

**Supporting Information
for**

Nonaromatic naphthocorroles

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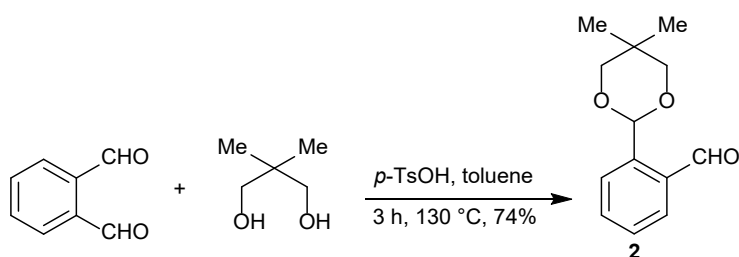
Table of Contents

1. General information	S2
2. Synthesis	S2
3. Crystallographic data	S6
4. Experimental methods	S8
5. Spectroscopic data	S8
6. Computational results	S11
7. Electrochemical data	S15
8. NMR Spectra	S18
9. Cartesian coordinates	S29
10. Additional references	S37

1. General Information

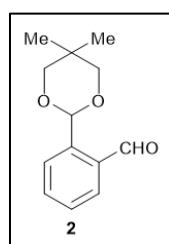
All reported NMR spectra (^1H , ^{13}C and ^{19}F NMR) were recorded using a Varian 500 and 600 or Bruker 500 spectrometers. Chemical shifts (δ ppm) were determined with TMS as the internal reference, J values are given in Hz. The ^1H NMR spectrum of pure deuterated THF (page 27) shows additional signals at around 2.5 and 11 ppm, which are observed in some NMR spectra registered in THF- d_8 . High resolution mass spectra (HRMS) were obtained via electron ionization (EI) source and an EBE double focusing geometry mass analyzer or spectrometer equipped with electrospray ion source with q-TOF type mass analyzer (ESI) or by atmospheric pressure chemical ionization (APCI). Chromatography was performed on silica gel 60 (230-400 mesh) and thin layer chromatography was performed on TLC plates (Merck, silica gel 60 F₂₅₄).

2. Synthesis



Scheme S1. Synthesis of 2-(5,5-dimethyl-1,3-dioxan-2-yl)benzaldehyde (**2**).

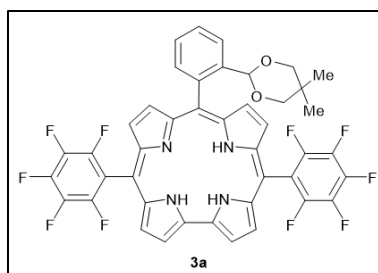
Synthesis of 2-(5,5-dimethyl-1,3-dioxan-2-yl)benzaldehyde (2**).** Round bottom flask was charged with phthalaldehyde (5.45 g, 41.0 mmol), 2,2-dimethylpropane-1,3-diol (4.25 g, 41.0 mmol) and $p\text{-TsOH}$ (0.025 g, 0.15 mmol). Following next, toluene was added (60 ml) and the reaction mixture was stirred at 130 °C (oil bath) for 3 h with Dean-Stark trap. After this time, the mixture was cooled to room temperature and the solvent was evaporated. Crude product was purified by column chromatography (silica, hexane/ethyl acetate 4:1) to afford product of analytical purity.



2-(5,5-dimethyl-1,3-dioxan-2-yl)benzaldehyde (2**).** Yellowish oil. Yield: 6.66 g (74%). ^1H NMR (CDCl_3 , 500 MHz): δ 10.43 (s, 1H, CHO) 7.90 (d, $J = 7.6$ Hz, 1H, Ar), 7.80 (d, $J = 7.7$ Hz, 1H, Ar), 7.61 (t, $J = 7.2$ Hz, 1H, Ar), 7.51 (t, $J = 7.5$ Hz, 1H, Ar), 6.02 (s, 1H, CH), 3.80 (d, $J = 11.1$ Hz, 2H, CH_2), 3.73 (d, $J = 11.0$ Hz, 2H, CH_2), 1.31 (s, 3H, CH_3), 0.82 (s, 3H, CH_3). ^{13}C NMR (CDCl_3 , 125 MHz): δ 192.1, 139.4, 133.7, 133.6, 130.2, 129.2, 127.2, 99.3, 78.0, 30.2, 23.4, 21.9. HRMS (EI): m/z calculated for $\text{C}_{13}\text{H}_{16}\text{O}_3$: 220.1099 [M^+]; found:

220.1095.

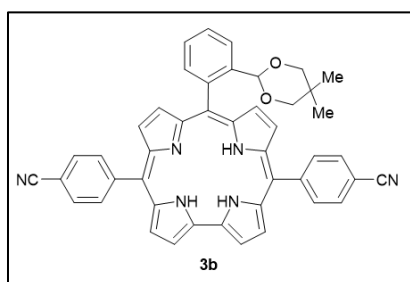
General procedure for the synthesis of corroles 3a-d. Dipyrromethane (**1a-d**) (2.0 mmol) and 2-(5,5-dimethyl-1,3-dioxan-2-yl)benzaldehyde (**2**) (1.0 mmol) were dissolved in MeOH (100 ml). Subsequently, solution of HCl_{aq} (36%, 5 ml in 100 ml of H_2O) was added and the reaction mixture was stirred at room temperature for 1 h. Then, the mixture was extracted by CHCl_3 . The combined organic layers were dried over Na_2SO_4 , filtered and diluted to 500 ml with CHCl_3 . DDQ (3.0 mmol) in toluene (6 ml) was added and the reaction mixture was stirred at room temperature for 15 minutes. The reaction mixture was concentrated to one-third of the initial volume and passed over by short silica column (DCM) and all fractions containing corrole were combined and evaporated. Further purification details are given below.



10-(2-(5,5-dimethyl-1,3-dioxan-2-yl)phenyl)-5,15-bis(pentafluorophenyl)corrole (3a).

Crude product was purified by column chromatography (silica, DCM/hexane 2:1) and crystallized from hot MeOH to afford product of analytical purity. Violet precipitate. Yield: 0.204 g (25%). M.p. 178-180 °C. ¹H NMR (CDCl₃, 600 MHz): δ 9.11 (d, *J* = 4.2 Hz, 2H, β-H), 8.66 (d, *J* = 4.6 Hz, 2H, β-H), 8.61-8.52 (m, 4H, β-H), 8.21 (dd, *J* = 8.1, 1.2 Hz, 1H, Ar), 7.93 (dd, *J* = 7.5, 0.9 Hz 1H, Ar),

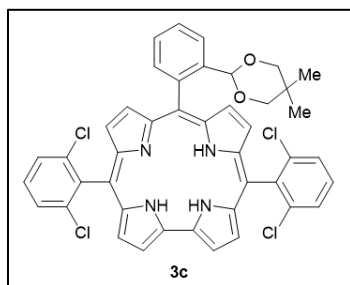
7.87 (td, *J* = 7.9, 1.2 Hz, 1H, Ar), 7.67 (td, *J* = 7.5, 1.4 Hz, 1H, Ar), 4.88 (s, 1H, CH), 3.32 (d, *J* = 11.6 Hz, 2H, CH₂), 2.49 (d, *J* = 11.2 Hz, 2H, CH₂), 1.23 (s, 3H, CH₃), 0.21 (s, 3H, CH₃). Signals from the inner NH groups were not visible. ¹⁹F NMR (CDCl₃, 470 MHz): δ -162.20 – -161.45 (m, 4F, Ar), -153.10 – -152.50 (m, 2F, Ar), -138.12 (d, *J* = 20.6 Hz, 2F, Ar), -137.84 (d, *J* = 20.2 Hz, 2F, Ar). HRMS (ESI): *m/z* calculated for C₄₃H₂₇F₁₀N₄O₂: 821.1974 [*M*+H⁺]; found: 821.1971.



10-(2-(5,5-dimethyl-1,3-dioxan-2-yl)phenyl)-5,15-bis(4-cyanophenyl)corrole (3b).

Crude product was purified by column chromatography (silica, DCM/hexane 95:5) and crystallized from DCM-cyclohexane to afford product of analytical purity. Violet precipitate. Yield: 0.258 g (37%). M.p. 250 °C (decomp). ¹H NMR (CDCl₃, 500 MHz): δ 9.05 (bs, 2H, β-H), 8.81 (bs, 2H, β-H), 8.60 (bs, 2H, β-H), 8.49 (bs, 6H, β-H+Ar), 8.21 (bs, 1H, Ar), 8.12 (bs, 4H, Ar), 7.88

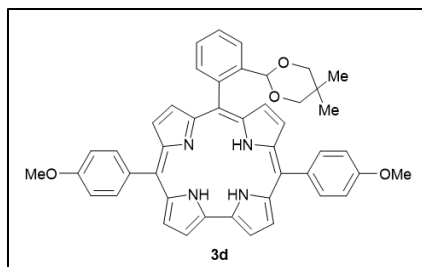
(bs, 2H, Ar), 7.67 (bs, 1H, Ar), 4.93 (s, 1H, CH), 3.31 (bs, 2H, CH₂), 2.51 (bs, 2H, CH₂), 1.23 (s, 3H, CH₃), 0.21 (s, 3H, CH₃), -2.32 (bs, 3H, NH). Some signals in the ¹³C NMR spectrum overlap. ¹³C NMR (CDCl₃, 125 MHz): δ 144.2, 144.1, 139.2, 135.6, 135.4, 134.3, 131.9, 129.3, 129.1, 127.4, 127.3, 126.2, 119.2, 117.1, 111.2, 110.0, 108.0, 100.0, 29.8, 26.7, 23.1, 21.3. HRMS (APCI): *m/z* calculated for C₄₅H₃₃N₆O₂: 689.2665 [*M*-H⁺]; found: 689.2666.



10-(2-(5,5-dimethyl-1,3-dioxan-2-yl)phenyl)-5,15-bis(2,6-dichlorophenyl)corrole (3c).

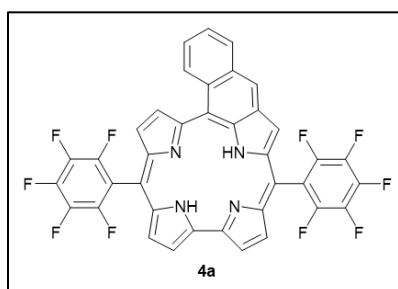
Crude product was purified by column chromatography (silica, DCM/hexane 2:1) and crystallized from DCM-cyclohexane to afford product of analytical purity. Violet precipitate. Yield: 0.216 g (28%). M.p. 215 °C (decomp). ¹H NMR (CDCl₃, 500 MHz): δ 8.97 (d, *J* = 3.9 Hz, 2H, β-H), 8.47 (d, *J* = 4.5 Hz, 2H, β-H), 8.43 (d, *J* = 4.5 Hz, 2H, β-H), 8.40 (d, *J* = 3.4 Hz, 2H, β-H), 8.17 (d, *J* = 7.6 Hz, 1H,

Ar), 7.96 (d, *J* = 7.4 Hz, 1H, Ar), 7.82 (t, *J* = 7.7 Hz, 1H, Ar), 7.77 (d, *J* = 3.3 Hz, 2H, Ar), 7.76 (d, *J* = 3.3 Hz, 2H, Ar), 7.68-7.59 (m, 3H, Ar), 4.90 (s, 1H, CH), 3.31 (d, *J* = 11.2 Hz, 2H, CH₂), 2.50 (d, *J* = 11.2 Hz, 2H, CH₂), 1.22 (s, 3H, CH₃), 0.20 (s, 3H, CH₃), -2.19 (bs, 3H, NH). Signals at around 1.43 and 0.97-0.86 originate from residual cyclohexane and hexane, respectively. ¹³C NMR (CDCl₃, 125 MHz): δ 140.2, 139.4, 138.6, 138.4, 137.2, 134.4, 130.4, 128.9, 128.13, 128.07, 127.5, 127.3, 126.0, 125.8, 125.7, 116.2, 108.0, 100.1, 29.8, 29.7, 24.1, 23.2, 21.3. Signals at around 31.9, 26.9, 22.7 and 14.1 originate from residual cyclohexane and hexane. HRMS (EI): *m/z* calculated for C₄₃H₃₂Cl₄N₄O₂: 776.1279 [*M*⁺]; found: 776.1257.



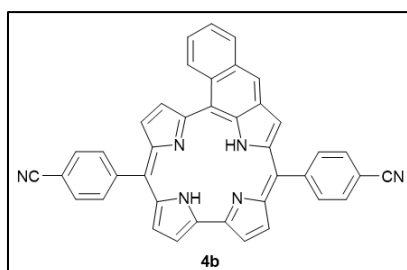
10-(2-(5,5-dimethyl-1,3-dioxan-2-yl)phenyl)-5,15-bis(4-methoxyphenyl)corrole (3d). Crude product was purified by column chromatography (silica, DCM/hexane 95:5) and crystallized from hot MeOH to afford product of analytical purity. Violet precipitate. Yield: 0.176 g (25%). M.p. 244 °C (decomp). ¹H NMR (CDCl₃, 600 MHz): δ 8.90 (bs, 2H, β-H), 8.82 (bs, 2H, β-H), 8.54 (bs, 2H, β-H), 8.36 (bs, 2H, β-H), 8.27 (bs, 4H, Ar), 8.21-8.13 (m, 1H, Ar), 7.94-7.87 (m, 1H, Ar), 7.86-7.79 (m, 1H, Ar), 7.67-7.60 (m, 1H, Ar), 7.40-7.27 (m, 4H, Ar), 4.94 (s, 1H, CH), 4.06 (s, 6H, OCH₃), 3.31 (d, *J* = 10.5 Hz, 2H, CH₂), 2.51 (d, *J* = 9.5 Hz, 2H, CH₂), 1.23 (s, 3H, CH₃), 0.20 (s, 3H, CH₃). Signals from the inner NH groups were not visible. HRMS (EI): *m/z* calculated for C₄₅H₄₀N₄O₄: 700.3050 [*M*⁺]; found: 700.3070.

General procedure for the synthesis of naphthocorroles 4a-d. Corrole (**3a-d**) (0.12 mmol) was dissolved in acetic acid (22 ml). Subsequently, TFA (11 ml) and 5% aq solution of H₂SO₄ (6 ml) were added and the reaction mixture was stirred at 50 °C (oil bath) for given time - **3a** - 2 h, **3b** and **3d** - 0.5 h and **3c** - 1 h under argon. Then, the mixture was cooled to room temperature, water was added, and then extracted by CHCl₃. Next, saturated solution of K₂CO₃ in water was added to the organic phase and extracted again by CHCl₃. The combined organic layers were dried over Na₂SO₄, filtered and evaporated. Further purification details are given below.



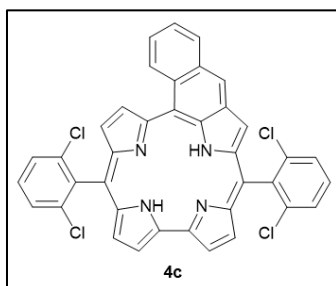
Naphthocorrole 4a. Crude product was purified by column chromatography (silica, DCM/hexane, 1:2) and crystallized from DCM/hexane to afford product of analytical purity. Dark precipitate. Yield: 0.038 g (44%). M.p. 315 °C (decomp). ¹H NMR (THF-*d*₈, 500 MHz): δ 16.39 (s, 1H, NH), 15.81 (s, 1H, NH), 8.10 (d, *J* = 8.9 Hz, 1H, Ar), 8.01 (s, 1H, Ar), 7.66 (d, *J* = 8.1 Hz, 1H, Ar), 7.51 (d, *J* = 4.8 Hz, 1H, β-H), 7.26 (t, *J* = 7.8 Hz, 1H, Ar), 7.15 (t, *J* = 7.4 Hz, 1H, Ar), 6.97 (d, *J* = 4.6 Hz, 1H, β-H), 6.95-6.88 (m, 2H, Ar), 6.72-6.68 (m, 2H, Ar),

6.38-6.32 (m, 1H, Ar). ¹⁹F NMR (THF-*d*₈, 470 MHz): δ -163.71 – -163.52 (m, 4F, Ar), -155.76 (t, *J* = 20.6 Hz, 1F, Ar), -155.48 (t, *J* = 20.8 Hz, 1F, Ar), -140.10 (dd, *J* = 22.6, 7.0 Hz, 2F, Ar), -139.52 (dd, *J* = 22.6, 7.0 Hz, 2F, Ar). HRMS (ESI): *m/z* calculated for C₃₈H₁₅F₁₀N₄: 717.1137 [*M*+H⁺]; found: 717.1136.

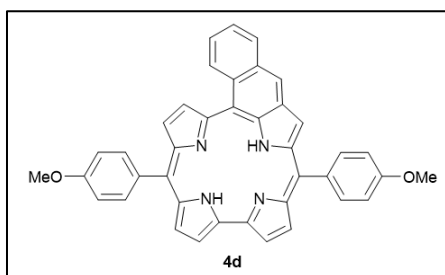


Naphthocorrole 4b. Crude product was purified by crystallization from DCM/hexane to afford product of analytical purity. Dark precipitate. Yield: 0.068 g (97%). M.p. 335 °C (decomp). ¹H NMR (THF-*d*₈, 500 MHz): δ 16.73 (s, 1H, NH), 16.14 (s, 1H, NH), 8.14 (d, *J* = 8.8 Hz, 1H, Ar), 8.01 (s, 1H, Ar), 7.90 (d, *J* = 8.1 Hz, 4H, Ar), 7.77 (dd, *J* = 8.0, 6.0 Hz, 4H, Ar), 7.67 (d, *J* = 7.9 Hz, 1H, Ar), 7.46 (d, *J* = 4.7 Hz, 1H, β-H), 7.24 (t, *J* = 7.4 Hz, 1H, Ar), 7.16 (t, *J* = 7.4 Hz, 1H,

Ar), 6.91 (d, *J* = 4.5 Hz, 1H, β-H), 6.88 (d, *J* = 4.6 Hz, 1H, β-H), 6.83 (d, *J* = 4.7 Hz, 1H, β-H), 6.65-6.61 (m, 2H, Ar), 6.33-6.29 (m, 1H, Ar). ¹³C NMR (THF-*d*₈, 125 MHz): δ 167.0, 159.6, 152.9, 152.3, 142.3, 141.3, 140.5, 137.4, 136.1, 135.6, 135.0, 134.6, 134.2, 133.3, 132.1, 131.9, 131.8, 131.7, 131.3, 131.0, 130.4, 128.5, 126.7, 126.1, 124.8, 123.5, 120.1, 117.9, 117.8, 116.3, 113.5, 113.1, 113.0, 111.0, 110.0. HRMS (APCI): *m/z* calculated for C₄₀H₂₃N₆: 587.1984 [*M*+H⁺]; found: 587.1987.

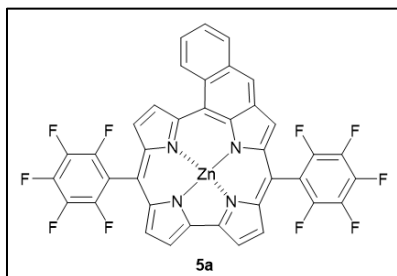


Naphthocorrole 4c. Crude product was purified by column chromatography (silica, DCM/hexane, 1:1) and crystallized from DCM/cyclohexane to afford product of analytical purity. Dark blue precipitate. Yield: 0.066 g (81%). M.p. 325 °C (decomp). ¹H NMR (THF-*d*₈, 500 MHz): δ 16.72 (s, 1H, NH), 16.14 (s, 1H, NH), 8.15 (d, *J* = 8.8 Hz, 1H, Ar), 7.92 (s, 1H, Ar), 7.64 (d, *J* = 8.1 Hz, 1H, Ar), 7.61-7.54 (m, 4H, Ar), 7.53-7.45 (m, 2H, Ar), 7.40 (d, *J* = 4.7 Hz, 1H, β-H), 7.21 (t, *J* = 7.1 Hz, 1H, Ar), 7.13 (t, *J* = 7.1 Hz, 1H, Ar), 6.84 (d, *J* = 4.5 Hz, 1H, β-H), 6.65 (d, *J* = 4.5 Hz, 1H, β-H), 6.63 (d, *J* = 4.7 Hz, 1H, β-H), 6.55 (dd, *J* = 3.8, 2.6 Hz, 1H, Ar), 6.36 (d, *J* = 1.6 Hz, 1H, Ar), 6.06-6.01 (m, 1H, Ar). ¹³C NMR (THF-*d*₈, 125 MHz): δ 168.5, 161.1, 154.9, 153.8, 142.5, 139.0, 137.2, 136.9, 136.7, 135.67, 135.66, 135.4, 135.3, 134.4, 133.14, 133.08, 131.9, 131.8, 131.5, 130.3, 129.4, 129.02, 128.98, 127.6, 126.9, 126.1, 124.4, 119.5, 114.6, 114.5, 111.7. HRMS (EI): *m/z* calculated for C₃₈H₂₀Cl₄N₄: 672.0442 [*M*⁺]; found: 672.0449.

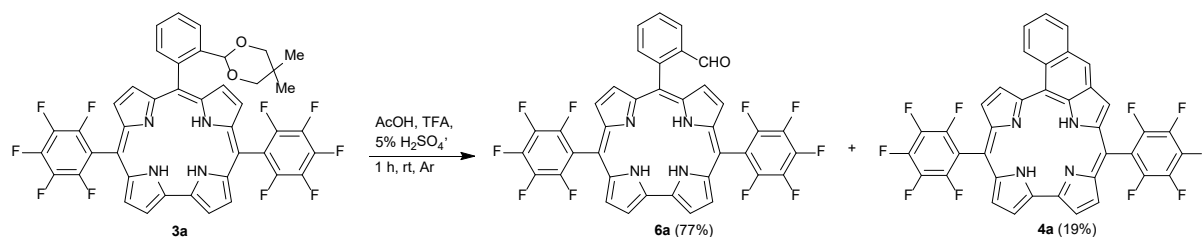


Naphthocorrole 4d. Crude product was purified by column chromatography (silica, DCM) and crystallized from DCM/cyclohexane to afford product of analytical purity. Dark precipitate. Yield: 0.060 g (83%). M.p. 238-240 °C. ¹H NMR (THF-*d*₈, 500 MHz): δ 17.02 (s, 1H, NH), 16.46 (s, 1H, NH), 8.22 (d, *J* = 8.9 Hz, 1H, Ar), 7.96 (s, 1H, Ar), 7.66 (d, *J* = 8.1 Hz, 1H, Ar), 7.54 (dd, *J* = 8.7, 2.4 Hz, 4H, Ar), 7.37 (d, *J* = 4.6 Hz, 1H, β-H), 7.21 (t, *J* = 7.1 Hz, 1H, Ar), 7.13 (t, *J* = 7.1 Hz, 1H, Ar), 7.07 (t, *J* = 8.2 Hz, 4H, Ar), 6.91 (d, *J* = 4.4 Hz, 1H, β-H), 6.88 (d, *J* = 4.6 Hz, 1H, β-H), 6.82 (d, *J* = 4.5 Hz, 1H, β-H), 6.66 (s, 1H, Ar), 6.55-6.50 (m, 1H, Ar), 6.37-6.32 (m, 1H, Ar), 3.89 (s, 6H, OCH₃). HRMS (ESI): *m/z* calculated for C₄₀H₂₉N₄O₂: 597.2291 [*M*+H⁺]; found: 597.2296.

Synthesis of naphthocorrole 5a. Round bottom flask was charged with compound **4a** (0.045 g, 0.063 mmol) and CHCl₃ (50 ml). Zinc acetate dihydrate was dissolved in MeOH (10 ml) and added to the reaction mixture, which was then stirred at 60 °C (oil bath) for 20 h under argon. After this time, the mixture was cooled to room temperature, water was added, extracted by DCM, dried over Na₂SO₄, filtered and the solvent was evaporated. Crude precipitate was crystallized from DCM/hexane to afford product of analytical purity.

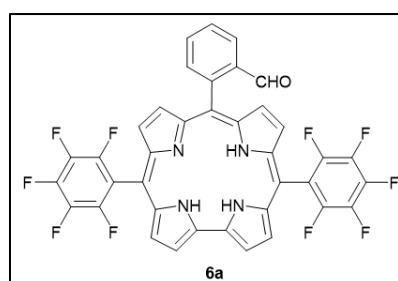


Naphthocorrole 5a. Brown precipitate. Yield: 0.041 g (84 %). M.p. 340 °C (decomp). ¹H NMR (THF-*d*₈, 500 MHz): δ 7.56 (d, *J* = 8.8 Hz, 1H, Ar), 7.29 (s, 1H, Ar), 7.11 (d, *J* = 7.9 Hz, 1H, Ar), 7.00 (d, *J* = 4.7 Hz, 1H, β-H), 6.86 (t, *J* = 7.2 Hz, 1H, Ar), 6.74 (t, *J* = 7.2 Hz, 1H, Ar), 6.51 (d, *J* = 4.6 Hz, 1H, β-H), 6.44 (d, *J* = 4.4 Hz, 1H, β-H), 6.40 (d, *J* = 4.7 Hz, 1H, β-H), 6.30 (d, *J* = 3.8 Hz, 1H, β-H), 6.02 (d, *J* = 3.8 Hz, 1H, β-H), 5.88 (s, 1H, Ar). ¹⁹F NMR (THF-*d*₈, 470 MHz): δ -164.40 (td, *J* = 23.5, 7.6 Hz, 2F, Ar), -164.02 (td, *J* = 23.4, 7.7 Hz, 2F, Ar), -156.98 (t, *J* = 20.6 Hz, 1F, Ar), -156.58 (t, *J* = 20.5 Hz, 1F, Ar), -141.12 (dd, *J* = 23.6, 7.8 Hz, 2F, Ar), -140.04 (dd, *J* = 23.6, 7.6 Hz, 2F, Ar). HRMS (EI): *m/z* calculated for C₃₈H₁₂F₁₀N₄Zn: 778.0194 [*M*⁺]; found: 778.0195.



Scheme S2. Synthesis of 10-(2-formylphenyl)-5,15-bis(pentafluorophenyl)corrole (**6a**).

Synthesis of 10-(2-formylphenyl)-5,15-bis(pentafluorophenyl)corrole (6a). Corrole **3a** (0.214 g, 0.26 mmol) was dissolved in acetic acid (50 ml). Subsequently, TFA (25 ml) and 5% aq solution of H₂SO₄ (12 ml) were added and the reaction mixture was stirred at room temperature for 1 h under argon. Then, water was added, and the resulting mixture was extracted by CHCl₃. Saturated solution of K₂CO₃ in water was added to the organic phase and extracted again by CHCl₃. The combined organic layers were dried over Na₂SO₄, filtered, and evaporated. The crude product was purified by column chromatography (silica, DCM/hexane, 2:1) and crystallized from hot MeOH to afford product of analytical purity.



10-(2-formylphenyl)-5,15-bis(pentafluorophenyl)corrole (6a). Violet precipitate. Yield: 0.147 g (77%). M.p. 203 °C (decomp). ¹H NMR (CDCl₃, 500 MHz): δ 9.49 (s, 1H, Ar), 9.15 (d, *J* = 4.1 Hz, 2H, β-H), 8.72 (d, *J* = 4.1 Hz, 2H, β-H), 8.59 (bs, 2H, Ar), 8.49 (d, *J* = 4.7 Hz, 2H, β-H), 8.42-8.36 (m, 1H, Ar), 8.16 (bs, 1H, Ar), 7.96-7.89 (m, 2H, Ar). Signals from the inner NH groups were not visible. ¹⁹F NMR (CDCl₃, 470 MHz): δ -161.90 – -161.30 (m, 4F, Ar), -152.48 (bs, 2F, Ar), -138.03 (d, *J* = 21.6 Hz, 2F, Ar), -137.59 (d, *J* = 21.7 Hz, 2F, Ar). HRMS (ESI): *m/z* calculated for C₃₈H₁₇F₁₀N₄O: 735.1243 [*M*+H⁺]; found: 735.1240.

Ar), -138.03 (d, *J* = 21.6 Hz, 2F, Ar), -137.59 (d, *J* = 21.7 Hz, 2F, Ar). HRMS (ESI): *m/z* calculated for C₃₈H₁₇F₁₀N₄O: 735.1243 [*M*+H⁺]; found: 735.1240.

3. Crystallographic Data

Table S1. Crystallographic data for compound **4a**.

Chemical formula	C ₃₈ H ₁₄ F ₁₀ N ₄	
Formula weight	716.53 g/mol	
Temperature	100 K	
Wavelength	1.54184 Å	
Crystal size	0.1 x 0.04 x 0.03 mm	
Crystal habit	violet block	
Crystal system	monoclinic	
Space group	P21/a	
Unit cell dimensions	a = 7.5781(3) Å	α = 90°
	b = 25.7071(9) Å	β = 104.588(4)°
	c = 14.9710(5) Å	γ = 90°
Volume	2822.49(18) Å ³	
Z	4	
Density	1.686 g/cm ³	
Absorption coefficient	1.289 mm ⁻¹	
F(000)	1440	
Index ranges	-9 ≤ h ≤ 9, -31 ≤ k ≤ 31, -18 ≤ l ≤ 18	
Diffractometer	Rigaku SuperNova	

Radiation source	CuK α	
Reflections collected	17379	
Independent reflections	5135 [R(int) = 0.0332]	
Tmin, Tmax	0.457, 1.000	
Absorption correction	multi-scan	
Refinement method	Full-matrix least-squares on F ²	
Restraints / parameters	0 / 519	
Goodness-of-fit on F²	1.220	
Final R indices	[F ² > 2 σ (F ²)]	R1 = 0.0737, wR2 = 0.1467
	all data	R1 = 0.0801, wR2 = 0.1493

Single crystal X-ray diffraction measurements were carried out on a Rigaku SuperNova diffractometer, at 100 K with Cu K α radiation (1.54184 Å). Violet crystal of approximate dimensions of 0.1 x 0.04 x 0.03 mm (block) was used. The structures were solved by direct methods and refined on F² by full-matrix least-squares. All non-hydrogen atoms were refined as anisotropic while hydrogen atoms were placed in calculated positions, and refined in riding mode.

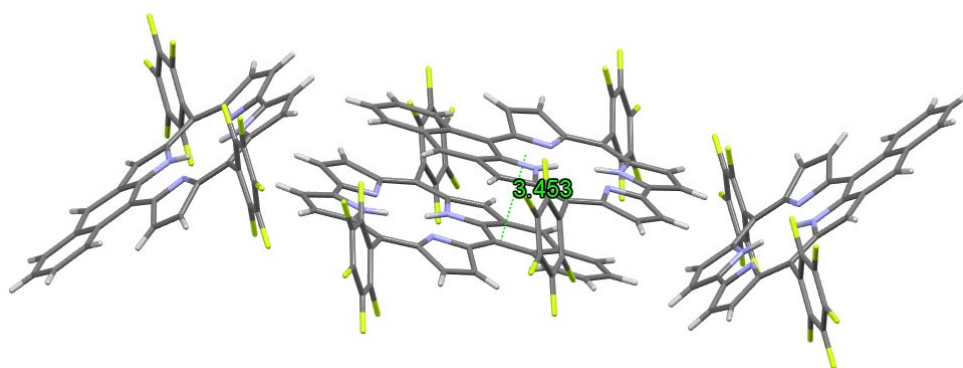


Figure S1. Packing diagram of crystal in elementary cell of compound **4a**.

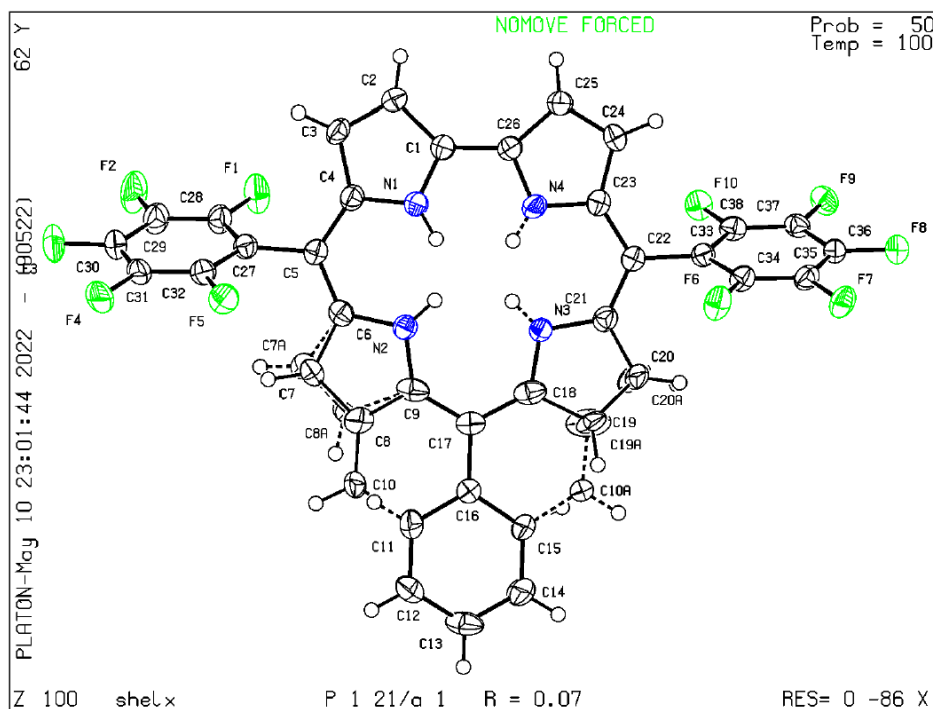
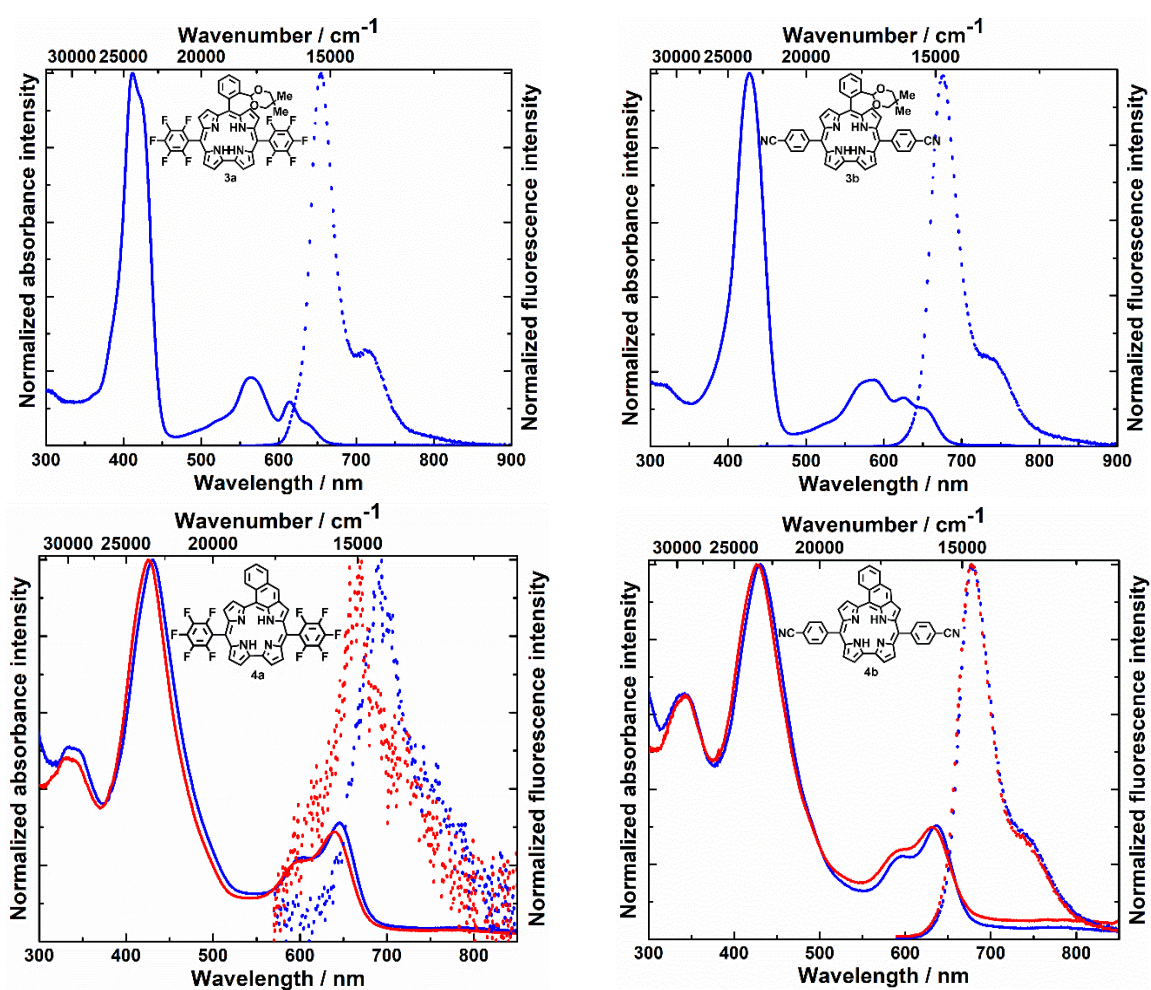


Figure S2. Thermal ellipsoid plot for compound **4a** with 50% probability level of ellipsoids contour.

4. Experimental Methods

Spectroscopic grade solvents were purchased from Sigma-Aldrich and used as obtained. For optical studies solutions of molecules at low concentrations, about few micromoles per liter, were used to avoid dimerization or reabsorption effects. All absorption and fluorescence spectra were taken at room temperature (21 °C). A Perkin Elmer UV/VIS Spectrometer model Lambda 35 was used for absorption spectra measurement. Fluorescence spectra were recorded with the FLS 1000 Spectrofluorometer from Edinburgh Instruments and corrected for the spectral response sensitivity of the photodetector. Fluorescence quantum yields (FQY) of molecules in solvents at 21 °C were determined using an integrating sphere. Molar absorptivity (absorption coefficient), ϵ was calculated from absorbance, A , of solution of given molar concentration, c , in cuvette of length, l , with a well-known formula $A=c \cdot \epsilon \cdot l$.

5. Spectroscopic Data



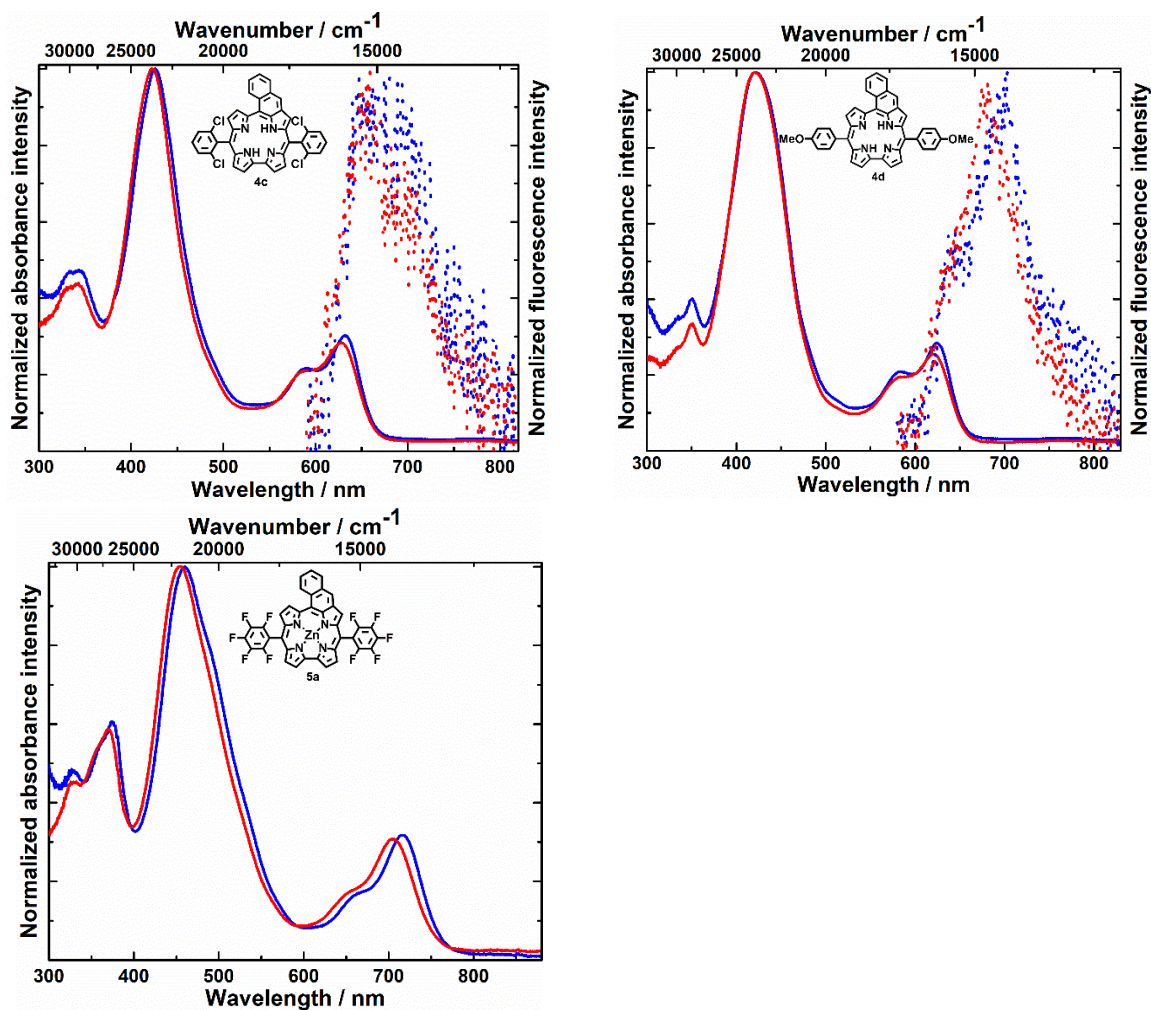


Figure S3. Absorption (solid line) and emission (dot line) spectra of compounds **3a-b** (excited at 405 and 420 nm respectively), **4a-d** (excited at 430 nm) and **5a** measured in toluene (blue) and DCM (red).

Table S2. Spectroscopic properties of compounds **3a-b**, **4a-d** and **5a** obtained in toluene and DCM.

Compound	Solvent	$\lambda_{\text{abs}}^{\text{max}}$ [nm]	$\lambda_{\text{em}}^{\text{max}}$ [nm]	ϵ [M ⁻¹ cm ⁻¹]	Stokes shift ^a [cm ⁻¹]	Φ_{F}
3a	toluene	412		115800		0.08 ^b
		564		21200		
		614		13600		
		640	655	6500	350	
3b	toluene	427		109000		0.17 ^b
		587		19500		
		624		14200		
		655	675	10800	450	
4a	toluene	335		26700		nd ^c
		431		52200		
		604		11500		
		645	689	16300	1000	
	DCM	334		26800		

		426		55700		nd ^c
		600		11800		
		640	667	16000	600	
4b	toluene	342		32700		<0.001 ^b
		431		49800		
		596		11100		
		636	677	15100	950	
	DCM	342		31400		<0.001 ^b
		426		48200		
		595		11500		
		632	677	14400	1050	
4c	toluene	346		25100		nd ^c
		426		53100		
		590		11500		
		631	681	16000	1200	
	DCM	343		25400		nd ^c
		423		57700		
		586		12100		
		628	659	16400	750	
4d	toluene	351		24900		nd ^c
		421		61900		
		583		12900		
		624	701	17600	1800	
	DCM	351		21600		nd ^c
		421		64300		
		583		12600		
		620	681	16400	1400	
5a	toluene	375		26900		nd ^c
		460		44400		
		716		14100		
	DCM	371		29600		nd ^c
		455		50300		
		705		15500		

^aStokes shift calculated as a difference between lowest energy absorption band and highest energy emission band expressed in cm⁻¹, ^bfluorescence quantum yield measured using an integrating sphere, ^cnot detected.

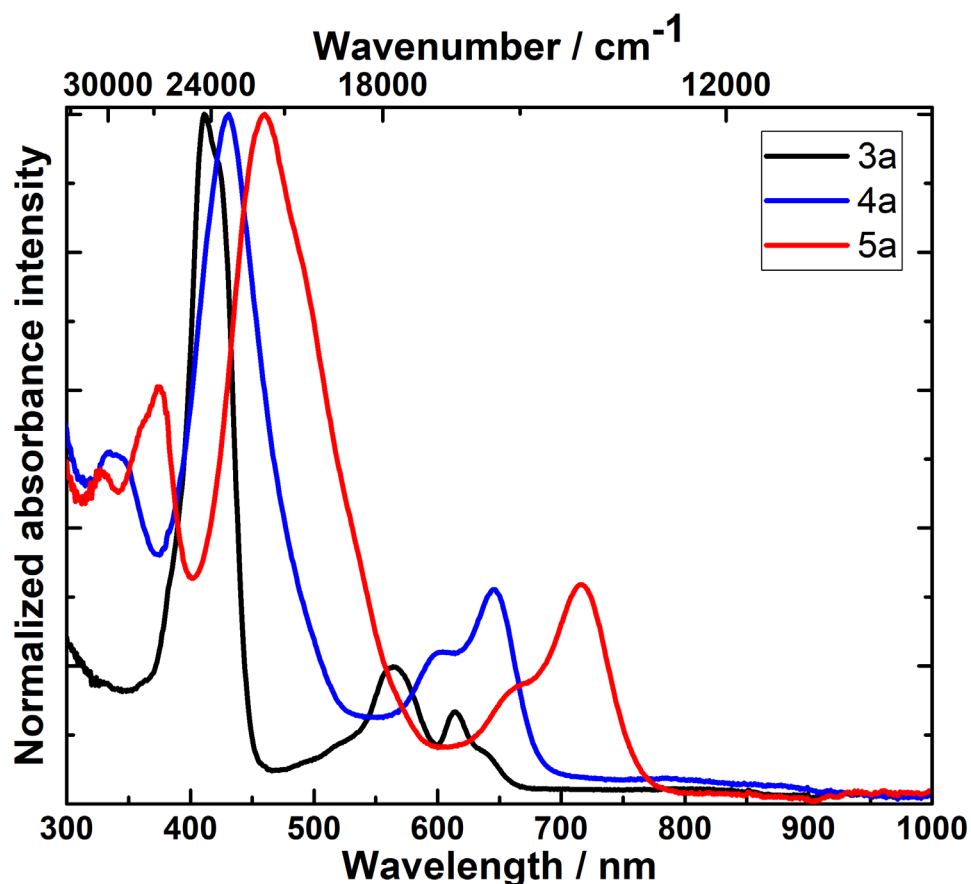


Figure S4. Absorption spectra of compounds **3a** (black), **4a** (blue) and **5a** (red) measured in toluene.

6. Computational Results

True minima for **4a** and **6a** have been determined using Gaussian16 at the B972/6-31G(d) level, using the SMD solvent to model the solvent (chloroform for **6a** and THF for **4a**).

The optimized geometry of **4a** turns out similar to the X-ray crystal structure.

The calculation of the magnetic response has been done still with the SMD model and the appropriate solvent, but at the B972/6-311+G(2d,p) level, and using the CSGT method^{S1} to distribute the origin, according to the Gaussian16 keywords NMR=CSGT output=(csgt,wfx).

The *.wfx file was then used in SYSMOIC to compute the current density and the current strengths, according to the CTOCD-DZ2 method.^{S2-S3} Selected results are reported in Figs. S5-S8 and Table S3-S4.

Isotropic nuclear shieldings, which can be obtained by integration of the current density and are an indirect indication of its quality, are reported in Table S3, together with the computed chemical shifts, obtained as $\delta_{\text{calc}} = A + B \sigma_{\text{iso}}$, where the values $A=31.29(5)$ ppm and $B=-0.974(5)$ have been determined by least squares refinement of σ_{iso} vs δ_{exp} . ($R^2=0.9996$), in analogy with ref. S4.

Table S3. Computed isotropic proton nuclear shieldings and chemical shifts for **4a**. All entries in ppm, but for the numbers of the proton, consistent with Cartesian coordinates, reported below.

#H	σ_{iso}	δ_{exp}	δ_{calc}
54	15.3506	16.39	16.36
24	15.9119	15.81	15.79
59	23.3644	8.10	8.14
66	23.4353	8.01	8.06
63	23.7539	7.66	7.74
28	23.9725	7.51	7.51
62	24.1332	7.26	7.35
64	24.2463	7.15	7.23
29	24.5338	6.97	6.94
25	24.5901	6.92(4)	6.88
26	24.6410	6.92(4)	6.83
27	24.7816	6.70(2)	6.68
30	24.8136	6.70(2)	6.65
31	25.2102	6.35(3)	6.24

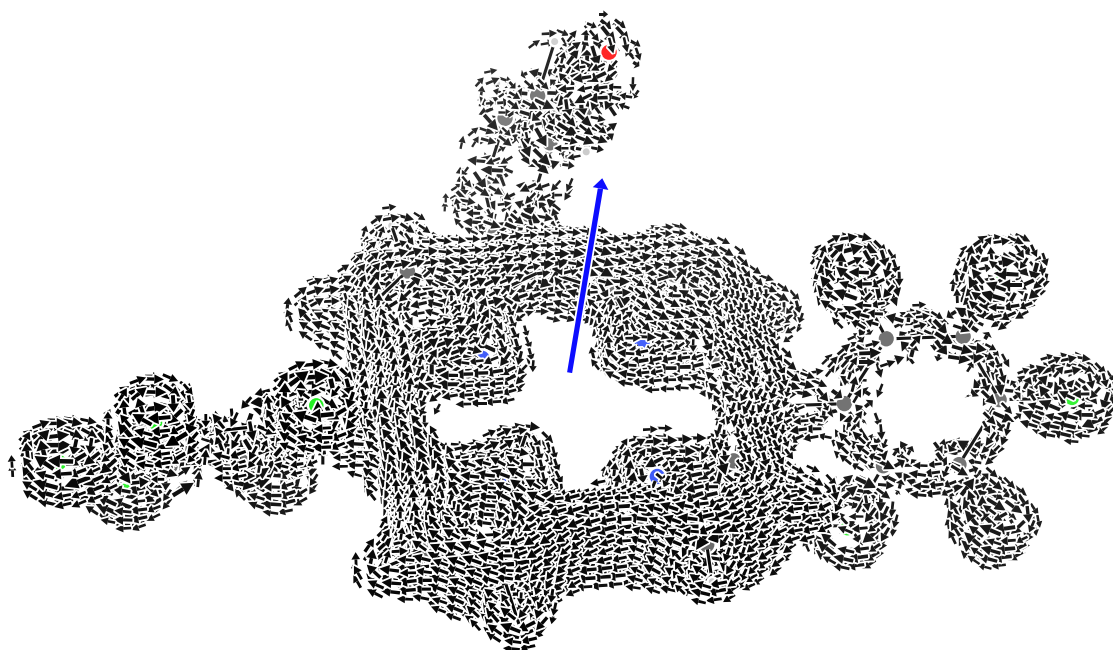


Figure S5. All-electron current density induced in **6a** by a unitary magnetic field (blue arrow) parallel to the Cartesian z -axis. Diatropic and paratropic currents are clockwise and anticlockwise, respectively. Currents lower/higher than 0.05/0.15 au are not shown.

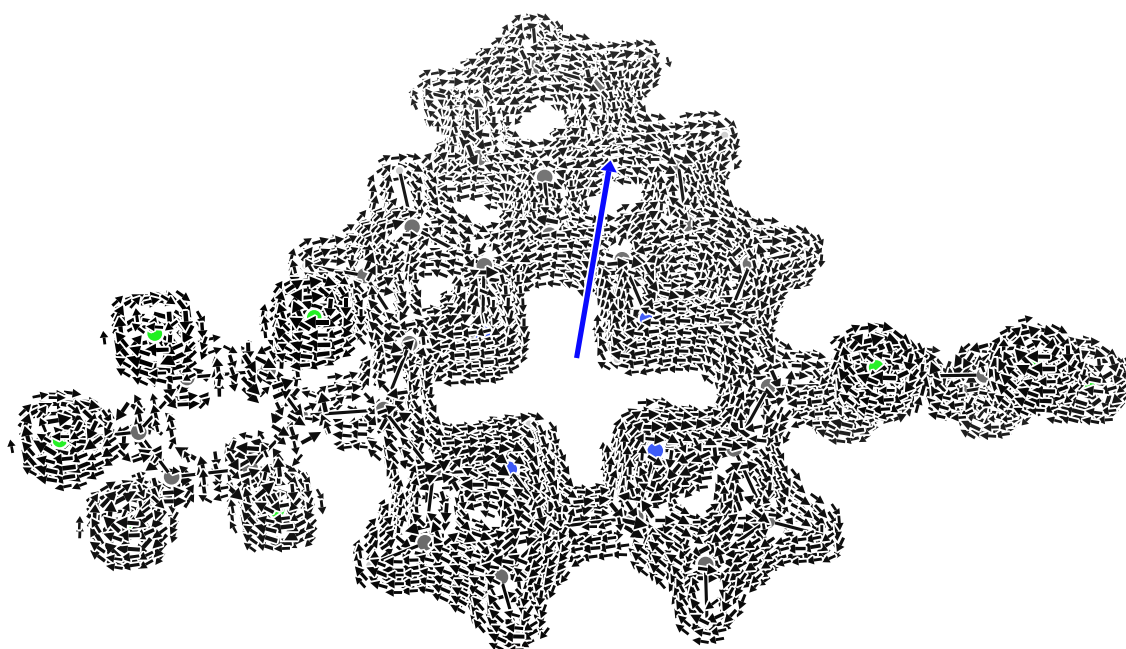


Figure S6. All-electron current density induced in **4a** by a unitary magnetic field (blue arrow) parallel to the Cartesian z -axis. Diatropic and paratropic currents are clockwise and anticlockwise, respectively. Currents lower/higher than 0.05/0.15 au are not shown.

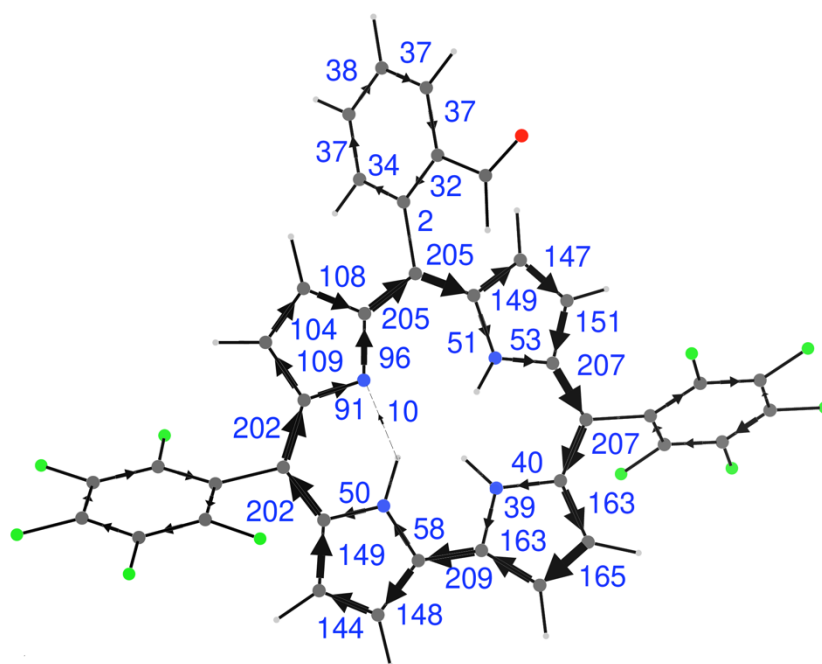


Figure S7. Bond current strengths for **6a**, computed in domains bisecting the bonds and extending up to $1 \cdot 10^{-3}$ au, expressed in percent units: a value of 100 equals the current strength of benzene (11.8 nA T^{-1} using the same method of calculation). The areas of the arrows are proportional to the current strength values. The magnetic field is oriented towards the reader, diatropic and paratropic currents are clockwise and anticlockwise, respectively.

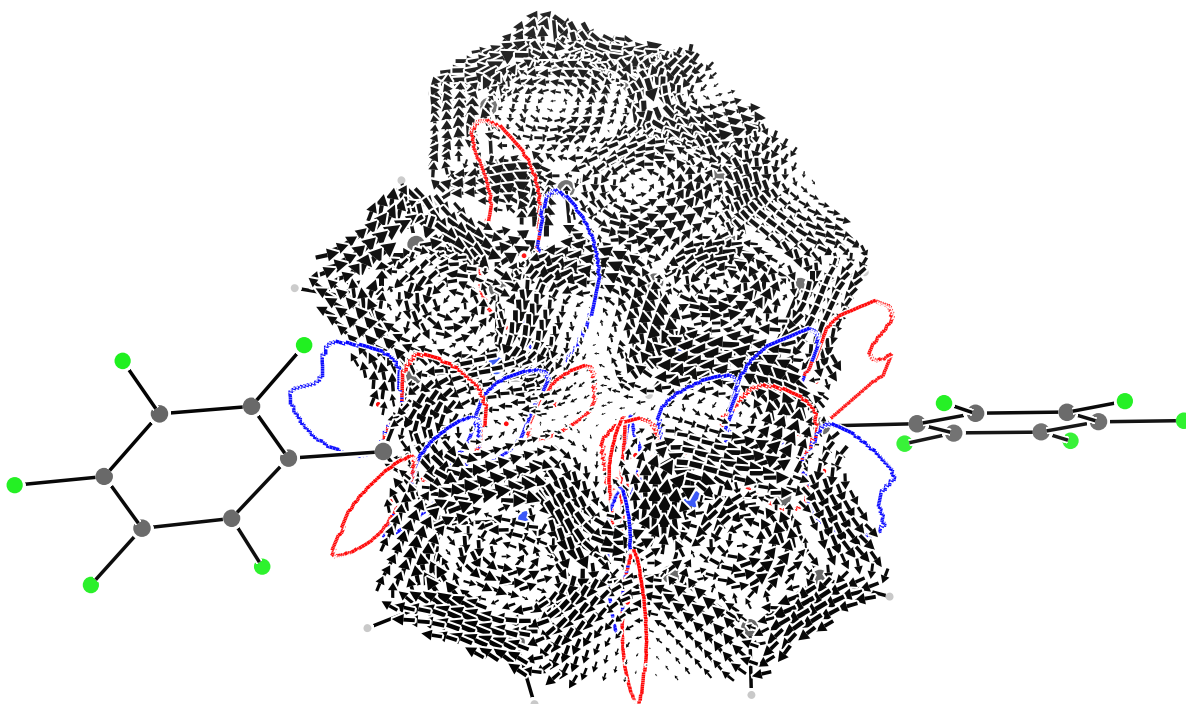
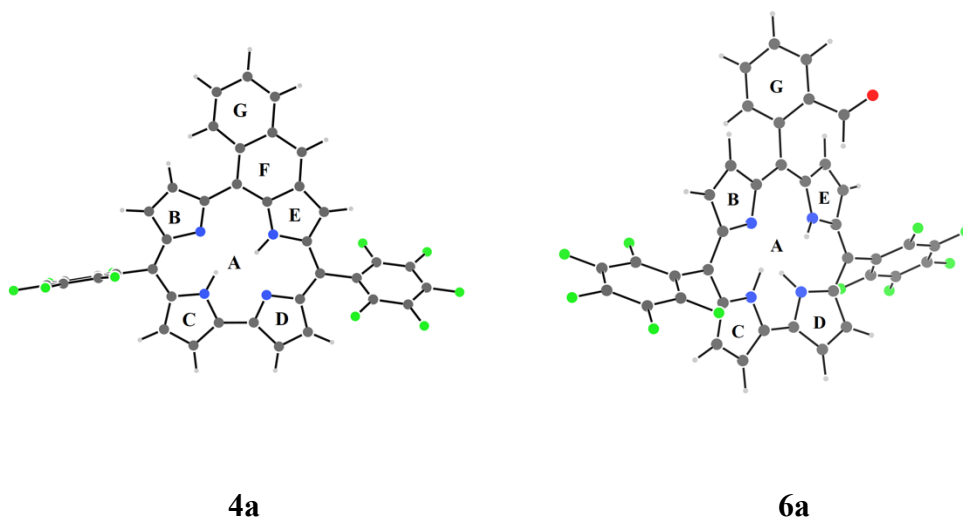


Figure S8. Current density computed on a surface placed 1 au above the rings of **4a**. The border of the integration domains used to produce the bond current strengths displayed in Fig. 3 are shown as blue and red closed curves.



Scheme S3. Ring labels of **4a** and **6a** needed for the interpretation of data in Table S4.

Table S4. Indicators of aromaticity for rings of **4a** and **6a**, all obtained at the B972/6-311+G(2d,p) level with implicit solvent (SMD, tetrahydrofuran for **4a**, chloroform for **6a**). Rings are labeled according to Scheme S3. $\overline{I}_0\%$ is the percentage of ring current strength of benzene signed according to the contribution given to the magnetizability: negative/positive for a diatropic/paratropic ring current. Ring current percentages and NICS^{S5} values have been computed with SYSMOIC, HOMA (Harmonic Oscillator Model of Aromaticity)^{S6} with Multiwfn.^{S7}

Ring	$\overline{I}_0\%$ ^a		NICS _{π,zz} (1) ^{b,c}		NICS _{zz} (1) ^c		HOMA	
	4a	6a	4a	6a	4a	6a	4a	6a
A	+14	-205	8.3	-37.6	12.3	-31.2	0.459 ^d (0.693)	0.714 ^d (0.845)
B	-33	-107	-6.6	-14.7	-8.6	-17.2	0.422	0.720
C	-54	-147	-13.0	-30.6	-16.7	-32.2	0.912	0.876
D	-24	-164	-2.8	-29.2	-6.4	-32.3	0.436	0.851
E	-33	-149	-5.1	-28.0	-8.0	-30.5	0.745	0.516
F	-31	--	-2.7	--	-0.8	--	0.573	--
G	-59	--	-16.1	-19.8	-15.0	-26.3	0.712	0.956

a) Values of $\overline{I}_0\%$ have been obtained from Fig. 3 and Fig. S5 averaging over bonds that should have the same current according to the current conservation.

b) For non-planar molecules the σ/π separation cannot be clear cut. A set of 23 and 24 orbitals has been selected for **4a** and **6a**, respectively, combining visual inspection and the low density value at the nuclei and at bond midpoints. Orbitals numbers are 180, 179, 178, 177, 176, 175, 174, 173, 172, 171, 170, 169, 167, 165, 164, 161, 158, 133, 131, 127, 126, 125, 124 for **4a**, 115, 116, 121, 122, 124, 127, 129, 130, 131, 165, 169, 170, 171, 173, 174, 175, 176, 177, 178, 179, 180, 183, 184, 185 for **6a**.

c) The magnetic shielding tensor σ_R at 1 Å above the average plane of ring R has been obtained by integration of the current density. Then the NICS_{zz} of ring R has been computed as $\text{NICS}_{zz}^R = -\mathbf{n}^T \sigma_R \mathbf{n}$, where \mathbf{n} is the unit column vector perpendicular to the average plane of ring R and T indicates transposition.

d) The HOMA of the macrocycle has been computed either following the outer path (the first entry) or the inner path passing through the 4 N atoms (value in parentheses).

7. Electrochemical Data

All compounds were tested in 0.1 M Tetrabutylammonium tetrafluoroborate (TBABF₄)/Benzonitrile solution (50 mM). The electrochemical measurements were performed with Bio-Logic VSP potentiostat. Cyclic voltammetry (CV) was conducted at scan rate of 100 mV/s under inert atmosphere. A 3-electrodes cell was placed in a sealed box and washed for an hour with Ar. Ar was bubbled into the solution 2 mins before the measurement. The working, counter, and pseudo-reference electrodes were Pt wire, glassy carbon rod and Ag wire, respectively. The reference potential was calibrated against ferrocene/ferrocenium redox couple by adding a small amount of ferrocene to the tested solution after the experiments. All potentials are reported vs. Fc/Fc⁺.

Spectroelectrochemistry: Since these compounds have nonaromatic character, they are expected to have fast and complicated electron transitions, and the shifts in the absorption spectra were relatively small. The most significant changes were found at the split Soret peaks of compounds **4a** and **4d**. This split peak can be deconvoluted into two main peaks with maxima at 432.4 nm and 451.0 nm for **4a** and, 426.2 nm and 442.9 nm for **4b**. Upon increasing the applied potential from beyond the reduction peak (in the CV), towards higher potentials, there is decrease in the intensity of the Soret peak located at the higher wavelength in parallel to increase in the intensity of the lower one.

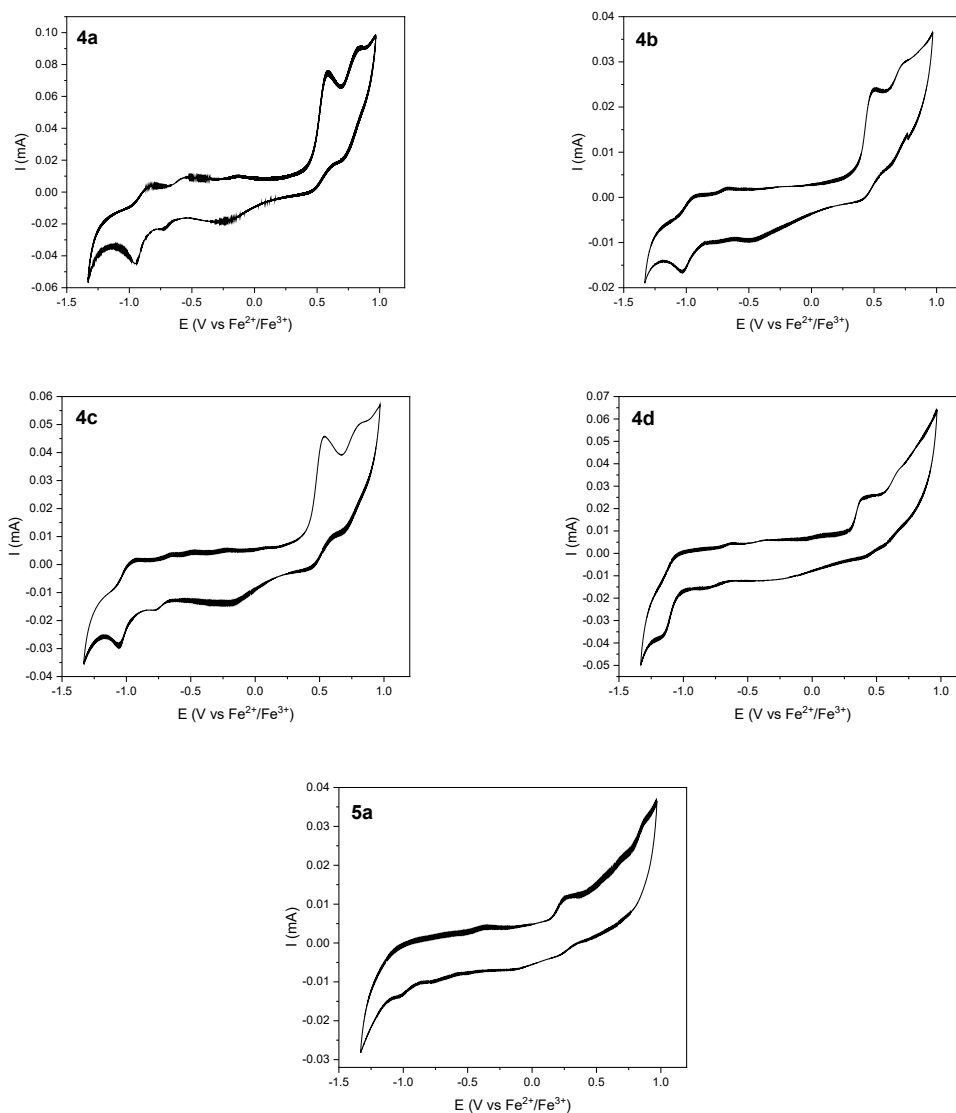


Figure S9. Cyclic voltammograms for compounds **4a-d** and **5a**.

Table S5. HOMO-LUMO energy values for compounds **4a-d** and **5a**.

compound	$E_{onset}^{Oxidation}(V)$	$E_{HOMO}(eV)$	$E_{onset}^{Reduction}(V)$	$E_{LUMO}(eV)$	$E_{gap}(eV)$
4a	0.443	-5.243	-0.85	-3.95	1.293
4b	0.376	-5.176	-0.905	-3.895	1.281
4c	0.408	-5.208	-0.953	-3.847	1.361
4d	0.307	-5.107	-1.049	-3.751	1.356
5a	0.141	-4.941	-0.913	-3.887	1.054

The HOMO and LUMO energies were calculated using the following equation:

$$E_{HOMO}^{LUMO}(eV) = -E_{onset}^{Ox/Red} - 4.8 eV$$

The HOMO-LUMO energy gap was calculated from the difference between E_{HOMO} to E_{LUMO} .^{S8-S9}

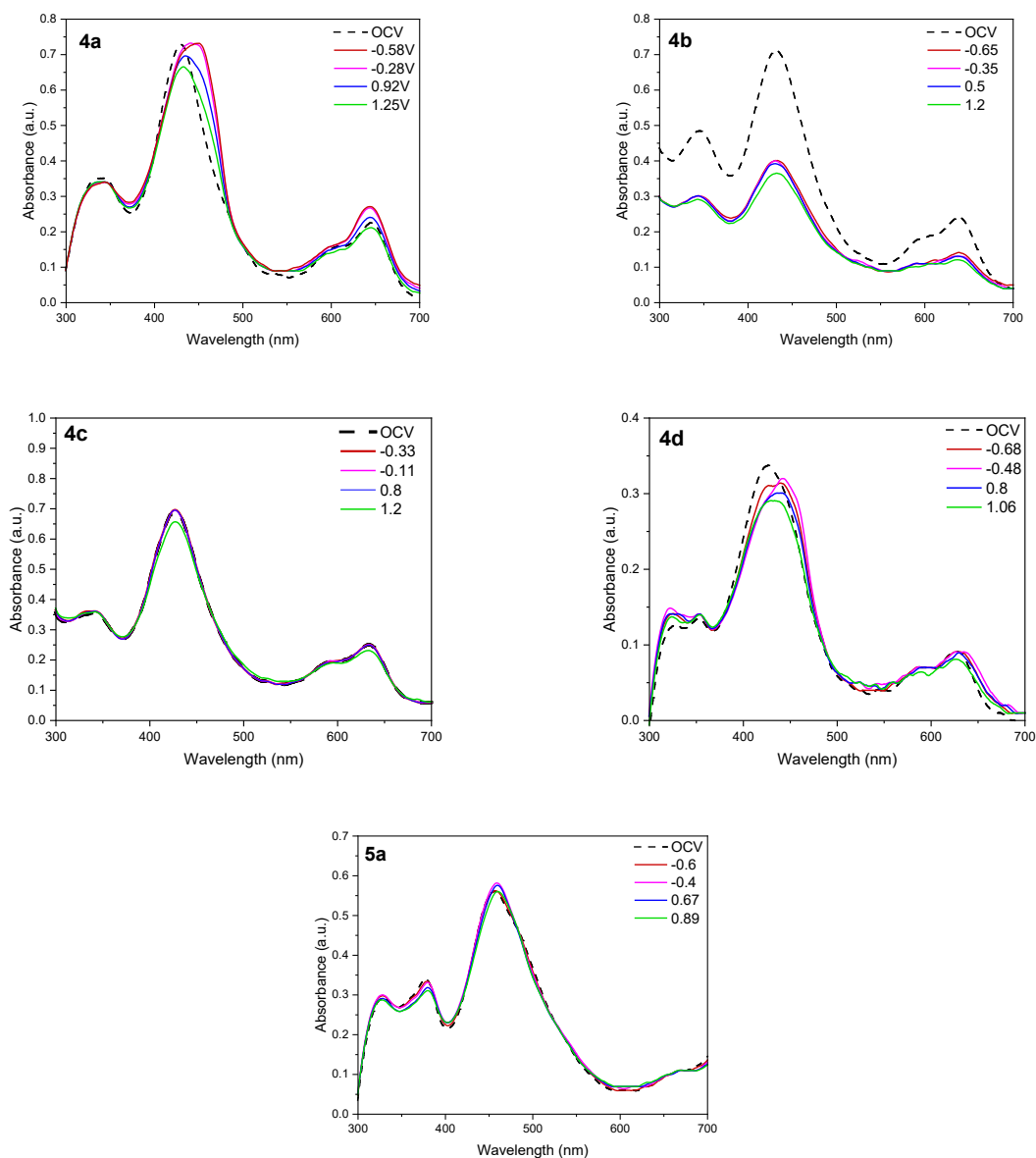
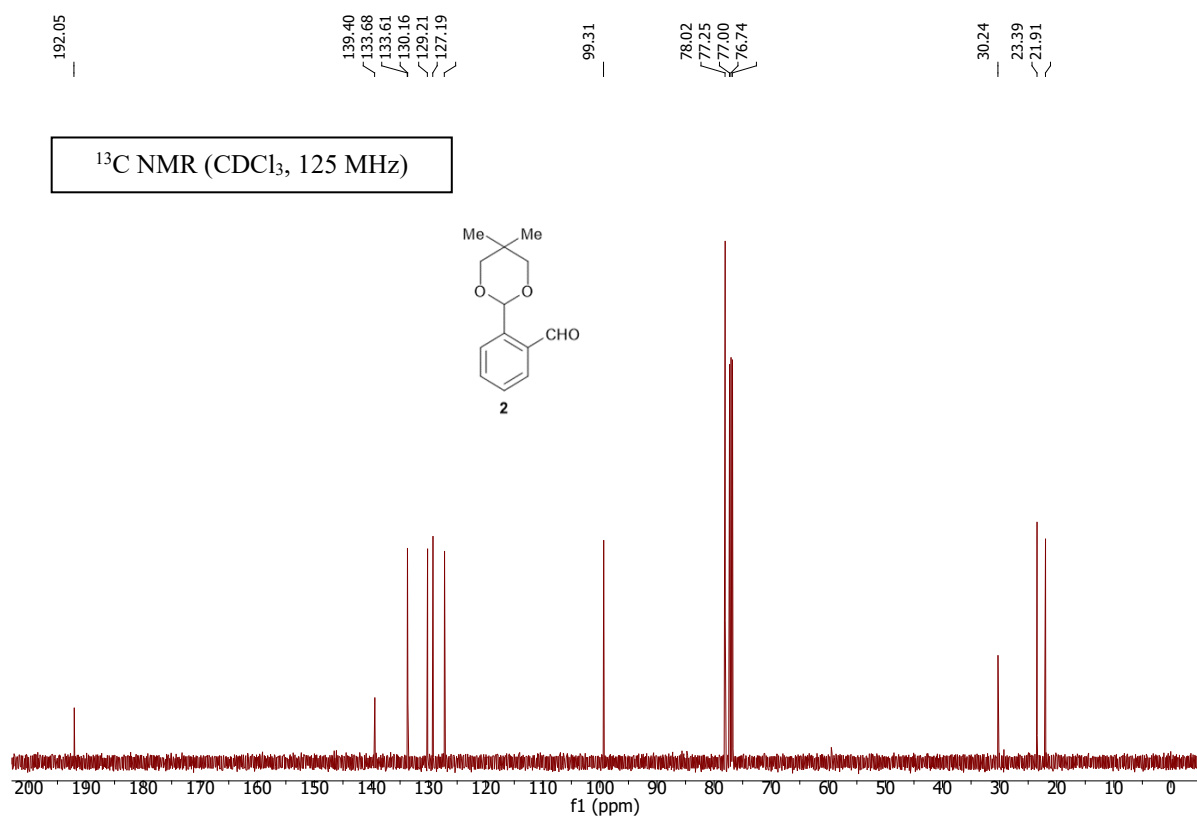
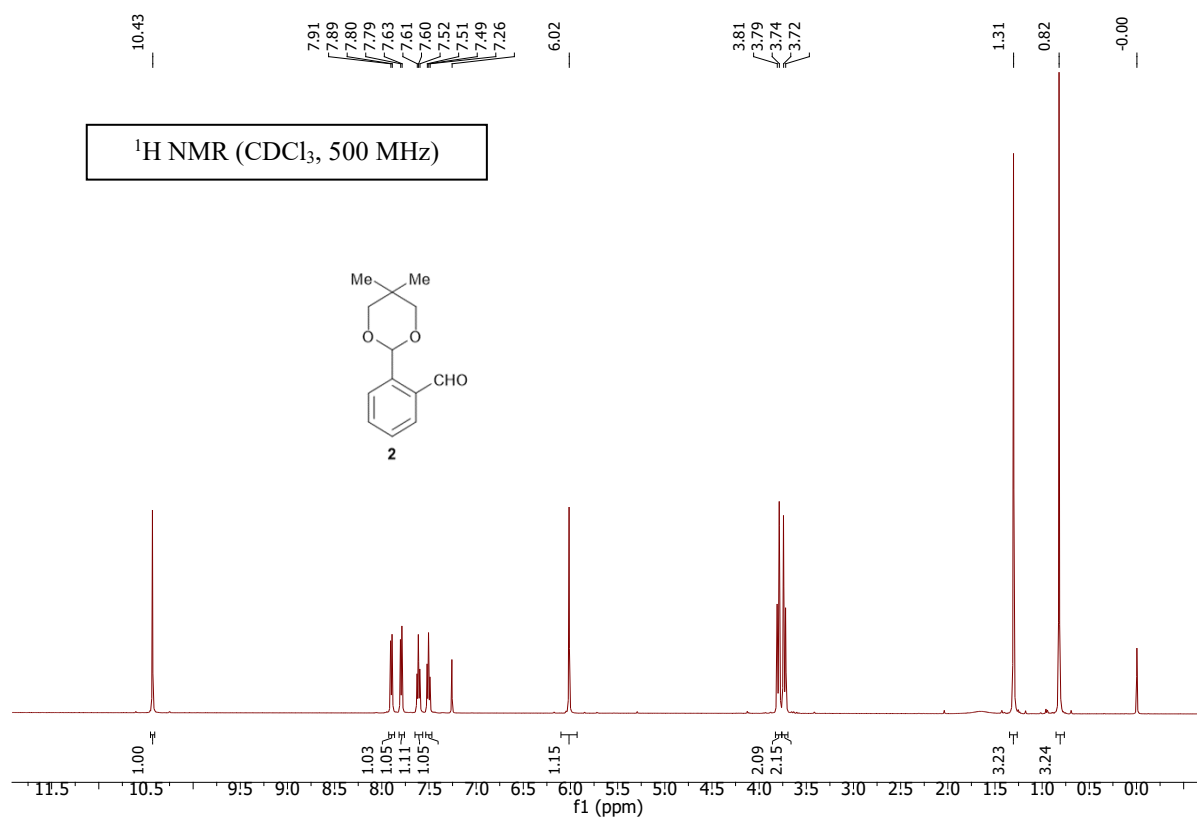
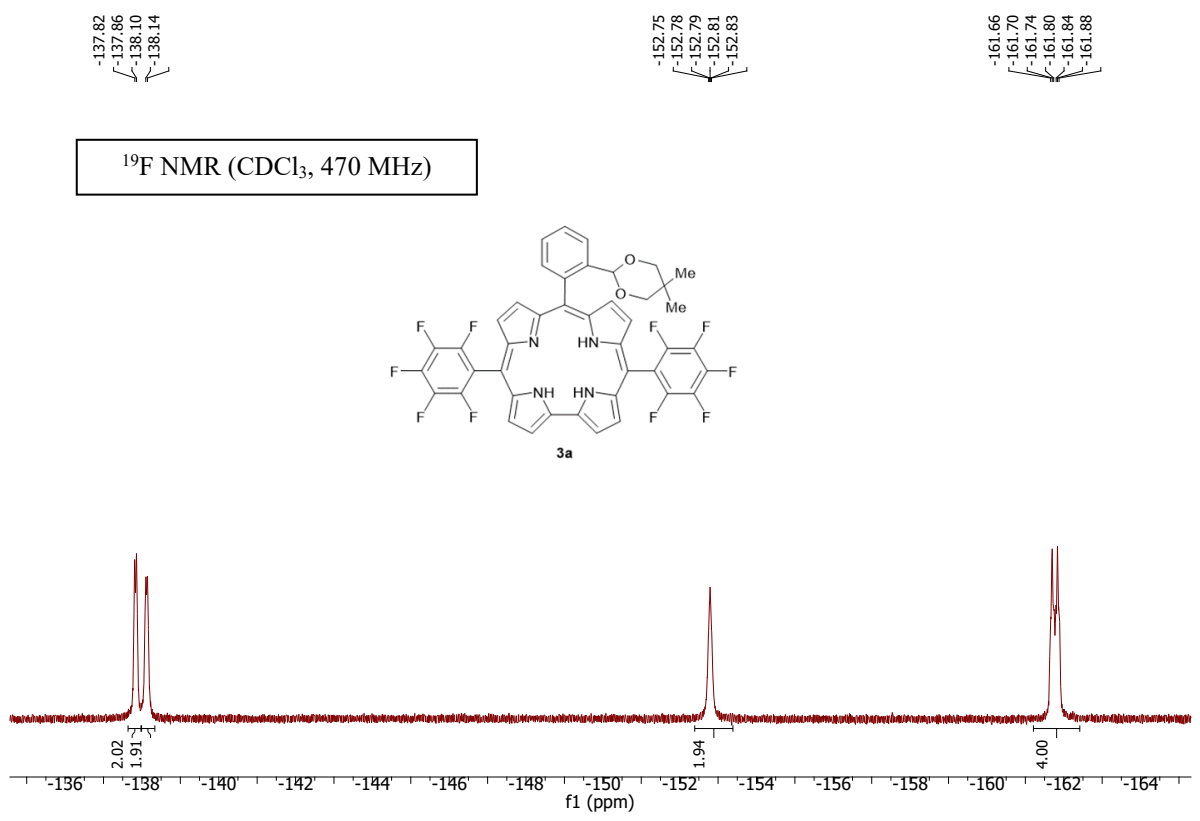
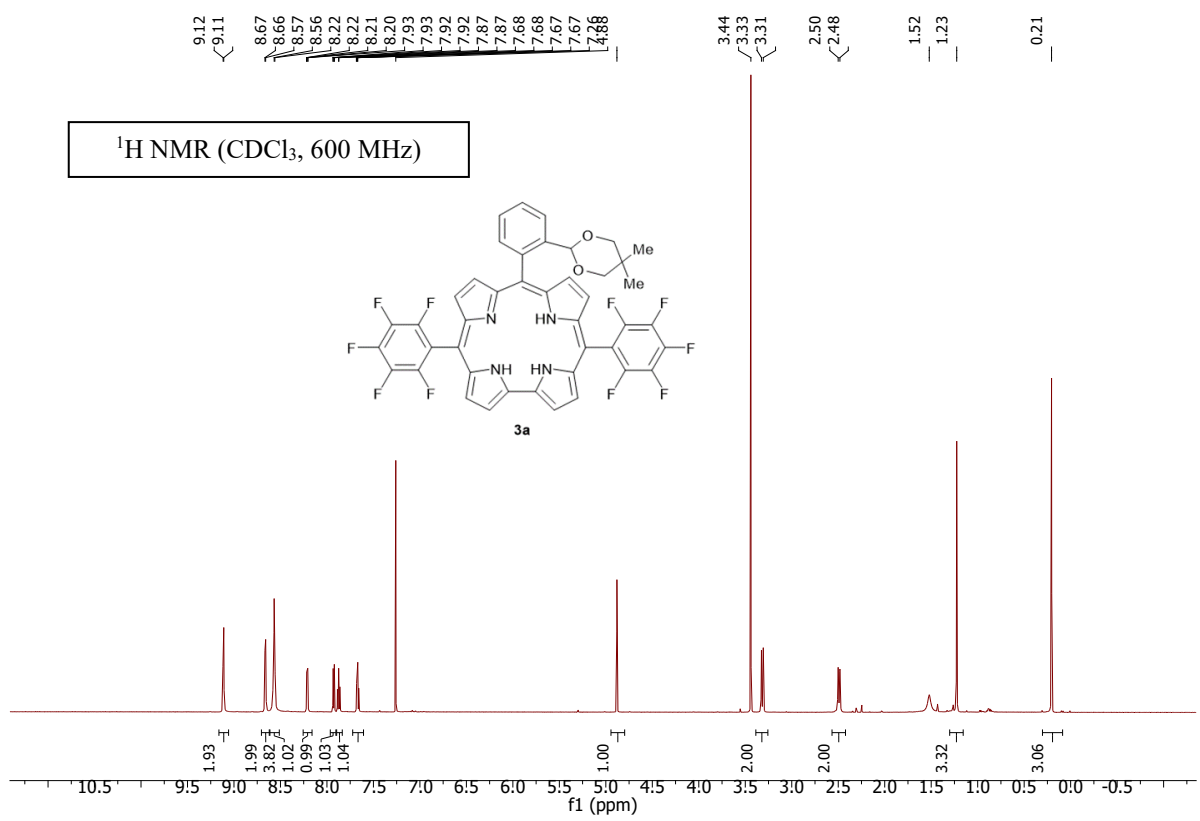


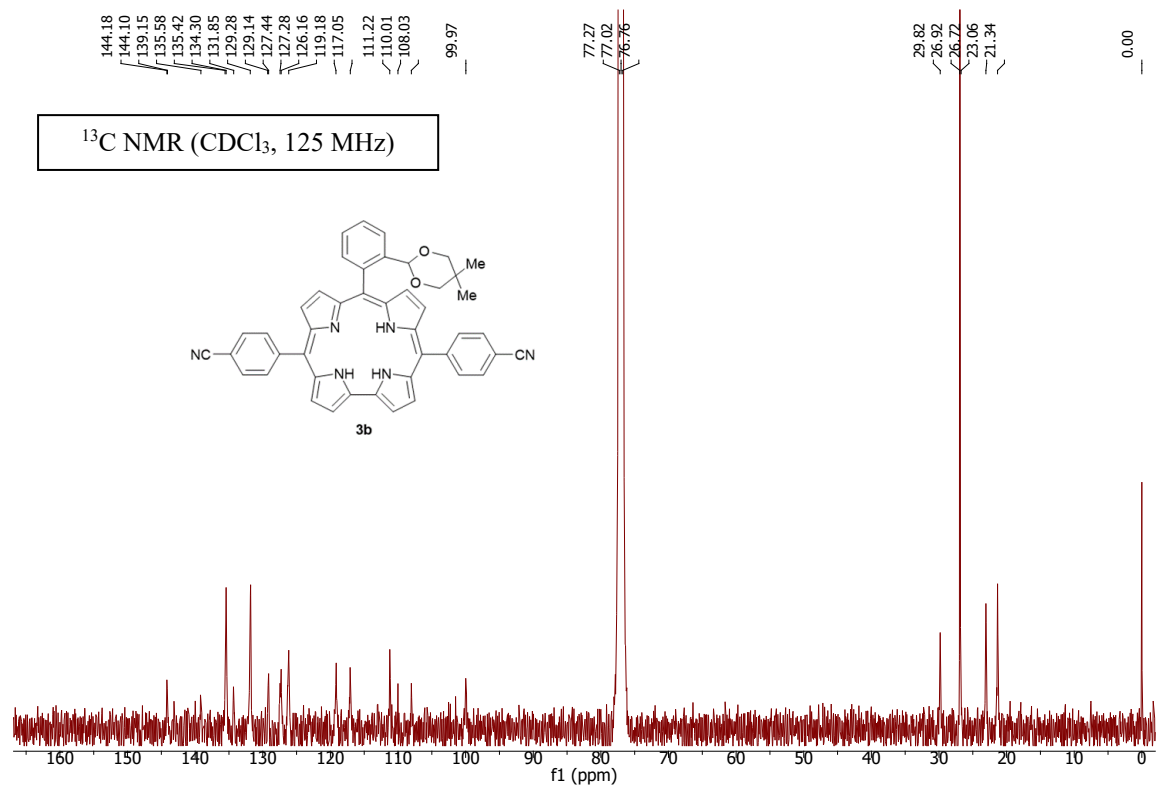
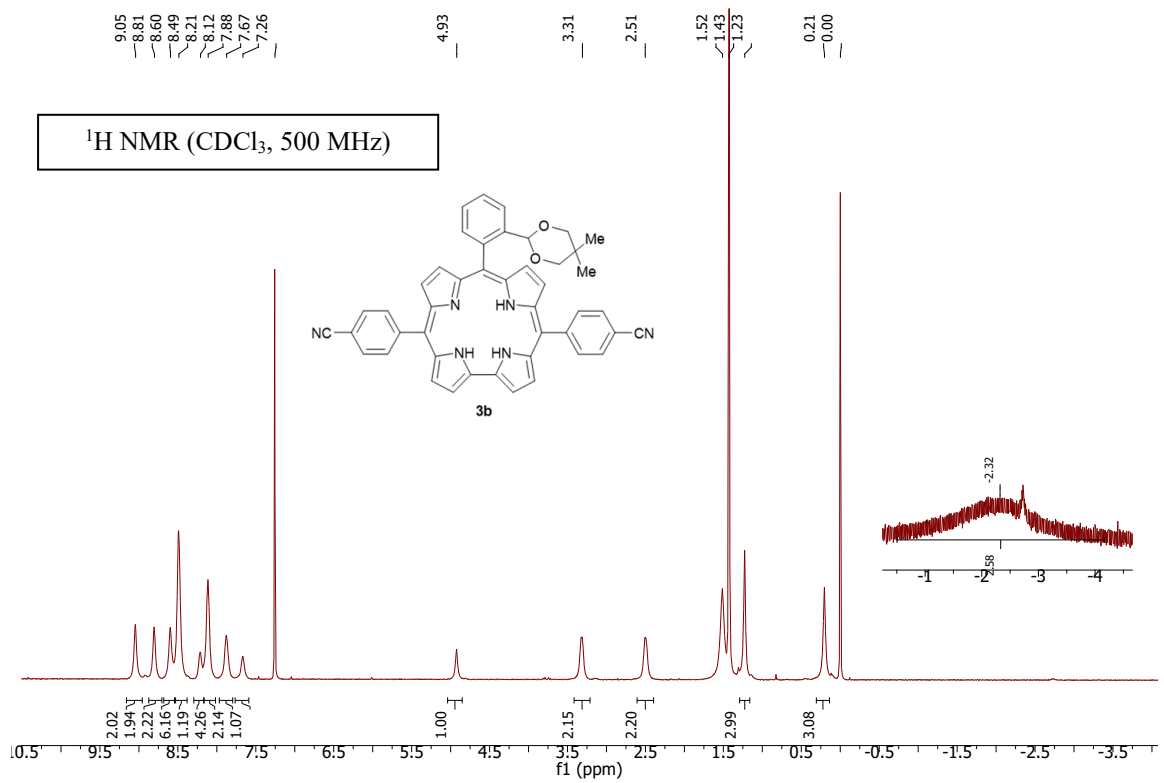
Figure S10. UV-visible spectroelectrochemical measurements for compounds 4a-d and 5a.

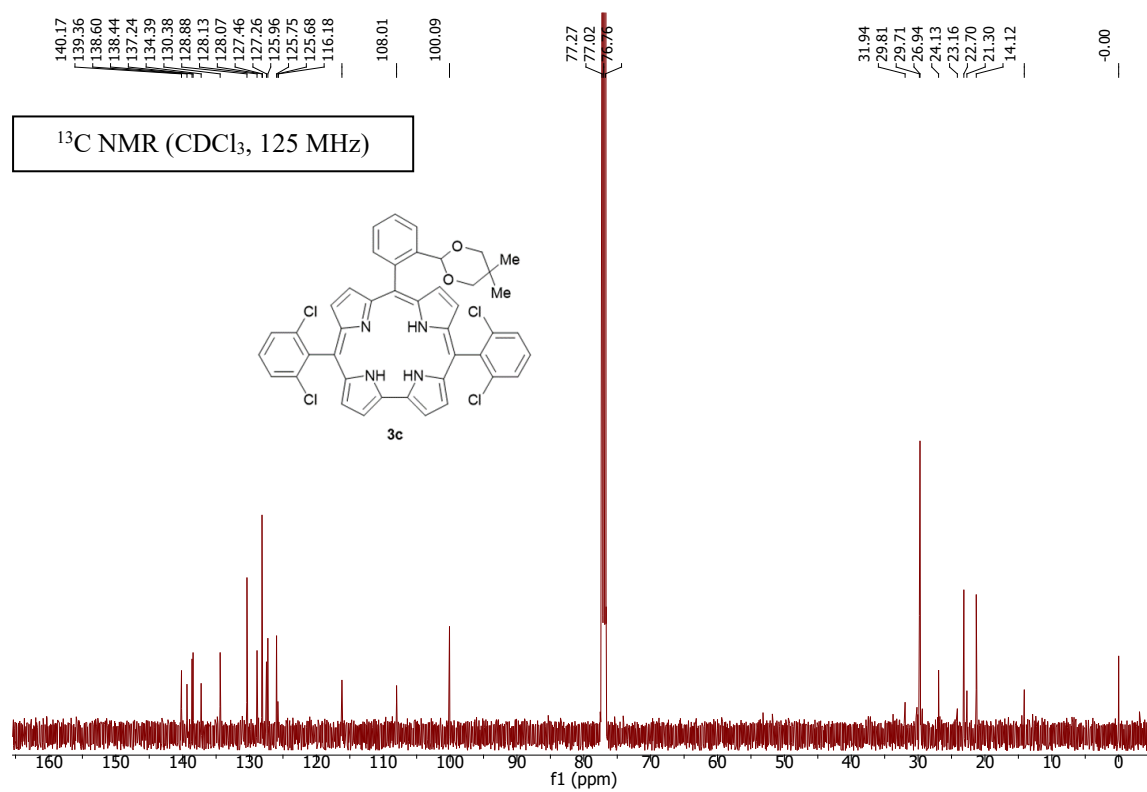
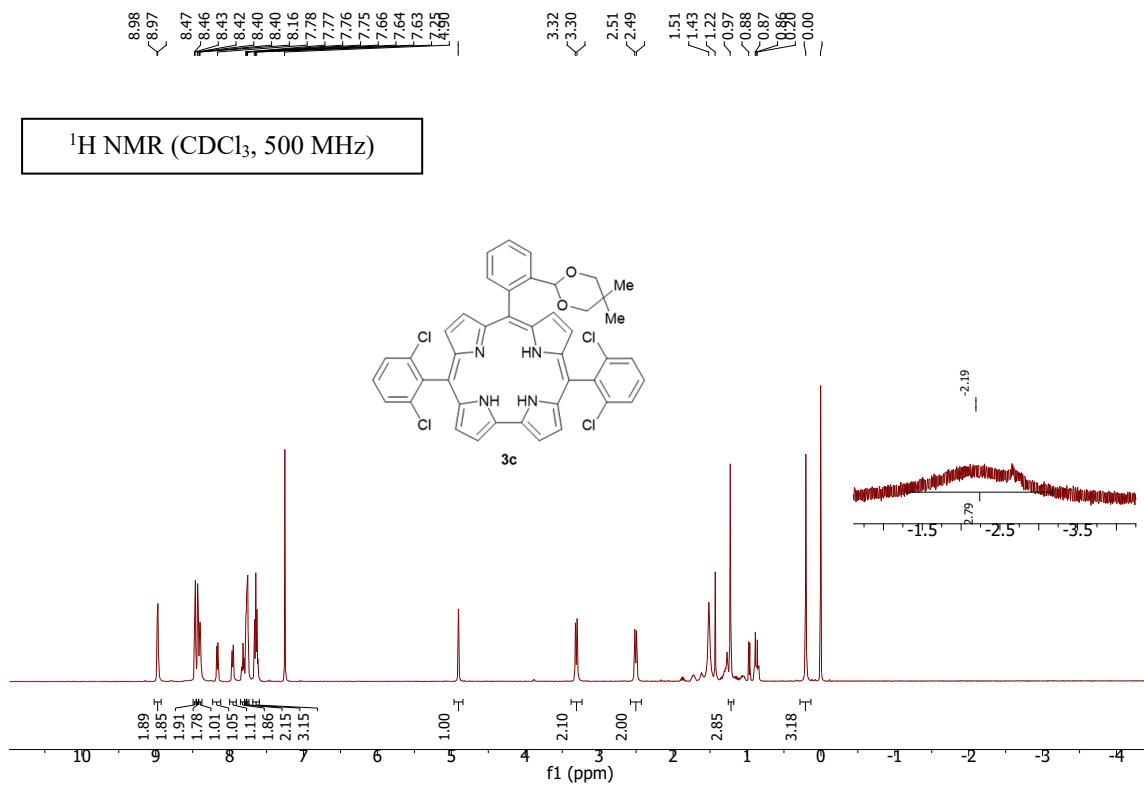
The samples were analyzed by using an ocean optics DH-2000-BAL deuterium halogen source spectrophotometer. A quartz three-electrode cell was used Ag wire as pseudo reference and Pt mesh and wire as working and counter electrodes, respectively. The electrode potential was held for 1min before and after the redox peaks after which the UV-Vis spectra were recorded.

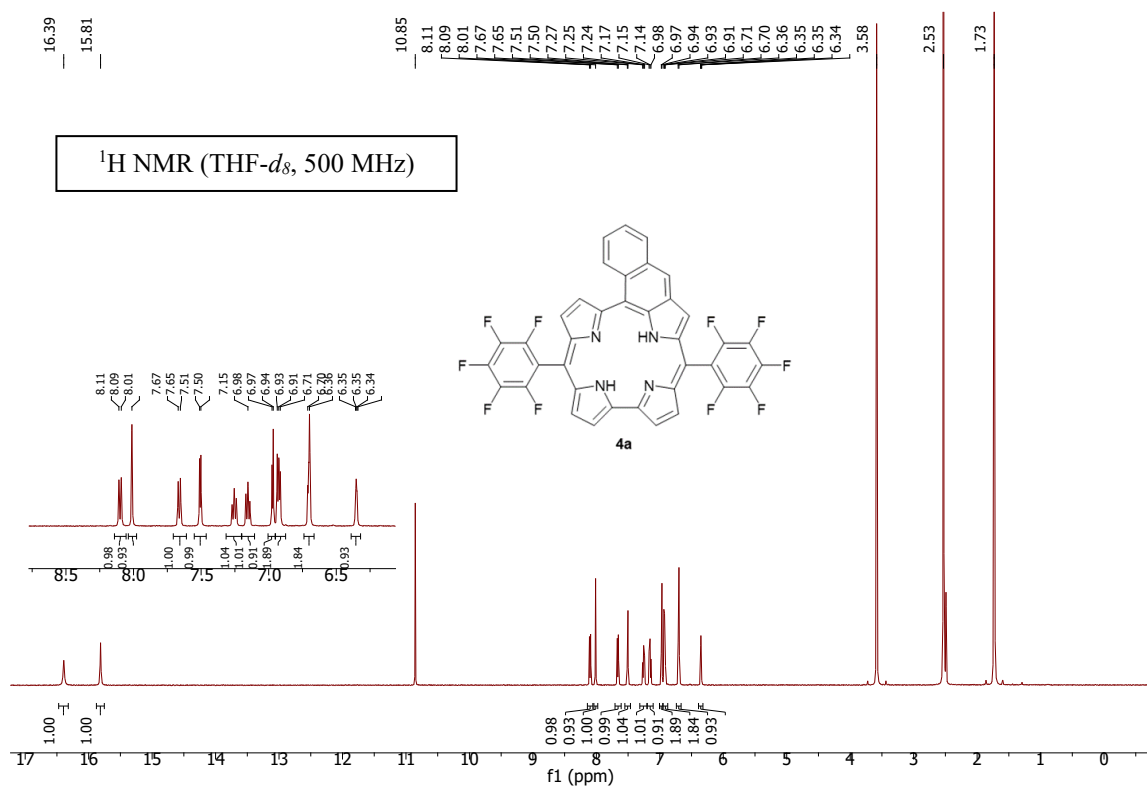
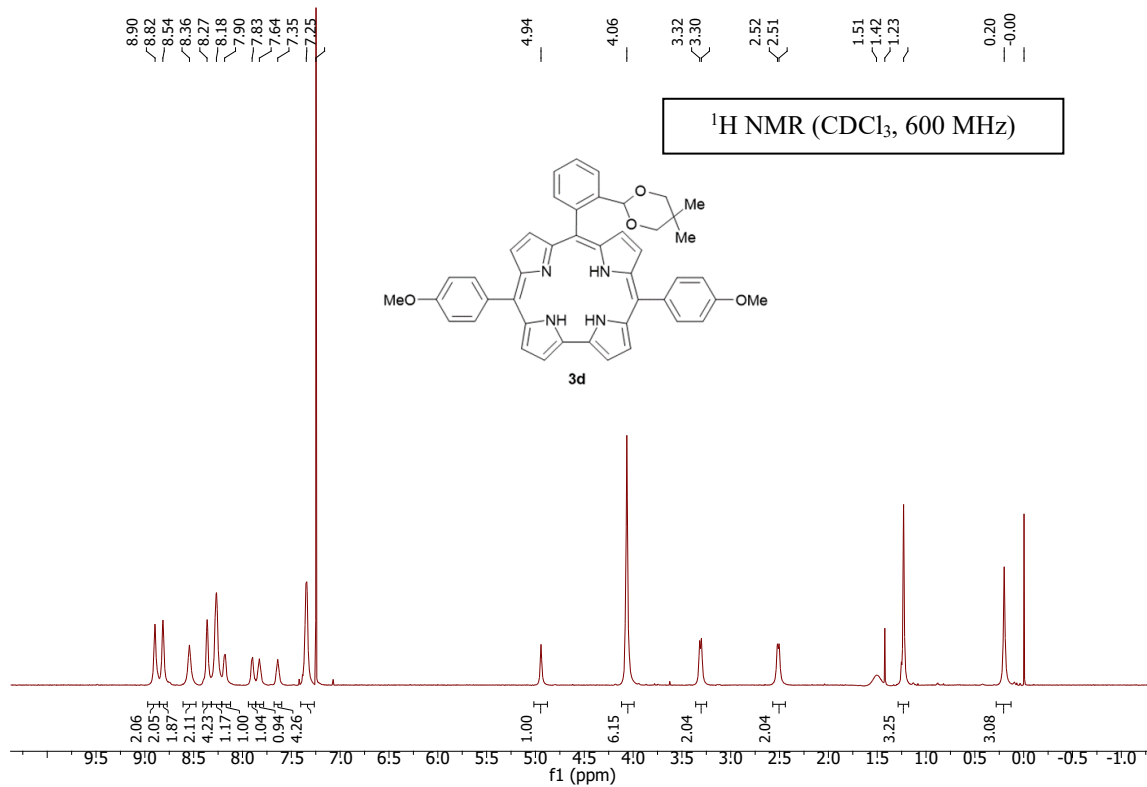
8. NMR Spectra

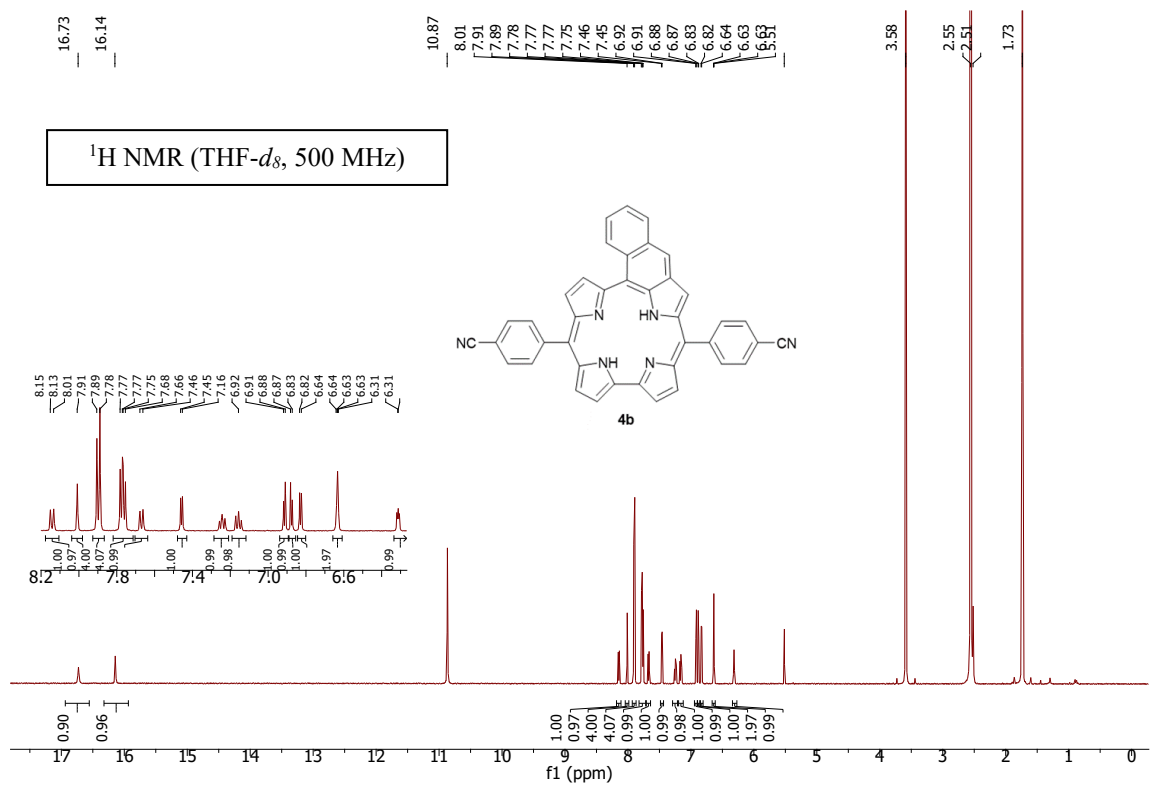
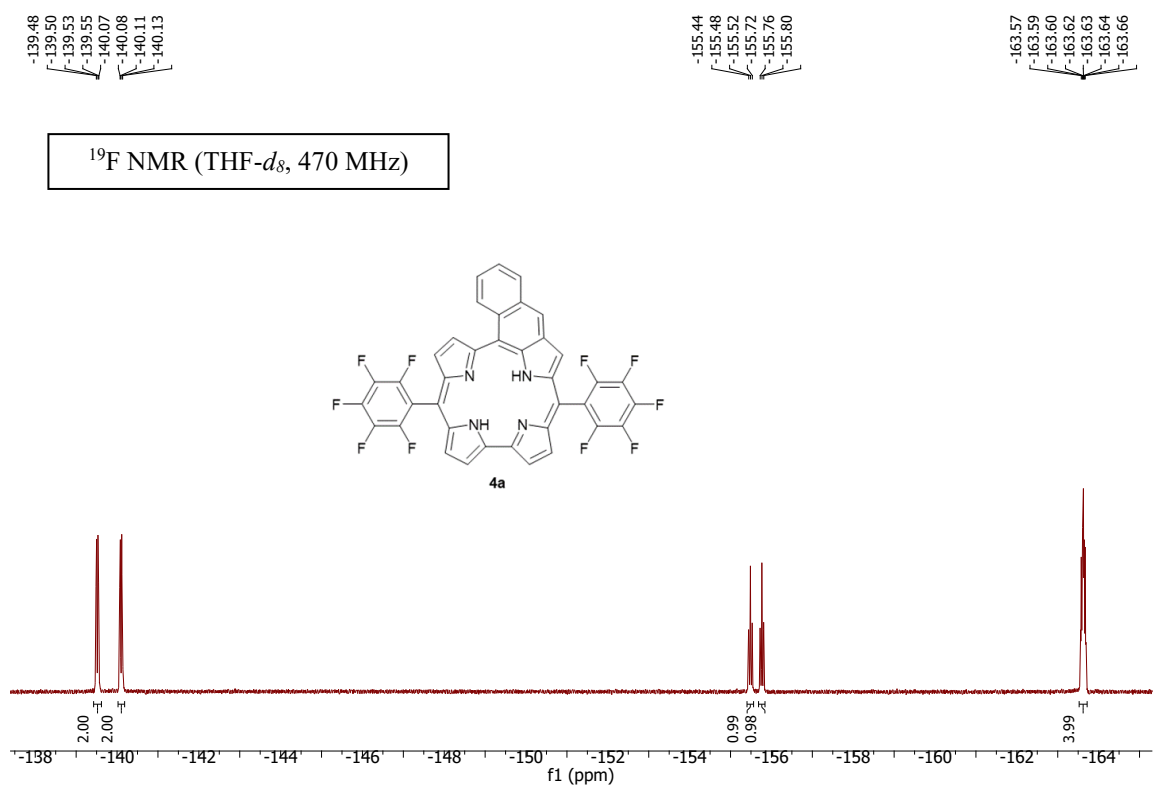


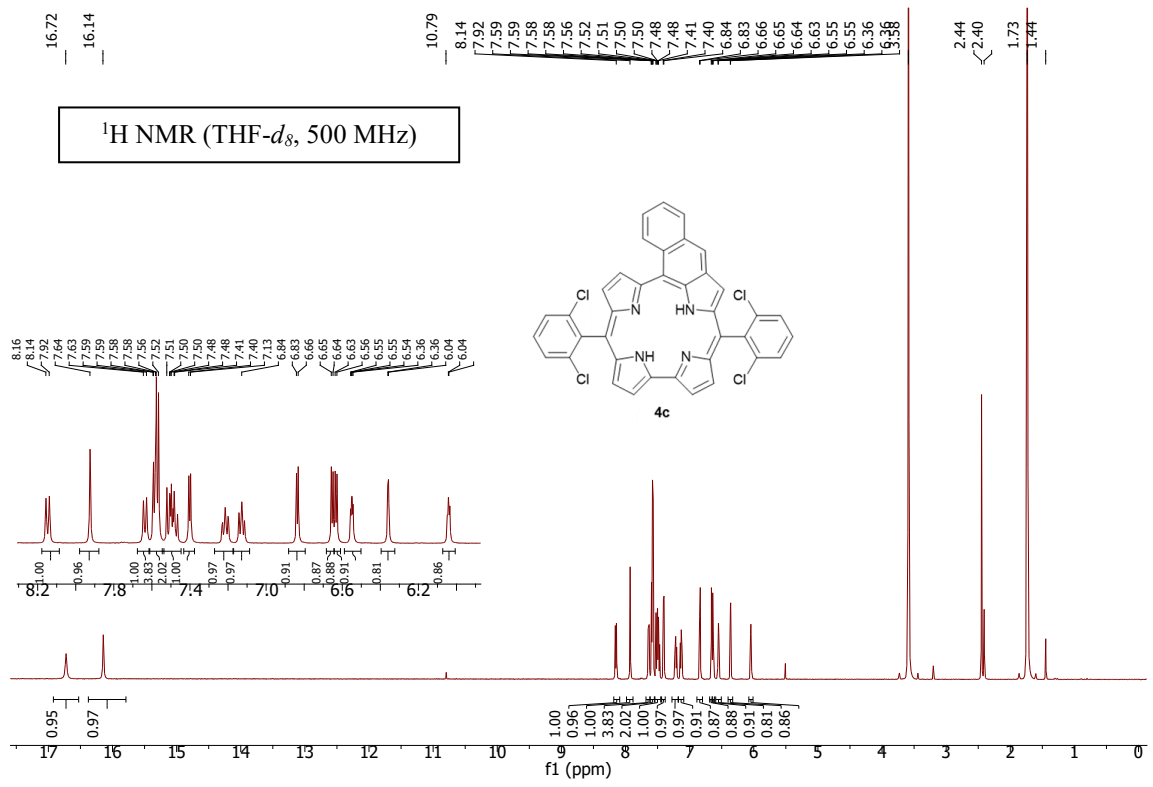
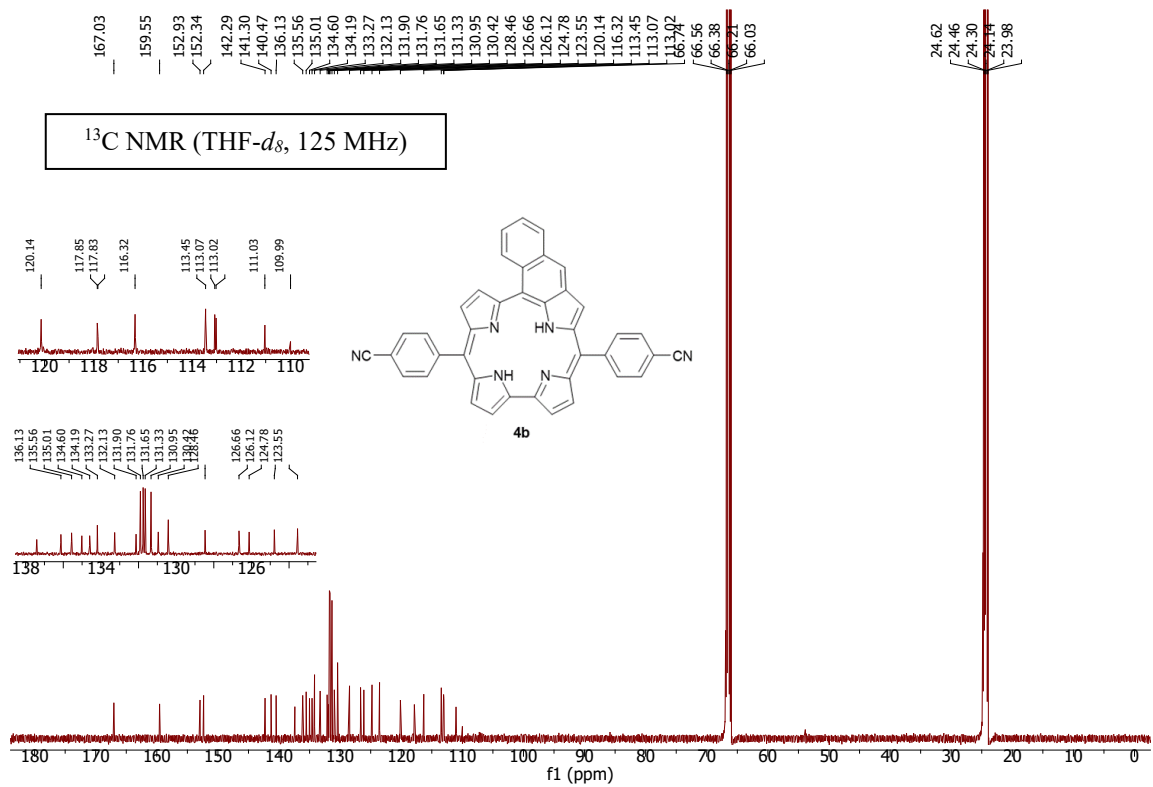


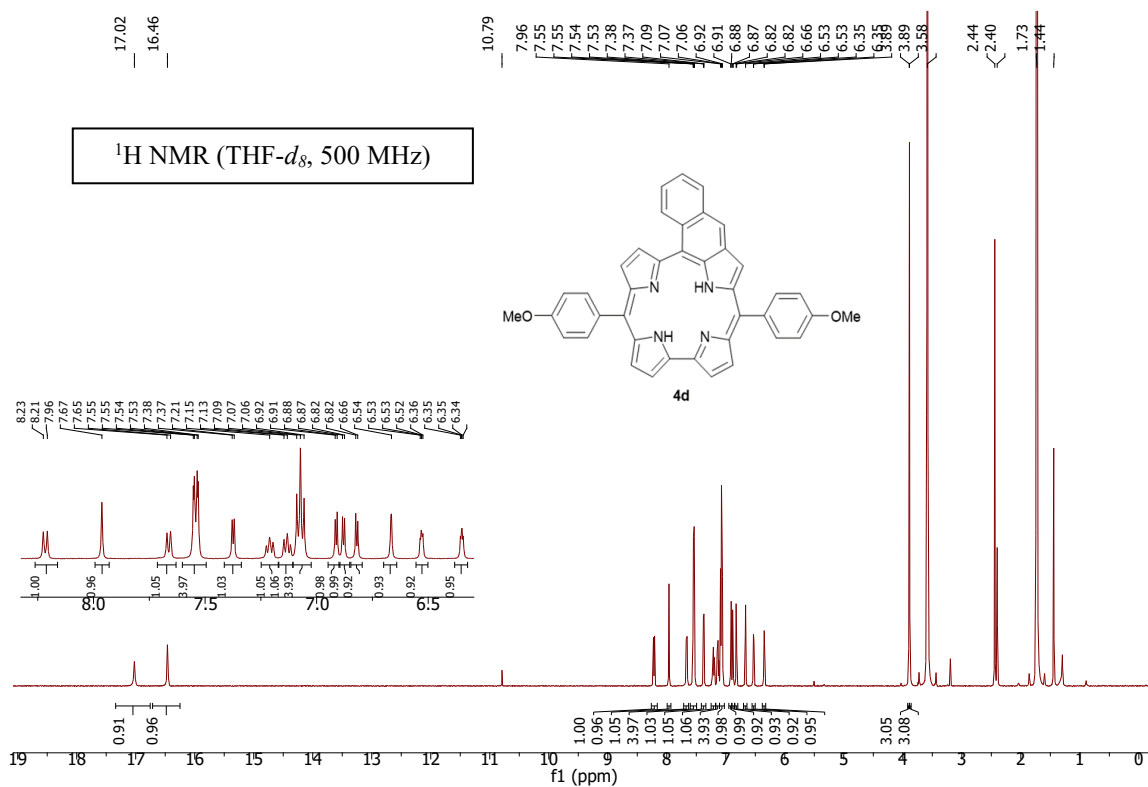
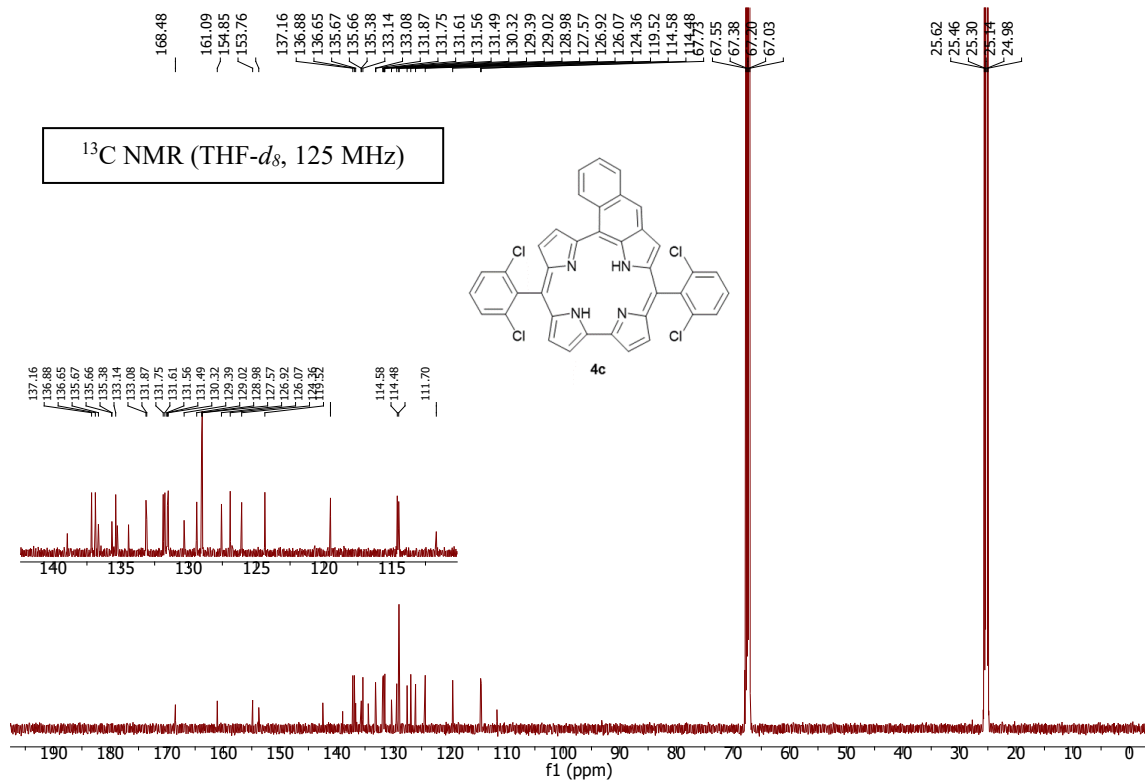


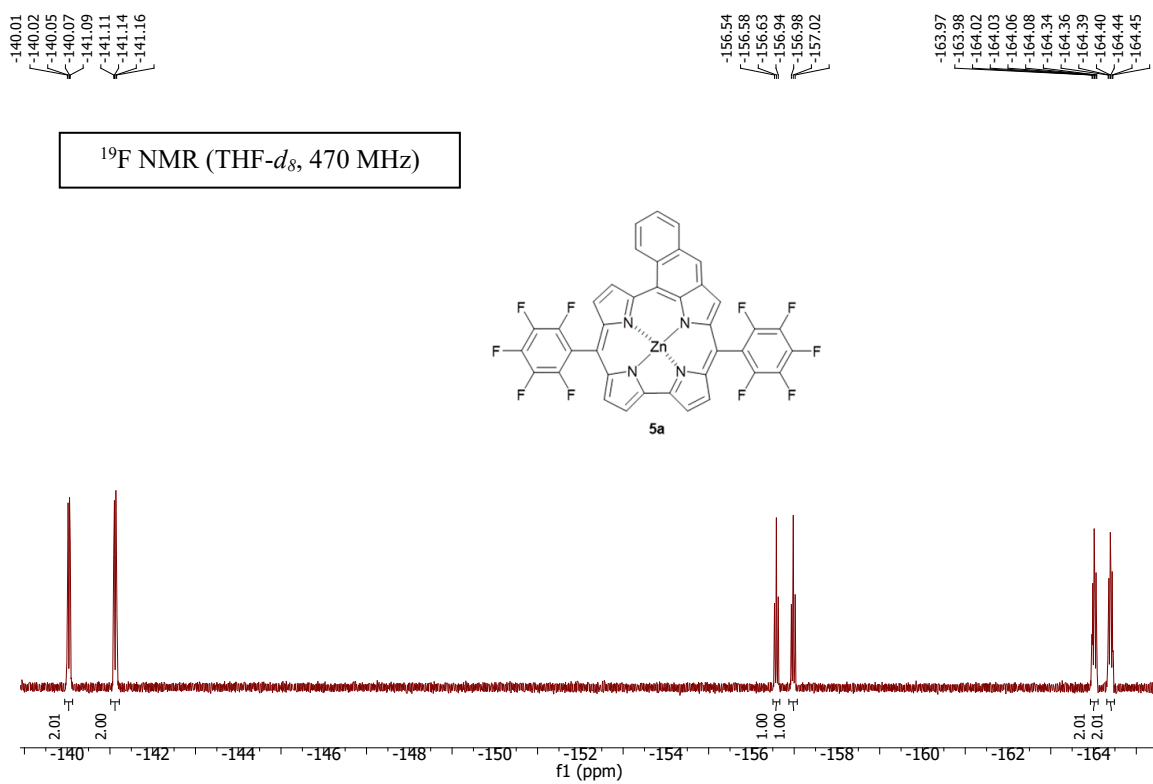
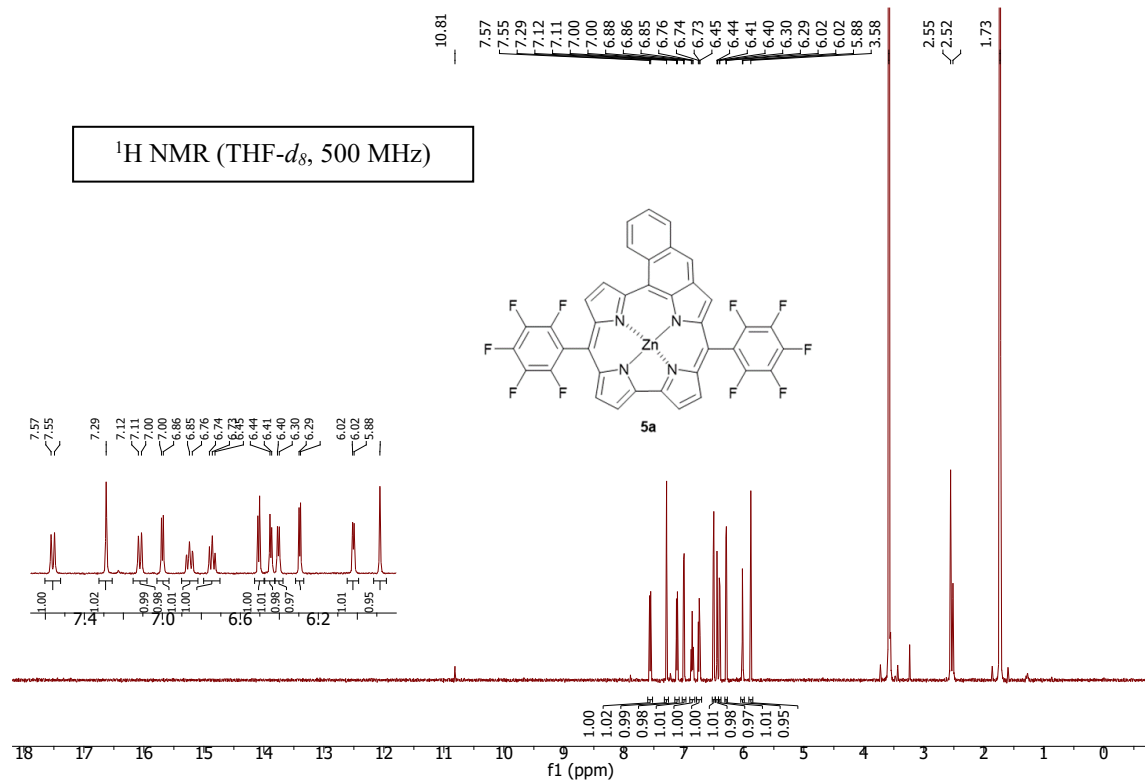


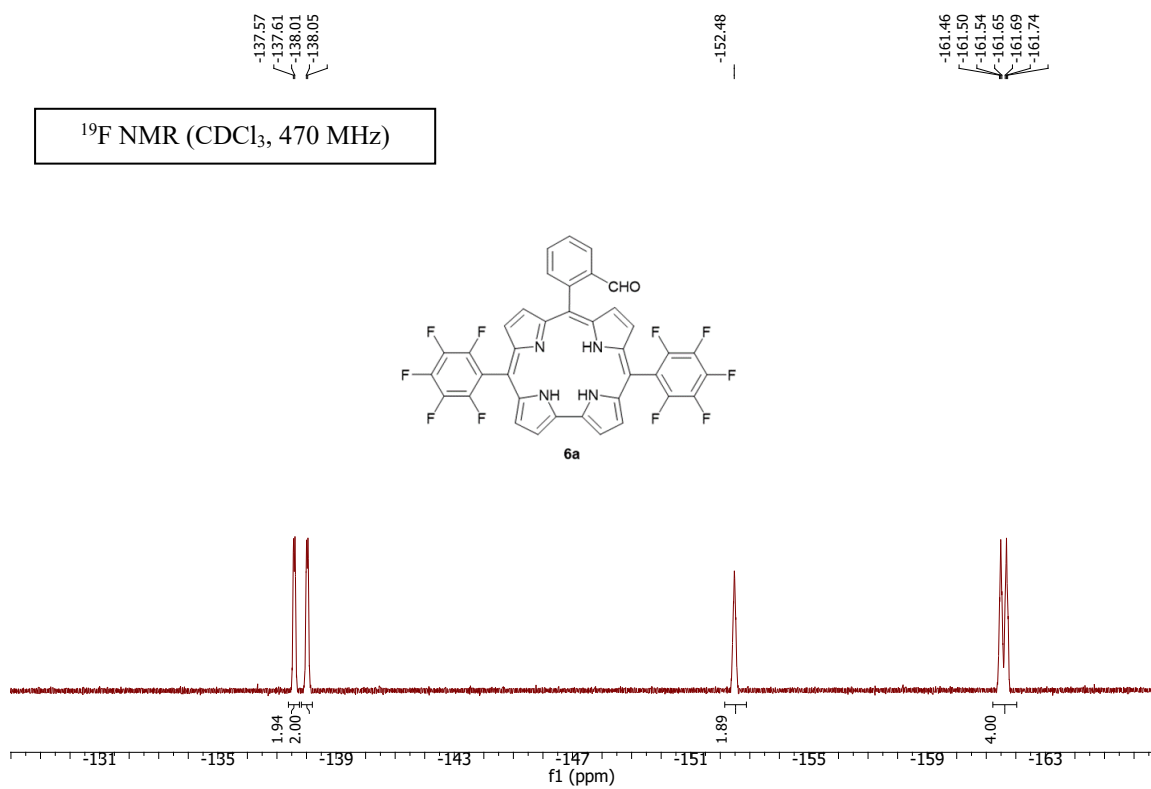
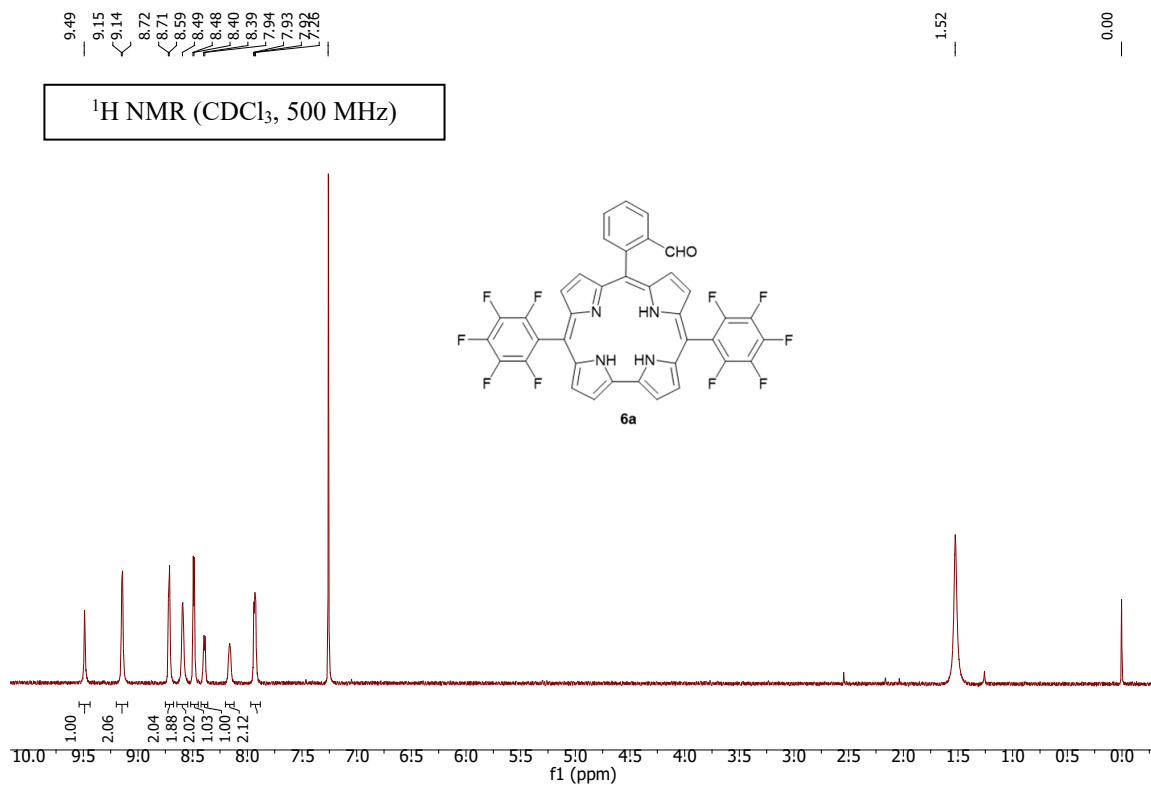


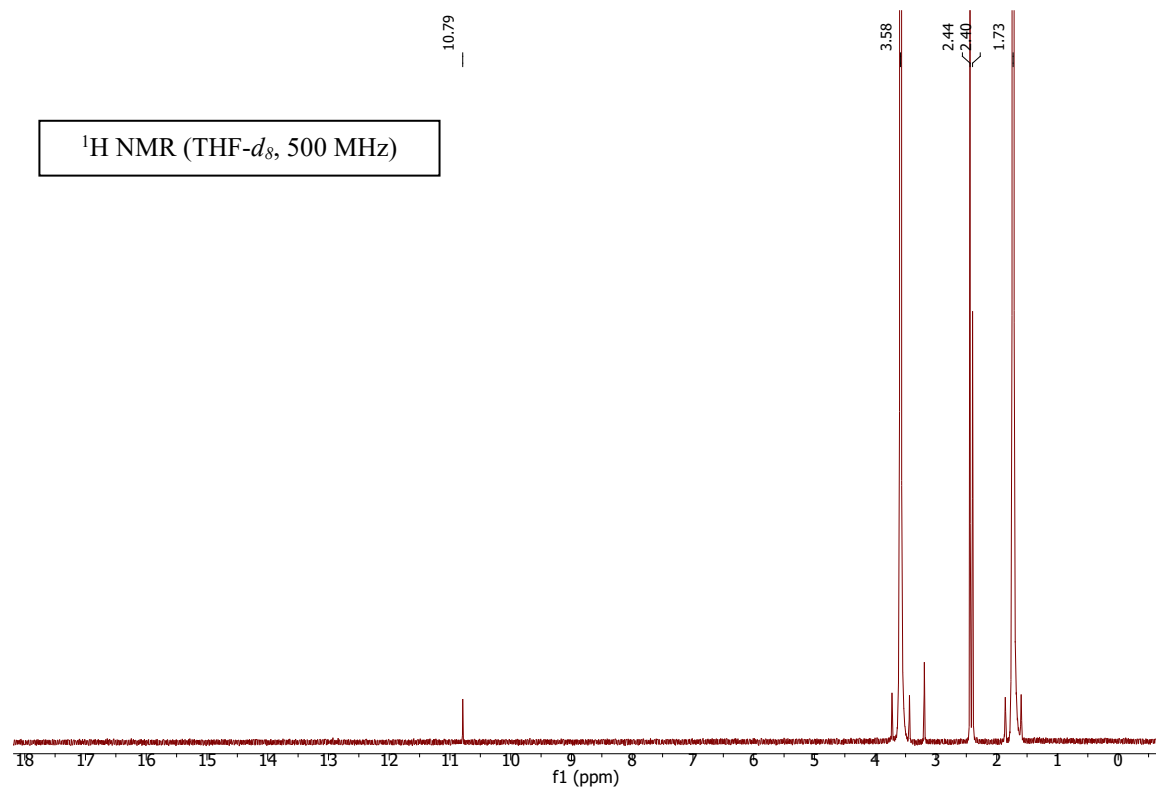












The ^1H NMR spectrum of pure deuterated THF with additional signals at around 2.5 and 11 ppm.

9. Cartesian Coordinates

4a

B972/6-31G(d) opt freq scrf=(solvent=chloroform,smd) E=-
2749.33727902

7	1.255625	-2.092332	-0.419046
7	1.465950	0.639127	-0.148347
7	-1.481873	0.597984	-0.160778
7	-1.366572	-2.023489	-0.215871
6	0.629435	-3.280184	-0.119616
6	2.587023	-2.123643	-0.086525
6	2.810670	0.335372	-0.275187
6	1.227875	1.981919	-0.328113
6	-1.286932	1.942532	-0.163142
6	-0.788351	-3.252087	-0.130877
6	-2.837965	0.390694	-0.075896
6	3.376540	-0.947947	-0.158370
6	-0.032028	2.602177	-0.272243
6	1.626905	-4.134713	0.389059
6	2.828251	-3.428120	0.408355
6	-2.721452	-2.086007	-0.121484
6	3.452996	1.574653	-0.582146
6	2.504039	2.564708	-0.614692
6	-3.458261	-0.881054	-0.063799
6	-2.563472	2.626981	-0.052137
6	-3.522252	1.664317	0.003886
6	-1.851554	-4.185615	-0.020474
6	-3.041753	-3.471852	-0.023497
1	0.778879	0.045553	0.287861
1	1.460172	-5.127795	0.780259
1	3.767311	-3.777930	0.811438
1	4.505398	1.684388	-0.798370
1	-2.709044	3.696425	-0.009375
1	-4.588736	1.811370	0.098244
1	-1.739846	-5.258354	0.040022
1	-4.037193	-3.885227	0.046425
6	-4.938235	-0.975250	0.030182
6	-5.570039	-1.494633	1.163021
6	-5.767710	-0.568723	-1.018207
6	-6.952133	-1.606856	1.254113
6	-7.152074	-0.664138	-0.946885
6	-7.746459	-1.187132	0.194640
6	4.847766	-1.080999	-0.078013
6	5.598678	-0.454983	0.924271
6	5.561801	-1.863256	-0.993793
6	6.979152	-0.586401	1.007038
6	6.940486	-2.014997	-0.924118
6	7.653129	-1.371975	0.080362
9	4.994308	0.286363	1.854817
9	7.657701	0.021714	1.979946

9	8.973885	-1.508011	0.154447
9	7.584253	-2.760151	-1.822819
9	4.923460	-2.479784	-1.991062
9	-7.519396	-2.103144	2.354083
9	-9.071007	-1.285607	0.272766
9	-7.910937	-0.268046	-1.969320
9	-5.237550	-0.075216	-2.139694
9	-4.845229	-1.896510	2.209975
1	-0.936762	-1.093222	-0.193314
6	-0.040511	4.092592	-0.418532
6	-0.489507	4.656781	-1.619443
6	0.416777	4.958555	0.598672
6	-0.475490	6.035230	-1.815583
1	-0.838981	4.002171	-2.410456
6	0.433998	6.344819	0.387212
6	-0.007938	6.885232	-0.811359
1	-0.824301	6.445600	-2.757520
1	0.790546	6.981897	1.189004
1	0.005856	7.958756	-0.965699
1	0.895332	-1.449298	-1.109219
1	2.668454	3.604152	-0.854326
6	0.840777	4.444830	1.920837
1	0.669445	3.369143	2.096575
8	1.330384	5.139240	2.792923

6a

opt freq 6-31g(d) b972 scrf=(smd,solvent=tetrahydrofuran)
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7	-1.513112	0.876405	-0.224486
7	-1.416483	-1.755885	-0.698185
6	0.590248	-2.976863	-0.673455
6	2.485453	-1.961919	-0.331562
6	2.771146	0.466612	0.074904
6	1.196943	2.090417	0.077089
6	-1.314262	2.153119	0.093709
6	-0.848856	-2.982665	-0.760966
6	-2.866233	0.610285	-0.012930
6	3.297304	-0.872987	-0.072423
6	-0.007234	2.811200	0.028600
6	1.615677	-4.010360	-0.729870
6	2.801960	-3.374432	-0.520385
6	-2.756754	-1.820281	-0.538223
6	3.457881	1.664440	0.224517
6	2.489223	2.707176	0.211078
6	-3.474316	-0.626187	-0.210868
6	-2.553529	2.755702	0.582501
6	-3.515587	1.804653	0.486719
6	-1.903965	-3.916044	-0.716529

6	-3.093810	-3.195018	-0.575565
1	0.742401	0.015109	-0.113684
1	1.457514	-5.064230	-0.910560
1	3.786602	-3.819152	-0.500031
1	4.526848	1.783194	0.309158
1	-2.664212	3.744910	0.998118
1	-4.554935	1.897343	0.764955
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1	-4.087029	-3.606796	-0.477681
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6	-5.512374	-0.756235	1.271544
6	-5.800710	-0.964143	-1.085989
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6	-7.171538	-1.127008	-0.917260
6	-7.711952	-1.102103	0.364123
6	4.765664	-1.060611	0.056935
6	5.317529	-1.711801	1.163114
6	5.651836	-0.605579	-0.922979
6	6.689199	-1.902896	1.294477
6	7.026491	-0.783642	-0.810631
6	7.545383	-1.435897	0.303097
9	4.528264	-2.164361	2.135724
9	7.185596	-2.523451	2.361811
9	8.856489	-1.613024	0.418738
9	7.845041	-0.343698	-1.763239
9	5.187563	0.010253	-2.009208
9	-7.397859	-0.897229	2.690239
9	-9.020209	-1.255546	0.537388
9	-7.966850	-1.302190	-1.970044
9	-5.314110	-0.987807	-2.325829
9	-4.745808	-0.590959	2.348313
1	-0.927181	-0.865796	-0.655068
6	0.136732	4.244470	-0.053602
6	-0.932312	5.110968	-0.408459
6	1.426353	4.868365	0.140474
6	-0.782082	6.478296	-0.450198
1	-1.880286	4.685742	-0.706425
6	1.537977	6.286917	0.116044
6	0.458110	7.084777	-0.154862
1	-1.627195	7.096004	-0.735707
1	2.515771	6.724403	0.292695
1	0.559227	8.163940	-0.180112
6	2.584023	4.085696	0.293749
1	3.544381	4.572199	0.433242

All-electron OLYP/STO-TZ2P optimized Cartesian coordinates (Å)

Table of Contents

Table of Contents
1. H ₂ (F10BC), C ₁
2. Zn(F10BC), C ₁
3. Au(F10TPC), C _{2v}

1. H₂(F10BC), C₁

C	3.670041000	0.274054000	5.852143000
C	3.855176000	1.332644000	4.964576000
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C	4.133045000	8.843585000	-2.681292000
C	4.639165000	0.012356000	6.819545000
C	4.789462000	10.700026000	-4.065499000
C	4.991724000	2.146655000	5.007644000
C	5.008784000	5.036938000	5.899000000
C	5.039419000	9.925187000	2.248723000
C	5.070159000	9.877118000	0.888375000
C	5.081893000	7.412300000	6.892901000
C	5.135029000	6.453930000	5.891786000
C	5.166031000	4.603257000	4.581825000
C	5.179763000	3.263776000	4.054778000
C	5.292347000	8.953550000	-1.906873000
C	5.352117000	6.860281000	4.523128000
C	5.352279000	8.757035000	6.575819000
C	5.362501000	3.002201000	2.702502000
C	5.380939000	1.743587000	1.963065000
C	5.414265000	9.727785000	7.614779000
C	5.469781000	8.612123000	2.728248000
C	5.488364000	8.537224000	0.531116000
C	5.506628000	8.197695000	4.126103000
C	5.543730000	8.032298000	-0.771892000
C	5.561709000	2.069851000	0.646321000
C	5.633065000	9.148894000	5.208709000
C	5.641609000	5.864536000	-2.256110000
C	5.662641000	3.523475000	0.600506000
C	5.682950000	4.520186000	-1.870593000
C	5.717907000	6.650276000	-1.073685000
C	5.782306000	0.807453000	6.891520000
C	5.786640000	4.484868000	-0.458176000
C	5.809265000	11.019931000	7.363698000
C	5.946085000	1.855613000	5.988852000
C	5.950112000	10.842225000	-3.306568000
C	6.115155000	10.468046000	5.015625000
C	6.187824000	9.972128000	-2.243982000
C	6.194957000	11.376123000	6.052932000
F	2.567895000	-0.481840000	5.791876000
F	2.753817000	9.566975000	-4.473304000
F	2.892000000	1.574502000	4.066007000
F	3.217540000	7.914213000	-2.377473000
F	4.474689000	-0.998297000	7.675803000
F	4.554008000	11.524507000	-5.089158000
F	6.715649000	0.549015000	7.814954000
F	6.829724000	11.804943000	-3.606449000
F	7.071897000	2.578201000	6.063292000
F	7.321067000	10.127624000	-1.548171000
H	4.696269000	10.743668000	2.862712000

H	4.787846000	10.655129000	0.192722000
H	4.844213000	4.405386000	6.758984000
H	4.876503000	7.134120000	7.924093000
H	5.168738000	9.410449000	8.625892000
H	5.260041000	0.755820000	2.386797000
H	5.485803000	5.599994000	2.781443000
H	5.531756000	6.248446000	-3.259915000
H	5.611294000	3.658472000	-2.519920000
H	5.618921000	1.395432000	-0.198887000
H	5.862465000	11.749291000	8.167521000
H	5.876326000	6.119869000	0.917265000
H	6.471118000	10.758846000	4.035820000
H	6.577449000	12.375252000	5.857316000
N	5.337772000	5.722022000	3.781032000
N	5.548420000	4.041598000	1.821656000
N	5.716696000	7.793184000	1.693006000
N	5.850793000	5.777357000	-0.044705000

2. Zn (F10BC), C₁

Zn	5.959287000	5.935083000	1.876146000
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C	3.662864000	0.327868000	5.668224000
C	3.923014000	1.377195000	4.790039000
C	3.980640000	9.154749000	-2.177998000
C	4.506784000	0.115566000	6.756561000
C	4.645426000	10.494772000	-4.063415000
C	5.023604000	7.408370000	6.904998000
C	5.030385000	2.220571000	4.944001000
C	5.032567000	5.059555000	5.838189000
C	5.149482000	6.474996000	5.888707000
C	5.190449000	10.000359000	2.250212000
C	5.221217000	9.896599000	0.882244000
C	5.295059000	8.766402000	6.632395000
C	5.307443000	9.705638000	7.699642000
C	5.309506000	3.316800000	3.989719000
C	5.310111000	8.862066000	-1.870605000
C	5.316589000	4.669481000	4.517489000
C	5.472152000	6.904559000	4.546040000
C	5.478599000	1.715965000	1.928300000
C	5.507590000	2.983644000	2.646893000
C	5.584601000	8.269714000	4.179245000
C	5.586177000	8.718008000	2.792922000
C	5.605431000	0.950288000	6.951342000
C	5.616670000	5.876765000	-2.267940000
C	5.618720000	8.551871000	0.555369000
C	5.621924000	9.201454000	5.287970000
C	5.655210000	1.999888000	0.593472000
C	5.659955000	7.975473000	-0.727623000
C	5.671293000	4.522506000	-1.955050000
C	5.683974000	11.013790000	7.500545000

C	5.812325000	3.436512000	0.487060000
C	5.860014000	6.600706000	-1.048383000
C	5.862161000	1.972751000	6.042247000
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C	6.061697000	10.539866000	5.146406000
C	6.088949000	11.419703000	6.212377000
C	6.296640000	9.406796000	-2.691482000
F	2.356790000	10.239620000	-3.529060000
F	2.603523000	-0.467196000	5.483661000
F	2.993350000	8.646098000	-1.427561000
F	3.058368000	1.577300000	3.786805000
F	4.264048000	-0.882540000	7.608427000
F	4.330847000	11.274056000	-5.101864000
F	6.410757000	0.757669000	8.000954000
F	6.944798000	10.719786000	-4.559915000
F	6.959964000	2.715805000	6.234544000
F	7.587946000	9.164224000	-2.429244000
H	4.761471000	7.109691000	7.917966000
H	4.775521000	4.408149000	6.660461000
H	4.857987000	10.855155000	2.818219000
H	4.958267000	10.662208000	0.165655000
H	5.039165000	9.353669000	8.693407000
H	5.329328000	0.739953000	2.369397000
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H	5.489071000	3.694442000	-2.628280000
H	5.674353000	1.290454000	-0.224303000
H	5.702997000	11.717493000	8.328474000
H	6.440972000	10.869647000	4.188213000
H	6.449276000	12.434066000	6.055658000
N	5.578505000	5.803345000	3.759731000
N	5.729398000	3.959560000	1.718888000
N	5.842390000	7.883360000	1.753074000
N	6.114594000	5.694587000	-0.071648000

3. Au (F10TPC) , C_{2v}

Au	0.000000000	0.000000000	-0.564480000
C	0.000000000	0.000000000	2.763159000
C	0.000000000	0.000000000	4.251915000
C	0.000000000	0.000000000	7.071163000
C	0.000000000	0.713333000	-3.323646000
C	0.000000000	1.257134000	2.127465000
C	0.000000000	1.828183000	-4.210501000
C	0.000000000	2.566292000	2.721302000
C	0.000000000	2.607481000	-2.054414000
C	0.000000000	2.790755000	0.450296000
C	0.000000000	2.986181000	-3.439344000
C	0.000000000	3.341588000	-0.848764000
C	0.000000000	3.492285000	1.706134000
C	0.000000000	4.823898000	-0.954884000

C	0.000000000	7.633064000	-1.135411000
C	0.000000000	-0.713333000	-3.323646000
C	0.000000000	-1.257134000	2.127465000
C	0.000000000	-1.828183000	-4.210501000
C	0.000000000	-2.566292000	2.721302000
C	0.000000000	-2.607481000	-2.054414000
C	0.000000000	-2.790755000	0.450296000
C	0.000000000	-2.986181000	-3.439344000
C	0.000000000	-3.341588000	-0.848764000
C	0.000000000	-3.492285000	1.706134000
C	0.000000000	-4.823898000	-0.954884000
C	0.000000000	-7.633064000	-1.135411000
C	1.192552000	0.000000000	4.978231000
C	1.193585000	5.545749000	-1.005514000
C	1.193585000	-5.545749000	-1.005514000
C	1.207686000	0.000000000	6.372652000
C	1.208848000	6.936931000	-1.092600000
C	1.208848000	-6.936931000	-1.092600000
C	-1.192552000	0.000000000	4.978231000
C	-1.193585000	5.545749000	-1.005514000
C	-1.193585000	-5.545749000	-1.005514000
C	-1.207686000	0.000000000	6.372652000
C	-1.208848000	6.936931000	-1.092600000
C	-1.208848000	-6.936931000	-1.092600000
F	0.000000000	0.000000000	8.407664000
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F	0.000000000	-8.966098000	-1.220864000
F	2.364963000	4.896120000	-0.966824000
F	2.364963000	-4.896120000	-0.966824000
F	2.365049000	0.000000000	7.043530000
F	2.365676000	0.000000000	4.330723000
F	2.365832000	7.607347000	-1.137187000
F	2.365832000	-7.607347000	-1.137187000
F	-2.364963000	4.896120000	-0.966824000
F	-2.364963000	-4.896120000	-0.966824000
F	-2.365049000	0.000000000	7.043530000
F	-2.365676000	0.000000000	4.330723000
F	-2.365832000	7.607347000	-1.137187000
F	-2.365832000	-7.607347000	-1.137187000
H	0.000000000	1.773619000	-5.290900000
H	0.000000000	2.755613000	3.785299000
H	0.000000000	4.004984000	-3.801068000
H	0.000000000	4.568957000	1.801346000
H	0.000000000	-1.773619000	-5.290900000
H	0.000000000	-2.755613000	3.785299000
H	0.000000000	-4.004984000	-3.801068000
H	0.000000000	-4.568957000	1.801346000
N	0.000000000	1.246706000	-2.054807000
N	0.000000000	1.443686000	0.766208000
N	0.000000000	-1.246706000	-2.054807000
N	0.000000000	-1.443686000	0.766208000

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