702000	-2.91959500	0.15710500
C	5.31989900	-4.05879900	0.23913500
H	4.89385200	-5.05302400	0.17075400
C	6.68757700	-3.94072600	0.41494800
H	7.29888300	-4.83622000	0.47679200
C	7.29089400	-2.67197600	0.51532700
H	8.36469500	-2.58825200	0.65233400
C	6.50599300	-1.54109100	0.43962100
H	6.95124000	-0.55269600	0.51590700
C	5.10265500	-1.63959400	0.26270700
C	4.29700000	-0.47487400	0.18044900
H	4.78836200	0.49029400	0.23772500
C	2.92218900	-0.51835900	0.03158700
C	3.08659900	1.87182700	-2.59974600
H	2.01314300	1.76939700	-2.79178900
H	3.50790400	0.86094100	-2.60997700
H	3.52609400	2.42944200	-3.43078300
C	3.84941800	3.90437300	1.11909200
H	4.03780200	4.42234300	2.05695900
C	3.15495400	2.69026400	1.14878400
C	2.67762200	2.12855800	2.46885400
H	3.01969300	2.74807800	3.30187300
H	3.04681700	1.11024200	2.62974300

H	1.58419200	2.07991700	2.51191500
C	-1.33047800	-0.55443100	-0.00046700
H	-1.88914100	-1.47081800	0.06737900
C	-4.47867100	-1.03068300	1.25362500
C	-5.49050700	-1.96796700	1.42604100
F	-7.58152500	-2.78857900	0.71655500
F	-5.71775200	0.88162200	-1.53520800
F	-3.43371300	-1.09010500	2.09920600
H	-7.53168100	-0.89639500	-1.09551300
H	-5.43341000	-2.70865600	2.21352400

Singlet open-shell structure of 2: Electronic energy = −2108.296224 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.626697 (Hartree/Particle)
Thermal correction to Energy = 0.667144
Thermal correction to Enthalpy = 0.668088
Thermal correction to Gibbs Free Energy = 0.552054
Sum of electronic and zero-point Energies = -2107.669527
Sum of electronic and thermal Energies = -2107.629080
Sum of electronic and thermal Enthalpies = -2107.628136
Sum of electronic and thermal Free Energies = -2107.744171

Atom	x	y	z
O	-1.09637100	-3.20019600	-0.66039400
C	5.07761600	5.76557700	-0.07954800
H	6.15737700	5.58296500	-0.00978100
H	4.80094000	6.39974900	0.76790600
H	4.90452100	6.33294600	-0.99897800
C	4.30271400	4.46900100	-0.07597500
C	4.03930000	3.78529400	-1.26608300
H	4.37653700	4.20963400	-2.20927000
C	3.35090300	2.56795000	-1.28393400
C	2.90292600	2.01553700	-0.06479800
C	2.16209800	0.70929400	-0.06313100
C	0.78159200	0.67486400	-0.13030800
C	0.04033500	1.91918600	-0.16533900
H	0.60349000	2.84383500	-0.22899700
C	-1.31326100	1.92823500	-0.08973800
C	-2.04367600	0.67537100	0.03146400
C	-3.40608900	0.95058100	0.11469100
C	-4.49068100	-0.02778900	0.26807200
C	-5.63263500	-0.03377700	-0.55151400
C	-6.68103100	-0.93657800	-0.42725100
C	-6.58377000	-1.89680800	0.57151800
C	-2.29632700	3.00994500	-0.08019500
C	-2.16142800	4.39219400	-0.14896100
H	-1.18059600	4.85107600	-0.24134900
C	-3.31114300	5.18772100	-0.09337400
H	-3.22304600	6.26872000	-0.14665000

C	-4.57409100	4.59807500	0.03517200
H	-5.45696900	5.22941000	0.08126900
C	-4.71990700	3.20999200	0.10518000
H	-5.70747600	2.77251200	0.20451200
C	-3.57909300	2.40477500	0.04249300
C	0.04660500	-0.59779500	-0.11653800
C	0.82432700	-1.85071400	-0.19235700
C	2.24807700	-1.80093000	-0.05455300
C	3.04338700	-2.98927800	-0.02774300
C	2.39066700	-4.22158200	-0.19078700
H	2.95226000	-5.14743900	-0.17404600
C	1.02927000	-4.28858700	-0.39884900
H	0.56848200	-5.25680800	-0.54309100
C	0.24247800	-3.12742300	-0.41616900
C	-1.68802500	-4.44065700	-1.05884700
H	-1.61876600	-5.16847000	-0.23908300
H	-1.14574700	-4.84785100	-1.92225000
C	-3.13816000	-4.16303500	-1.41264100
H	-3.20400000	-3.43437200	-2.22482900
H	-3.68403700	-3.77006000	-0.55068600
H	-3.62440100	-5.08870800	-1.73544200
C	4.48702000	-2.91959500	0.15710500
C	5.31989900	-4.05879900	0.23913500
H	4.89385200	-5.05302400	0.17075400
C	6.68757700	-3.94072600	0.41494800
H	7.29888300	-4.83622000	0.47679200
C	7.29089400	-2.67197600	0.51532700
H	8.36469500	-2.58825200	0.65233400
C	6.50599300	-1.54109100	0.43962100
H	6.95124000	-0.55269600	0.51590700
C	5.10265500	-1.63959400	0.26270700
C	4.29700000	-0.47487400	0.18044900
H	4.78836200	0.49029400	0.23772500
C	2.92218900	-0.51835900	0.03158700
C	3.08659900	1.87182700	-2.59974600
H	2.01314300	1.76939700	-2.79178900
H	3.50790400	0.86094100	-2.60997700
H	3.52609400	2.42944200	-3.43078300
C	3.84941800	3.90437300	1.11909200
H	4.03780200	4.42234300	2.05695900
C	3.15495400	2.69026400	1.14878400
C	2.67762200	2.12855800	2.46885400
H	3.01969300	2.74807800	3.30187300
H	3.04681700	1.11024200	2.62974300
H	1.58419200	2.07991700	2.51191500
C	-1.33047800	-0.55443100	-0.00046700
H	-1.88914100	-1.47081800	0.06737900
C	-4.47867100	-1.03068300	1.25362500
C	-5.49050700	-1.96796700	1.42604100
F	-7.58152500	-2.78857900	0.71655500
F	-5.71775200	0.88162200	-1.53520800

F	-3.43371300	-1.09010500	2.09920600
H	-7.53168100	-0.89639500	-1.09551300
H	-5.43341000	-2.70865600	2.21352400

Triplet open-shell structure of 2: Electronic energy = −2108.274834 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.624578 (Hartree/Particle)
Thermal correction to Energy = 0.665182
Thermal correction to Enthalpy = 0.666126
Thermal correction to Gibbs Free Energy = 0.548768
Sum of electronic and zero-point Energies = -2107.650256
Sum of electronic and thermal Energies = -2107.609652
Sum of electronic and thermal Enthalpies = -2107.608708
Sum of electronic and thermal Free Energies = -2107.726066

Atom	x	y	z
O	-1.09362300	-3.16408200	-0.68094800
C	5.02682200	5.81643200	-0.12633500
H	6.11199100	5.65757300	-0.08917700
H	4.76132500	6.43848400	0.73373400
H	4.81494300	6.38675400	-1.03589500
C	4.28079000	4.50298600	-0.11038000
C	3.99353500	3.82427000	-1.29779600
H	4.29080600	4.26429100	-2.24738400
C	3.33158000	2.59211800	-1.30393400
C	2.93708300	2.01600500	-0.07729600
C	2.21577100	0.70142000	-0.06566600
C	0.78504800	0.67580000	-0.10499800
C	0.05708200	1.90174500	-0.11057700
H	0.61261000	2.83184800	-0.15400100
C	-1.31551300	1.90365700	-0.04125600
C	-2.02325000	0.66719100	0.06229200
C	-3.45344600	0.95759600	0.14302600
C	-4.52822600	-0.02434300	0.27225400
C	-5.68201500	-0.01031200	-0.53520300
C	-6.71815200	-0.92857100	-0.43338500
C	-6.60118700	-1.92464300	0.52798700
C	-2.30014000	2.98111300	-0.03119200
C	-2.15850800	4.36353600	-0.08488400
H	-1.17447900	4.81734400	-0.16206400
C	-3.30303600	5.16587900	-0.03329800
H	-3.20426900	6.24656000	-0.07530600
C	-4.58026900	4.59012100	0.07894300
H	-5.45413000	5.23329000	0.12373200
C	-4.73987600	3.21001400	0.13399200
H	-5.73120800	2.77962200	0.22134300
C	-3.60019900	2.38445100	0.07177100
C	0.07727300	-0.57453200	-0.10277500
C	0.83623200	-1.82438900	-0.17576600
C	2.26313300	-1.78385900	-0.04343600

C	3.04564300	-2.98190000	-0.00107300
C	2.37908400	-4.20497700	-0.13711100
H	2.93070600	-5.13647400	-0.10565700
C	1.01190200	-4.26700100	-0.35013700
H	0.54818500	-5.23498400	-0.48593200
C	0.23983800	-3.10607700	-0.39656200
C	-1.68423300	-4.40556500	-1.07560200
H	-1.64530700	-5.12096100	-0.24287700
H	-1.11917000	-4.83109400	-1.91522300
C	-3.12064000	-4.12326100	-1.47830500
H	-3.15588100	-3.40483300	-2.30152500
H	-3.69124100	-3.71633300	-0.63910000
H	-3.60266000	-5.04983400	-1.80481900
C	4.49688500	-2.92975400	0.16863200
C	5.30989700	-4.07746500	0.26786900
H	4.86630100	-5.06592800	0.23016900
C	6.68477800	-3.98223700	0.42202900
H	7.28042600	-4.88704800	0.49737300
C	7.30955200	-2.72127400	0.48221000
H	8.38672300	-2.65229300	0.60175100
C	6.54445100	-1.57858700	0.39095400
H	7.00864000	-0.59712000	0.43827300
C	5.13287400	-1.65212500	0.23625600
C	4.35165200	-0.48237800	0.14789600
H	4.85309000	0.47816600	0.18672400
C	2.94501400	-0.50283300	0.02067400
C	3.04469400	1.89668700	-2.61522700
H	1.97152600	1.72606400	-2.75289300
H	3.52955400	0.91558900	-2.66105300
H	3.40388200	2.49116100	-3.45949200
C	3.87967300	3.91750000	1.09341000
H	4.08726000	4.43119700	2.02974400
C	3.21426000	2.68752100	1.13295600
C	2.79943200	2.09736000	2.46141200
H	3.08715100	2.75360100	3.28708200
H	3.26462700	1.11974600	2.62787700
H	1.71595000	1.94510000	2.51129800
C	-1.34063400	-0.53622000	0.02084400
H	-1.88476100	-1.46044700	0.09794800
C	-4.49679000	-1.06617300	1.21991600
C	-5.49806300	-2.01671400	1.36875400
F	-7.58851800	-2.82910900	0.65068300
F	-5.78769700	0.93684100	-1.48540000
F	-3.44706200	-1.13874900	2.05730800
H	-7.57539700	-0.87369500	-1.09208600
H	-5.42752300	-2.78280900	2.13038900

Singlet closed-shell structure of 3: Electronic energy = −2306.730124 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.610542 (Hartree/Particle)
Thermal correction to Energy = 0.652943
Thermal correction to Enthalpy = 0.653887
Thermal correction to Gibbs Free Energy = 0.534040
Sum of electronic and zero-point Energies = -2306.119582
Sum of electronic and thermal Energies = -2306.077181
Sum of electronic and thermal Enthalpies = -2306.076237
Sum of electronic and thermal Free Energies = -2306.196084

Atom	x	y	z
O	-0.91364800	-3.19296000	0.19828400
C	5.59848600	5.61099100	0.20545900
H	6.67283700	5.39199700	0.16289000
H	5.41948700	6.17240700	1.12743200
H	5.36697700	6.26475500	-0.64052800
C	4.78017200	4.34207700	0.16300000
C	4.32719200	3.81785200	-1.05045500
H	4.54823200	4.34792700	-1.97424900
C	3.59210700	2.62934800	-1.11622900
C	3.29645800	1.94028600	0.07920400
C	2.50930700	0.66159400	0.03664400
C	1.12817700	0.67506400	0.09990400
C	0.44850600	1.94985600	0.18005600
H	1.05631600	2.84652400	0.22515400
C	-0.90387000	2.02599900	0.17220200
C	-1.69957800	0.81027300	0.08767100
C	-3.04722900	1.16520600	0.04406000
C	-4.20655600	0.26882100	-0.04432200
C	-5.21694500	0.45737200	-1.00269900
C	-6.34439800	-0.35469800	-1.07599700
C	-6.49400300	-1.41113900	-0.18148300
C	-1.82410400	3.15914300	0.20390900
C	-1.61302400	4.52996500	0.30940600
H	-0.60646000	4.93379900	0.37835900
C	-2.72022800	5.38435200	0.33055200
H	-2.57338900	6.45711800	0.41191500
C	-4.01766700	4.86389700	0.25182700
H	-4.86749600	5.54013100	0.27397900
C	-4.23936300	3.48868000	0.14550400
H	-5.25284700	3.10587800	0.08860300
C	-3.13971400	2.62601000	0.11590100
C	0.33803100	-0.56527000	0.05096200
C	1.06868900	-1.85207700	0.00536000
C	2.50024300	-1.84455900	-0.09079100
C	3.26021300	-3.05365400	-0.17952800
C	2.56500400	-4.27192400	-0.14623800
H	3.09786900	-5.21226800	-0.21145400
C	1.19458500	-4.30780800	-0.02012800
H	0.70075200	-5.26898900	0.01127900
C	0.43948200	-3.12741900	0.06075800
C	-1.55167500	-4.46472800	0.37690300

H	-1.11515100	-4.97364900	1.24596900
H	-1.38207900	-5.09234400	-0.50778300
C	-3.03265000	-4.21604800	0.58404300
H	-3.47225300	-3.74192500	-0.29789700
H	-3.20326100	-3.57160600	1.44742700
H	-3.54682300	-5.16711400	0.75197100
C	4.71196900	-3.02635500	-0.29815600
C	5.50936500	-4.18866600	-0.41009100
H	5.04938200	-5.16988800	-0.41341800
C	6.88635400	-4.10955100	-0.52127100
H	7.46944600	-5.02171300	-0.60693500
C	7.53654300	-2.85974300	-0.52485300
H	8.61745000	-2.80785700	-0.61221400
C	6.78782000	-1.70761000	-0.41702000
H	7.26823400	-0.73288800	-0.41781600
C	5.37555300	-1.76673900	-0.30313300
C	4.60480400	-0.58325300	-0.18844900
H	5.12721800	0.36698800	-0.18112600
C	3.22440400	-0.58720100	-0.08560000
C	3.11642700	2.11183600	-2.45478400
H	2.02269200	2.09982900	-2.51431900
H	3.45500000	1.08579400	-2.63282900
H	3.49034900	2.73742700	-3.26925200
C	4.47389200	3.64395100	1.33441900
H	4.81031400	4.03713500	2.29128200
C	3.74257000	2.45189100	1.31669200
C	3.43009300	1.74071300	2.61372700
H	3.88756400	2.25740500	3.46126100
H	3.79999000	0.70995300	2.60590400
H	2.35076400	1.68850800	2.79303200
C	-1.04305900	-0.45218000	0.03146200
H	-1.64871500	-1.33819200	-0.03047800
C	-4.39966800	-0.80210200	0.84224500
C	-5.51439800	-1.63235300	0.78211400
F	-7.56700300	-2.20619800	-0.24817800
F	-5.65017100	-2.64639900	1.65037400
F	-7.27461200	-0.14008100	-2.01513500
F	-5.10818800	1.44412800	-1.90539100
F	-3.49592800	-1.05390100	1.80400000

Singlet open-shell structure of 3: Electronic energy = −2306.730124 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.610542 (Hartree/Particle)
Thermal correction to Energy = 0.652943
Thermal correction to Enthalpy = 0.653887
Thermal correction to Gibbs Free Energy = 0.534040
Sum of electronic and zero-point Energies= -2306.119582
Sum of electronic and thermal Energies = -2306.077181
Sum of electronic and thermal Enthalpies = -2306.076237

Sum of electronic and thermal Free Energies = -2306.196084

Atom	x	y	z
O	-0.91364800	-3.19296000	0.19828500
C	5.59848600	5.61099100	0.20545900
H	6.67283700	5.39199700	0.16288900
H	5.41948800	6.17240600	1.12743300
H	5.36697600	6.26475500	-0.64052700
C	4.78017200	4.34207700	0.16300000
C	4.32719200	3.81785200	-1.05045500
H	4.54823200	4.34792700	-1.97424900
C	3.59210700	2.62934800	-1.11622900
C	3.29645800	1.94028600	0.07920400
C	2.50930700	0.66159400	0.03664400
C	1.12817700	0.67506400	0.09990400
C	0.44850600	1.94985600	0.18005600
H	1.05631600	2.84652400	0.22515400
C	-0.90387000	2.02599900	0.17220200
C	-1.69957800	0.81027300	0.08767100
C	-3.04722900	1.16520600	0.04406000
C	-4.20655600	0.26882100	-0.04432200
C	-5.21694500	0.45737200	-1.00269900
C	-6.34439800	-0.35469800	-1.07599700
C	-6.49400300	-1.41113900	-0.18148400
C	-1.82410400	3.15914300	0.20390900
C	-1.61302400	4.52996500	0.30940600
H	-0.60646000	4.93379900	0.37836000
C	-2.72022800	5.38435200	0.33055200
H	-2.57338900	6.45711800	0.41191500
C	-4.01766700	4.86389700	0.25182700
H	-4.86749600	5.54013000	0.27397900
C	-4.23936300	3.48868000	0.14550400
H	-5.25284700	3.10587800	0.08860300
C	-3.13971400	2.62601000	0.11590100
C	0.33803100	-0.56527000	0.05096200
C	1.06868900	-1.85207700	0.00536000
C	2.50024300	-1.84455900	-0.09079100
C	3.26021300	-3.05365400	-0.17952800
C	2.56500400	-4.27192400	-0.14623800
H	3.09786900	-5.21226800	-0.21145400
C	1.19458500	-4.30780800	-0.02012700
H	0.70075200	-5.26898900	0.01127900
C	0.43948200	-3.12741900	0.06075800
C	-1.55167500	-4.46472800	0.37690300
H	-1.11515100	-4.97364900	1.24596900
H	-1.38207900	-5.09234400	-0.50778300
C	-3.03265000	-4.21604800	0.58404400
H	-3.47225300	-3.74192500	-0.29789700
H	-3.20326100	-3.57160600	1.44742800
H	-3.54682300	-5.16711400	0.75197100

C	4.71196900	-3.02635500	-0.29815600
C	5.50936500	-4.18866600	-0.41009100
H	5.04938200	-5.16988800	-0.41341800
C	6.88635400	-4.10955100	-0.52127100
H	7.46944600	-5.02171300	-0.60693500
C	7.53654300	-2.85974300	-0.52485300
H	8.61745000	-2.80785700	-0.61221400
C	6.78782000	-1.70761000	-0.41702100
H	7.26823400	-0.73288800	-0.41781600
C	5.37555300	-1.76673900	-0.30313300
C	4.60480400	-0.58325300	-0.18844900
H	5.12721800	0.36698800	-0.18112600
C	3.22440400	-0.58720100	-0.08560000
C	3.11642700	2.11183600	-2.45478400
H	2.02269200	2.09982900	-2.51431900
H	3.45500000	1.08579400	-2.63282900
H	3.49034900	2.73742700	-3.26925200
C	4.47389200	3.64395100	1.33441900
H	4.81031400	4.03713500	2.29128200
C	3.74257000	2.45189100	1.31669200
C	3.43009300	1.74071300	2.61372700
H	3.88756400	2.25740500	3.46126100
H	3.79999000	0.70995300	2.60590400
H	2.35076400	1.68850800	2.79303300
C	-1.04305900	-0.45218000	0.03146300
H	-1.64871500	-1.33819200	-0.03047800
C	-4.39966900	-0.80210200	0.84224500
C	-5.51439800	-1.63235300	0.78211400
F	-7.56700300	-2.20619800	-0.24817800
F	-5.65017100	-2.64639900	1.65037400
F	-7.27461200	-0.14008100	-2.01513500
F	-5.10818700	1.44412800	-1.90539100
F	-3.49592800	-1.05390100	1.80400000

Triplet open-shell structure of 3: Electronic energy = −2306.707754 Hartree

No. of Imaginary Frequency = Zero

Zero-point correction = 0.608421 (Hartree/Particle)
Thermal correction to Energy = 0.650973
Thermal correction to Enthalpy = 0.651917
Thermal correction to Gibbs Free Energy = 0.530623
Sum of electronic and zero-point Energies = -2306.099333
Sum of electronic and thermal Energies = -2306.056781
Sum of electronic and thermal Enthalpies = -2306.055836
Sum of electronic and thermal Free Energies = -2306.177131

Atom	x	y	z
O	-0.91039500	-3.17532600	0.15336900
C	5.53567000	5.67221300	0.22772700

H	6.61537500	5.48051700	0.18733400
H	5.34025500	6.22586000	1.15114000
H	5.29095600	6.32349700	-0.61670200
C	4.74909200	4.38347900	0.17795700
C	4.33701700	3.83865900	-1.04121200
H	4.56666800	4.36660700	-1.96433500
C	3.63351000	2.63157900	-1.11242600
C	3.32624300	1.94273900	0.08062500
C	2.56122300	0.65346500	0.03180500
C	1.13202200	0.67371200	0.07879500
C	0.46276800	1.93071300	0.13956200
H	1.06254000	2.83323600	0.16362400
C	-0.90737300	2.00007200	0.14529600
C	-1.67893500	0.79943100	0.09020000
C	-3.09268200	1.17257100	0.04902800
C	-4.24298800	0.27341900	-0.02248100
C	-5.27843000	0.46227700	-0.95718700
C	-6.39670400	-0.36269400	-1.01491200
C	-6.51526000	-1.43016200	-0.12837100
C	-1.82946800	3.13037500	0.16199300
C	-1.61223800	4.50145500	0.24289900
H	-0.60366700	4.90096400	0.29878500
C	-2.71432900	5.36267800	0.25797800
H	-2.55729100	6.43531700	0.32129200
C	-4.02424800	4.85643300	0.19937200
H	-4.86432400	5.54409500	0.21953100
C	-4.25841000	3.48850900	0.11769200
H	-5.27469800	3.11229500	0.07741900
C	-3.16068000	2.60618900	0.08964900
C	0.37185900	-0.54693100	0.04047400
C	1.08592300	-1.82902200	-0.01287700
C	2.52185200	-1.82692000	-0.09695600
C	3.27517400	-3.04165000	-0.19142800
C	2.57245400	-4.25027200	-0.18702700
H	3.09959800	-5.19322400	-0.26069100
C	1.19451500	-4.28521900	-0.07704700
H	0.70138800	-5.24707600	-0.06632900
C	0.44580400	-3.11152700	0.01883300
C	-1.54783600	-4.45122000	0.28898700
H	-1.11552000	-4.98710800	1.14392800
H	-1.37291400	-5.05161800	-0.61352600
C	-3.03024100	-4.21152300	0.49697900
H	-3.46623600	-3.70726600	-0.37013200
H	-3.20579100	-3.59910500	1.38253800
H	-3.54432700	-5.16832100	0.62875800
C	4.73450000	-3.02923600	-0.28696300
C	5.51709200	-4.19716100	-0.39695000
H	5.04497400	-5.17267300	-0.41758200
C	6.89991000	-4.13887700	-0.48348000
H	7.47120100	-5.05844000	-0.56792400
C	7.56455700	-2.89707300	-0.46261800

H	8.64766300	-2.85776100	-0.53036700
C	6.83051100	-1.73573000	-0.35626100
H	7.32482500	-0.76812100	-0.33891800
C	5.41181100	-1.77238200	-0.26706600
C	4.66036300	-0.58665200	-0.15840400
H	5.18830400	0.35996300	-0.13938400
C	3.24959900	-0.57035000	-0.07577100
C	3.21012200	2.08365100	-2.45619800
H	2.12313500	1.96249000	-2.51579800
H	3.64941200	1.09756200	-2.64201900
H	3.52082100	2.74990200	-3.26528000
C	4.43343600	3.68711700	1.34783600
H	4.73925500	4.09549100	2.30876000
C	3.73167800	2.47733600	1.32239700
C	3.41425000	1.76203400	2.61577500
H	3.79564800	2.32036800	3.47477800
H	3.85853400	0.76112600	2.63790300
H	2.33474400	1.63208800	2.74839800
C	-1.05185600	-0.43559700	0.03377400
H	-1.64568800	-1.32988800	-0.02151400
C	-4.40349300	-0.81385100	0.85416100
C	-5.51204000	-1.65191600	0.81153700
F	-7.58164300	-2.23306600	-0.17783800
F	-5.62170400	-2.67210300	1.67431900
F	-7.34829200	-0.14960200	-1.93144800
F	-5.20032200	1.45538400	-1.85530900
F	-3.47872300	-1.06095100	1.79529700

4. Appendix:

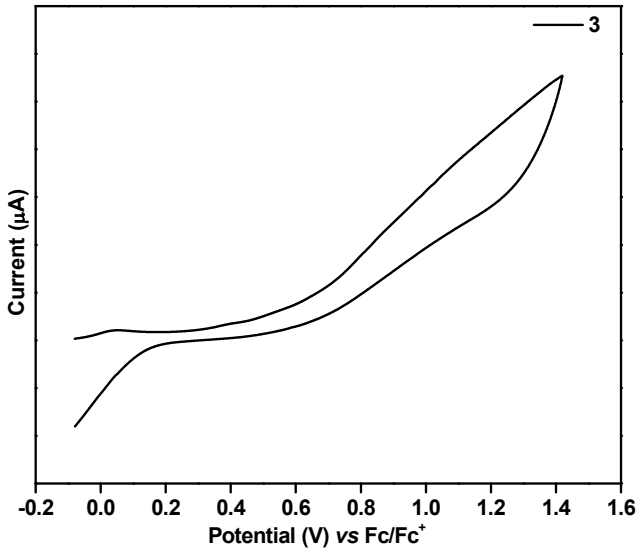

Fig. S21: Anodic scan of **3**, revealing no well-resolved oxidation in the CV experiment.

We have not calculated the HOMO energy of **3**, as the oxidation peak cannot be clearly defined from the CV scan. Thus, the electrochemical HOMO-LUMO gap is not calculated.

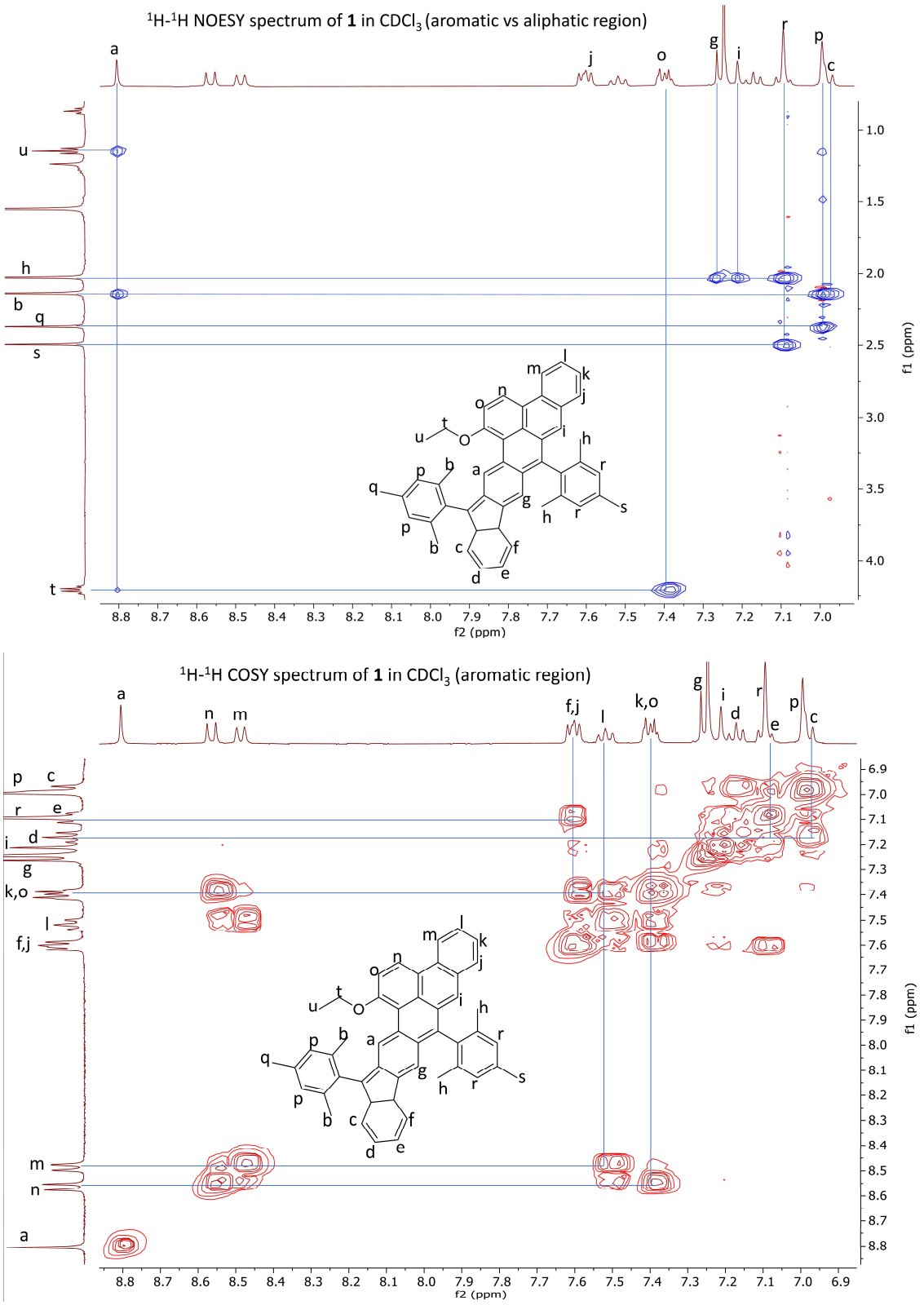

Fig. S22. 2D gNOESY (top) and 2D gCOSY (bottom) spectra of **1** in $CDCl_3$ at 298 K.

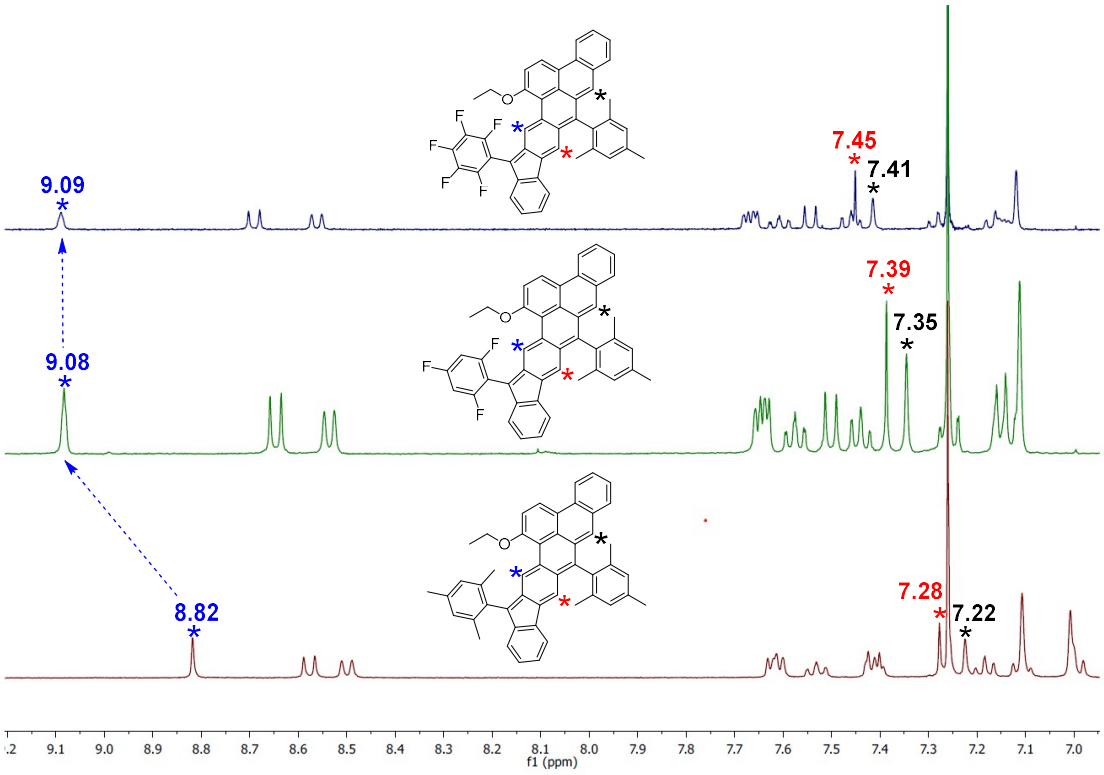

Fig. S23 Partial ^{1}H NMR spectra of compounds **1**, **2** and **3** showing a downfield chemical shift of core protons for the starred (*) singlets as core aromaticity is enhanced from **1** to **3**.

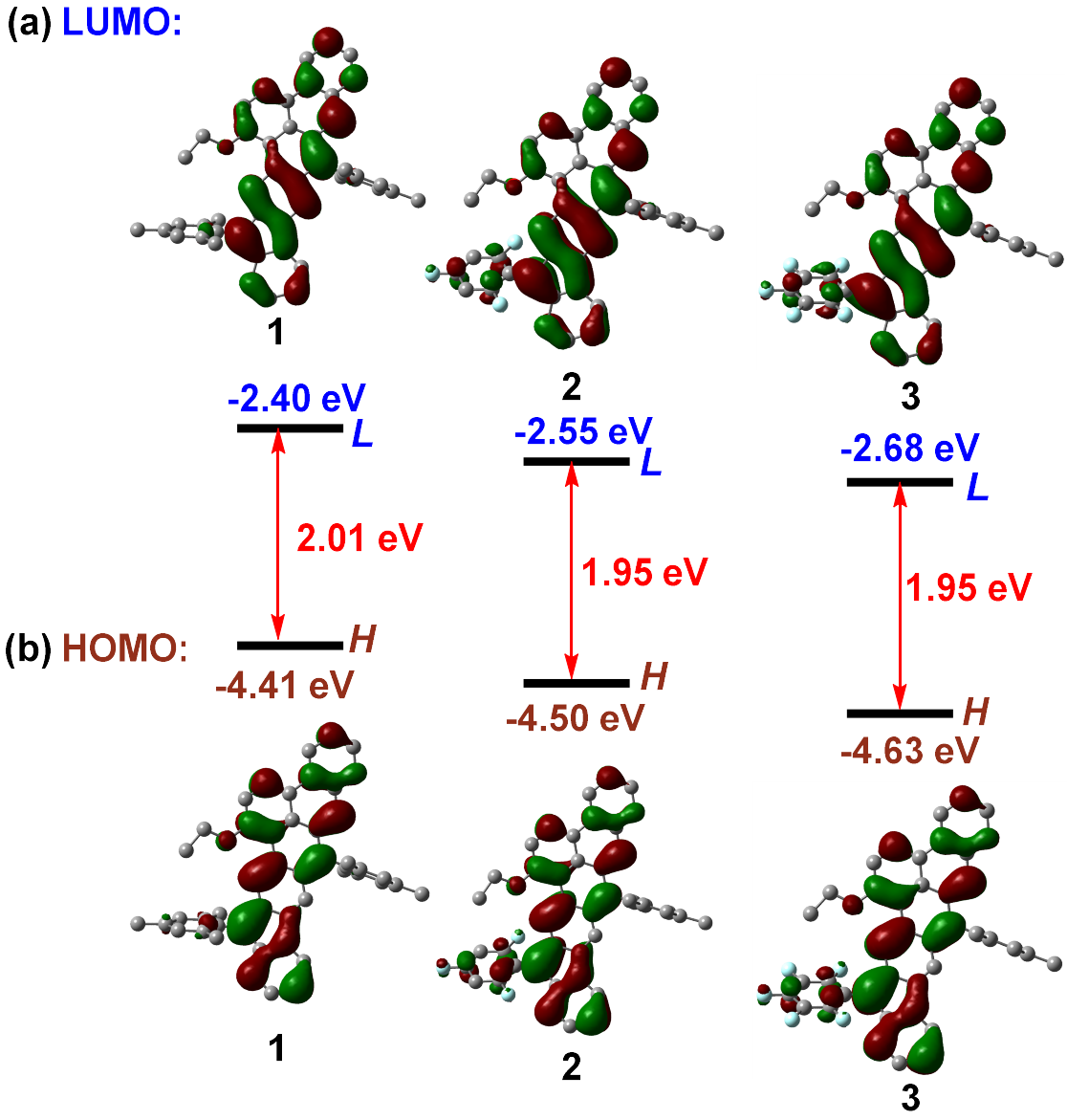

Fig. S24 Frontier molecular orbital profiles of **1**, **2**, and **3**.

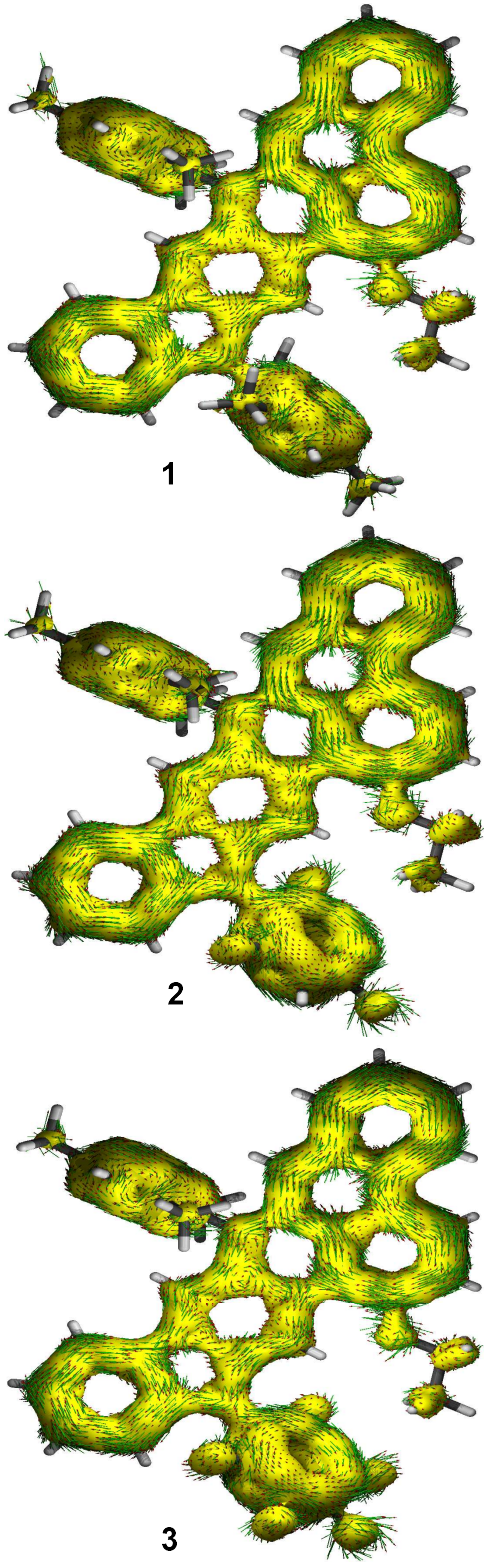

Fig. S25 Current–density vectors for **1-3** plotted onto the ACID isosurface of 0.02.

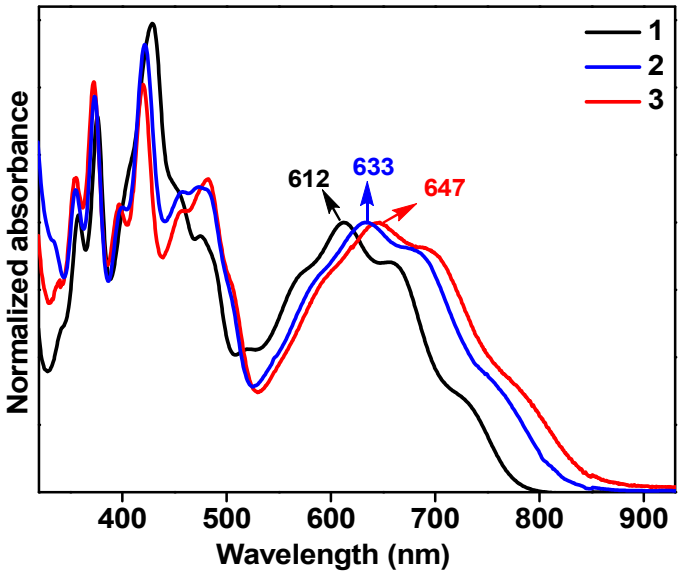

Fig. S26 Normalized absorbance plots for **1**-**3**.

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