Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

69451 Weinheim, Germany

Internally 1,4-Phenylene-bridged *meso*-Aryl Substituted Expanded Porphyrins; Decaphyrin and Octaphyrin Cases

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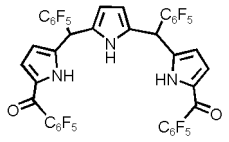
I. General Information

Silica gel column chromatography was performed on Wakogel C-200, C-300, and C-400. UV-visible spectra were recorded on a Shimadzu UV-3100PC spectrometer. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded on a JEOL ECA-600 spectrometer (operating as 600.17 MHz for ^{1}H, 150.91 MHz for ^{13}C, and 564.73 MHz for ^{19}F) using the residual solvent as the internal reference for ^{1}H (δ = 7.26 ppm), ^{13}C (δ = 77.16 ppm), and hexafluorobenzene as external reference for ^{19}F (δ = −162.9 ppm). Mass spectra were recorded on a BRUKER microTOF using positive or negative mode ESI-TOF method for solutions of samples in acetonitrile.

II. Experimental Procedures



S1

1,14-Bis(pentafluorobenzoyl)-5,10-bis(pentafluorophenyl)tripyrrane (S1).

To a solution of 5,10-bis(pentafluorophenyl)tripyrrane[1] (1.2 g, 2.1 mmol) in dry toluene (20 mL), under inert atmosphere were added a solution of EtMgBr prepared from Mg (51 mg, 21 mmol) and bromoethane (1.6 mL, 21 mmol) in dry THF (20 mL) through a syringe over a period of 5 min with constant stirring. A mild exothermic reaction was initiated and the solution was allowed to stir for 5 min at room temperature. Pentafluorobenzoyl chloride (3.1 mL, 21 mmol) was added and stirring was continued for further 2.5 h. The reaction was quenched by addition of a saturated aqueous ammonium chloride solution (50 mL). The reaction mixture was extracted three times with ethyl acetate (20 mL). Combined organic layer was washed twice with water, then with brine and dried over anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure and separation of the residue by silica gel column chromatography gave **S1** (1.0 g, 50%) as a diastereoisomeric mixture by elution with a 1:1 mixture of hexane and dichloromethane.

S1: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): (major diastereomer) 10.22 (br s, 2H, NH), 8.29 (br s, 1H, NH), 6.65 (s, 2H, β-pyrrole), 6.10 (s, 2H, β-pyrrole), 6.03 (s, 2H, β-pyrrole), and 5.90 (s, 2H, *meso*-H). (minor diastereomer) 10.34 (br s, 2H, NH), 8.50 (br s, 1H, NH), 6.65 (s, 2H, β-pyrrole), 6.07 (s, 2H, β-pyrrole), 6.00 (s, 2H, β-pyrrole), and 5.88 (s, 2H, *meso*-H); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm): (major diastereomer) –141.1 (m, 4F, *o*-F), –142.1 (d, 4F, *o*-F), –151.6 (t, 2F, *p*-F), –154.1 (d, 2F, *p*-F), –160.8 (m, 4F, *m*-F), and –161.0 (m, 4F, *m*-F). (minor diastereomer) –141.1 (m, 4F, *o*-F), –142.1 (d, 4F, *o*-F), –151.7 (t, 2F, *p*-F), –154.2 (d, 2F, *p*-F), –160.8 (m, 4F, *m*-F), and –161.0 (m, 4F, *m*-F); ESI-MS: 944.0469 $[M–H]^-$, Calcd. for $C_{40}H_{10}F_{20}N_3O_2$ 944.0459.

1,4-Phenylene-bridged [46]decaphyrin (4a).

The dibenzoyltripyrrane **S1** (200 mg, 0.21 mmol) was reduced with excess $NaBH_4$ in a 3:1 mixture of THF and methanol (40 mL). After 30 min, the reaction was quenched by addition of a 1:1 mixture of dichloromethane and water (50 mL) and the organic layer was separated, and further washed with water and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to yield diol **2** in a quantitative yield. This compound was found to be unstable at ambient temperature and hence must be used immediately. The diol **2** was dissolved in a solution of **1a** (39 mg, 0.1 mmol) in dry CH_2Cl_2 (100 mL). After the solution was stirred under inert and dark atmosphere for 15 min, *p*-toluenesulfonic acid (20 mg, 0.11 mmol) was added and stirring was continued for 60 min. DDQ (60 mg, 0.26 mmol) was added and the resulting solution was opened to the air with constant stirring for further 60 min. The reaction mixture was passed through a basic alumina column to remove the tar products followed by evaporation of solvent under reduced pressure. The residue was purified by silica gel chromatography using a 3:1 mixture of hexane and dichloromethane. A pale orange band eluted as a marker, which was followed by a reddish brown band. Recrystallization from dichloromethane and heptane provided **4a** as bluish green crystals (16 mg, 7%).

4a: ^{1}H NMR (600 MHz, $CDCl_3$, 233 K) δ (ppm): 9.01 (br s, 2H, NH), 7.36 (d, 4H, J = 4.4 Hz, β-pyrrole), 7.31 (d, 4H, J = 4.4 Hz, β-pyrrole), 7.19 (d, 4H, J = 4.4 Hz, β-pyrrole), 6.84 (d, 4H, J = 4.4 Hz, β-pyrrole), 5.84 (br s, 4H, NH), 3.78 (s, 4H, Ph-H), and 1.2 (s, 4H, β-pyrrole); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm): –136.9 (br s, 8F, *o*-F), –137.8 (d, 4F, *o*-F), –139.0 (d, 4F, *o*-F), –151.2 (br s, 4F, *p*-F), –153.5 (t, 4F, *p*-F), –160.5 (m, 8F, *m*-F), and –162.4 (m, 8F, *m*-F); ESI-MS: 2179.2163 $[M+H]^+$, Calcd. for $C_{104}H_{31}F_{40}N_{10}$ 2179.2094; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 505 (17.9), 593 (6.8), 800 (12.7), and 856 (10.9).

1,4-Phenylene-bridged [44]decaphyrin (5a).

DDQ (10 mg, 44 μmol) was added to a solution of **4a** (10 mg, 4.6 μmol) in dichloromethane (10 mL). An immediate color change from dark red to dark green was observed. Stirring was continued for 15 min and the solution was passed through a basic alumina column. The solvent was evaporated under reduced pressure and the residue was passed through a short

silica gel column with a 1:1 mixture of hexane and dichloromethane as an eluent. Evaporation of the dark green fraction to dryness yielded **5a** in a quantitative yield. Crystals with brownish metallic luster were obtained by slow vapor diffusion of heptane into a solution of **5a** in dichloromethane.

5a: ^{1}H NMR (600 MHz, CD_2Cl_2, 298 K) δ (ppm): 13.59 (br s, 4H, NH), 8.98 (s, 4H, Ph-H), 7.78 (s, 4H, β-pyrrole), 6.82 (d, 4H, J = 4.62 Hz, β-pyrrole), 6.36 (m, 8H, β-pyrrole), and 6.30 (d, 4H, J = 4.62 Hz, β-pyrrole); ^{19}F NMR (565 MHz, CD_2Cl_2, 298 K) δ (ppm): –139.1 - –139.2 (m, 8F, *o*-F), –139.4 (m, 8F, *o*-F), –153.7 (m, 4F, *p*-F), –156.1 (m, 4F, *p*-F), –162.2 (m, 8F, *m*-F), –164.7 (m, 4F, *m*-F), and –165.3 (m, 4F, *m*-F); ESI-MS: 2177.2037 $[M+H]^+$, Calcd. for $C_{104}H_{29}F_{40}N_{10}$ 2177.1938; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 454 (13.9), and 619 (11.0).

Deutrated-1,4-phenylene-bridged [46]decaphyrin (4b).

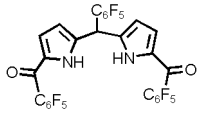
Following the synthetic procedure of **4a**, the reaction of diol **2** with **1b** gave **4b**.

4b: ^{1}H NMR (600 MHz, $CDCl_3$, 233 K) δ (ppm): 9.01 (br s, 2H, NH), 7.36 (d, 4H, J = 4.4 Hz, β-pyrrole), 7.31 (d, 4H, J = 4.4 Hz, β-pyrrole), 7.18 (d, 4H, J = 4.4 Hz, β-pyrrole), 6.84 (d, 4H, J = 4.4 Hz, β-pyrrole), 5.84 (br s, 4H, NH), and 1.20 (s, 4H, β-pyrrole); ESI-MS: 2183.2399 $[M+H]^+$, Calcd. for $C_{104}H_{27}F_{40}N_{10}D_4$ 2183.2351.

Deutrated-1,4-phenylene-bridged [44]decaphyrin (5b).

Following the synthetic procedure of **5a**, the oxidation **4b** with DDQ gave **5b**.

5b: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 13.60 (br s, 4H, NH), 7.79 (s, 4H, β-pyrrole), 6.82 (d, 4H, J = 4.62 Hz, β-pyrrole), 6.36 (m, 8H, β-pyrrole), and 6.30 (d, 4H, J = 4.62 Hz, β-pyrrole); ESI-MS: 2181.2180 $[M+H]^+$, Calcd. for $C_{10}H_{25}F_{40}N_{10}D_4$ 2181.2184.



S2

1,9-Bis(pentafluorobenzoyl)-5-pentafluorophenyldipyrromethane[2] **(S2)**.

A solution of EtMgBr prepared from Mg (2.4 g, 99 mmol) and bromoethane (7.2 mL, 110

mmol) in dry THF (100 mL) and pentafluorobenzoyl chloride (14 mL, 96 mmol) were both added slowly to a solution of 5-pentafluorophenyldipyrromethane (6.3 g, 20 mmol) in toluene (150 mL) under N_2 atmosphere. Then the reaction mixture was stirred for 1.5 h at room temperature. After the reaction was quenched with 0.5 M HCl (200 mL), the products were extracted with ethyl acetate (200 mL). The organic phase was washed with brine and dried over anhydrous Na_2SO_4. After the removal of the solvent, recrystallization from dichloromethane/hexane afforded **S2** as a white solid (6.3 g, 45%).

S2: ^{1}H NMR (600 MHz, DMSO-d_6, 298 K) δ (ppm) 12.71 (br s, 2H, NH), 6.88 (s, 2H, β-pyrrole), 6.05 (s, 1H, *meso*-H), and 6.02 (s, 2H, β-pyrrole); ^{19}F NMR (565 MHz, DMSO-d_6, 298 K) δ (ppm) –143.0 (d, 2F, *o*-F), –144.6 (d, 4F, *o*-F), –155.3 (t, 2F, *p*-F), –158.2 (t, 1F, *p*-F), –163.2 (t, 4F, *m*-F), and –164.7 (t, 2F, *m*-F). ^{13}C NMR (150 MHz, DMSO-d_6, 298K) δ (ppm) 171.2 (2C, carbonyl-C), 145.9 and 144.3 (2C, *o*-C at *meso*-C_6F_5), 144.1 and 142.5 (4C, *o*-C), 142.5 and 140.8 (2C, *p*-C), 141.2 and 139.5 (1C, *p*-C at *meso*-C_6F_5), 140.2 (2C, pyrrole), 138.1 and 136.5 (4C, *m*-C), 138.1 and 136.5 (4C, *m*-C at *meso*-C_6F_5), 131.3 (2C, pyrrole), 128.8 (2C, pyrrole), 128.1 (2C, pyrrole), 114.1 (2C, *ipso*-C), 113.9 (1C, *ipso*-C at *meso*-C_6F_5), and 32.9 (1C, *meso*-C). ESI-MS: 699.0198 $[M–H]^-$, Calcd. for $C_{29}H_5F_{15}N_2O_2$ 699.0195.

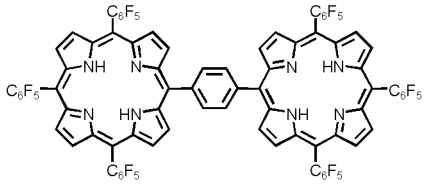
***p*-Quinodimethane-bridged octaphyrins (6a)** and **(7a)**.

The dibenzoyldipyrromethane **S2** (2.8 g, 4.0 mmol) was reduced with excess $NaBH_4$ in a 10:1 mixture of THF and methanol (150 mL). The organic layer was separated and washed with water and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to yield **3** in a quantitative yield, which was then dissolved in a 10:3 mixture of dichloromethane and THF (300 mL) that contained **1a** (730 mg, 2.0 mmol). After the solution was stirred under inert atmosphere for 15 min, methanesulfonic acid (13 μL, 0.20 mmol) was added and the resulting solution was stirred for 1 h. *p*-Chloranil (2.5 g, 10 mmol) was added and the resulting solution was opened to the air with constant stirring for further 2 h. The reaction mixture was passed through a basic alumina column followed by evaporation of solvent under reduced pressure. The residue was subjected to silica gel column chromatography using a 5:1

mixture of hexane and dichloromethane. The product **6a** eluted first as a violet band (17 mg, 0.6%), which was followed by **7a** as a violet band (14 mg, 0.5%), and 1,4-phenylene-linked diporphyrin **S3** as a reddish brown band. Recrystallization from dichloromethane and acetonitrile gave violet crystals of **6a**, while violet crystals of **7a** were obtained by recrystallization from dichloromethane and methanol.

6a: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.57 (br s, 4H, NH), 8.26 (d, 4H, J = 2.7 Hz, β-pyrrole), 7.59 (d, 4H, J = 4.1 Hz, β-pyrrole), 7.46 (d, 4H, J = 4.1 Hz, β-pyrrole), 7.23 (d, 4H, J = 3.7 Hz, β-pyrrole), 5.09 (s, 4H, quinodimethane-H), and 2.71 (s, 4H, endo-*meso*-H); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm): –138.1 (d, 4F, *o*-F), –138.5 (d, 4F, *o*-F), –141.2 (d, 4F, *o*-F), –152.4 (t, 4F, *p*-F), –155.8 (t, 2F, *p*-F), –161.5 (m, 4F, *m*-F), –161.7 (m, 4F, *m*-F), and –162.0 (m, 4F, *m*-F); ESI-MS: 1693.1920 $[M+H]^+$, Calcd. for $C_{82}H_{27}F_{30}N_8$; 1693.1874; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 394 (5.3), 593 (10.9), and 895 (3.9).

7a: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.20 (br s, 2H, NH), 8.47 (d, 2H, J = 4.1 Hz, β-pyrrole), 8.24 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.84 (br s, 2H, NH), 7.73 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.65 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.58 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.42 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.33 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.24 (d, 2H, J = 4.1 Hz, β-pyrrole) 6.42 (s, 1H, exo-*meso*-H), 5.21 (s, 2H, quinodimethane-H), 4.85 (s, 2H, quinodimethane-H), and 2.45 (s, 1H, endo-*meso*-H); ^{19}F NMR (565 MHz, $CDCl_3$, 293 K) δ (ppm) –137.6 (d, 2F, *o*-F), –138.1 (d, 2F, *o*-F), –138.5 (m, 6F, *o*-F), –141.6 (d, 2F, *o*-F), –152.6 (m, 4F, *p*-F), –156.1 (m, 2F, *p*-F), –161.6 (m, 4F, *m*-F), –161.8 (m, 4F, *m*-F), –162.1 (m, 2F, *m*-F), and –162.4 (m, 2F, *m*-F); ESI-MS: 1693.1915 $[M+H]^+$, Calcd. for $C_{82}H_{27}F_{30}N_8$ 1693.1874; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 392 (4.7), 593 (9.5), and 898 (3.4).



S3

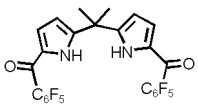
S3: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.41 (d, 4H, J = 3.7 Hz, β-pyrrole), 9.03 (d, J = 3.7 Hz, β-pyrrole), 8.96 (d, 4H, β-pyrrole), 8.94 (d, 4H, β-pyrrole), 8,69 (s, 4H, Ph-H), and –2.68 (s, 4H, NH); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm): –137.5 (m, 12F, *o*-F), –152.5 (t, 6F, *p*-F), and –162.4 (m, 12F, *m*-F); ESI-MS: 1691.1742 $[M+H]^+$, Calcd. for $C_{82}H_{25}F_{30}N_8$ 1691.1718; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 423 (51), 510 (4.9), and 586 (1.5).

Deuterated-*p*-quinodimethane-bridged octaphyrins (6b) and (7b).

Following the synthetic procedure of **6a** and **7a**, the reaction of diol **3** with **1b** gave **6b** and **7b**.

6b: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.52 (br s, 4H, NH), 8.27 (d, 4H, J = 4.1 Hz, β-pyrrole) 7.60 (d, 4H, J = 4.1 Hz, β-pyrrole), 7.46 (d, 4H, J = 4.6 Hz, β-pyrrole), 7.24 (d, 4H, β-pyrrole) and 2.69 (s, 2H, endo-*meso*-H).

7b: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.43 (br s, 2H, NH), 8.36 (d, 2H, J = 4.2 Hz, β-pyrrole), 8.31 (br s, 2H, NH), 8.07 (d, 2H, J = 4.2 Hz, β-pyrrole), 7.66 (d, 2H, J = 4.2 Hz, β-pyrrole), 7.60 (d, 2H, J = 4.2 Hz, β-pyrrole), 7.50 (d, 2H, J = 4.2 Hz, β-pyrrole), 7.33 (d, 2H, J = 4.1 Hz, β-pyrrole), 7.27 (d, 2H, J = 4.2 Hz, β-pyrrole), 7.18 (d, 2H, J = 4.2 Hz, β-pyrrole) 6.42 (s, 1H, exo-*meso*-H), and 2.45 (s, 1H, endo-*meso*-H).



S4

5,5-Dimethyl-1,9-bis(pentafluorobenzoyl)dipyrromethane (S4).

Following the synthetic procedure of **S2**, the reaction of 5,5-dimethyldipyrromethane[3] (4.6 g, 26 mmol) with EtMgBr prepared from Mg (3.2 g, 130 mmol) and EtBr (9.8 mL, 130 mmol) followed by the reaction with pentafluorobenzoyl chloride (19 mL, 130 mmol) gave **S4** as a white solid (4.2 g, 29%).

S4: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.72 (br s, 2H, NH), 6.66 (s, 2H, β-pyrrole), 6.24 (s, 2H, β-pyrrole), and 1.83 (s, 6H, Me); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm) –141.8 (m, 4F, *o*-F), –152.1 (t, 2F, *p*-F), and –161.3 (t, 4F, *m*-F); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ (ppm) 172.3

(2C, carbonyl-C), 148.9 (2C, pyrrole), 145.0 and 143.3 (4C, *o*-C),143.3 and 141.6 (2C, *p*-C), 138.5 and 136.9 (4C, *m*-C), 131.7 (2C, pyrrole), 122.9 (2C, pyrrole), 114.0 (2C, *ipso*-C), 109.5 (2C, pyrrole), 36.5 (1C, *meso*-C), and 27.8 (2C, Me) ESI-MS: 561.0651 $[M–H]^-$, Calcd. for $C_{25}H_{11}F_{10}N_2O_2$ 561.0666.

***p*-Quinodimethane-bridged calix-octaphyrin (9).**

A solution of **S4** (1.0 g, 1.8 mmol) in a 10:1 mixture of THF and methanol (110 mL) was reduced with excess $NaBH_4$. The organic layer was separated, and washed with water and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure to yield diol **8** in a quantitative yield, which was then immediately dissolved in a 2:1 mixture of dichloromethane and THF (90 mL) that contained **1a** (330 mg, 0.9 mmol). After the solution was stirred under inert atmosphere for 15 min, methanesulfonic acid (12 μL, 0.18 mmol) was added and the resulting solution was stirred for 1.5 h. DDQ (1.6 g, 7.2 mmol) was added and the resulting solution was opened to the air with constant stirring for further 2 h. The reaction mixture was passed through a basic alumina column followed by evaporation of solvent under reduced pressure. The residue was subjected to silica gel column chromatography using a 19:1 mixture of hexane and ethyl acetate. The calix-octaphyrin **9** eluted first as a violet band (33 mg, 3%). Recrystallization from dichloromethane and methanol gave violet crystals of **9**.

9: ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ (ppm): 9.15 (br s, 4H, NH), 8.20 (d, 4H, J = 4.8 Hz, β-pyrrole), 7.72 (d, 4H, J = 4.1 Hz, β-pyrrole), 7.47 (d, 4H, J = 4.8 Hz, β-pyrrole), 7.31 (d, 4H, J = 4.1 Hz, β-pyrrole), 4.65 (s, 4H, quinodimethane-H), 1.39 (s, 6H, exo-Me) and –1.03 (s, 6H, endo-Me); ^{19}F NMR (565 MHz, $CDCl_3$, 298 K) δ (ppm): –138.0 (d, 4F, *o*-F), –138.6 (d, 4F, *o*-F), –153.1 (t, 4F, *p*-F) –161.9 (m, 4F, *m*-F), and –162.1 (m, 4F, *m*-F); ESI-MS: 1417.2786 $[M+H]^+$, Calcd. for $C_{74}H_{37}F_{20}N_8$ 1417.2827; UV-Vis (CH_2Cl_2) λ_{max} nm (ε x 10^{-4}): 392 (4.3), 588 (9.8), and 894 (3.5).

1) R. Taniguchi, S. Shimizu, M. Suzuki, J.–Y. Shin, H. Furuta, A. Osuka, *Tetrahedron Lett*. **2002**, *44*, 2505.

2) P. D. Rao, S. Dhanalekshmi, B. J. Litter, J. S. Lindsey, *J. Org. Chem*. **2000**, *65*, 7323.

3) B. J. Litter, M. A. Miller, C.-H. Hung, R. W. Wagner, D. F. O'Shea, P. D. Boyle, J. S. Lindsey, *J. Org. Chem*. **1999**, *64*, 1391.

III. ^{1}H and ^{19}F NMR Spectra of 4a, 5a, 6a, 7a, and 9

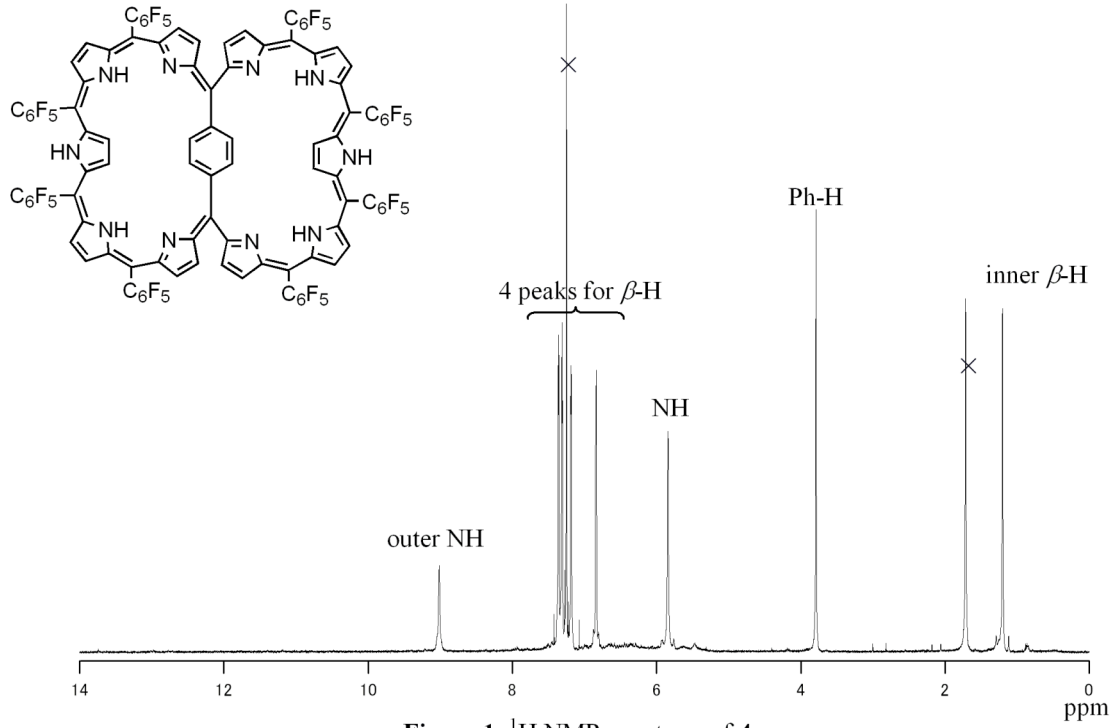


Figure 1. ^{1}H NMR spectrum of **4a**

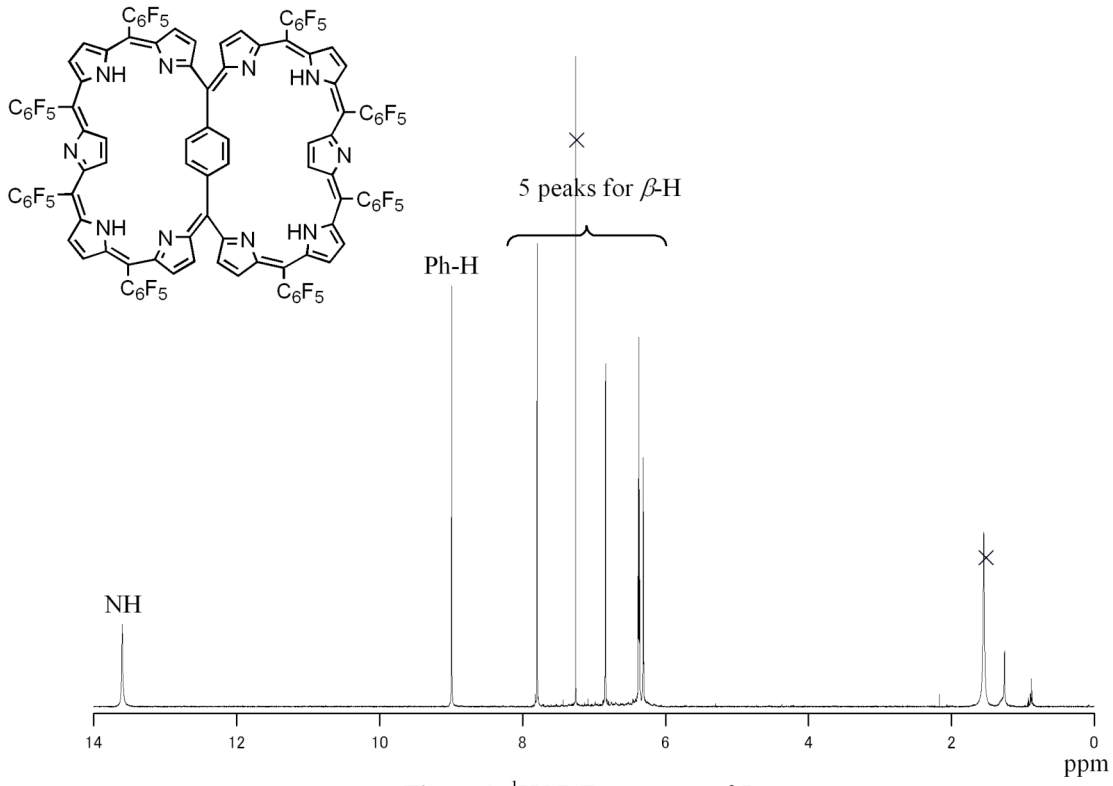


Figure 2. ^{1}H NMR spectrum of **5a**

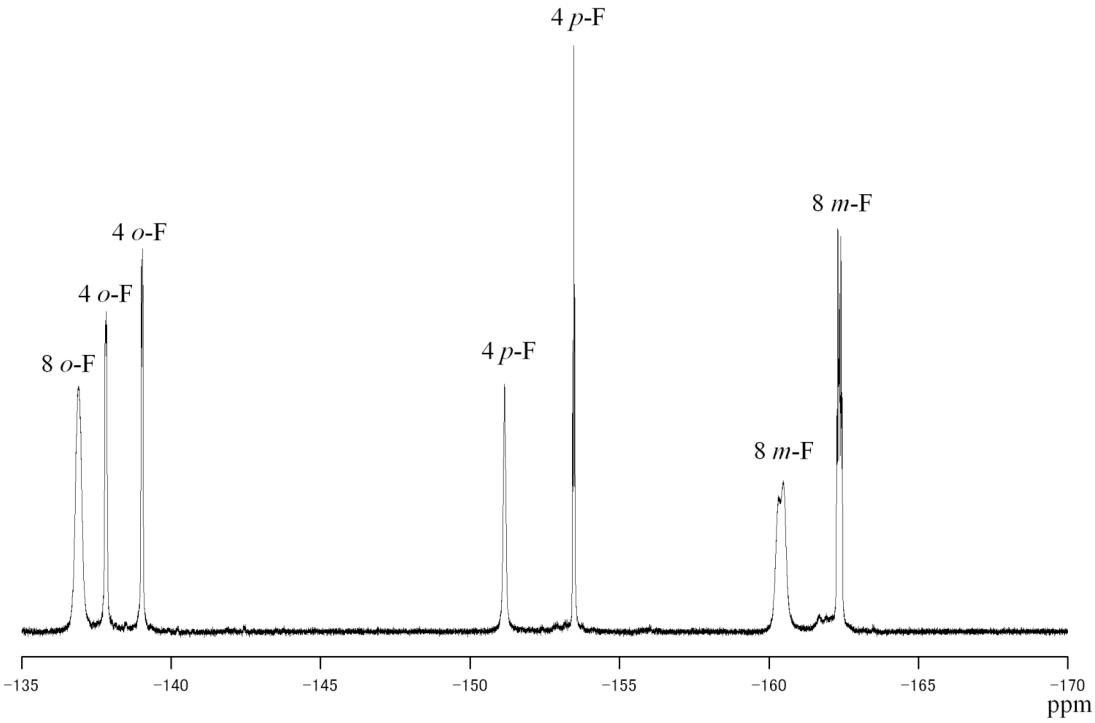


Figure 3. ^{19}F NMR spectrum of **4a**

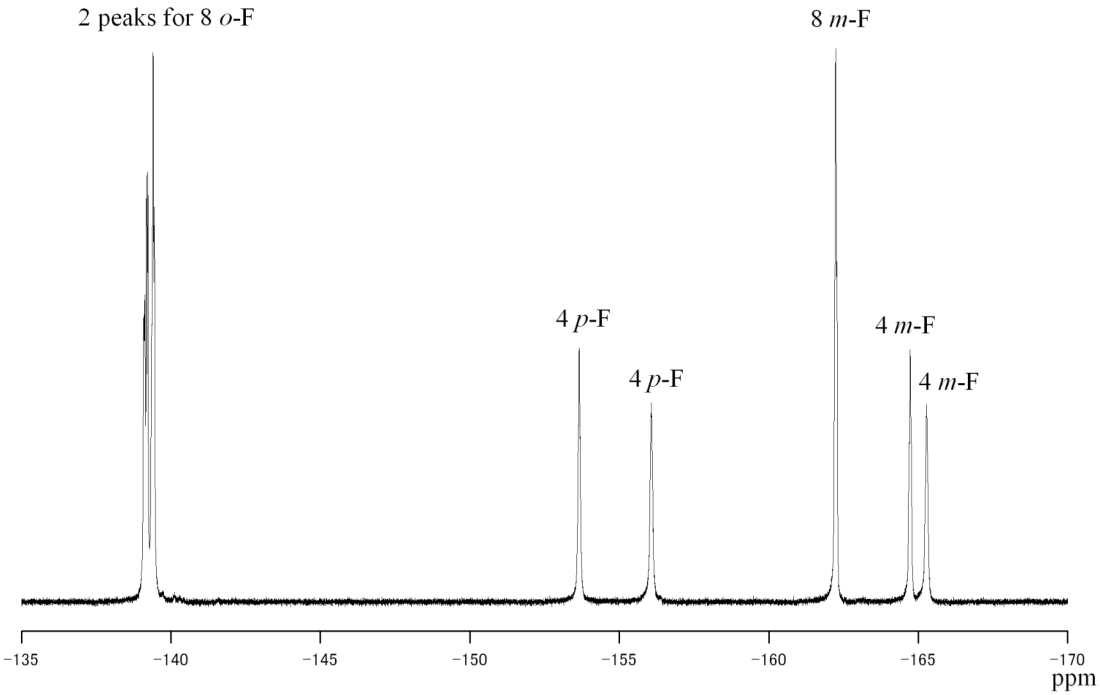


Figure 4. ^{19}F NMR spectrum of **5a**

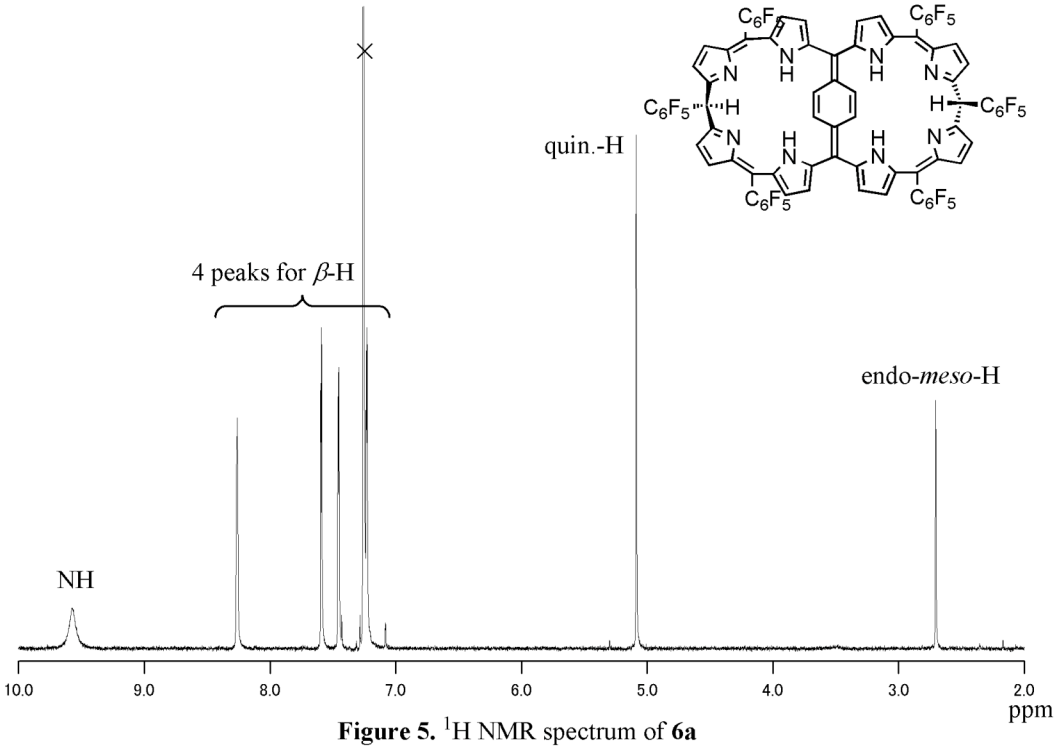


Figure 5. ^{1}H NMR spectrum of **6a**

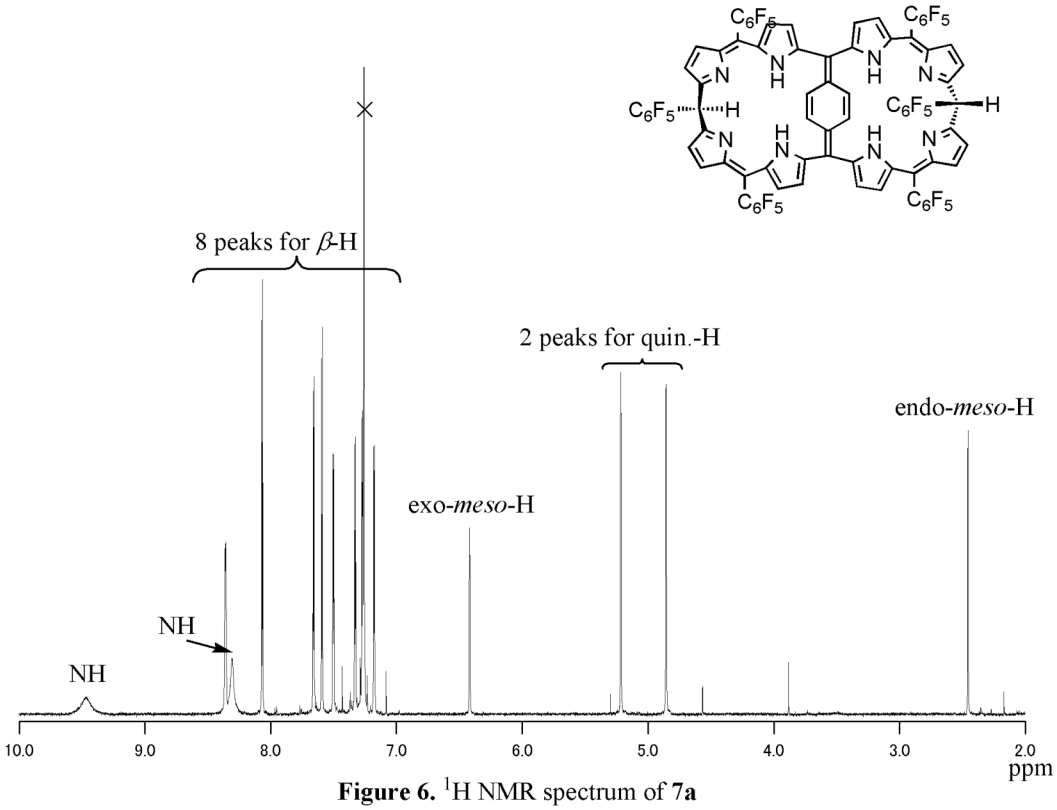


Figure 6. ^{1}H NMR spectrum of **7a**

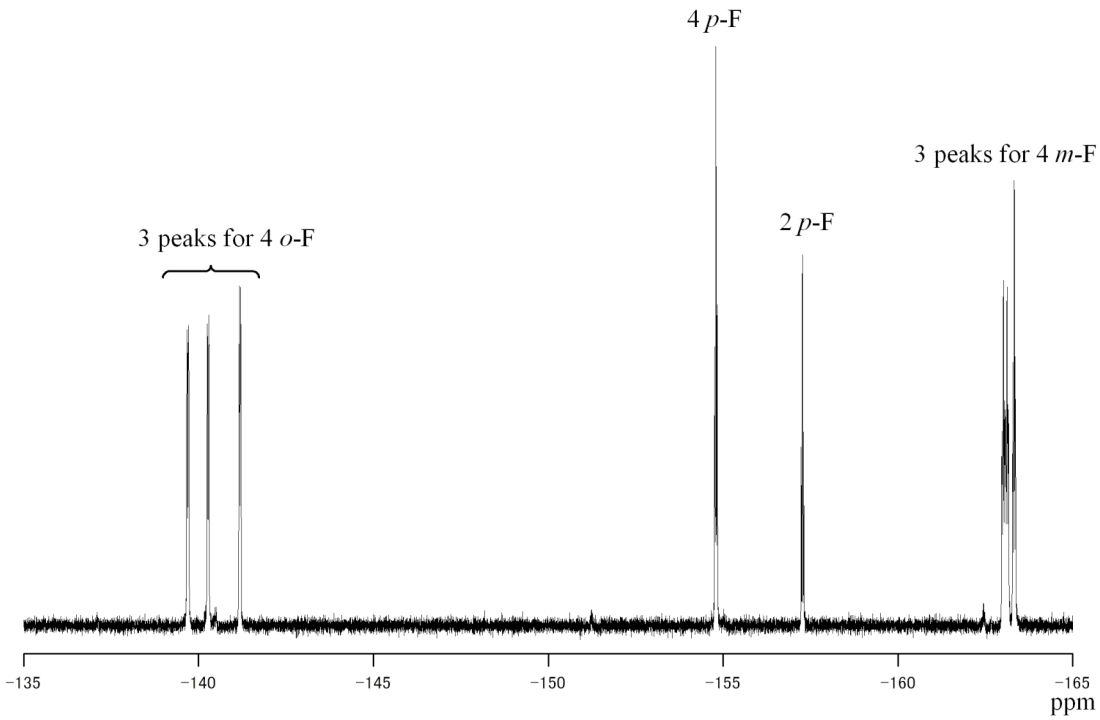


Figure 7. ^{19}F NMR spectrum of **6a**

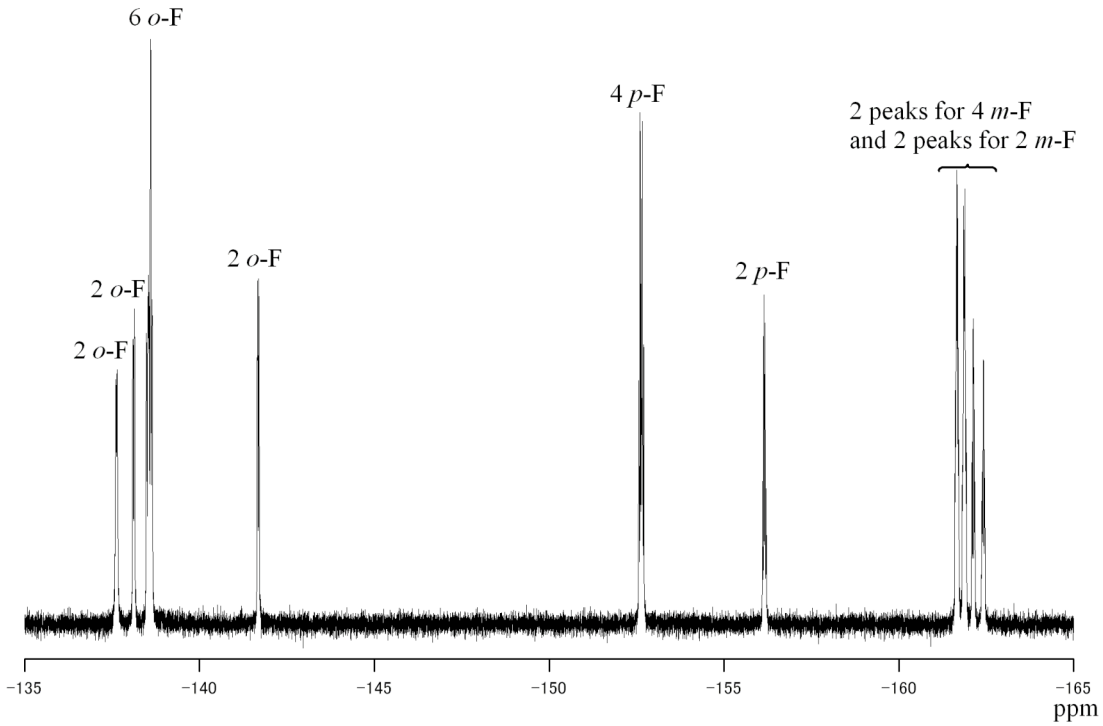


Figure 8. ^{19}F NMR spectrum of **7a**

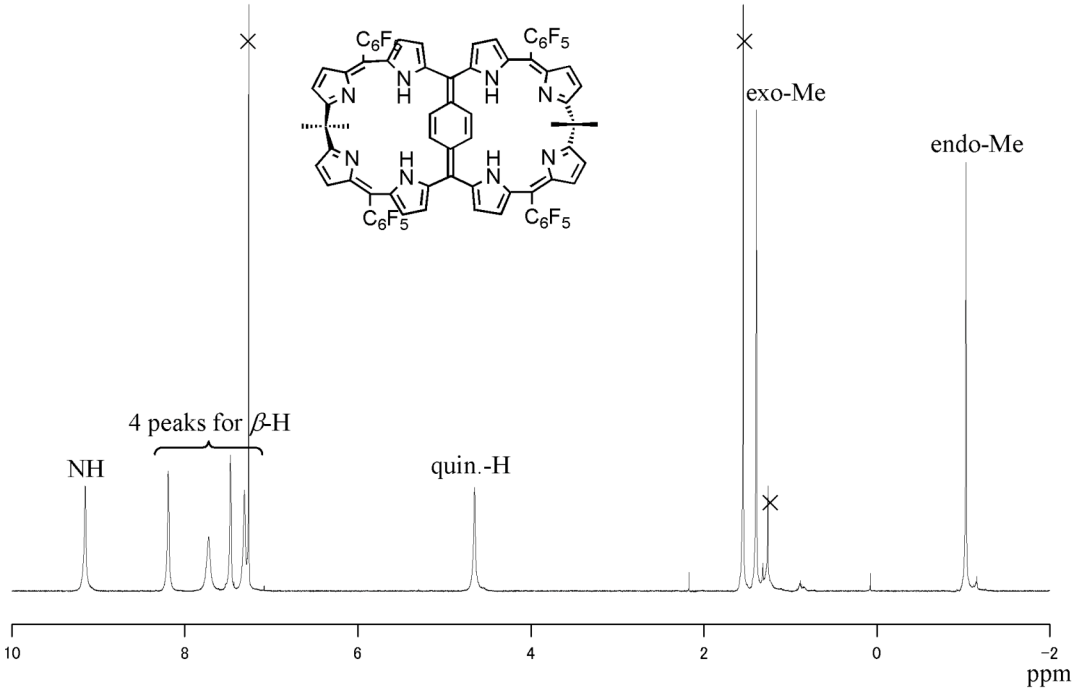


Figure 9. ^{1}H NMR spectrum of **9**

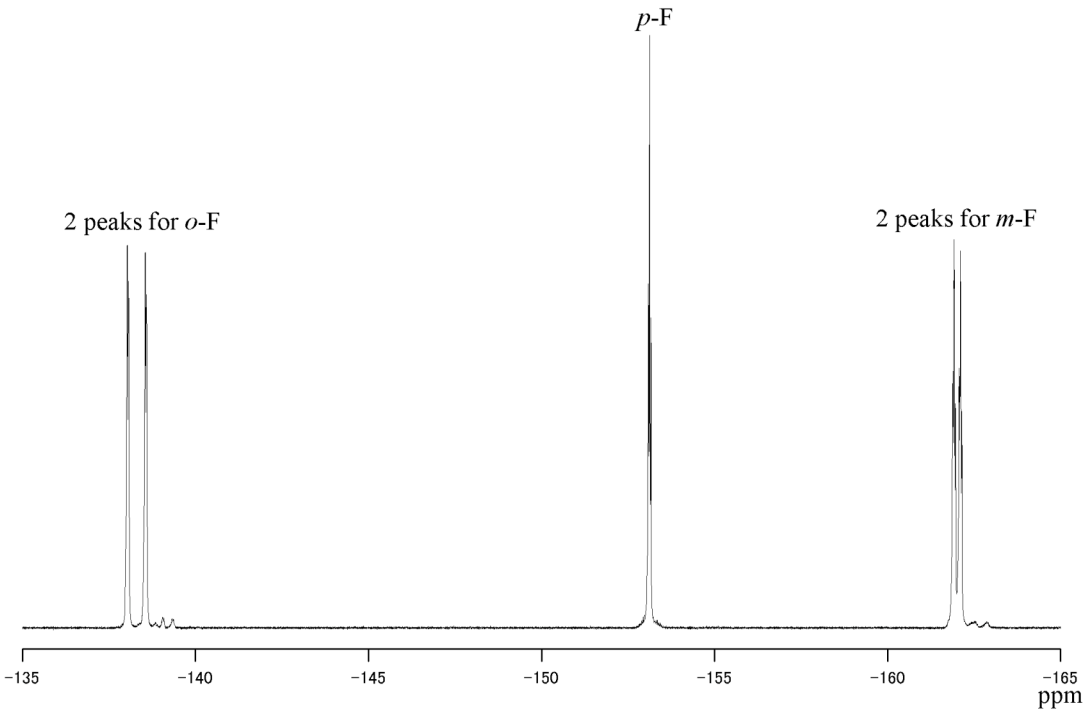
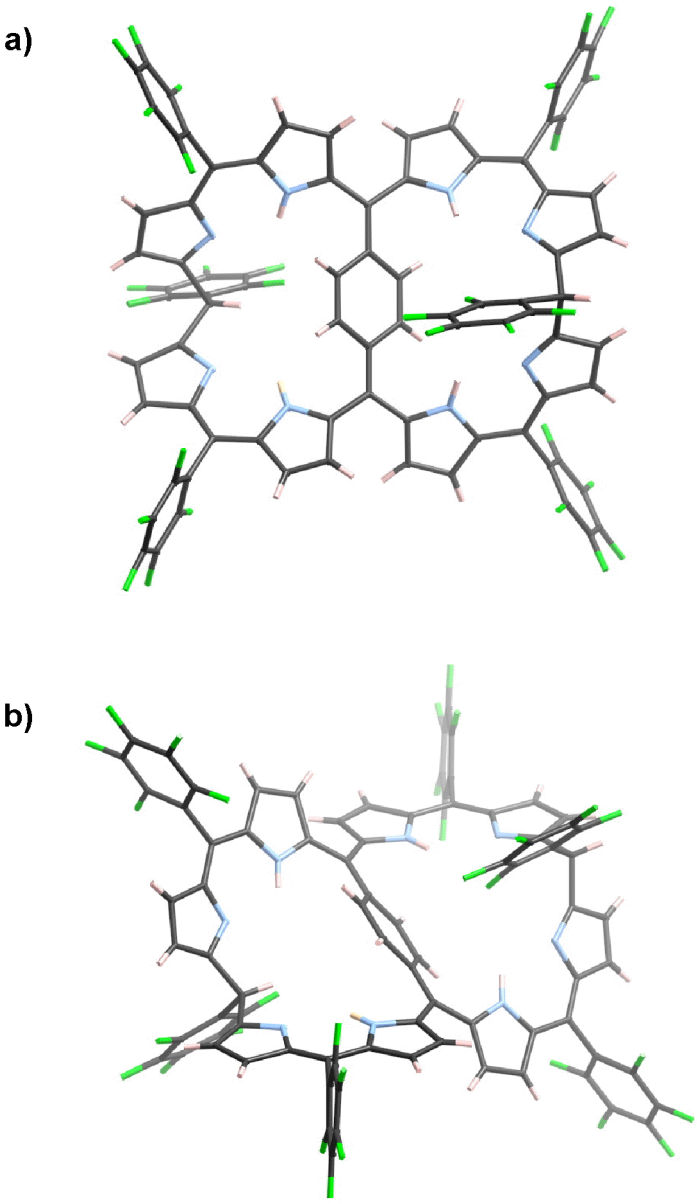


Figure 10. ^{19}F NMR spectrum of **9**

IV. Preliminary X-ray structure of 7a



a) top view b) side view

Crystallographic data for **7a**: $C_{84}H_{28}Cl_6F_{30}N_8$, M_w = 1761.43, Monoclinic, space group $P2_1/n$ (No.14), a = 18.918(6), b = 10.750(5), c = 20.695(8) Å, β = 117.204(16)°, V = 3743(2) Å^3, D_c = 1.563 mg/mm^3, Z = 2, R_1 = 0.1363, R_w (all data) = 0.4157, GOF = 1.423 (I>2.0 $\sigma(I)$).

V. Absorption Spectra of 6a, 7a, and 9