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Mallory Reaction of Stilbene Imines: Corannulene Substrates Provide an Exception to the Rule in Oxidative Photocyclizations of Diarylethenes

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General Methods and Materials

All reagents were obtained from commercial suppliers and were used without further purification. Benzophenone imine with the methoxy groups was synthesized following a procedure given in: WO 2007/55698 (A1), "Improved method for making amino acid glycosides and glycopeptides" by Robin Polt. The trifluoromethyl imine was synthesized following a procedure given in: WO2009113409, "Process for stereoselective preparation of diamino acid derivatives", by Shu Kobayashi, Yasuhiro Yamashita and Kazutaka Seki. Solvents were purified by standard procedures. All reactions with air- and moisture-sensitive reagents were carried out in flame-dried reaction vessels under nitrogen atmosphere. Reactions were monitored by thin-layer chromatography (TLC) on silica gel-coated aluminum plates (60 F254, Merck) and visualized with UV light (λ = 254 and 366 nm). Column chromatography purifications were carried out on silica gel 40−63 mesh as the stationary phase. ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV-300, Bruker BBFO-400, Bruker AV-400 or Bruker AV-500 spectrometers. Chemical shifts are recorded in parts per million (ppm) relative to tetramethylsilane (δ = 0.00 ppm) and chloroform (δ = 7.26 ppm). ^{1}H NMR splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublets), m (multiplet), etc. ^{13}C NMR chemical shifts are reported relative to $CDCl_3$ (δ = 77.00 ppm). High−resolution mass spectra (HRMS) were recorded by using Waters Q−Tof Premier spectrometer in ESI+ mode with TOF mass analyser. Voltammetric measurements were performed using a Metrohm Autolab PGSTAT302N potentiostat in a three-electrode setup. A 1 mm diameter planar disk glassy carbon disk (GC, Cypress Systems) was used as a working electrode in conjunction with a platinum wire counter electrode (Metrohm) and a silver wire miniature reference electrode (eDAQ) connected to the test solution via a salt bridge containing 0.5 M tetra-n-butylammonium hexafluorophosphate (nBu$_4$NPF$_6$) in DMF (Tedia). nBu$_4$NPF$_6$ was synthesized through a standard procedure according to the literature (Kissinger, P.; Heineman, W. R. Laboratory Techniques in Electroanalytical Chemistry, Second ed.; CRC Press, 1996) and used as the supporting electrolyte. All voltammetric experiments were conducted under an argon atmosphere at room temperature in a Faraday cage. Prior to each scan, the working electrode was cleaned by polishing it with an alumina oxide (grain size 0.3 μm) slurry on a Buehler Ultrapad polishing cloth, rinsing it with acetone, and then drying it with a lint free tissue. In accordance with IUPAC recommendations, the absolute potentials were calibrated using ferrocene (Fc) as an internal reference which was added to the test solution at the end of the measurements.

Compound 3. Yield: 61% (125 mg). Yellow solid. ^{1}H NMR (300 MHz, CD_2Cl_2) δ 7.73 (d, J = 8.4 Hz, 2H), 7.52-7.36 (m, 3H), 7.32-7.23 (m, 3H), 7.18-7.07 (m, 4H), 6.91 (t, J = 7.4 Hz, 1H), 6.69 (d, J = 7.4 Hz, 2H). ^{13}C NMR (75 MHz, CD_2Cl_2) δ 168.38, 151.94, 140.01, 136.76, 131.09, 129.77, 129.60, 128.83, 128.53, 128.28, 123.35, 121.07. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{19}H_{15}N$, 258.1283; found, 258.1288.

Compound 5. Yield: 81% (165 mg). Orange solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.24 (d, *J* = 9.1 Hz, 1H), 8.13 (d, *J* = 7.8 Hz, 2H), 8.04 (d, *J* = 9.1 Hz, 1H), 8.00-7.86 (m, 6H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.50 (t, *J* = 7.2 Hz, 2H), 7.18-7.07 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.68, 146.65, 139.88, 136.89, 132.07, 131.99, 131.43, 129.96, 129.37, 129.04, 128.72, 128.27, 127.82, 127.74, 127.13, 126.47, 126.02, 125.52, 125.40, 125.33, 125.04, 124.87.123.70, 122.92, 117.94.

Compound 9. Yield: 71% (92 mg). Yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 – 7.85 (m, 3H), 7.81 – 7.73 (m, 5H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.56 – 7.41 (m, 5H), 7.36 – 7.28 (m, 3H), 6.88 (s, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 170.02, 150.72, 139.84, 136.81, 136.42, 136.32, 135.90, 135.63, 133.17, 132.76, 132.53, 131.45, 131.17, 130.43, 130.35, 130.09, 129.98, 129.23, 128.68, 128.52, 127.68, 127.63, 127.46, 127.44, 127.40, 127.29, 126.72, 126.65, 125.33. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{33}H_{19}N$, 430.1596; found, 430.1593.

Compound 11. Yield: 71% (105 mg). Yellow solid. ^{1}H NMR (300 MHz, CD_2Cl_2) δ 7.88 – 7.70 (m, 8H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.28 (s, 1H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.93 (s, 1H), 6.81 (d, *J* = 8.3 Hz, 2H), 3.91 (s, 3H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.18, 162.51, 160.33, 153.81, 151.39, 136.42, 136.36, 135.96, 135.63, 132.97, 132.79, 131.98, 131.80, 131.45, 131.13, 130.34, 127.60, 127.58, 127.45, 127.26, 126.65, 126.51, 125.43, 114.51, 113.91, 113.79, 55.88, 55.55. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{35}H_{23}NO_2$, 490.1807; found, 490.1799.

Compound 13. Yield: 50% (85 mg). Yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.99 (d, *J* = 8.2 Hz, 2H), 7.88 – 7.81 (m, 4H), 7.79 – 7.73 (m, 5H), 7.64 – 7.60 (m, 3H), 7.57 (d, *J* = 8.2 Hz, 2H), 6.8 (s, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.18, 149.42, 142.44, 139.80, 136.47, 136.26, 136.02, 135.72, 133.61, 133.21, 132.88, 132.23, 131.54, 131.35, 131.18, 130.73, 130.45, 130.20, 127.90, 127.84, 127.77, 127.57, 127.49, 127.37, 126.96, 126.70, 125.92, 125.88, 125.85, 125.61, 124.96, 123.16, 122.90, 114.18. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{35}H_{17}F_6N$, 566.1343; found, 566.1340.

Compound 10. Yield: 94% (42 mg). Yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.52 (d, *J* = 8.4 Hz, 1H), 8.76 (d, *J* = 8.7 Hz, 1H), 8.70 (d, *J* = 8.7 Hz, 1H), 8.37 (d, *J* = 8.3 Hz, 1H), 8.08 – 7.86 (m, 9H), 7.79 – 7.73 (m, 1H), 7.68 – 7.56 (m, 3H). ^{13}C NMR (101 MHz, C_6D_5Cl) δ 159.27, 144.25, 140.46, 138.12, 136.80, 135.73, 135.58, 135.36, 134.89, 134.63, 133.98, 131.79, 131.18, 131.06, 130.85, 130.50, 130.38, 129.90, 128.97, 128.72, 127.97, 127.80, 127.70, 127.36, 127.11, 127.02, 126.93, 125.95, 124.15. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{33}H_{17}N$, 428.1439; found, 428.1452.

Compound 12. Yield: 99% (64 mg). Light yellow solid. ^{1}H NMR (300 MHz, CD_2Cl_2) δ 8.79 (d, *J* = 8.7 Hz, 2H), 8.64 (d, *J* = 8.8 Hz, 1H), 8.31 (d, *J* = 9.1 Hz, 1H), 8.00 – 7.74 (m, 8H), 7.32 (dd, *J* = 9.1, 2.4 Hz, 1H), 7.14 (d, *J* = 8.7 Hz, 2H), 4.18 (s, 3H), 3.94 (s, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 161.69, 160.83, 158.72, 144.70, 138.23, 137.71, 136.84, 135.89, 135.04, 134.86, 132.77, 132.18, 131.90, 131.46, 131.32, 130.96, 130.30, 128.96, 128.45, 128.04, 127.92, 127.70, 127.55, 127.16, 126.57,

123.37, 121.45, 118.71, 114.16, 107.42, 56.21, 55.86. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{35}H_{21}NO_2$, 488.1651; found, 488.1661

Compound 14. Yield: 71% (40 mg). White solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.84 (s, 1H), 8.74 (d, *J* = 8.7 Hz, 1H), 8.62 (d, *J* = 8.7 Hz, 1H), 8.45 (d, *J* = 8.6 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 8.05 (d, *J* = 8.7 Hz, 2H), 7.98 – 7.88 (m, 7H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 157.66, 144.87, 143.22, 138.22, 137.06, 135.72, 135.67, 135.06, 134.77, 132.52, 132.20, 132.15, 131.52, 131.47, 131.30, 131.22, 129.70, 129.52, 129.40, 129.15, 128.58, 128.49, 128.28, 128.01, 127.90, 127.68, 127.29, 126.79, 126.26, 125.96, 125.92, 125.88, 125.84, 125.75, 125.70, 124.48, 123.41, 123.33, 123.30. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{35}H_{15}F_6N$, 564.1187; found, 564.1177

Compound 16. Yield: 62% (79 mg). Brown solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 – 7.68 (m, 8H), 7.54 – 7.21 (m, 18H), 3.62 (t, *J* = 7.1 Hz, 2H), 1.68 – 1.55 (m, 2H), 1.35 - 1.17 (m, 30H), 0.86 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.29, 169.70, 151.82, 136.22, 135.50, 134.95, 131.47, 130.83, 129.85, 129.18, 128.63, 128.46, 127.88, 125.79, 125.64, 112.13, 37.95, 32.14, 29.90, 29.86, 29.83, 29.81, 29.70, 29.56, 29.47, 28.99, 27.07, 22.90, 14.32. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{66}H_{63}N_3O_2$, 930.4999; found, 930.4984.

Compound 18. Yield: 76% (54 mg). Orange oily. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.86 – 7.78 (m, 8H), 7.40 – 7.31 (m, 6H), 7.01 – 6.93 (m, 4H), 6.85 – 6.77 (m, 4H), 3.89 (s, 6H), 3.71 (s, 6H), 3.61 (t, *J* = 7.2 Hz, 2H), 1.65 – 1.60 (m, 2H), 1.32 – 1.21 (m, 30H), 0.86 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.80, 169.47, 162.65, 160.45, 152.68, 136.03, 135.62, 135.01, 132.69, 132.48, 131.94, 131.64, 130.99, 128.71, 128.06, 125.99, 125.84, 113.89, 112.07, 55.80, 55.60, 38.08, 32.37, 30.13, 30.09, 30.07, 29.97, 29.79, 29.70, 29.19, 27.34, 23.13, 14.31. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{70}H_{71}N_3O_6$, 1050.5421; found, 1050.5432.

Compound 20. Yield: 46% (55 mg). Orange gummy. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.2 Hz, 4H), 7.82 (s, 4H), 7.74 (d, *J* = 8.0 Hz, 4H), 7.59 (d, *J* = 7.7 Hz, 4H), 7.51 (d, *J* = 7.7 Hz, 4H), 7.32 (s, 2H), 3.61 (t, *J* = 7.3 Hz, 2H), 1.68 – 1.56 (m, 2H), 1.35 – 1.16 (m, 30H), 0.87 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.42, 167.57, 150.65, 141.60, 139.00, 136.35, 135.50, 134.91, 133.54, 133.28, 131.73, 131.64, 131.46, 131.06, 130.44, 130.02, 129.93, 129.07, 127.67, 125.80, 125.49, 125.09, 124.84, 122.94, 122.67, 111.96, 38.03, 32.13, 31.80, 29.90, 29.86, 29.82, 29.78, 29.68, 29.56, 29.40, 28.97, 27.09, 22.90, 14.31. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{70}H_{59}F_{12}N_3O_2$, 1202.4494; found, 1202.4513.

Compound 17. Yield: 99% (70 mg). Light brown solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.90 (d, *J* = 8.3 Hz, 2H), 8.75 (d, *J* = 8.6 Hz, 2H), 8.32 (d, *J* = 8.2 Hz, 2H), 8.18 (d, *J* = 8.6 Hz, 2H), 8.12 (d, *J* = 8.3 Hz, 4H), 7.92 – 7.86 (m, 2H), 7.78 – 7.72 (m, 2H), 7.71 – 7.60 (m, 6H), 3.43 (t, *J* = 7.3 Hz, 2H), 1.40 – 1.31 (m, 2H), 1.29 – 1.08 (m, 30H), 0.86 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.39, 160.79, 145.19, 139.66, 138.93, 137.45, 136.87, 132.47, 132.40, 132.15, 131.77, 131.29, 131.09, 130.52, 129.67, 128.88, 128.84, 127.69, 127.13, 126.24, 125.70, 124.99, 123.25, 38.41, 32.33, 30.07, 30.05, 30.01, 29.97, 29.91, 29.83, 29.75, 29.50, 28.64, 27.19, 23.09, 14.28. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{66}H_{59}N_3O_2$, 926.4686; found, 926.4749.

Compound 19. Yield: 97% (50 mg). Orange solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.68 (d, *J* = 8.5 Hz, 2H), 8.26 (d, *J* = 9.1 Hz, 2H), 8.16-8.10 (m, 4H), 8.07 (d, *J* = 8.5 Hz, 4H), 7.38 (dd, *J* = 9.1, 2.4 Hz, 2H), 7.21 (d, *J* = 8.6 Hz, 4H), 4.1 (s, 6H), 3.99 (s, 6H), 3.47 (t, *J* = 7.1 Hz, 2H), 1.52 – 1.45 (m, 2H), 1.33 – 1.17 (m, 30H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.47, 161.13, 159.82,159.60, 145.74, 138.89, 138.57, 137.03, 132.46, 132.09, 132.03, 131.83, 131.54, 130.63, 130.04, 129.29, 126.02, 125.37, 122.11, 120.56, 119.28, 114.18, 111.68, 56.03, 55.86, 38.25, 32.36, 30.11, 30.08, 30.04, 30.01, 29.93, 29.78, 29.70, 29.05, 27.34, 23.12,14.31. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{70}H_{67}N_3O_6$, 1046.5108; found, 1046.5072.

Compound 21. Yield: 44% (20 mg). Yellow gummy. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.26 (s, 2H), 8.69 (d, *J* = 8.6 Hz, 2H), 8.36 (d, *J* = 8.7 Hz, 2H), 8.20 (d, *J* = 8.0 Hz, 4H), 8.12 (d, *J* = 8.6 Hz, 2H), 7.94 (d, *J* = 8.3 Hz, 6H), 3.43 (t, *J* = 7.0 Hz, 2H), 1.54 – 1.47 (m, 2H), 1.27 – 1.20 (m, 30H), 0.86 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.30, 159.23, 145.88, 142.16, 139.07, 137.77, 136.13, 132.80, 132.24, 132.00, 131.75, 131.31, 131.21, 131.09, 130.81, 130.78, 130.52, 130.26, 130.21, 130.17, 129.02, 128.57, 127.77, 126.50, 125.94, 125.91, 125.89, 125.86, 125.69, 125.41, 125.38, 125.00, 124.53, 124.27, 123.77, 123.74, 123.36, 123.23, 123.21, 38.36, 32.13, 29.90, 29.86, 29.82, 29.78, 29.56, 29.53, 29.45, 28.69, 26.95, 22.89, 14.31. HRMS (ESI) (m/z): $[M+H]^+$ calcd for $C_{70}H_{55}F_{12}N_3O_2$, 1198.4181; found, 1198.4199.

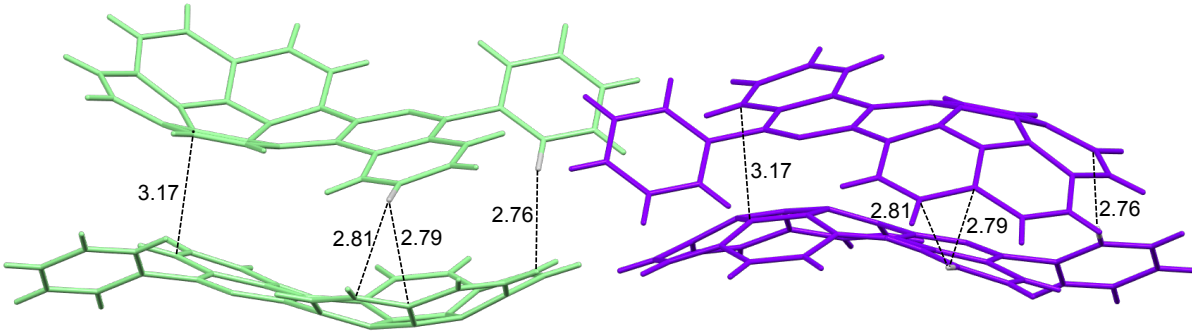

Figure S1. Molecular packing in a unit cell of **10**. The distances are given in Å.

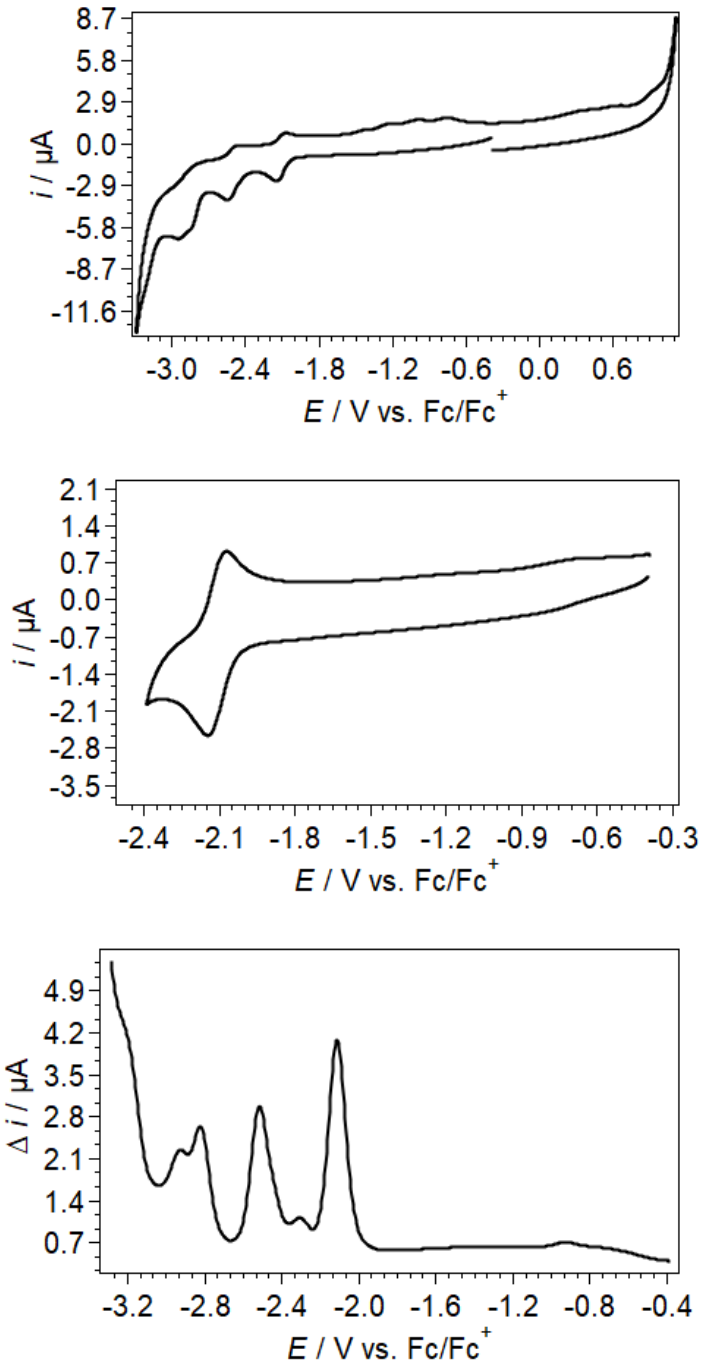

Figure S2. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **10** with 0.1 M nBu$_4$NPF$_6$/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

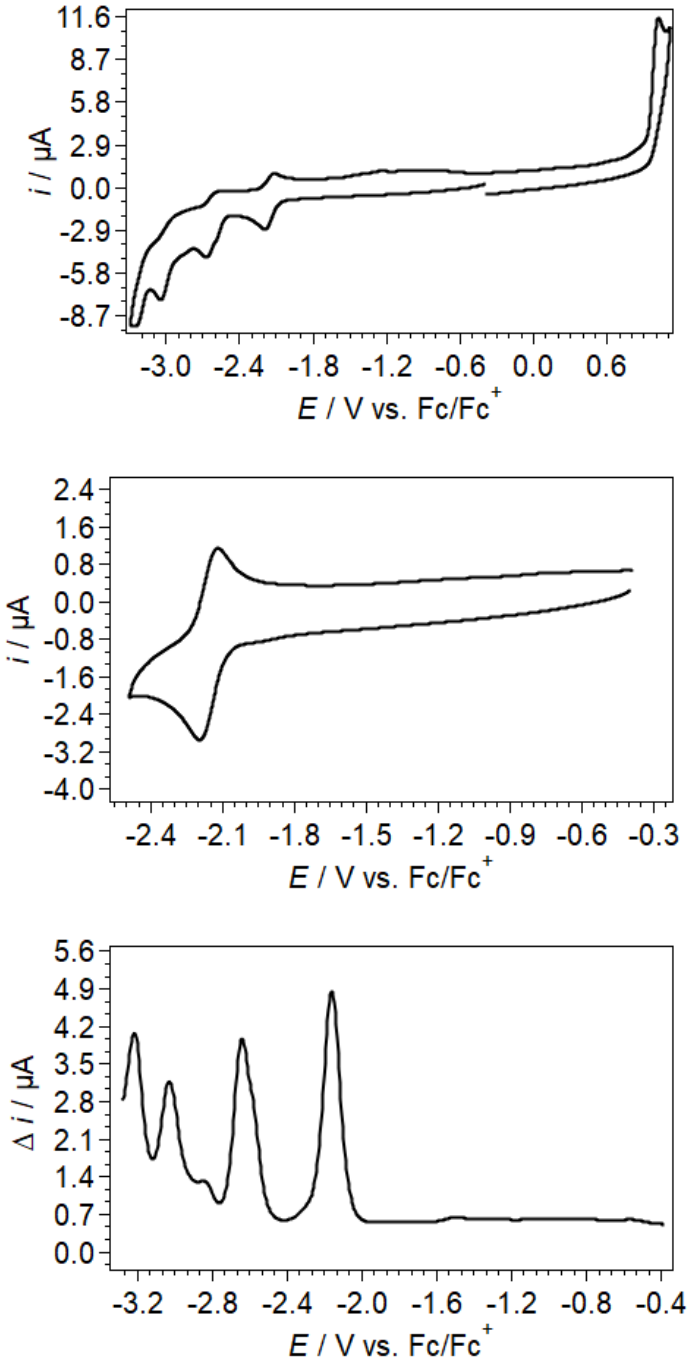

Figure S3. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **12** with 0.1 M *n*Bu_4NPF_6/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

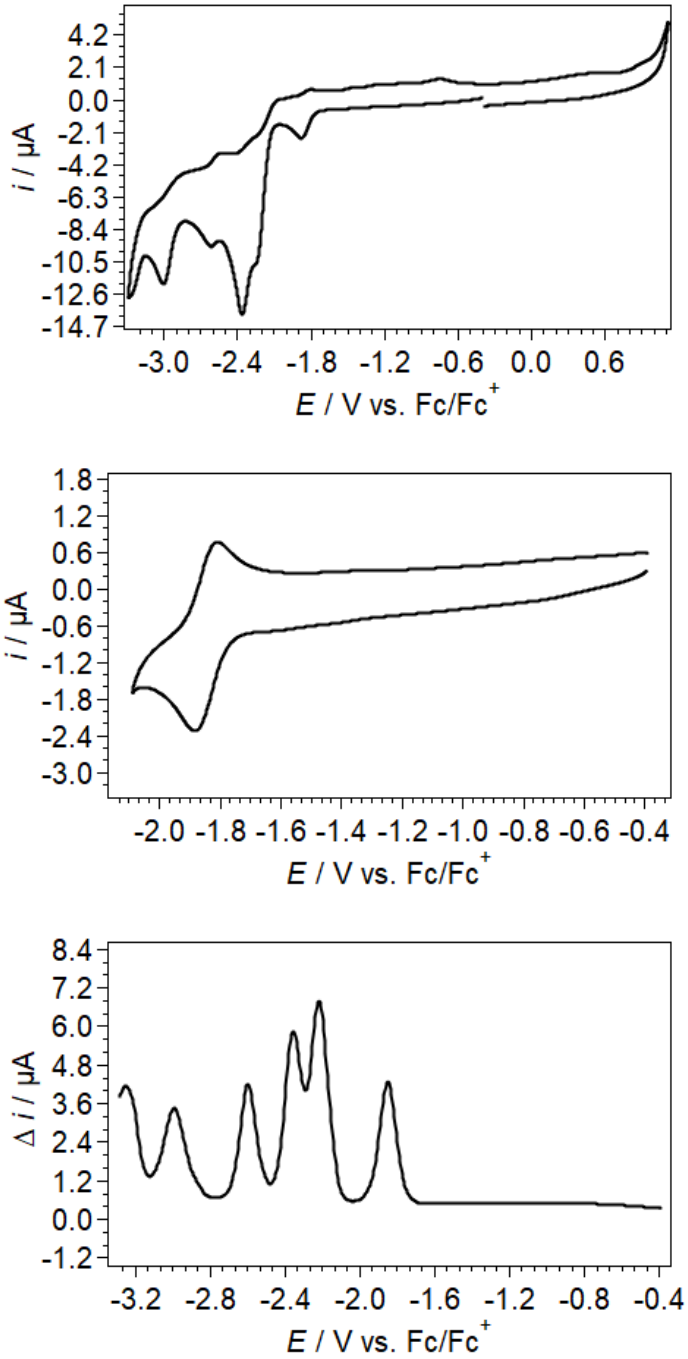

Figure S4. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **14** with 0.1 M nBu$_4$NPF$_6$/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

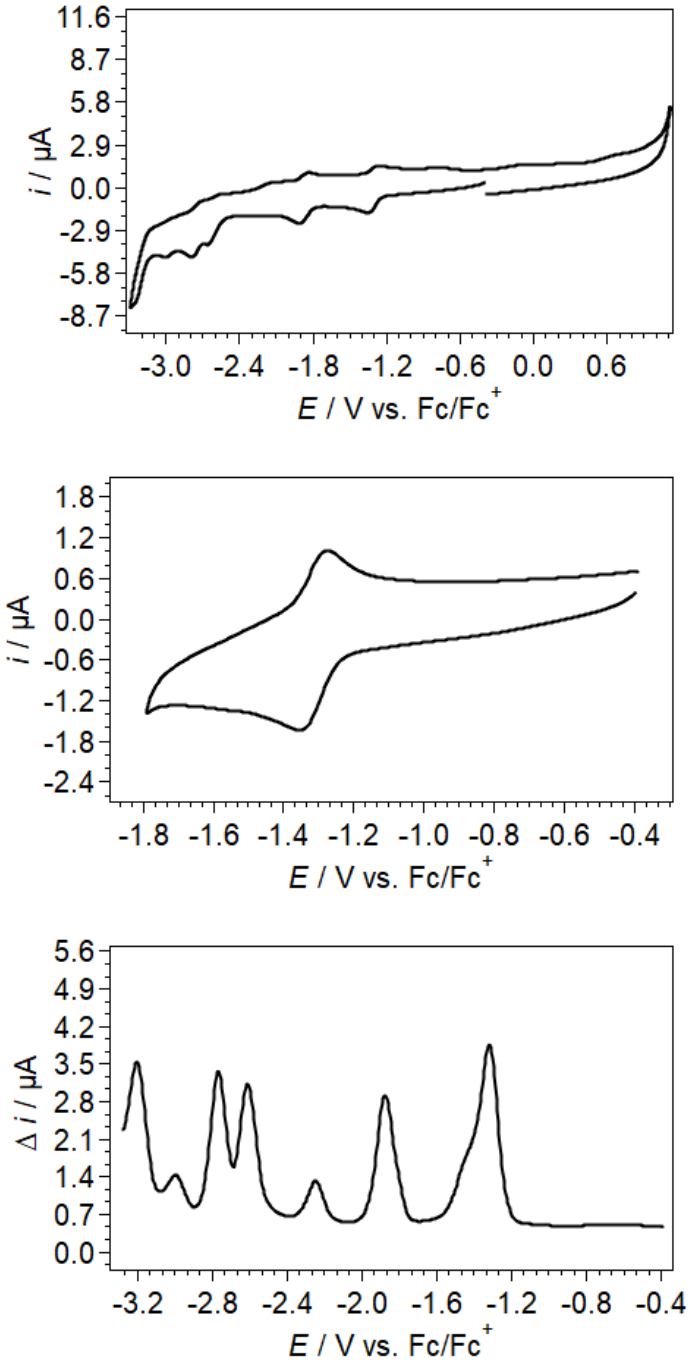

Figure S5. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **17** with 0.1 M *n*Bu_4NPF_6/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

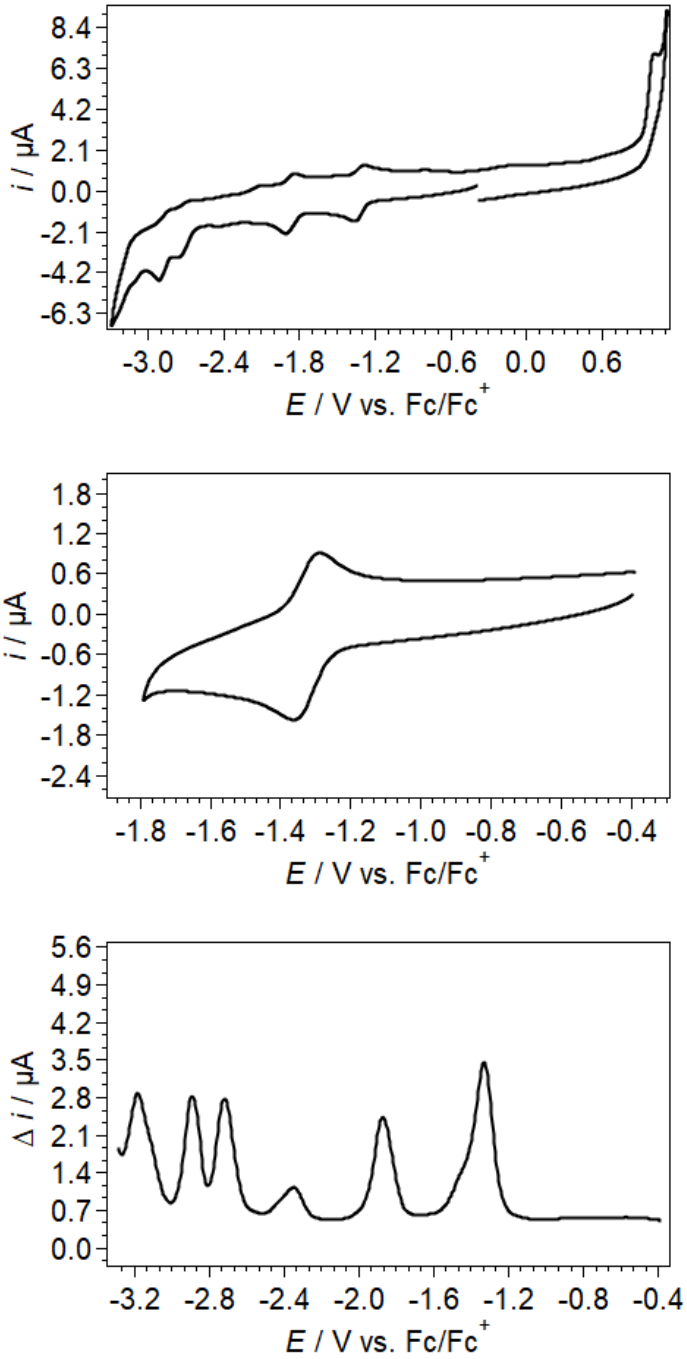

Figure S6. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **19** with 0.1 M nBu$_4$NPF$_6$/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

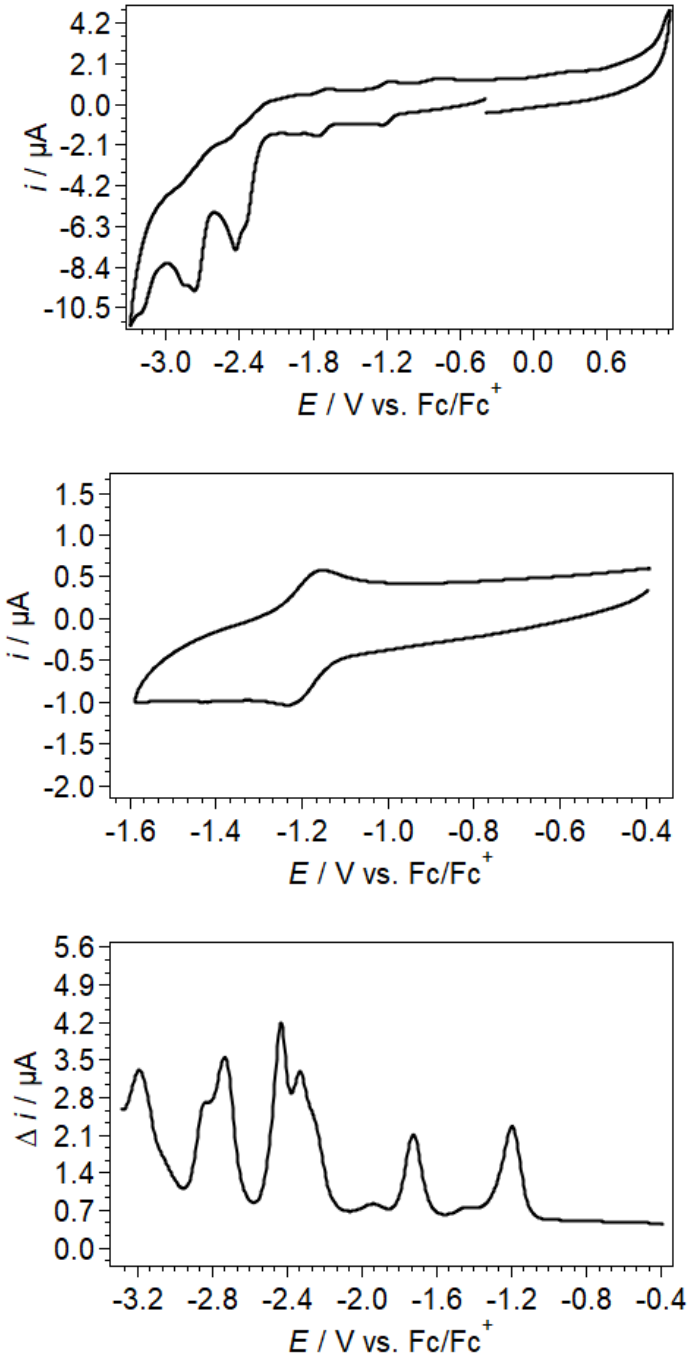

Figure S7. Overall cyclic (upper), first reduction (middle) and square-wave (bottom) voltammograms showing reduction processes of 1 mM compound **21** with 0.1 M *n*Bu_4NPF_6/DMF at 0.1 V s^{-1} using 1 mm diameter GC working electrode at 298±2 K in a Faraday cage.

Computational Details

To examine the electronic properties of the azahelicenes, we performed DFT calculations with the *Gaussian 16* suite of programs (Revision A.03).[1] The calculations were carried out with dispersion-corrected ωB97X-D exchange-correlation functional.[2] The ultrafine integration grid was used in all DFT computations. The nature of the stationary points was characterized by harmonic vibrational frequency calculations. No imaginary frequencies were seen for the

reported minima, while the transition states associated with the bowl-inversion had one negative Hessian eigenvalue.The Gibbs free energies reported in the present study were derived by combining ωB97X-D/Def2TZVPP electronic energies with the thermal and solvation contributions obtained at the ωB97X-D/Def2SVP level, according to the following formula below:

$$G = E_0' + (G_0 - E_0) + (G_{sol} - E_0) + \Delta G_{conc}.$$

In this formula, E_0' and E_0 are electronic energies calculated using Def2TZVPP and Def2SVP basis sets, respectively.[3] The G_0 is the gas-phase Gibbs free energy obtained from calculations at the ωB97X-D/Def2SVP level of theory (T = 298.15 K). The thermal contributions were estimated within the ideal gas−rigid rotor−harmonic oscillator approximation. The G_{sol} is the solution-phase Gibbs free energy which was derived from a single point energy calculation at the ωB97X-D/Def2SVP level using the implicit SMD solvation model (solvent = DMF as it was used for voltammetric measurements).[4] Although stoichiometry remains unchanged in the investigated conformational interconversion, we added ΔG_{conc} (1.89 kcal/mol) to the Gibbs free energy as it is conceptually substantiated when shifting from ideal gas standard state (p = 1 atm) to the standard concentration in solution phase (c = 1 mol/dm^3).

Computational Results

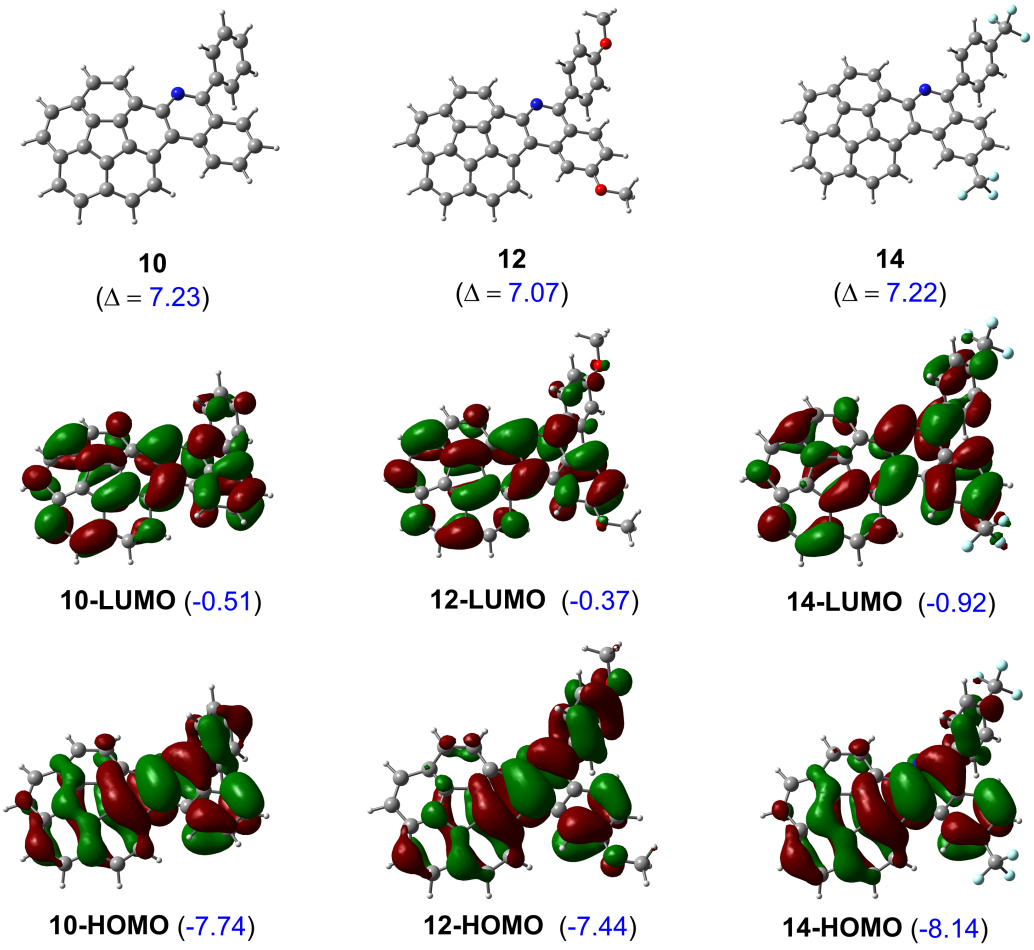

Figure S8. Frontier molecular orbitals of the single azahelicenes (isovalue = 0.03). Orbital energies calculated at the ωB97X-D/Def2TZVPP level and the HOMO-LUMO energy gaps (Δ) are given in parenthesis (in eV).

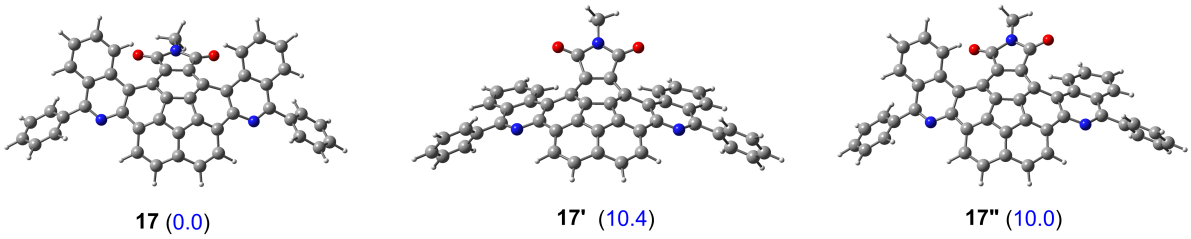

Figure S9. Computationally identified conformers for truncated **17** along with the relative stabilities given in parenthesis (in kcal/mol) with respect to **17**.

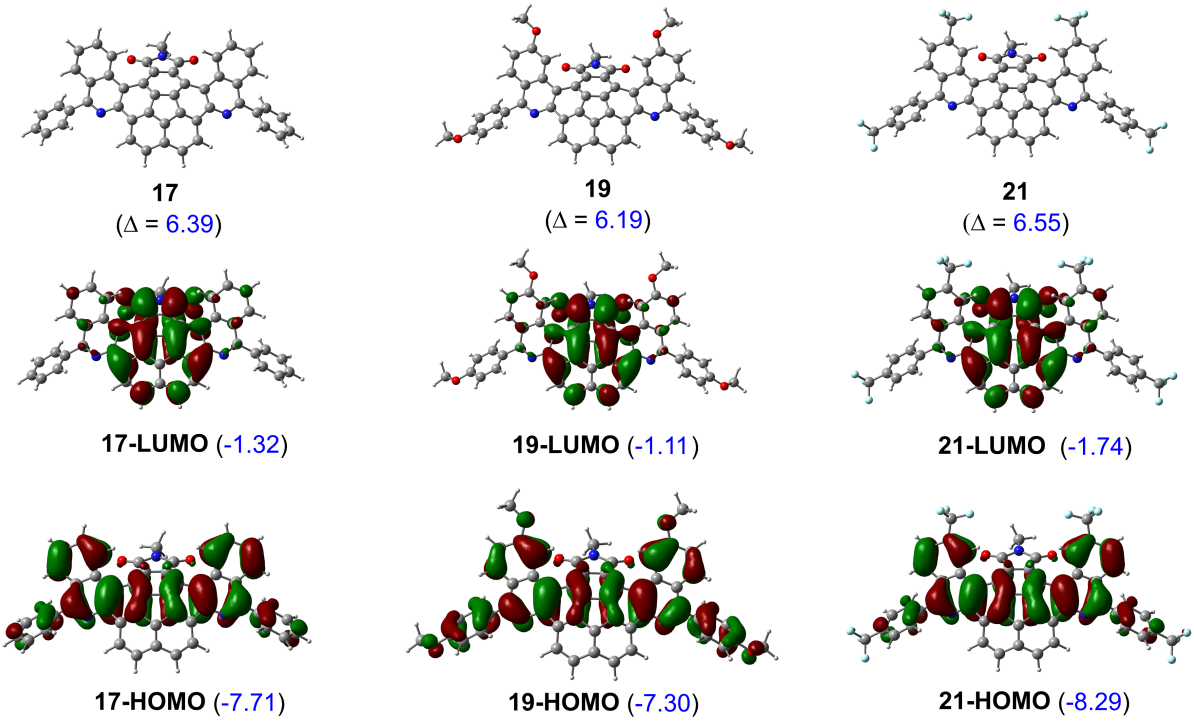

Figure S10. Frontier molecular orbitals of the double azahelicenes (isovalue = 0.03). Orbital energies calculated at the ωB97X-D/Def2TZVPP level and the HOMO-LUMO energy gaps (Δ) are given in parenthesis (in eV). For computations, the long $C_{18}H_{37}$ alkyl chain was simplified to Me-group.

To assess the sensitivity of the frontier molecular orbital energy trend, we calculated the HOMO and LUMO energies using larger and smaller basis sets, Def2TZVPP and Def2SVP, respectively. Table S1 compares the calculated orbital energies. The difference between the energies obtained with the two basis sets is minor. Consequently, the established trend is independent of the basis set and remains general.

Table S1. Summary of orbital energies calculated using Def2TZVPP and Def2SVP basis sets.

Compound	**Def2TZVPP**		**Def2SVP**	
	HOMO (eV)	LUMO (eV)	HOMO (eV)	LUMO (eV)
10	-7.74	-0.51	-7.76	-0.48
12	-7.44	-0.37	-7.44	-0.34
14	-8.14	-0.92	-8.17	-0.90
17	-7.71	-1.32	-7.73	-1.30
19	-7.30	-1.11	-7.30	-1.08
21	-8.28	-1.74	-8.31	-1.72

Computed energy components of the reported structures

Table S2. Compilation of energies (in Hartree) computed for optimized structures at the ωB97X-D/Def2SVP level of theory. For the definition of various energy components, see Computational details section.

Structure	E_0'	G_0	E_0	G_{sol} (DMF)	G
10	-1322.5203	-1320.7983	-1321.1489	-1321.1783	-1322.1962
10'	-1322.5191	-1320.7971	-1321.1474	-1321.1771	-1322.1954
10-TS	-1322.5032	-1320.7814	-1321.1326	-1321.1620	-1322.1783
12	-1551.5921	-1549.5493	-1549.9592	-1549.9923	-1551.2124
14	-1996.7298	-1994.2028	-1994.5506	-1994.5783	-1996.4067
17	-2197.0767	-2194.2352	-2194.7753	-2194.8205	-2196.5787
17'	-2197.0563	-2194.2155	-2194.7535	-2194.8005	-2196.5622
17''	-2197.0578	-2194.2169	-2194.7557	-2194.8025	-2196.5628
17-TS	-2197.0579	-2194.2154	-2194.7561	-2194.8022	-2196.5603
19	-3545.4971	-3541.0461	-3541.5803	-3541.6221	-3545.0015
21	-2655.2197	-2651.7375	-2652.3951	-2652.4480	-2654.6120

Cartesian coordinates of the reported structures

Cartesian coordinates of the optimized geometries are given below in standard XYZ format (units are in Å). The first line indicates the total number of atoms and the second line is the name of the molecule as presented in the article.

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10
C -5.780530 0.427582 0.920390
C -5.182510 1.673393 0.961164
H -5.673358 2.470757 1.525635
C -3.877670 1.915214 0.379961
C -2.901542 2.925139 0.692323
C -1.557319 2.772113 0.383285
H -0.871396 3.527185 0.769050
C -1.039617 1.599990 -0.288777
C 0.331585 1.063116 -0.362141
C 0.542074 -0.341516 -0.471856
C -0.572856 -1.268070 -0.680110
C -0.615557 -2.689886 -0.455094
C -1.816354 -3.365922 -0.307325
H -1.789451 -4.429524 -0.055458
C -3.085450 -2.678186 -0.348988
C -4.364826 -3.060399 0.210215
C -5.339811 -2.126642 0.514704
H -6.248696 -2.466683 1.018479
C -5.137748 -0.710285 0.295295
C -4.003308 -0.400779 -0.425052
C -3.387786 0.876088 -0.386765
C -2.017438 0.720289 -0.699363
C -1.784512 -0.671585 -0.915146
C -3.009583 -1.356839 -0.746723

H	-4.538375	-4.104174	0.485767
H	-3.198238	3.796642	1.282094
H	-6.724211	0.283704	1.453558
H	0.326613	-3.222797	-0.312879
N	1.764938	-0.907390	-0.301476
C	2.826260	-0.180707	-0.088216
C	2.787058	1.259244	-0.167255
C	1.516238	1.882410	-0.313938
C	3.961927	2.054475	-0.187880
C	1.480459	3.290122	-0.501677
C	3.889382	3.419450	-0.337405
H	4.934790	1.567955	-0.114234
C	2.634221	4.039310	-0.502747
H	0.529094	3.779474	-0.703856
H	4.802476	4.017358	-0.361217
H	2.578027	5.117930	-0.664626
C	4.082807	-0.928353	0.205189
C	4.410697	-2.047526	-0.569758
C	4.910805	-0.581532	1.280459
C	5.557194	-2.786801	-0.293571
H	3.749494	-2.330361	-1.390863
C	6.052665	-1.328930	1.563110
H	4.647407	0.266942	1.916318
C	6.382709	-2.428378	0.772459
H	5.807224	-3.651394	-0.912309
H	6.683799	-1.053877	2.410945
H	7.280239	-3.010999	0.991317

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10'

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C	5.230646	1.677009	-0.806939
H	5.742420	2.483112	-1.339503
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C	-0.546561	-0.342982	0.409366
C	0.560510	-1.276477	0.628027
C	0.604743	-2.695460	0.386105
C	1.807383	-3.373125	0.262079
H	1.784754	-4.433637	-0.002933
C	3.076923	-2.690385	0.351960
C	4.372679	-3.067125	-0.171871
C	5.360050	-2.131428	-0.427335
H	6.284039	-2.465878	-0.906797
C	5.155741	-0.718517	-0.188810
C	3.999034	-0.417790	0.499084

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C	2.008416	0.706116	0.731318
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H	4.552492	-4.106473	-0.459861
H	3.262899	3.811184	-1.155598
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H	-0.335634	-3.224074	0.218043
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H	-2.559319	5.142988	0.251246
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C	-4.170242	-1.955902	-1.090807
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H	-3.285136	-2.174134	-1.691634
C	-6.400109	-1.413060	0.487936
H	-5.189444	0.111326	1.414407
C	-6.457364	-2.423837	-0.470165
H	-5.374603	-3.491201	-2.004248
H	-7.265939	-1.208289	1.121364
H	-7.372323	-3.006358	-0.598207

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10-TS

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C	3.116591	4.467278	0.418644
H	4.233708	2.741976	1.001108
C	1.893900	4.942810	-0.095980
H	-0.040711	4.466444	-0.817059
H	3.940377	5.158519	0.606288
H	1.771448	6.006191	-0.312772
C	-0.599512	-0.742561	-0.780201
C	-0.506044	-2.186558	-0.906579

C	-1.807803	-0.273162	-1.166655
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H	0.421132	-2.683671	-0.613755
C	-2.859097	-1.057397	-1.639783
C	-2.212737	1.074199	-1.179999
C	-2.835883	-2.411736	-1.811282
H	-1.385467	-4.049464	-1.467050
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C	5.340874	-1.488844	1.183635
H	3.841182	-1.258088	-0.358234
C	5.817484	-1.024638	2.409867
H	5.532164	0.395100	4.012191
H	5.834600	-2.326757	0.686614
H	6.684720	-1.497493	2.875906

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H	-5.637137	2.493701	1.564295
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C	-1.021367	1.608749	-0.290433
C	0.344964	1.063485	-0.377046
C	0.547428	-0.340017	-0.504526
C	-0.576215	-1.256243	-0.712798
C	-0.626553	-2.679886	-0.500594

C	-1.830133	-3.350272	-0.349320
H	-1.807719	-4.416220	-0.106879
C	-3.095373	-2.654586	-0.374768
C	-4.373015	-3.033776	0.190556
C	-5.339956	-2.096797	0.510662
H	-6.247182	-2.435948	1.018124
C	-5.130977	-0.679682	0.302528
C	-3.999582	-0.370900	-0.423055
C	-3.375696	0.901722	-0.378458
C	-2.008800	0.740451	-0.703009
C	-1.786254	-0.650396	-0.932178
C	-3.014231	-1.330057	-0.760604
H	-4.551157	-4.078914	0.458093
H	-3.155483	3.808578	1.309719
H	-6.702469	0.314042	1.481336
H	0.313680	-3.219167	-0.370060
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C	2.803100	1.235891	-0.200727
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C	3.974084	2.028293	-0.234125
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C	3.920898	3.397540	-0.364010
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C	2.664781	4.034242	-0.494563
H	0.568763	3.802366	-0.671458
H	4.848623	3.968175	-0.397036
C	4.089526	-0.959274	0.132501
C	4.382841	-2.098147	-0.620360
C	4.963610	-0.613157	1.175530
C	5.524459	-2.858856	-0.376279
H	3.694531	-2.392633	-1.414695
C	6.097508	-1.366490	1.438047
H	4.737558	0.246054	1.811205
C	6.394108	-2.493162	0.657999
H	5.721790	-3.733627	-0.995908
H	6.772535	-1.109201	2.255800
O	7.521887	-3.159208	0.977911
O	2.514604	5.362421	-0.658917
C	3.648213	6.186645	-0.717512
H	4.235975	6.144013	0.215608
H	4.302648	5.925107	-1.566778
H	3.282016	7.210835	-0.856880
C	7.866219	-4.306902	0.250941
H	8.028719	-4.082186	-0.817713
H	8.803356	-4.681581	0.680164
H	7.095636	-5.092795	0.336609

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C	-5.784824	0.424684	0.885436
C	-5.189537	1.671889	0.922147
H	-5.685862	2.472289	1.477201
C	-3.880989	1.911731	0.348472
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C	-1.562961	2.775235	0.360148
H	-0.885055	3.538903	0.743139
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C	0.332043	1.060080	-0.361708
C	0.546403	-0.345954	-0.466314
C	-0.564819	-1.276369	-0.673472
C	-0.607312	-2.697199	-0.442662
C	-1.808788	-3.372537	-0.297432
H	-1.782642	-4.435053	-0.041359
C	-3.077941	-2.685584	-0.348638
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H	-6.249964	-2.470130	0.996868
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C	-3.997737	-0.409513	-0.442922
C	-3.384453	0.868255	-0.407711
C	-2.011626	0.712111	-0.707833
C	-1.775540	-0.680850	-0.914773
C	-3.000960	-1.366225	-0.752220
H	-4.535343	-4.108924	0.483264
H	-3.212228	3.803769	1.236941
H	-6.732024	0.282839	1.412710
H	0.333430	-3.230966	-0.294810
N	1.771766	-0.904112	-0.294359
C	2.830966	-0.174207	-0.084030
C	2.787741	1.263709	-0.164552
C	1.515007	1.878254	-0.312306
C	3.958653	2.067005	-0.181757
C	1.469570	3.285815	-0.497097
C	3.881255	3.428815	-0.325703
H	4.935731	1.589639	-0.107399
C	2.617509	4.039115	-0.490299
H	0.518778	3.774112	-0.697360
H	4.788424	4.035137	-0.344170
C	4.088505	-0.919995	0.210194
C	4.418551	-2.037571	-0.565622
C	4.915663	-0.571311	1.284219
C	5.564372	-2.774303	-0.292351
H	3.761638	-2.321827	-1.389080
C	6.058663	-1.313164	1.567740
H	4.654764	0.276831	1.920759
C	6.387757	-2.411770	0.775313
H	5.823510	-3.633803	-0.912847
H	6.695434	-1.036455	2.409280
C	7.600724	-3.245907	1.102253

C	2.561035	5.532184	-0.697523
F	1.310570	5.980202	-0.825728
F	3.233766	5.894533	-1.794366
F	3.116705	6.178995	0.333119
F	8.164979	-3.750148	0.000544
F	8.533600	-2.536788	1.744830
F	7.283200	-4.281489	1.888408

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C	-5.742883	0.650669	1.224059
C	-5.159043	1.945511	1.207214
C	-3.744798	2.102796	0.807537
C	-2.688130	2.936068	1.292155
C	-1.329383	2.734068	0.977693
C	-0.860142	1.674640	0.138684
C	0.483604	1.108333	-0.103306
C	0.635230	-0.295568	-0.258001
C	-0.529821	-1.173509	-0.413860
C	-0.618372	-2.598978	-0.248026
C	-1.840310	-3.235587	-0.096952
H	-1.848356	-4.308663	0.112016
C	-3.083214	-2.502378	-0.084531
C	-4.358225	-2.862017	0.487928
C	-5.297315	-1.904910	0.838929
H	-6.209461	-2.203917	1.358761
C	-5.052003	-0.502645	0.636596
C	-3.925017	-0.194627	-0.079512
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C	-1.721850	-0.521308	-0.591122
C	-2.966457	-1.167505	-0.434314
H	-4.557003	-3.906823	0.741132
H	0.307035	-3.170514	-0.155190
N	1.849370	-0.895869	-0.235975
C	2.949647	-0.192585	-0.189276
C	2.932652	1.240675	-0.334672
C	1.671778	1.895550	-0.286546
C	4.100839	1.997730	-0.614644
C	1.623087	3.287808	-0.553196
C	4.021609	3.349886	-0.845639
H	5.062797	1.489189	-0.682563
C	2.767344	3.996999	-0.822647
H	0.657040	3.790862	-0.581215
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C	4.214650	-0.962110	-0.025469
C	4.396803	-2.148601	-0.746674
C	5.200857	-0.562055	0.885451
C	5.553829	-2.904204	-0.581611

H	3.614766	-2.468890	-1.437385
C	6.353631	-1.325718	1.058346
H	5.054240	0.342168	1.480669
C	6.536260	-2.493942	0.320182
H	5.689433	-3.821870	-1.158123
H	7.110092	-1.008620	1.779404
H	7.442312	-3.089382	0.452334
C	-6.040807	3.039852	1.506882
C	-7.323926	2.762428	2.052236
C	-5.730667	4.378846	1.156590
C	-7.670689	1.383004	2.281959
C	-8.238638	3.828664	2.258696
C	-6.633516	5.391926	1.365062
H	-4.775841	4.596601	0.679111
N	-6.940837	0.408148	1.808214
C	-8.897298	0.983566	3.026972
C	-7.897813	5.118586	1.929994
H	-9.233615	3.610641	2.647389
H	-6.378426	6.412940	1.074165
C	-9.694669	-0.056636	2.533815
C	-9.237245	1.580596	4.247797
H	-8.615303	5.928057	2.078064
C	-10.824621	-0.471608	3.232363
H	-9.412303	-0.535065	1.594336
C	-10.362424	1.156308	4.951967
H	-8.602946	2.368005	4.661358
C	-11.162633	0.134973	4.442538
H	-11.445021	-1.276282	2.831790
H	-10.610739	1.622691	5.907767
H	-12.047341	-0.193633	4.992308
C	-2.740467	3.898818	2.447211
C	-0.518970	3.566741	1.933433
N	-1.429118	4.258457	2.723980
O	-3.687946	4.277408	3.086755
O	0.675996	3.620734	2.070717
C	-1.058791	5.118352	3.821714
H	-1.430247	6.139810	3.657750
H	-1.479341	4.741079	4.764436
H	0.036199	5.128806	3.881296

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C	-0.759116	0.114047	0.504116
C	-0.090977	1.381926	0.551402
C	1.136831	1.605269	-0.233643
C	2.076109	2.693415	-0.471263
C	3.394046	2.493823	-0.891373
C	3.966025	1.176562	-1.137036
C	5.306724	0.563670	-1.173138
C	5.457397	-0.828750	-1.480769

C	4.306134	-1.729723	-1.568778
C	4.225220	-3.165856	-1.427835
C	3.026958	-3.807839	-1.139094
H	3.050395	-4.886933	-0.965291
C	1.781162	-3.084982	-0.971733
C	0.522099	-3.427950	-0.339605
C	-0.400953	-2.464336	0.048755
H	-1.301110	-2.769366	0.586110
C	-0.156745	-1.052977	-0.144174
C	0.960106	-0.772793	-0.873854
C	1.591167	0.493695	-0.905860
C	2.931291	0.290669	-1.333693
C	3.098799	-1.096966	-1.556716
C	1.884011	-1.748364	-1.284465
H	0.311512	-4.471567	-0.091150
H	5.148320	-3.747207	-1.472408
N	6.669040	-1.424996	-1.615653
C	7.776562	-0.756209	-1.452365
C	7.777719	0.616487	-1.018312
C	6.521948	1.245466	-0.787787
C	8.976040	1.335149	-0.768779
C	6.528305	2.491058	-0.111613
C	8.941185	2.582203	-0.192463
H	9.931642	0.882400	-1.032932
C	7.703019	3.139013	0.186298
H	5.589488	2.926728	0.216730
H	9.868710	3.125578	-0.002265
H	7.672786	4.094851	0.712973
C	9.035653	-1.519708	-1.698289
C	9.195778	-2.188204	-2.917579
C	10.030033	-1.642997	-0.719978
C	10.341092	-2.939802	-3.166126
H	8.407359	-2.114415	-3.669176
C	11.170757	-2.405198	-0.965228
H	9.899964	-1.157810	0.250081
C	11.332714	-3.048322	-2.191309
H	10.458368	-3.448504	-4.125423
H	11.934146	-2.502143	-0.190231
H	12.229204	-3.641446	-2.384637
C	-0.631583	2.329412	1.500039
C	-1.909483	2.086095	2.077539
C	0.086465	3.464257	1.953356
C	-2.526923	0.807712	1.837863
C	-2.503983	3.077120	2.901748
C	-0.481362	4.376341	2.810191
H	1.121949	3.597076	1.654441
N	-1.939223	-0.118535	1.132603
C	-3.852428	0.436891	2.416089
C	-1.810588	4.211577	3.249163
H	-3.519894	2.926274	3.266354

H	0.101316	5.236728	3.145103
C	-4.849115	-0.055705	1.565710
C	-4.104702	0.502611	3.792018
H	-2.275999	4.966368	3.885896
C	-6.084242	-0.445720	2.076355
H	-4.641964	-0.133106	0.496569
C	-5.337243	0.100961	4.303671
H	-3.322317	0.848879	4.471196
C	-6.332344	-0.366148	3.446575
H	-6.856891	-0.819174	1.400831
H	-5.517824	0.147247	5.379797
H	-7.299719	-0.676259	3.847664
C	1.750889	4.149440	-0.677519
C	3.919934	3.822584	-1.368237
N	2.912353	4.752082	-1.147868
O	0.693160	4.708802	-0.549182
O	4.964193	4.071624	-1.912128
C	2.995802	6.129506	-1.570315
H	3.715644	6.685654	-0.952881
H	3.316298	6.188442	-2.619749
H	1.998653	6.572753	-1.459791

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C	-5.814299	1.424337	-0.118931
C	-5.062476	2.484776	0.476283
C	-3.629443	2.657815	0.147197
C	-2.568567	3.526124	0.597904
C	-1.202773	3.189202	0.543536
C	-0.701327	2.013903	-0.121024
C	0.585949	1.285072	-0.158304
C	0.598614	-0.121550	-0.393982
C	-0.584553	-0.823377	-0.898325
C	-0.862049	-2.234254	-0.994846
C	-2.141021	-2.714804	-1.240803
H	-2.298431	-3.796653	-1.237955
C	-3.275757	-1.830444	-1.385683
C	-4.697164	-2.068405	-1.251965
C	-5.596622	-1.042934	-0.994878
H	-6.649659	-1.277012	-0.826403
C	-5.154339	0.318384	-0.816763
C	-3.840876	0.537406	-1.109828
C	-3.104344	1.663427	-0.658192
C	-1.728416	1.350543	-0.765352
C	-1.635799	-0.003492	-1.205321
C	-2.936281	-0.493013	-1.424170
H	-5.074709	-3.094101	-1.277387
H	-0.050409	-2.938494	-0.802462
N	1.693718	-0.881180	-0.146698
C	2.829029	-0.341129	0.205389

C	3.029070	1.084809	0.137088
C	1.883577	1.902704	-0.067035
C	4.318469	1.676722	0.142146
C	2.082741	3.280255	-0.331947
C	4.472094	3.025885	-0.073908
H	5.195792	1.043272	0.275577
C	3.342391	3.829147	-0.331825
H	1.227827	3.899982	-0.595380
H	5.470376	3.467707	-0.085319
H	3.469472	4.890215	-0.555448
C	3.908981	-1.280861	0.615108
C	4.091582	-2.472728	-0.097228
C	4.706904	-1.031650	1.739244
C	5.070128	-3.383301	0.289823
H	3.452061	-2.672506	-0.958729
C	5.678733	-1.949705	2.132497
H	4.550530	-0.122370	2.324199
C	5.867588	-3.123561	1.404888
H	5.210587	-4.304087	-0.280501
H	6.287214	-1.748640	3.016817
H	6.632967	-3.840258	1.710601
C	-5.773454	3.224982	1.495616
C	-7.194184	3.146798	1.548348
C	-5.125874	3.943928	2.531442
C	-7.843284	2.151990	0.736301
C	-7.907900	3.983371	2.446123
C	-5.836692	4.682654	3.446590
H	-4.049183	3.859953	2.646735
N	-7.159152	1.305819	0.016899
C	-9.325549	1.976403	0.712426
C	-7.241854	4.757339	3.365811
H	-8.997207	3.993245	2.410844
H	-5.306081	5.214993	4.238436
C	-9.989643	1.986011	-0.519570
C	-10.061266	1.736520	1.879522
H	-7.799259	5.392967	4.056390
C	-11.366845	1.790529	-0.581039
H	-9.411871	2.145355	-1.432182
C	-11.437960	1.529541	1.815794
H	-9.549314	1.687985	2.843268
C	-12.094902	1.564278	0.586851
H	-11.874654	1.809717	-1.547750
H	-11.998957	1.333180	2.732045
H	-13.174542	1.406640	0.538124
C	-2.644021	4.945553	1.085915
C	-0.487981	4.211335	1.389805
N	-1.391146	5.244622	1.609103
O	-3.560359	5.720921	1.003752
O	0.625459	4.183188	1.845502
C	-1.050449	6.484335	2.262353

H	-1.939816	7.126085	2.240059
H	-0.746768	6.303186	3.303132
H	-0.223665	6.986301	1.739969

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C	5.293897	1.142469	6.424976
C	5.910090	-0.161884	6.445060
N	5.887937	2.225592	6.980586
C	7.019527	2.131056	7.624979
C	7.579447	0.850037	7.968654
C	6.991573	-0.308788	7.388568
C	8.601670	0.706172	8.943027
C	7.413356	-1.575491	7.865908
C	9.017311	-0.539434	9.347841
H	9.028899	1.597995	9.401739
C	8.401211	-1.689573	8.813842
H	6.909517	-2.472932	7.517543
H	9.793958	-0.637709	10.108738
H	8.693131	-2.678938	9.171600
C	5.348745	-1.288169	5.658818
C	5.690456	-2.641987	5.247998
C	4.135057	-0.980228	5.104060
C	4.784602	-3.539646	4.643757
C	3.232336	-1.874857	4.502833
C	3.497956	0.273684	5.185955
C	3.392501	-3.226956	4.355331
C	2.050950	-1.160313	4.222423
C	3.973731	1.375554	5.815713
C	2.224207	0.161362	4.630615
C	2.138762	-3.899341	3.933602
C	0.888367	-1.682119	3.760765
C	3.021426	2.469951	5.814087
C	1.254187	1.126524	4.650869
C	0.975844	-3.136767	3.549418
C	-0.172058	-0.694918	3.687021
C	1.738402	2.350900	5.272351
H	3.306125	3.417057	6.276849
C	-0.002516	0.625616	4.112803
H	-1.150086	-0.999209	3.308773
H	1.078852	3.219700	5.344164
H	-0.867639	1.290681	4.047829
C	7.655604	3.416095	8.028712
C	9.025442	3.642886	7.843082
C	6.859518	4.447438	8.541962
C	9.589678	4.871566	8.180548
H	9.651026	2.859232	7.409518
C	7.426350	5.669869	8.889930
H	5.788555	4.274655	8.661406
C	8.793360	5.884802	8.711689

H	10.656905	5.039446	8.020854
H	6.796927	6.462690	9.299921
H	9.236956	6.845897	8.980807
C	1.929785	-5.324241	4.019946
C	0.766975	-5.899983	3.435784
C	2.776511	-6.169103	4.781306
C	-0.188849	-5.012047	2.827028
C	0.527815	-7.292499	3.572961
C	2.521451	-7.513435	4.904591
H	3.613981	-5.738223	5.323240
N	-0.110233	-3.718623	2.986816
C	-1.349108	-5.507414	2.035082
C	1.395804	-8.088843	4.280496
H	-0.378245	-7.721408	3.144555
H	3.184354	-8.134374	5.510434
C	-2.612713	-4.937866	2.234623
C	-1.192900	-6.485037	1.044022
H	1.193768	-9.155885	4.391984
C	-3.703350	-5.357983	1.479223
H	-2.724323	-4.158812	2.990722
C	-2.283344	-6.896180	0.279971
H	-0.205187	-6.911145	0.853538
C	-3.542008	-6.339509	0.500809
H	-4.686250	-4.914232	1.651876
H	-2.146213	-7.651353	-0.496928
H	-4.397373	-6.665674	-0.094896
C	5.591859	-4.682725	4.090652
C	7.069074	-3.220834	5.076509
N	6.916455	-4.443233	4.437329
O	8.133733	-2.732134	5.354829
O	5.219004	-5.607699	3.416160
C	8.026175	-5.262462	4.013318
H	8.746614	-4.663412	3.439140
H	8.544715	-5.697223	4.879755
H	7.625227	-6.066370	3.384134

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C	-5.742642	0.678191	1.248508
C	-5.143172	1.966624	1.277408
C	-3.727186	2.125527	0.885747
C	-2.665200	2.938739	1.394482
C	-1.309123	2.733851	1.077115
C	-0.849244	1.690608	0.212642
C	0.488585	1.115684	-0.038628
C	0.627868	-0.284171	-0.241867
C	-0.544274	-1.145059	-0.433395
C	-0.648358	-2.574367	-0.316922
C	-1.877496	-3.202313	-0.191116
H	-1.897786	-4.281820	-0.020431

C	-3.112315	-2.456125	-0.156278
C	-4.393358	-2.822389	0.398201
C	-5.324156	-1.868366	0.778235
H	-6.241445	-2.177154	1.282938
C	-5.063458	-0.462710	0.624819
C	-3.929812	-0.141447	-0.074614
C	-3.252356	1.111067	0.069701
C	-1.894567	0.905936	-0.248031
C	-1.728487	-0.473780	-0.590071
C	-2.980335	-1.111521	-0.459669
H	-4.604257	-3.873110	0.613613
H	0.269699	-3.160112	-0.242139
N	1.837312	-0.893206	-0.232531
C	2.942857	-0.202973	-0.144341
C	2.941865	1.234025	-0.226997
C	1.686512	1.893385	-0.174329
C	4.121240	1.996983	-0.444326
C	1.648704	3.296161	-0.379234
C	4.058144	3.356544	-0.605791
H	5.083041	1.489283	-0.516518
C	2.801986	4.007628	-0.580233
H	0.690261	3.809631	-0.413180
H	4.967233	3.933433	-0.783965
C	4.198124	-0.991813	0.002678
C	4.380413	-2.145191	-0.769939
C	5.170627	-0.645563	0.947861
C	5.524500	-2.919171	-0.623221
H	3.607912	-2.428883	-1.486208
C	6.313297	-1.424735	1.104908
H	5.023547	0.227767	1.586754
C	6.495497	-2.556986	0.312820
H	5.661968	-3.813794	-1.232952
H	7.059626	-1.156513	1.853906
C	-6.010904	3.056481	1.620120
C	-7.293766	2.781197	2.160119
C	-5.675257	4.401952	1.322893
C	-7.660416	1.400042	2.333155
C	-8.185478	3.856809	2.421488
C	-6.552063	5.419928	1.590552
H	-4.724963	4.626267	0.843276
N	-6.944913	0.434049	1.821904
C	-8.891937	0.988547	3.063446
C	-7.821608	5.151078	2.154956
H	-9.182863	3.645063	2.806880
C	-9.705261	-0.018374	2.529256
C	-9.218474	1.537414	4.308791
H	-8.516983	5.969996	2.346825
C	-10.837746	-0.445893	3.210361
H	-9.433454	-0.464605	1.571511
C	-10.347060	1.104060	4.998897

H	-8.571514	2.293987	4.757751
C	-11.162678	0.118619	4.445824
H	-11.469831	-1.227351	2.784992
H	-10.586723	1.526697	5.975505
C	-2.713226	3.879585	2.569260
C	-0.496240	3.544891	2.051410
N	-1.399152	4.224411	2.853705
O	-3.666373	4.247732	3.206486
O	0.698650	3.592275	2.194289
C	-1.001714	5.076231	3.950025
H	-0.444412	5.947005	3.577943
H	-1.913422	5.410293	4.459363
H	-0.363141	4.524455	4.653833
C	2.758822	5.499501	-0.792410
C	-6.188948	6.849731	1.279913
C	7.757723	-3.374051	0.431022
C	-12.420666	-0.317659	5.154279
F	-12.640324	-1.627660	5.005676
F	-13.495268	0.316112	4.669121
F	-12.370815	-0.062711	6.464424
F	8.658284	-3.011679	-0.490665
F	8.336769	-3.228383	1.625897
F	7.520013	-4.677171	0.253377
F	3.294292	5.836065	-1.971608
F	1.514484	5.980994	-0.765013
F	3.459579	6.138002	0.149868
F	-4.985965	6.956538	0.712232
F	-7.077371	7.404682	0.447362
F	-6.178629	7.593595	2.390478

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C	-5.745415	0.750247	1.203644
C	-5.140068	2.033535	1.245109
C	-3.719938	2.186271	0.871979
C	-2.657592	2.984550	1.402916
C	-1.297669	2.776540	1.095957
C	-0.833051	1.744412	0.220839
C	0.503898	1.169304	-0.026572
C	0.642116	-0.227721	-0.236909
C	-0.533541	-1.082100	-0.440754
C	-0.644002	-2.511766	-0.331549
C	-1.875992	-3.136953	-0.218992
H	-1.900716	-4.217167	-0.051973
C	-3.109447	-2.387805	-0.192277
C	-4.396688	-2.751143	0.350128
C	-5.327343	-1.795030	0.725782
H	-6.250230	-2.100975	1.222158
C	-5.061211	-0.389205	0.581182
C	-3.920061	-0.070185	-0.107318

C	-3.238955	1.178609	0.049855
C	-1.879938	0.970555	-0.256628
C	-1.715059	-0.407582	-0.604940
C	-2.970268	-1.042203	-0.488069
H	-4.612900	-3.802048	0.560445
H	0.272617	-3.099106	-0.250510
N	1.847610	-0.848362	-0.221236
C	2.956403	-0.161373	-0.127470
C	2.957507	1.275805	-0.214760
C	1.704771	1.951473	-0.164660
C	4.128005	2.035795	-0.448537
C	1.670510	3.342422	-0.374315
C	4.078259	3.399731	-0.622161
H	5.088348	1.526245	-0.530707
C	2.828943	4.065392	-0.586761
H	0.724670	3.881037	-0.397939
H	5.000706	3.946539	-0.816145
C	4.206562	-0.950402	0.029569
C	4.372732	-2.141887	-0.695405
C	5.201594	-0.588878	0.940246
C	5.505958	-2.920465	-0.538540
H	3.587504	-2.446946	-1.389268
C	6.344105	-1.370473	1.118686
H	5.078045	0.308952	1.550127
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C	-6.010844	3.133258	1.569315
C	-7.304460	2.848283	2.092116
C	-5.673408	4.466395	1.271322
C	-7.675498	1.468103	2.267386
C	-8.196125	3.923752	2.317201
C	-6.556247	5.501790	1.513032
H	-4.714343	4.712284	0.818462
N	-6.954716	0.500058	1.763805
C	-8.911159	1.062036	2.987085
C	-7.838148	5.224460	2.046908
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C	-9.697405	0.012861	2.483236
C	-9.283960	1.640021	4.202441
H	-8.559768	6.022759	2.218732
C	-10.829972	-0.415336	3.153273
H	-9.398295	-0.463493	1.547972
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C	-11.202805	0.181596	4.367796
H	-11.451951	-1.221294	2.760470
H	-10.664477	1.679325	5.848154
C	-2.713643	3.897248	2.597689
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O	-3.666238	4.248209	3.245124
O	0.701932	3.585056	2.267507
C	-1.008632	5.039525	4.028815
H	-1.922896	5.335973	4.557027
H	-0.358189	4.464877	4.703362
H	-0.464553	5.936071	3.699283
O	2.684936	5.391539	-0.777409
O	-6.134758	6.740386	1.190538
O	-12.318462	-0.301175	4.950443
O	7.572500	-3.360817	0.458450
C	-6.984790	7.836170	1.393602
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H	-7.909410	7.757188	0.795701
C	3.816446	6.184243	-1.013721
H	3.457528	7.214056	-1.129736
H	4.526288	6.149679	-0.169208
H	4.342849	5.886741	-1.937326
C	-12.741796	0.243952	6.169878
H	-13.656197	-0.291188	6.453275
H	-11.987640	0.106199	6.964352
H	-12.971925	1.320102	6.079951
C	8.603907	-3.045272	1.352890
H	8.247530	-3.020474	2.397522
H	9.358091	-3.835501	1.255002
H	9.071819	-2.074351	1.113062

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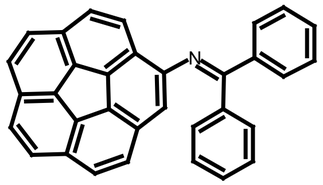
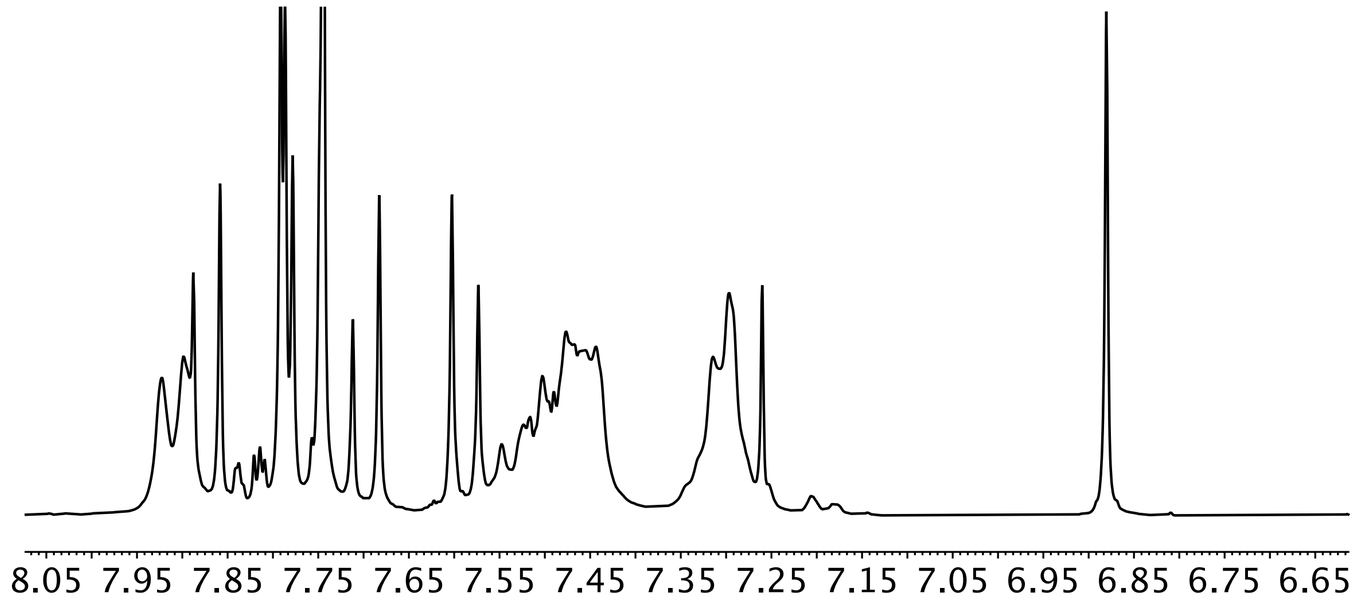
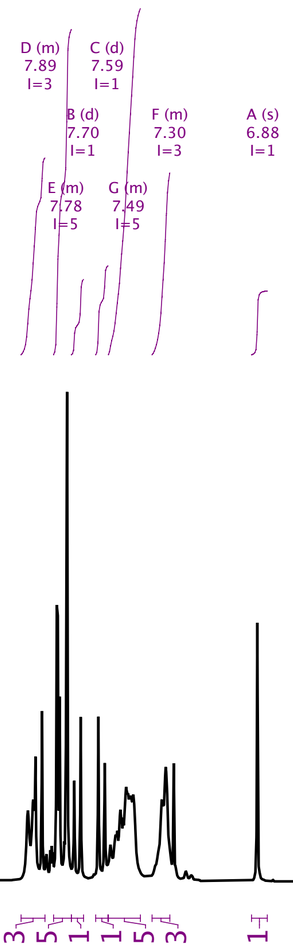
[3] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.*, **2005**, *7*, 3297.

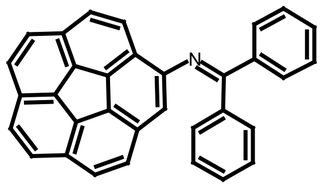
[4] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-6396.



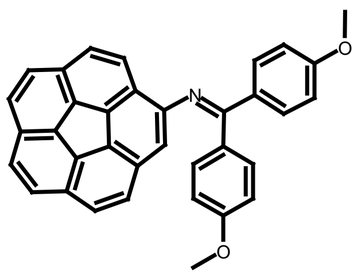
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 – 7.85 (m, 3H), 7.81 – 7.73 (m, 5H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.56 – 7.41 (m, 5H), 7.36 – 7.28 (m, 3H), 6.88 (s, 1H).



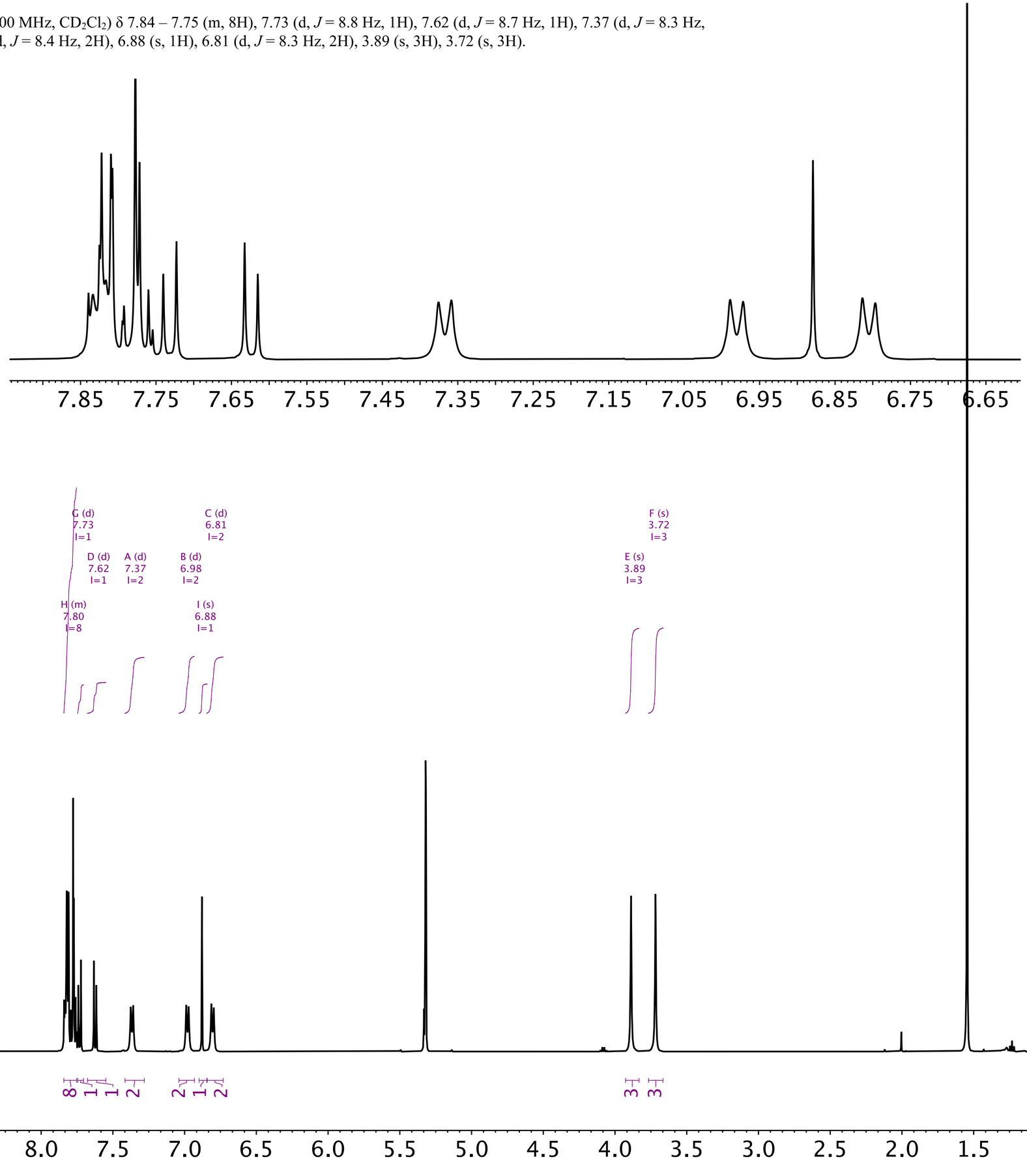


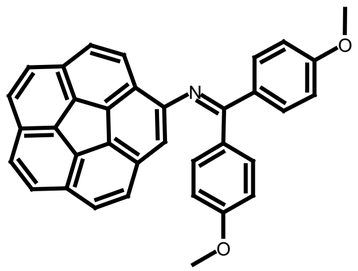


^{13}C NMR (101 MHz, CD_2Cl_2) δ 170.18, 150.88, 140.00, 138.26, 136.97, 136.58, 136.48, 136.06, 135.79, 133.34, 132.92, 132.70, 131.62, 131.34, 130.59, 130.51, 130.25, 130.14, 129.39, 128.85, 128.69, 127.84, 127.80, 127.63, 127.60, 127.56, 127.45, 126.88, 126.81, 125.50.

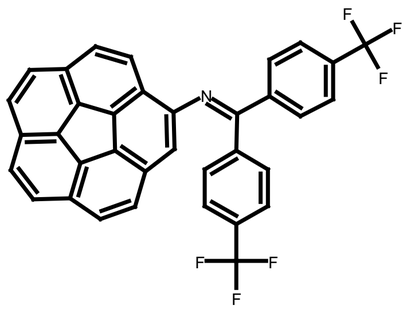


^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.84 – 7.75 (m, 8H), 7.73 (d, *J* = 8.8 Hz, 1H), 7.62 (d, *J* = 8.7 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.88 (s, 1H), 6.81 (d, *J* = 8.3 Hz, 2H), 3.89 (s, 3H), 3.72 (s, 3H).

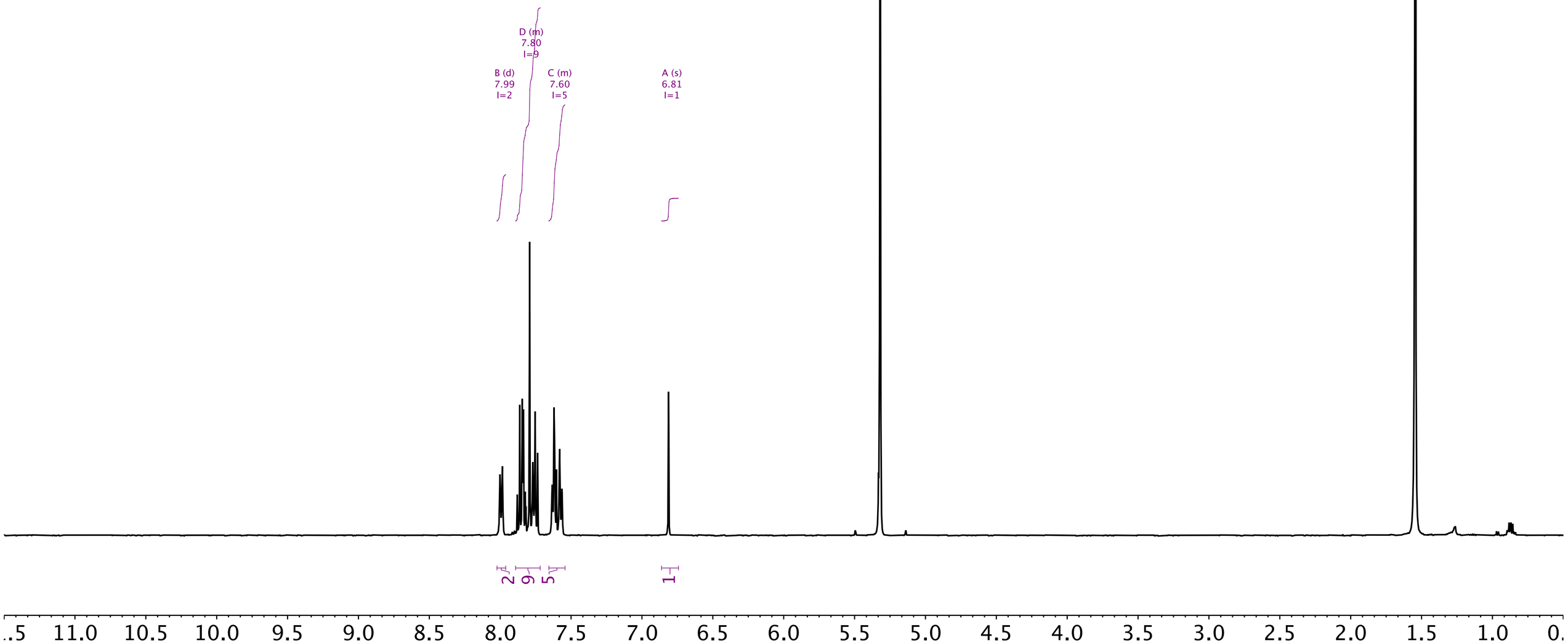


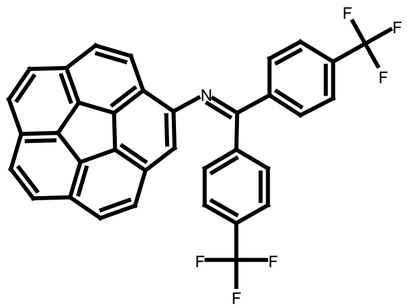


^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.34, 162.68, 160.52, 153.98, 151.53, 136.59, 136.53, 136.13, 135.79, 133.14, 132.96, 132.15, 131.97, 131.62, 131.29, 130.50, 127.78, 127.75, 127.62, 127.43, 126.82, 126.68, 125.60, 114.68, 114.08, 113.96, 56.05, 55.72, 54.54.

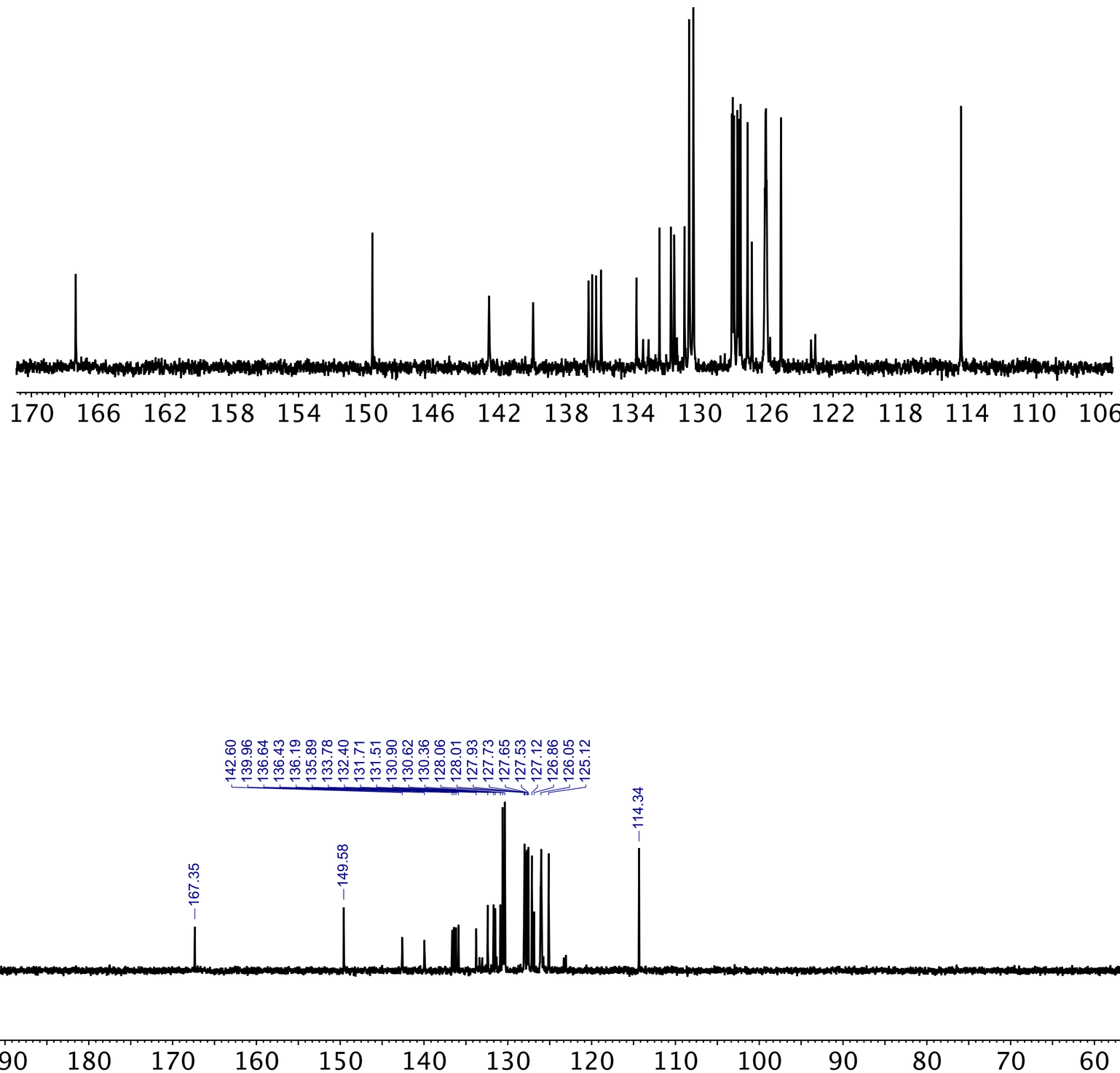


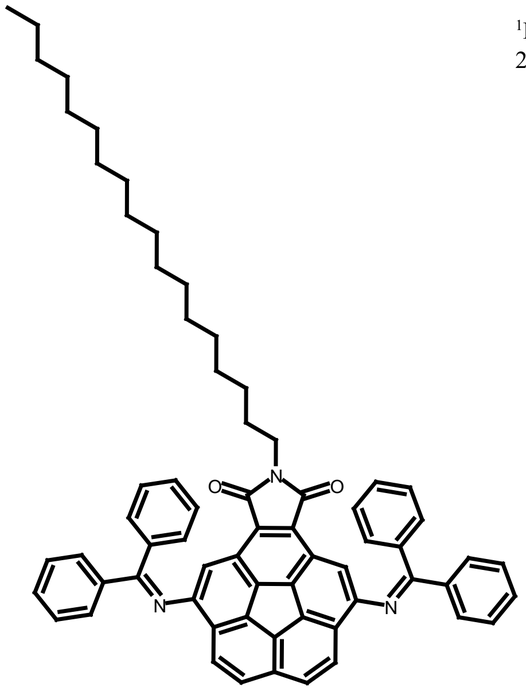
^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.99 (d, J = 8.1 Hz, 2H), 7.89 – 7.72 (m, 9H), 7.66 – 7.54 (m, 5H), 6.81 (s, 1H).



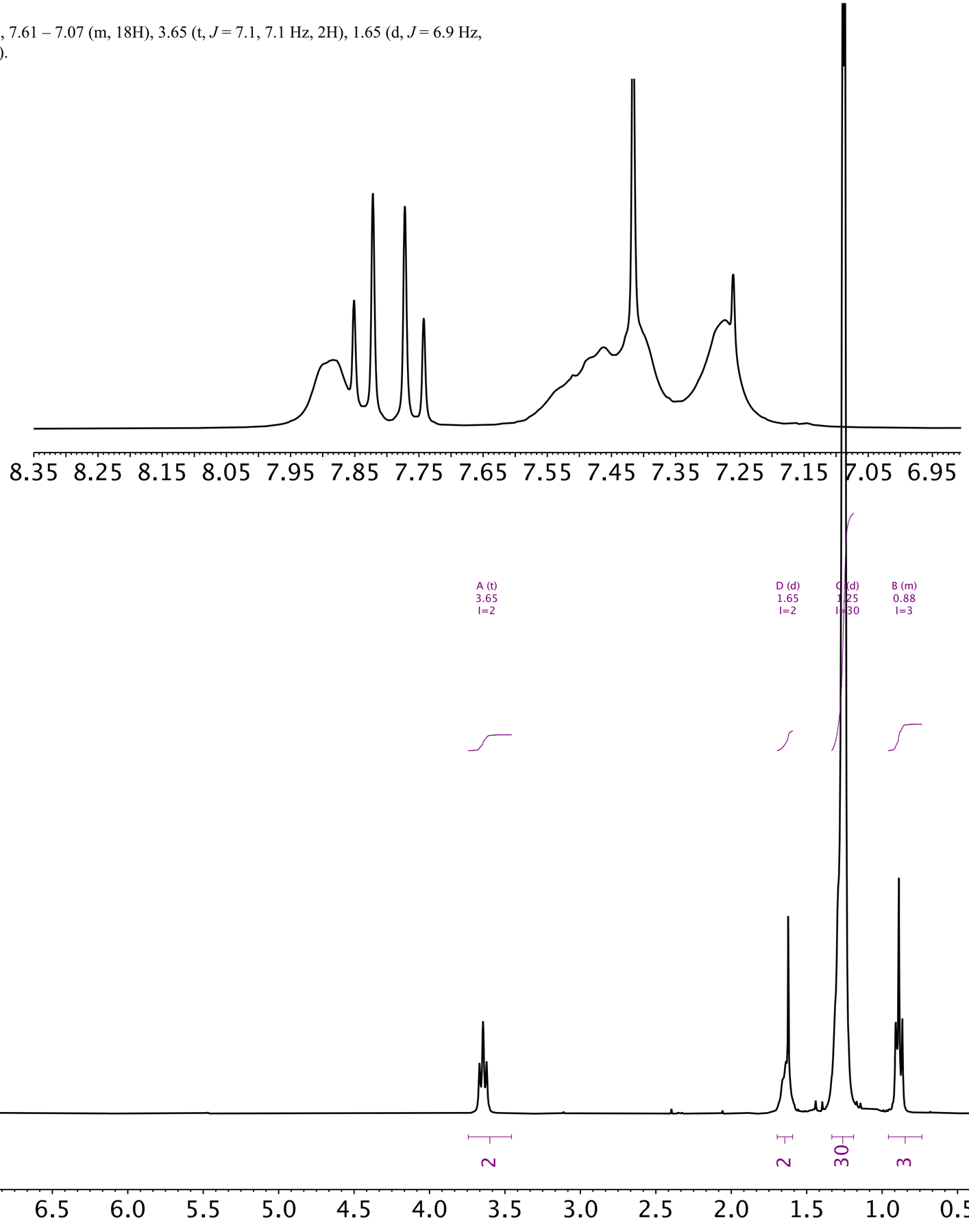


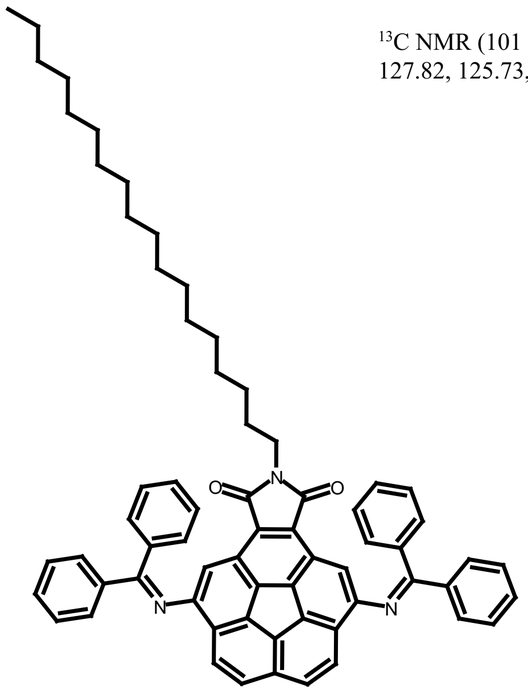
^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.35, 149.58, 142.60, 139.96, 136.64, 136.43, 136.19, 135.89, 133.78, 132.40, 131.71, 131.51, 130.90, 130.62, 130.36, 128.06, 128.01, 127.93, 127.73, 127.65, 127.53, 127.12, 126.86, 126.05(q), 125.12, 114.34.



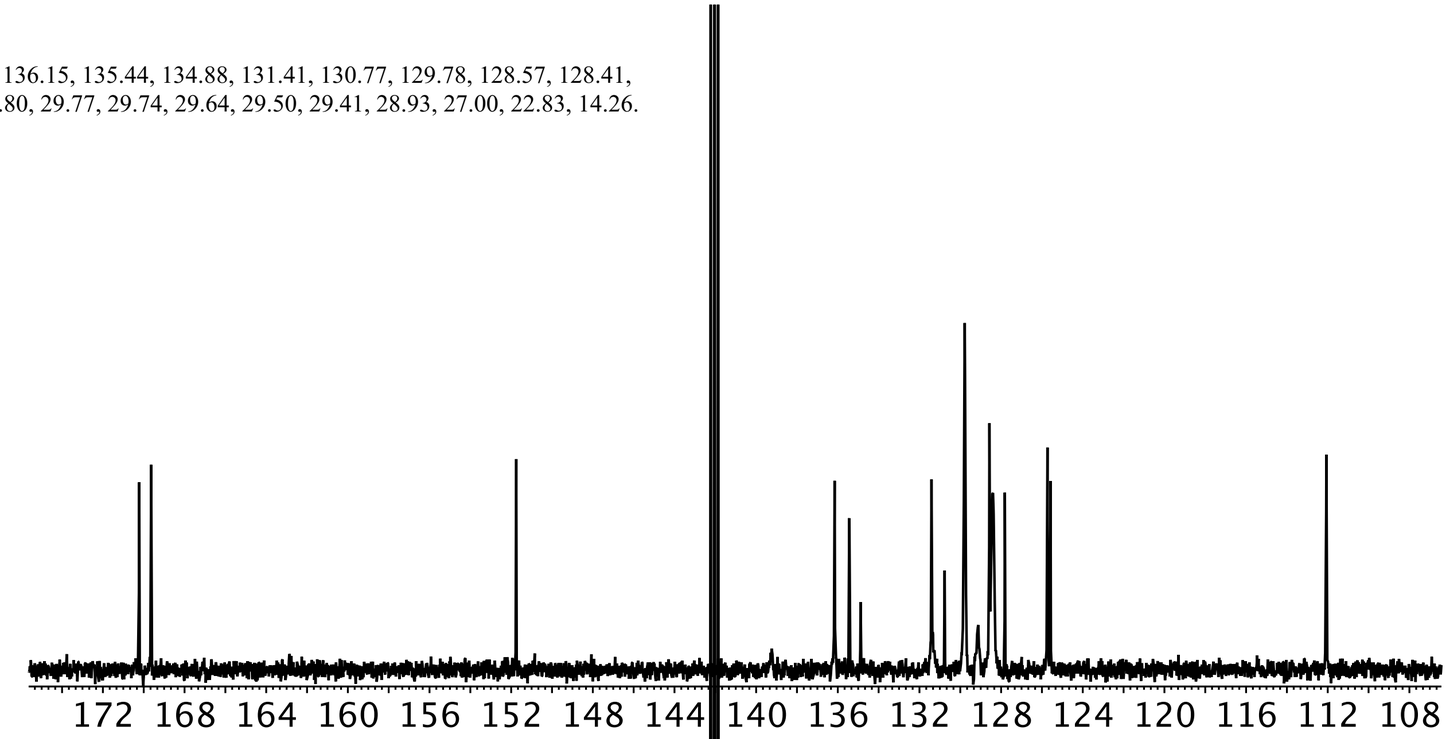


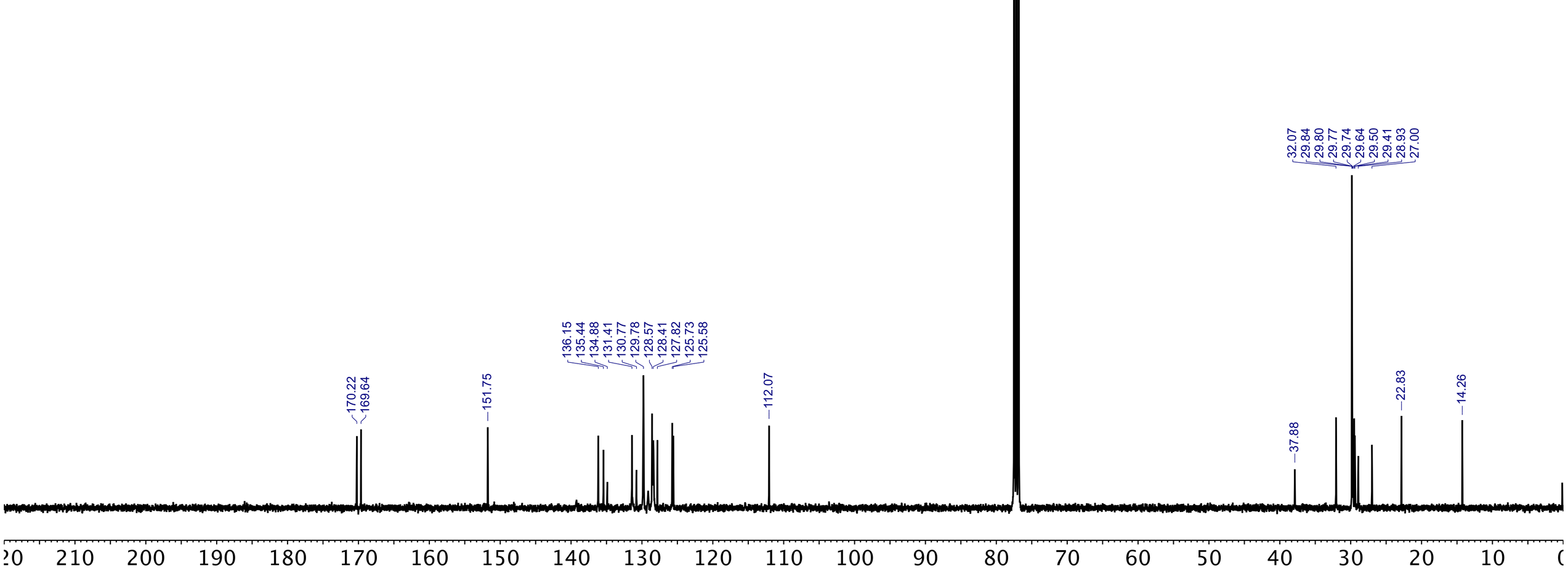
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.01 – 7.68 (m, 8H), 7.61 – 7.07 (m, 18H), 3.65 (t, J = 7.1, 7.1 Hz, 2H), 1.65 (d, J = 6.9 Hz, 2H), 1.25 (d, J = 4.9 Hz, 30H), 0.96 – 0.74 (m, 3H).

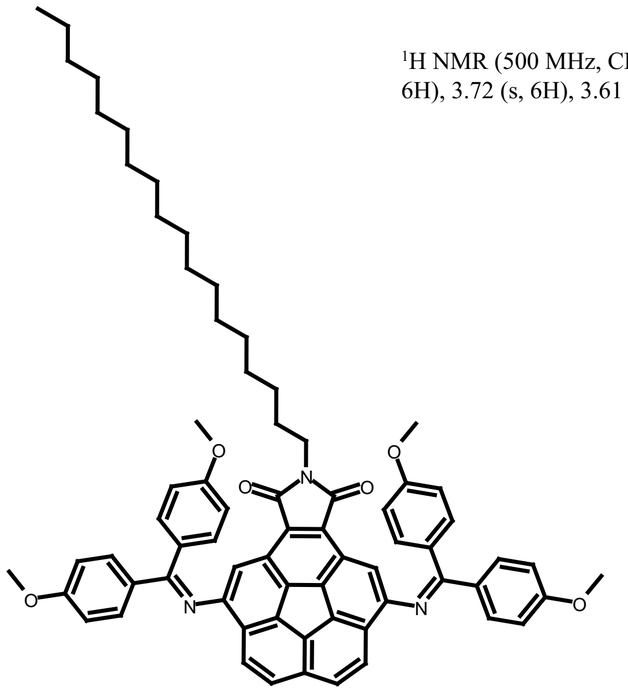




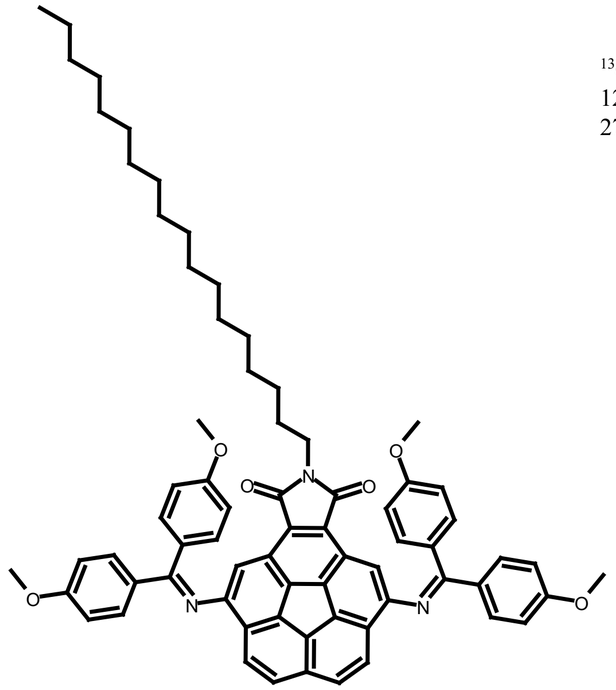
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.22, 169.64, 151.75, 136.15, 135.44, 134.88, 131.41, 130.77, 129.78, 128.57, 128.41, 127.82, 125.73, 125.58, 112.07, 37.88, 32.07, 29.84, 29.80, 29.77, 29.74, 29.64, 29.50, 29.41, 28.93, 27.00, 22.83, 14.26.



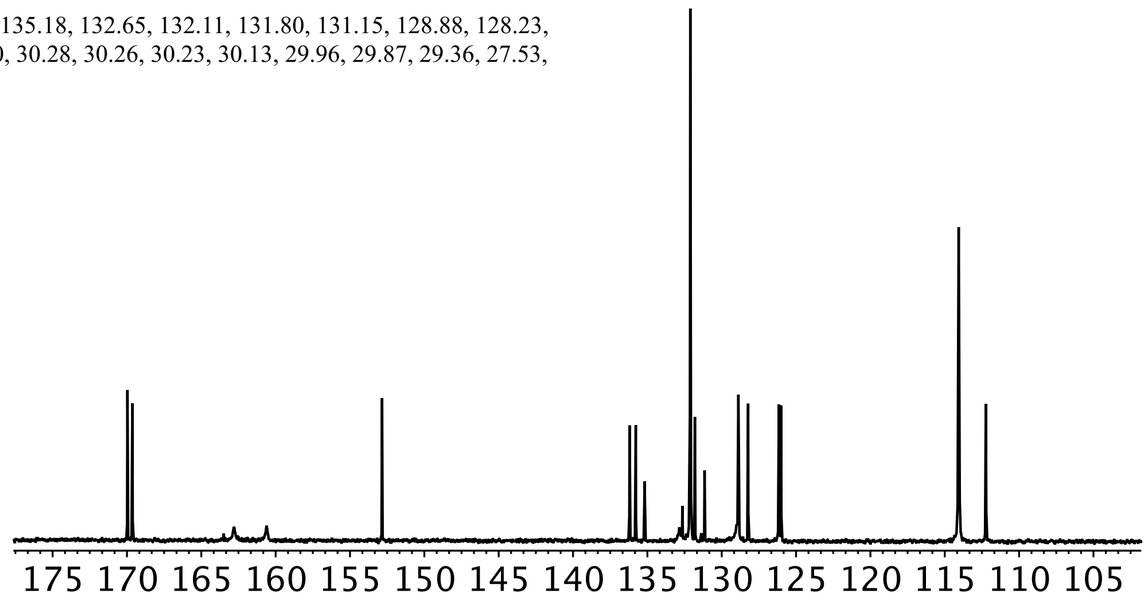


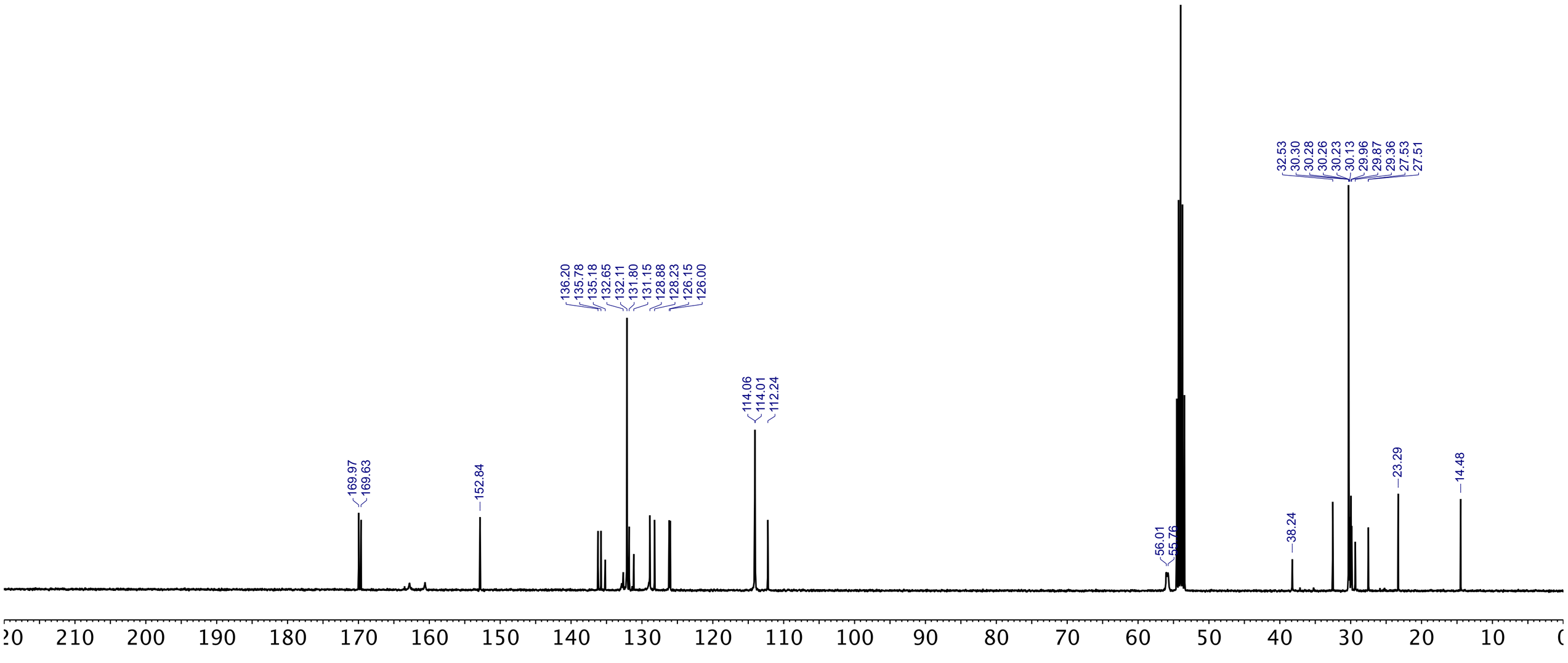


^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.92 – 7.73 (m, 8H), 7.46 – 7.27 (m, 6H), 7.07 – 6.93 (m, 4H), 6.88 – 6.70 (m, 4H), 3.89 (s, 6H), 3.72 (s, 6H), 3.61 (t, *J* = 7.2, 7.2 Hz, 2H), 1.68 – 1.59 (m, 2H), 1.34 – 1.20 (m, 31H), 0.87 (t, *J* = 6.9, 6.9 Hz, 4H).

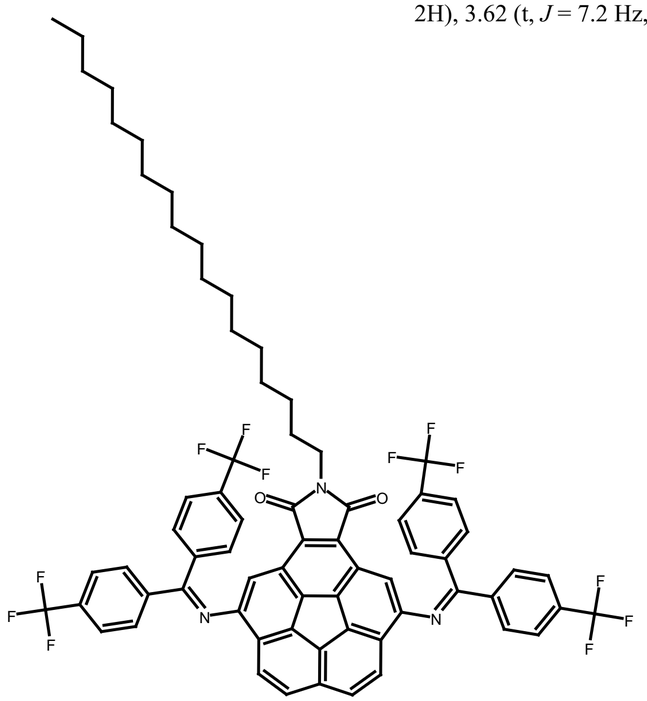


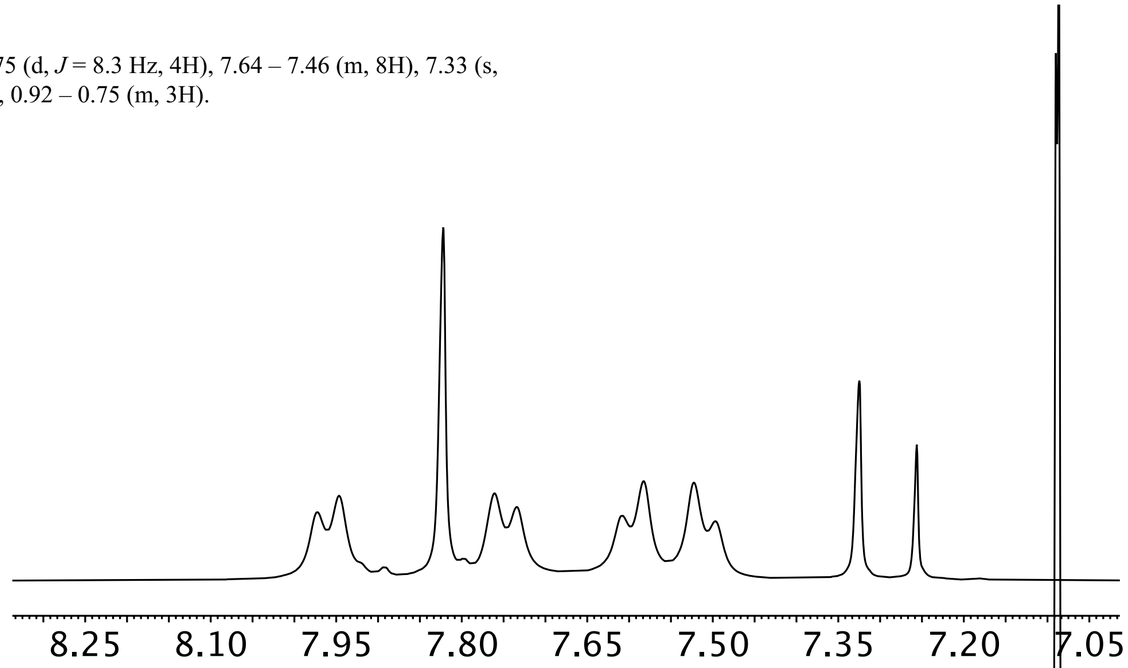
^{13}C NMR (101 MHz, CD_2Cl_2) δ 169.97, 169.63, 152.84, 136.20, 135.78, 135.18, 132.65, 132.11, 131.80, 131.15, 128.88, 128.23, 126.15, 126.00, 114.06, 114.01, 112.24, 56.01, 55.76, 38.24, 32.53, 30.30, 30.28, 30.26, 30.23, 30.13, 29.96, 29.87, 29.36, 27.53, 27.51, 23.29, 14.48.

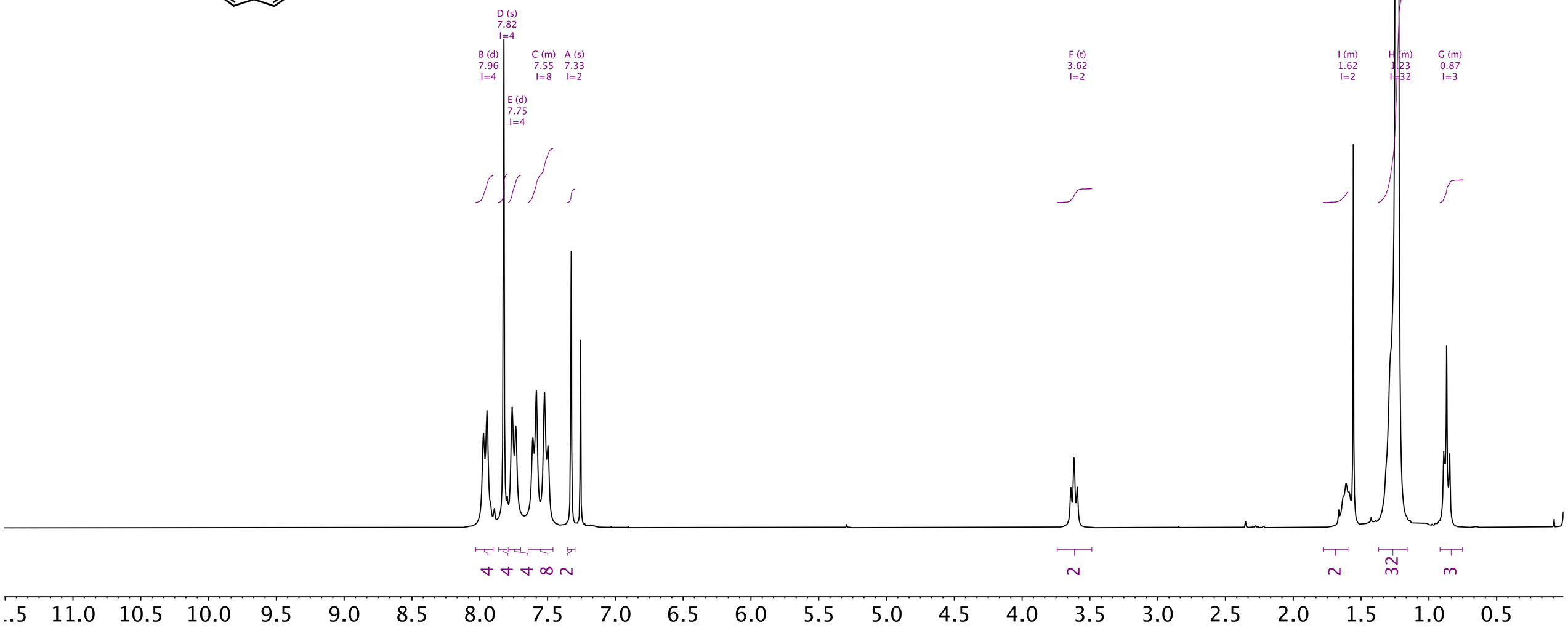




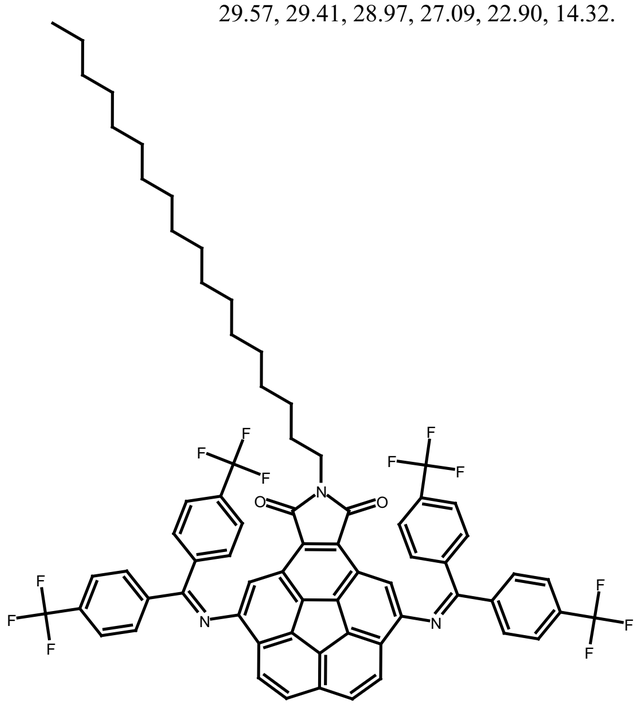
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.1 Hz, 4H), 7.82 (s, 4H), 7.75 (d, *J* = 8.3 Hz, 4H), 7.64 – 7.46 (m, 8H), 7.33 (s, 2H), 3.62 (t, *J* = 7.2 Hz, 2H), 1.78 – 1.60 (m, 2H), 1.37 – 1.16 (m, 32H), 0.92 – 0.75 (m, 3H).

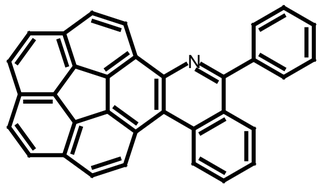




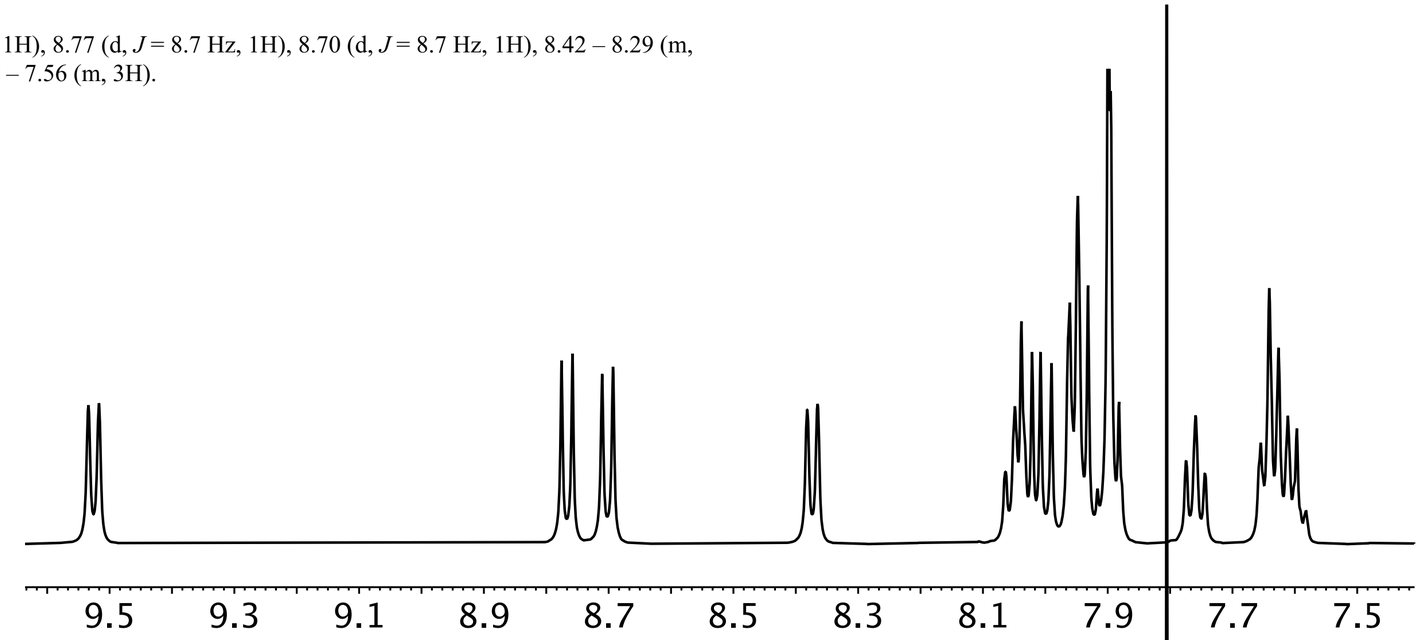


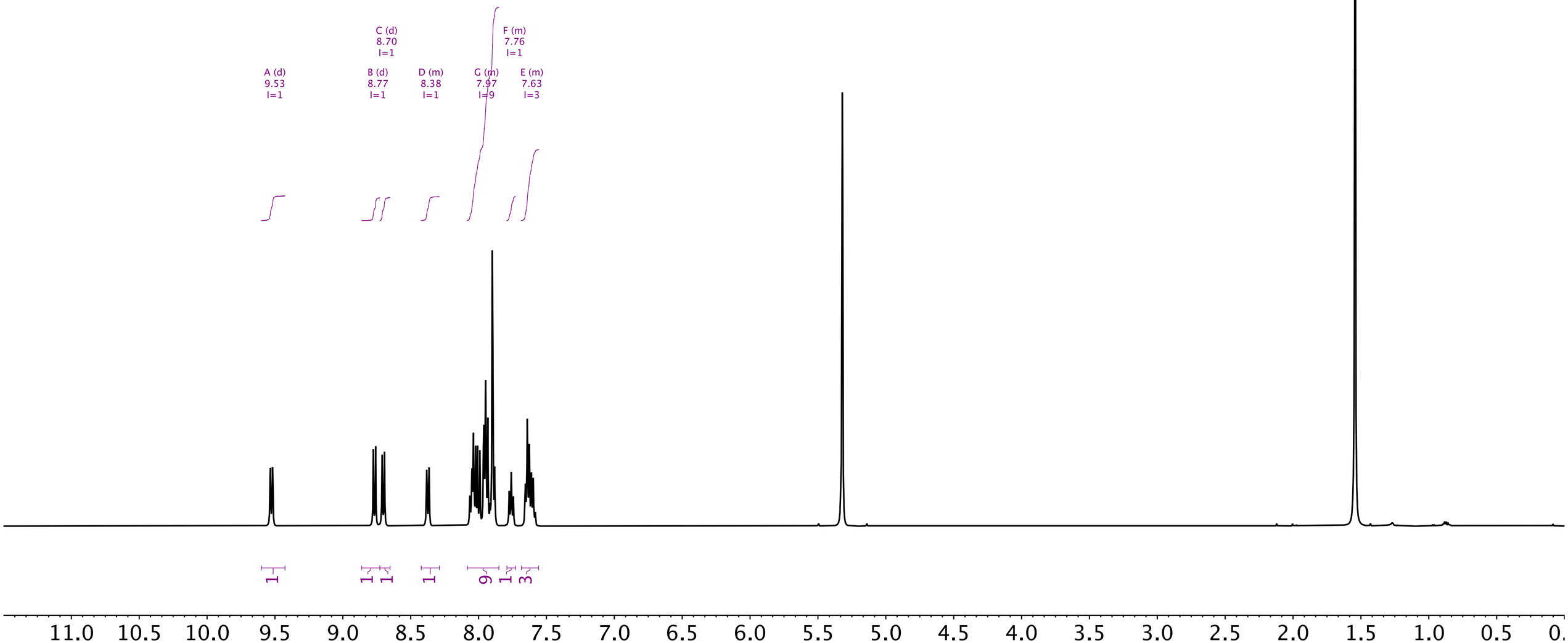
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.43, 167.58, 150.65, 141.61, 139.01, 136.36, 135.51, 134.91, 131.65, 131.07, 130.44, 130.02, 129.94, 129.08, 127.68, 125.80, 125.52, 125.50, 111.97, 60.61, 38.04, 32.13, 31.81, 29.91, 29.87, 29.83, 29.80, 29.68, 29.57, 29.41, 28.97, 27.09, 22.90, 14.32.

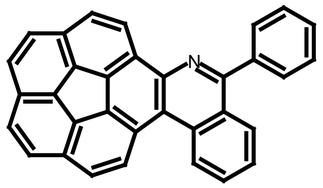




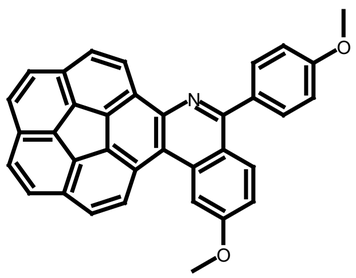
[1]H NMR (500 MHz, CD_2Cl_2) δ 9.53 (d, *J* = 8.4 Hz, 1H), 8.77 (d, *J* = 8.7 Hz, 1H), 8.70 (d, *J* = 8.7 Hz, 1H), 8.42 – 8.29 (m, 1H), 8.08 – 7.85 (m, 9H), 7.79 – 7.73 (m, 1H), 7.68 – 7.56 (m, 3H).



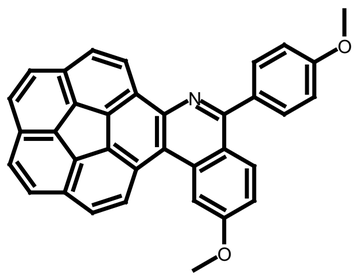




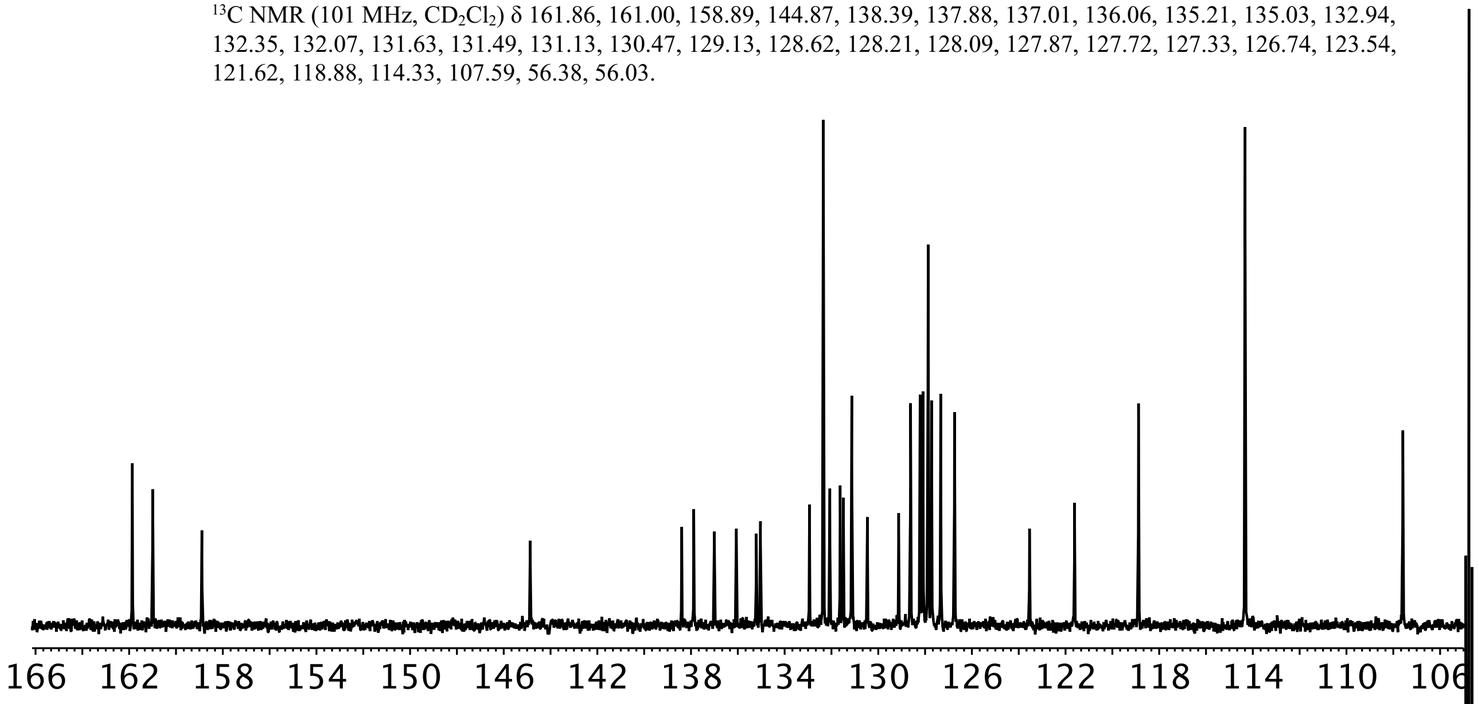
^{13}C NMR (101 MHz, C_6D_5Cl) δ 159.27, 144.25, 140.47, 138.13, 136.80, 135.74, 135.59, 135.37, 134.90, 134.63, 133.99, 131.80, 131.19, 131.06, 130.86, 130.51, 130.38, 129.90, 128.98, 128.72, 127.97, 127.81, 127.70, 127.37, 127.12, 127.02, 126.93, 125.96, 124.16.

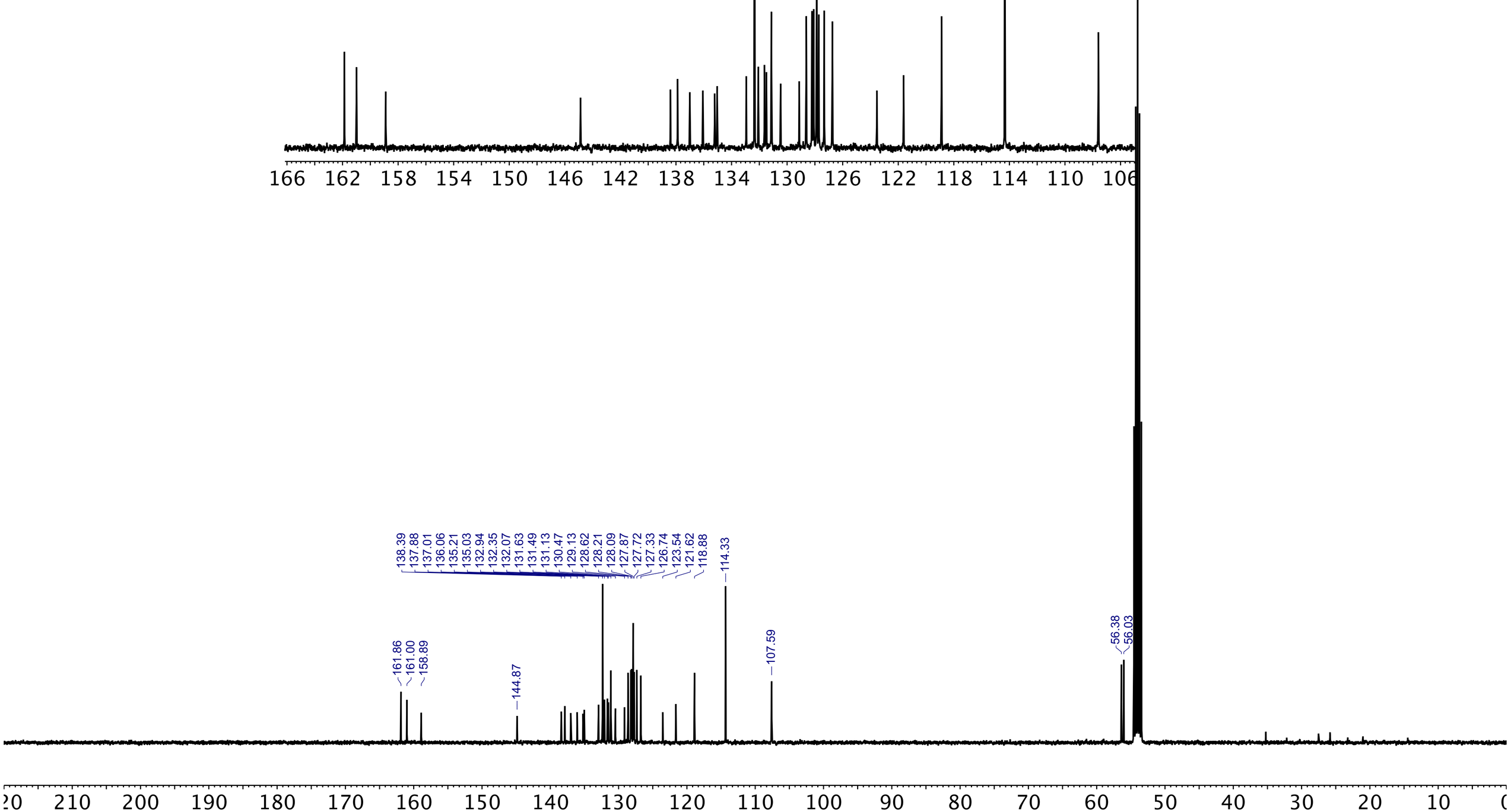


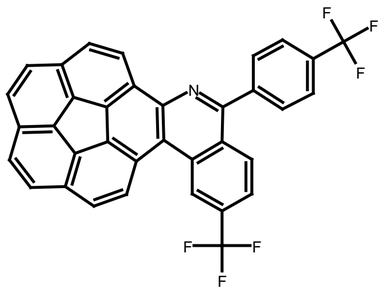
^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.83 (d, *J* = 2.5 Hz, 1H), 8.74 (dd, *J* = 16.0, 8.7 Hz, 2H), 8.32 (d, *J* = 9.1 Hz, 1H), 8.01 (dd, *J* = 14.9, 8.7 Hz, 2H), 7.96 – 7.84 (m, 6H), 7.37 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.19 – 7.09 (m, 2H), 4.21 (s, 3H), 3.94 (s, 3H).



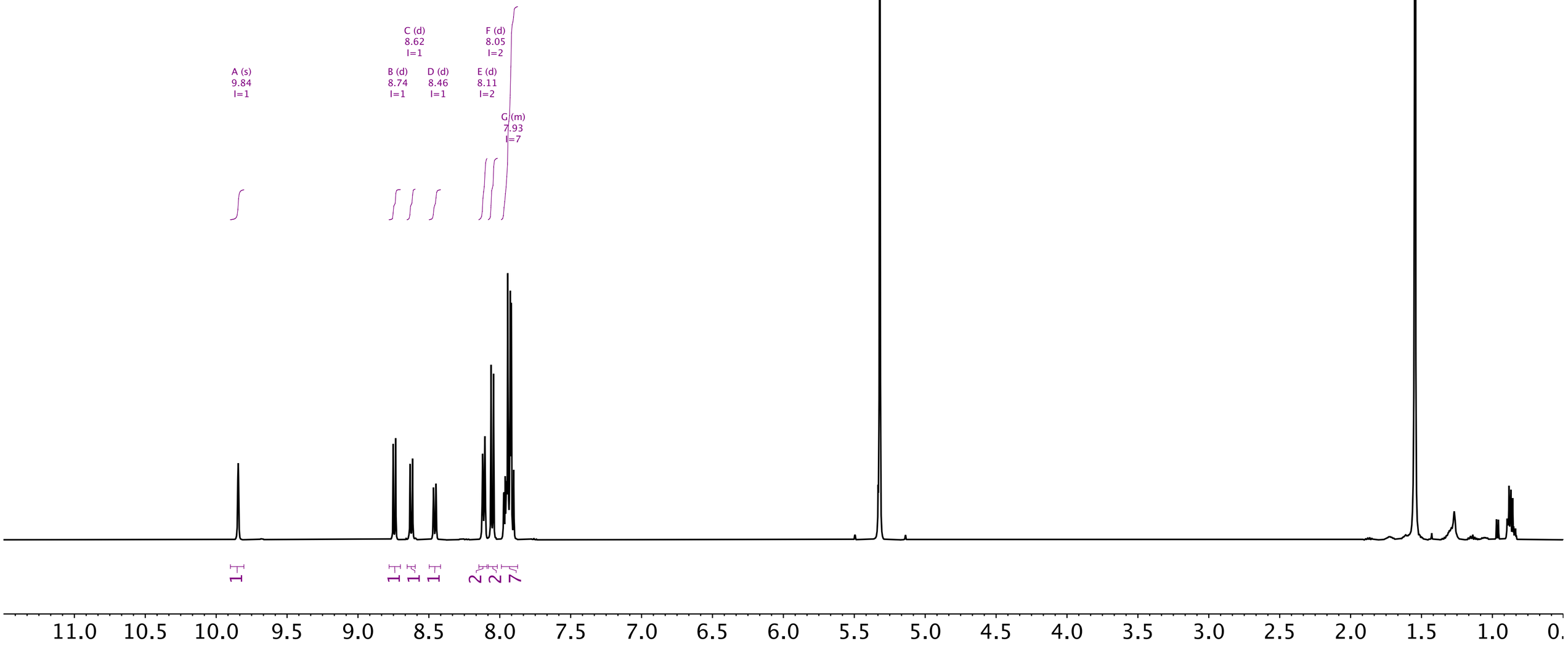
^{13}C NMR (101 MHz, CD_2Cl_2) δ 161.86, 161.00, 158.89, 144.87, 138.39, 137.88, 137.01, 136.06, 135.21, 135.03, 132.94, 132.35, 132.07, 131.63, 131.49, 131.13, 130.47, 129.13, 128.62, 128.21, 128.09, 127.87, 127.72, 127.33, 126.74, 123.54, 121.62, 118.88, 114.33, 107.59, 56.38, 56.03.

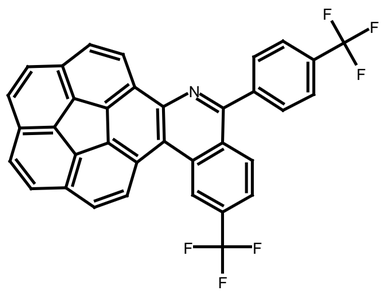




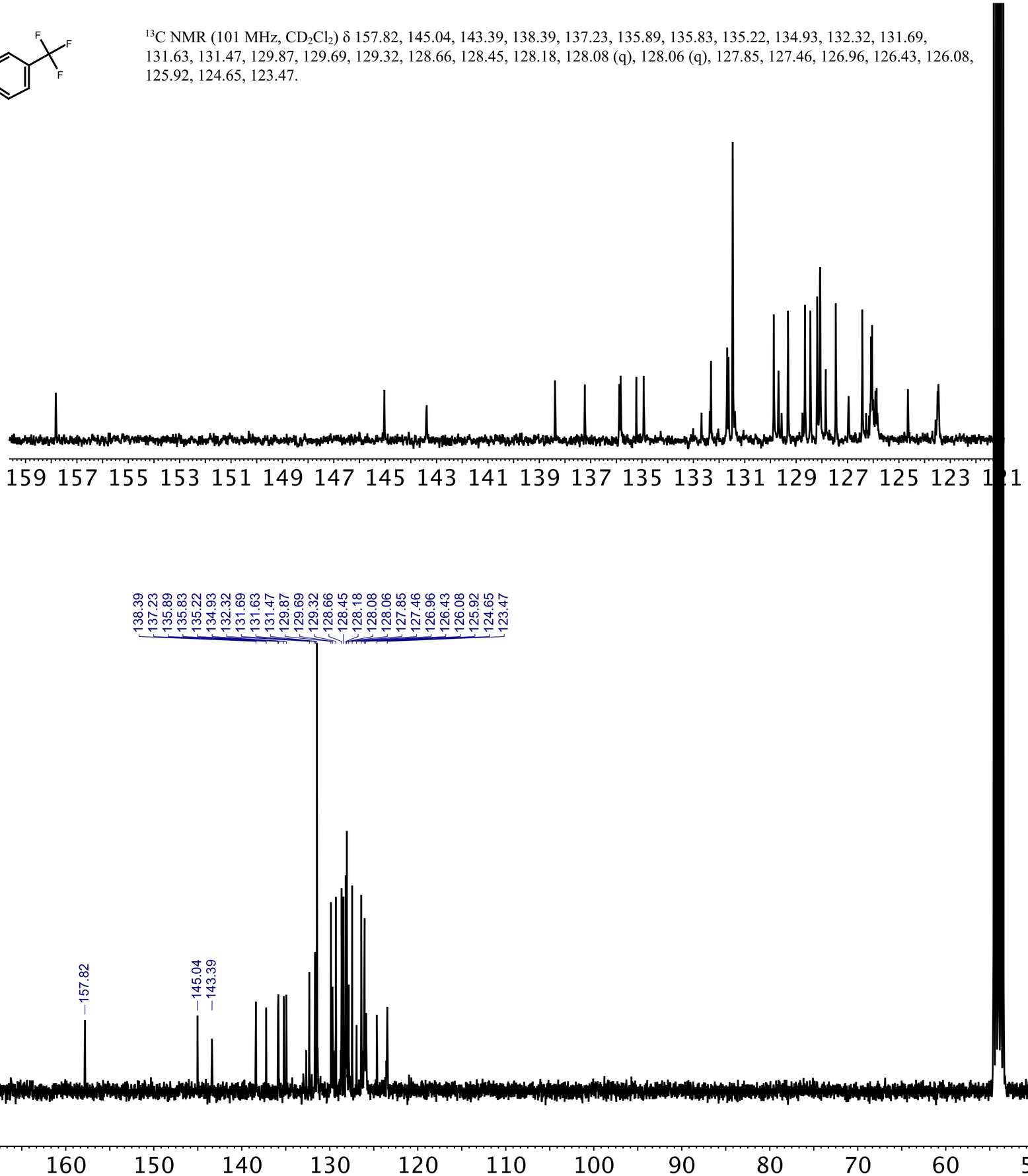


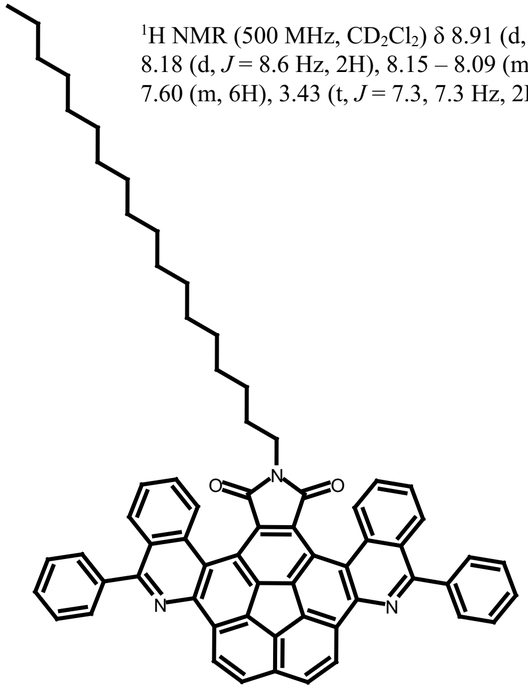
^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.84 (s, 1H), 8.74 (d, *J* = 8.7 Hz, 1H), 8.62 (d, *J* = 8.7 Hz, 1H), 8.46 (d, *J* = 8.7 Hz, 1H), 8.11 (d, *J* = 8.0 Hz, 2H), 8.05 (d, *J* = 8.7 Hz, 2H), 7.99 – 7.87 (m, 7H).





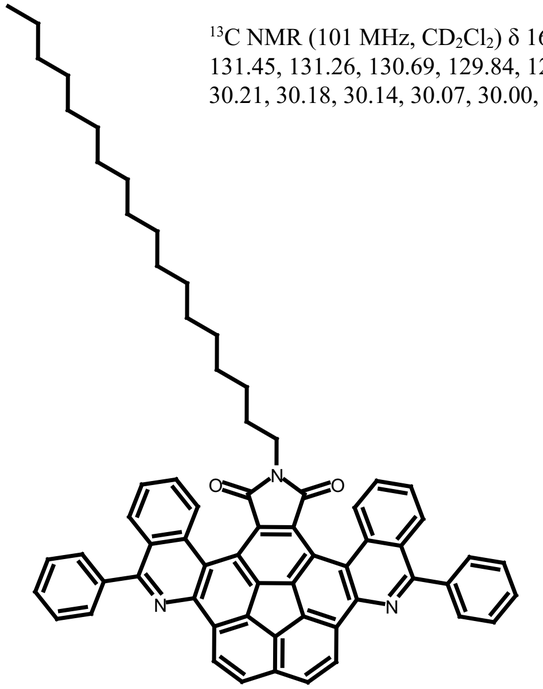
^{13}C NMR (101 MHz, CD_2Cl_2) δ 157.82, 145.04, 143.39, 138.39, 137.23, 135.89, 135.83, 135.22, 134.93, 132.32, 131.69, 131.63, 131.47, 129.87, 129.69, 129.32, 128.66, 128.45, 128.18, 128.08 (q), 128.06 (q), 127.85, 127.46, 126.96, 126.43, 126.08, 125.92, 124.65, 123.47.

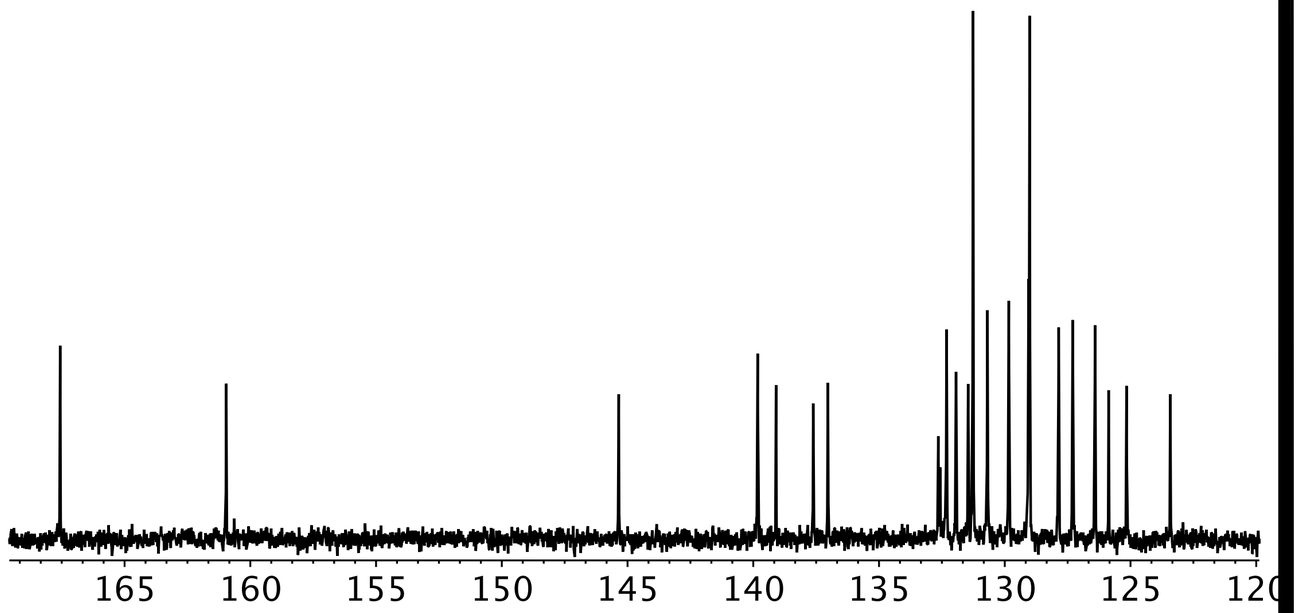


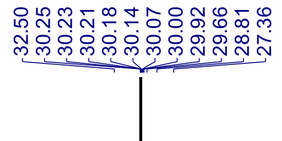


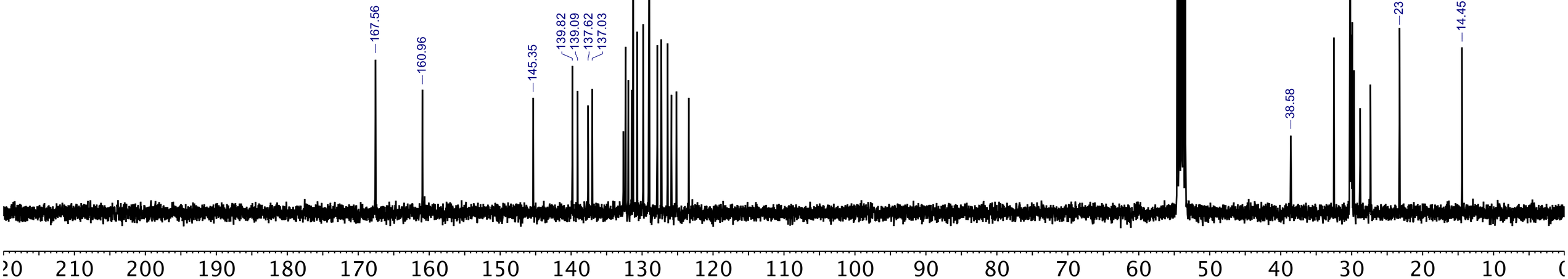
^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.91 (d, *J* = 8.4, 1.0, 1.0 Hz, 2H), 8.75 (d, *J* = 8.6 Hz, 2H), 8.32 (dt, *J* = 8.2, 1.0, 1.0 Hz, 2H), 8.18 (d, *J* = 8.6 Hz, 2H), 8.15 – 8.09 (m, 4H), 7.90 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 2H), 7.75 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 2H), 7.72 – 7.60 (m, 6H), 3.43 (t, *J* = 7.3, 7.3 Hz, 2H), 1.40 – 1.31 (m, 2H), 1.29 – 1.08 (m, 30H), 0.86 (t, *J* = 7.0, 7.0 Hz, 3H).

^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.56, 160.96, 145.35, 139.82, 139.09, 137.62, 137.03, 132.64, 132.57, 132.31, 131.94, 131.45, 131.26, 130.69, 129.84, 129.05, 129.01, 127.86, 127.30, 126.41, 125.87, 125.16, 123.42, 38.58, 32.50, 30.25, 30.23, 30.21, 30.18, 30.14, 30.07, 30.00, 29.92, 29.66, 28.81, 27.36, 23.26, 14.45.

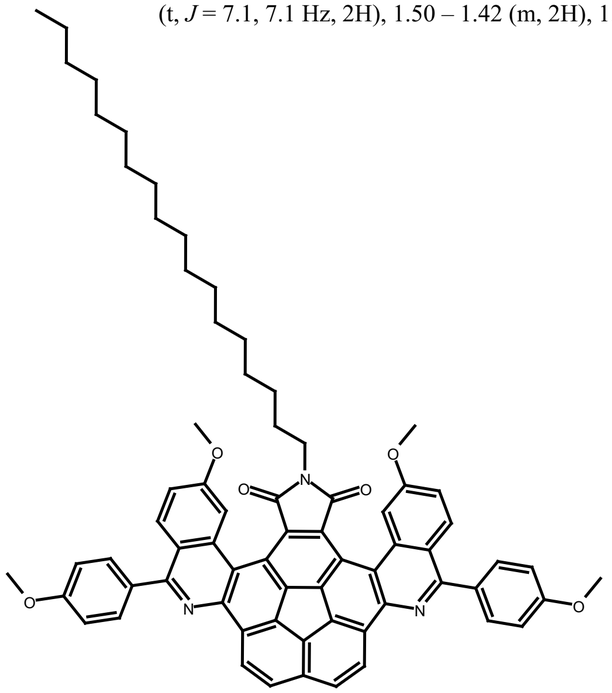


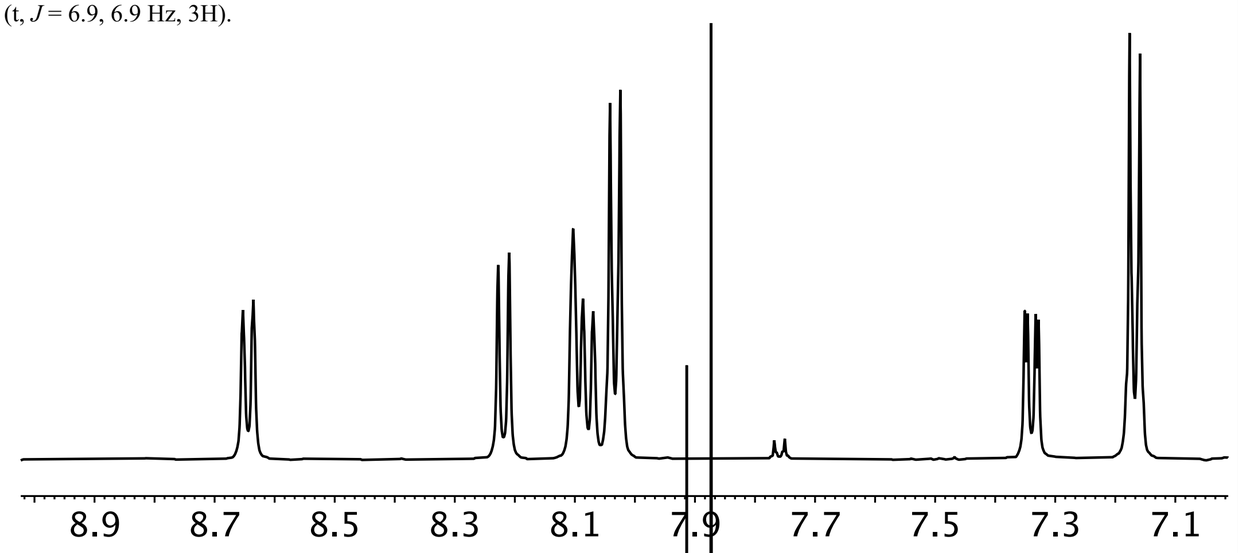


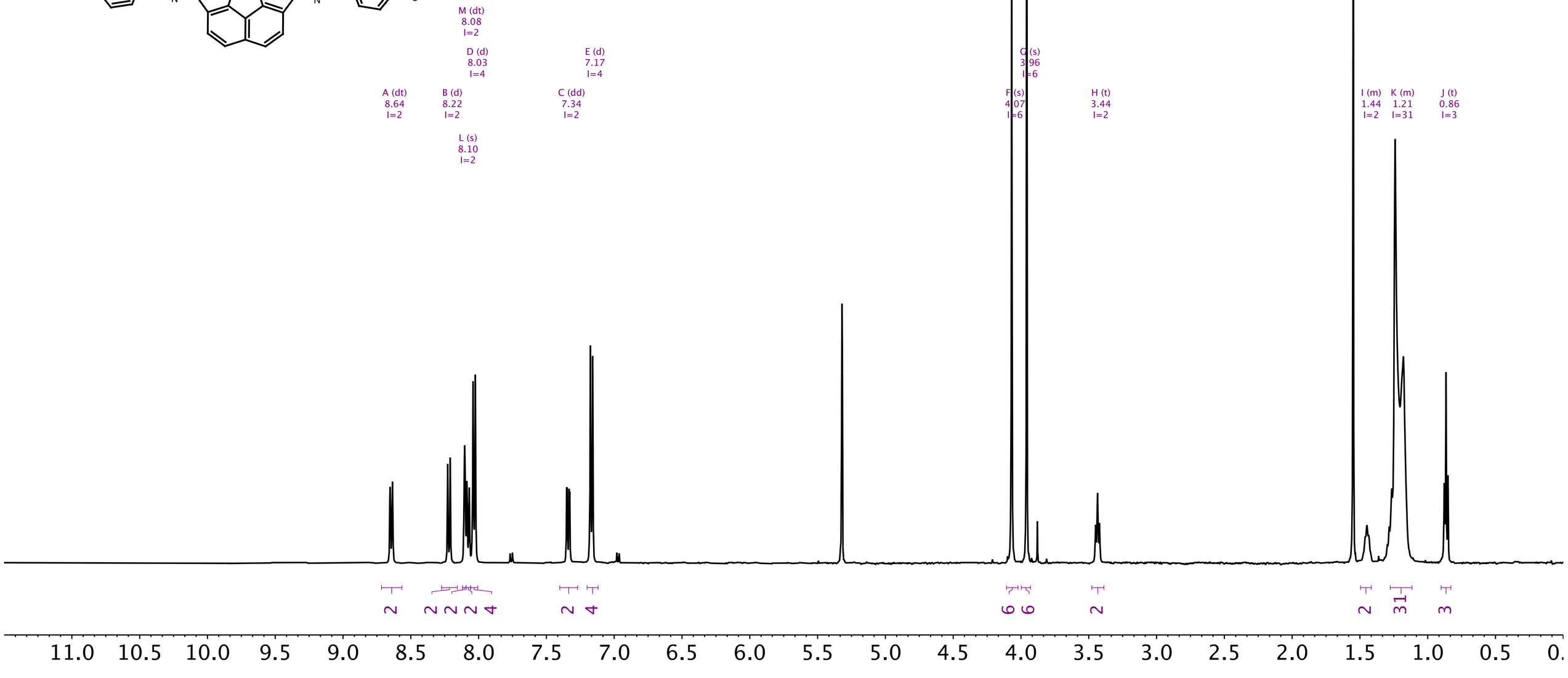




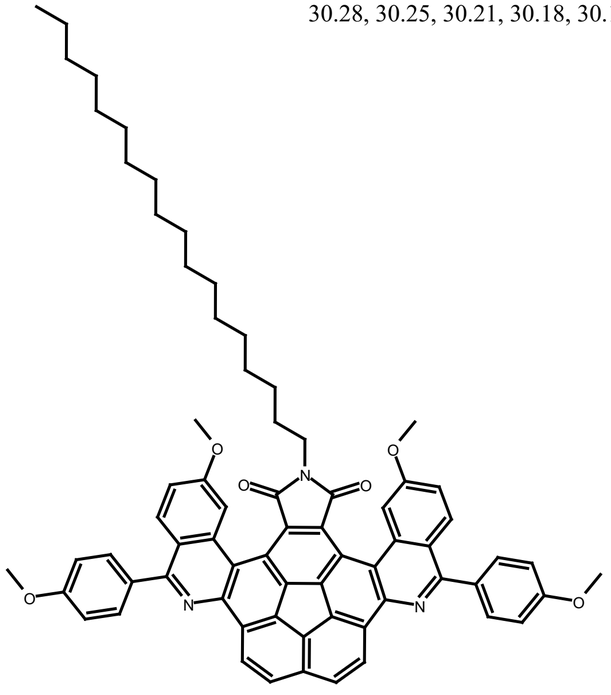
^{1}H NMR (500 MHz, CD_2Cl_2) δ 8.64 (dt, *J* = 8.6, 1.3, 1.3 Hz, 2H), 8.22 (d, *J* = 9.1 Hz, 2H), 8.10 (s, 2H), 8.08 (dt, *J* = 8.6, 1.3, 1.3 Hz, 2H), 8.03 (d, *J* = 8.7 Hz, 4H), 7.34 (dd, *J* = 9.2, 2.5 Hz, 2H), 7.17 (d, *J* = 8.7 Hz, 4H), 4.07 (s, 6H), 3.96 (s, 6H), 3.44 (t, *J* = 7.1, 7.1 Hz, 2H), 1.50 – 1.42 (m, 2H), 1.28 – 1.12 (m, 31H), 0.86 (t, *J* = 6.9, 6.9 Hz, 3H).

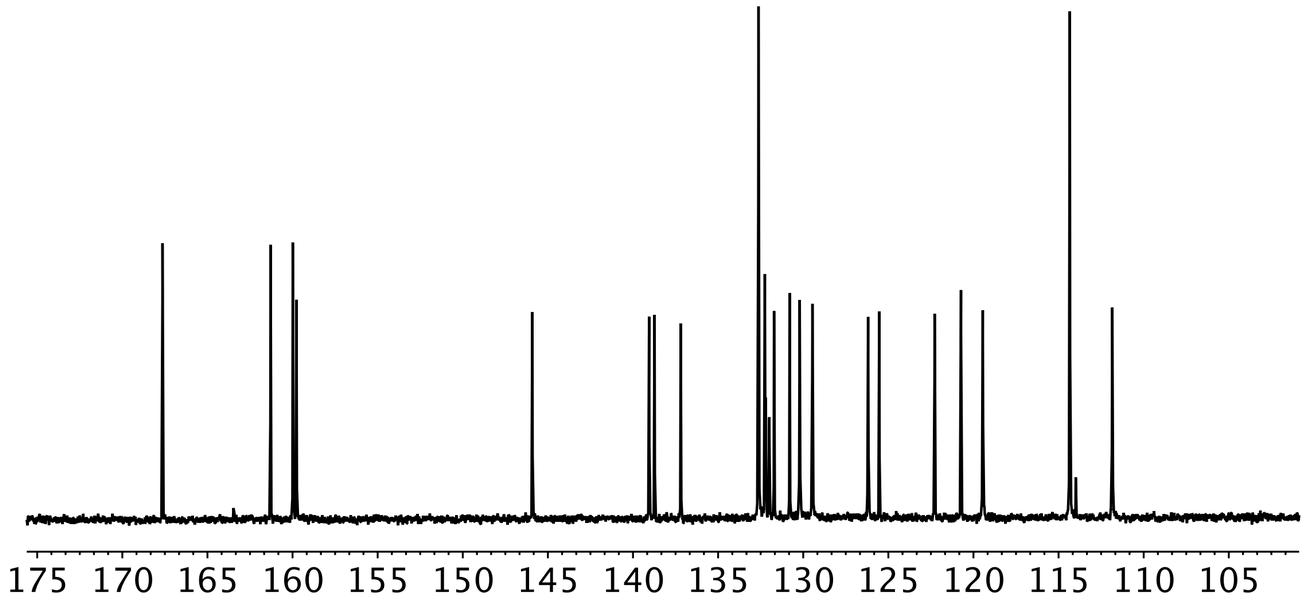


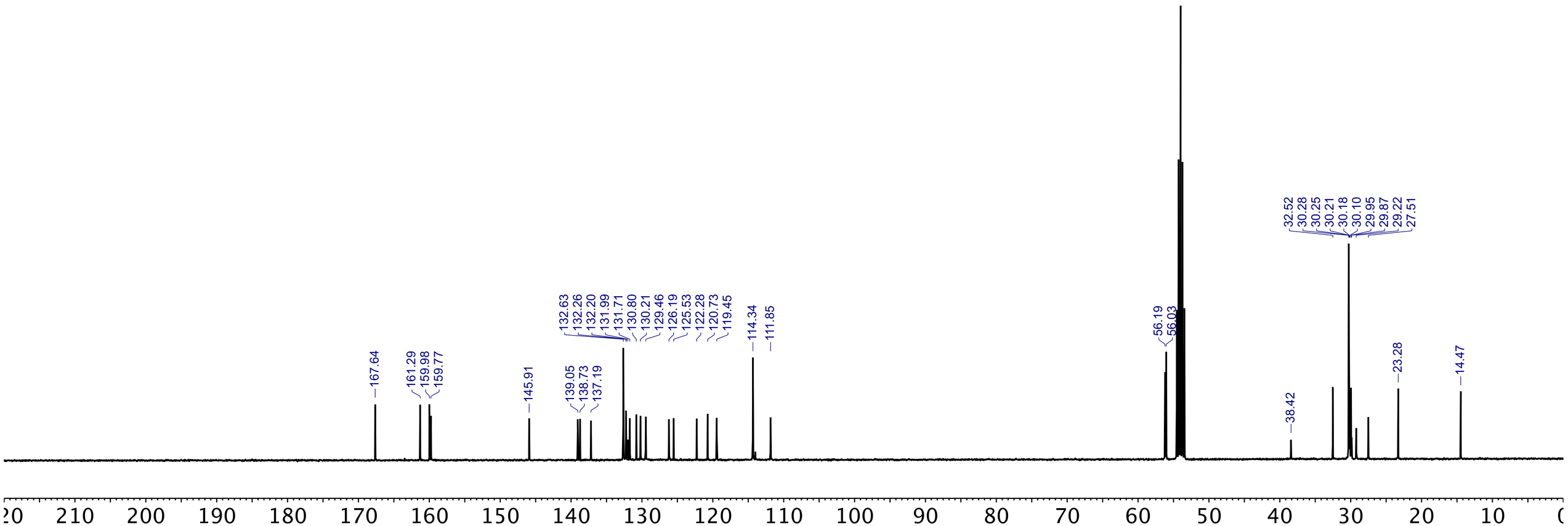




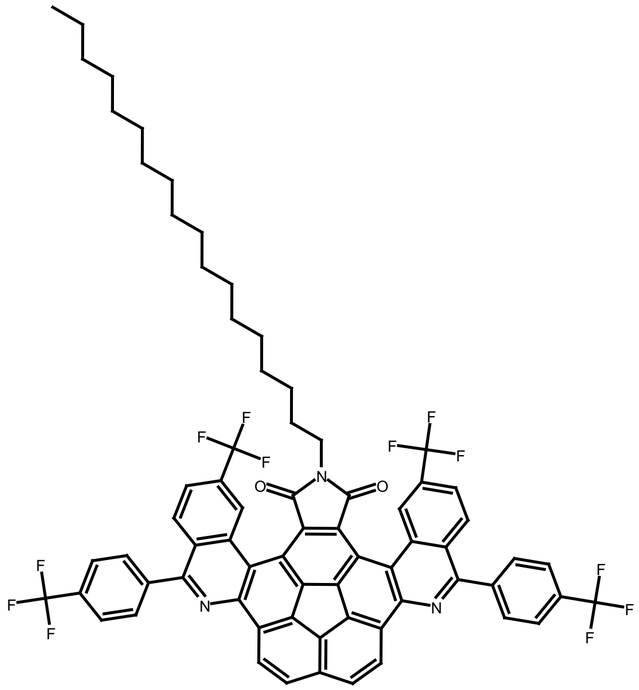
^{13}C NMR (101 MHz, CD_2Cl_2) δ 167.64, 161.29, 159.98, 159.77, 145.91, 139.05, 138.73, 137.19, 132.63, 132.26, 132.20, 131.99, 131.71, 130.80, 130.21, 129.46, 126.19, 125.53, 122.28, 120.73, 119.45, 114.34, 111.85, 56.19, 56.03, 38.42, 32.52, 30.28, 30.25, 30.21, 30.18, 30.10, 29.95, 29.87, 29.22, 27.51, 23.28, 14.47.

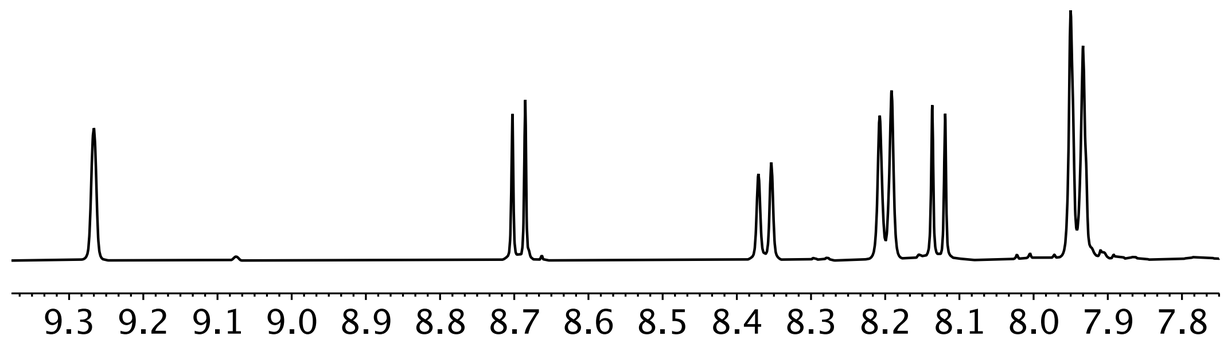


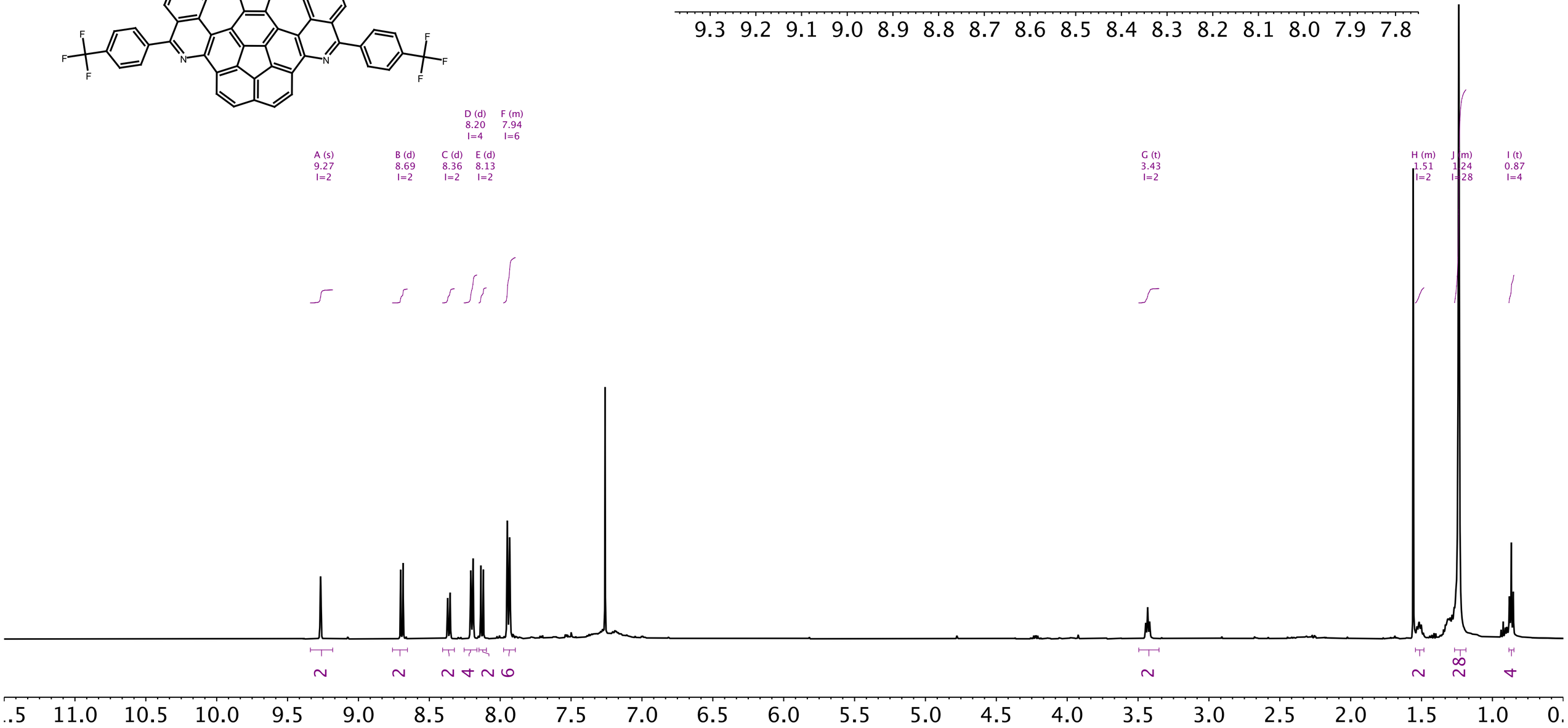




^{1}H NMR (500 MHz, $CDCl_3$) δ 9.27 (s, 2H), 8.69 (d, *J* = 8.7 Hz, 2H), 8.36 (d, *J* = 8.7 Hz, 2H), 8.20 (d, *J* = 8.0 Hz, 4H), 8.13 (d, *J* = 8.6 Hz, 2H), 7.94 (dd, *J* = 8.7, 1.9 Hz, 6H), 3.43 (t, *J* = 7.0 Hz, 2H), 1.51 (q, *J* = 7.4 Hz, 2H), 1.24 (s, 28H), 0.87 (t, *J* = 6.9 Hz, 4H).







^{13}C NMR (126 MHz, $CDCl_3$) δ 167.24, 159.17, 145.83, 142.10, 139.01, 137.71, 136.07, 132.74, 132.18, 131.95, 131.69, 131.25, 131.15, 130.75, 130.72, 130.46, 130.15, 127.71, 126.44, 125.82, 125.63, 125.35, 125.32, 124.94, 123.68, 123.30, 123.17, 123.15, 38.30, 32.06, 29.84, 29.79, 29.76, 29.72, 29.50, 29.46, 29.39, 28.63, 26.88, 22.83, 14.25.