Electronic Supplementary Material (ESI) for Chemical Science.

Supplementary Information for:

"Nonspherical Anion Sequestration by C-H Hydrogen Bonding"

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Experimental section

General considerations. All manipulations were performed under an atmosphere of dry, oxygen-free N_2 by means of standard Schlenk or glovebox techniques (MBraun glovebox equipped with a –35 °C freezer), unless otherwise noted. All glassware was oven dried for a minimum of 10 h and cooled in an evacuated antechamber prior to use in the drybox. Anhydrous and anaerobic tetrahydrofuran (THF), hexanes, and dichloromethane (DCM) were dried and deoxygenated on dual high-performance columns within a Glass Contour 800L Solvent Purification System and stored over 4 Å molecular sieves prior to use. All fluorinated chemicals were purchase through commercial suppliers and used without further purification. Additional dry, oxygen-free solvents were stored within an Mbraun glovebox and kept over 4 Å molecular sieves. Chemicals and solvents were purchased from commercial suppliers and used as received. TBA and $[n\text{-}Bu_4N]^+$ are used throughout this document to refer to the tetra-*n*-butylammonium cation. Compound **S1** was synthesized according to published procedures.[1]

^{1}H-, ^{13}C- and ^{19}F nuclear magnetic resonance (NMR) spectra were obtained using a Bruker Avance 400 MHz spectrometer. Chemical shifts for protons are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are referenced to residual protium in the NMR solvent ($CHCl_3$: δ 7.26 and $(CH_3)_2SO$: δ 2.50). Chemical shifts for carbon are reported in ppm downfield from TMS and are referenced to the carbon resonances of the solvent ($CDCl_3$: δ 77.2). Data are presented as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, br = broad), coupling constants in Hertz, and integration. Some ^{1}H NMR and ^{13}C NMR were recorded at high temperatures to enhance signal resolution.

High-resolution mass spectrometry (HRMS) was performed on a Thermo Scientific Q-Exactive Oribtrap instrument equipped with a Dionex Ultimate 3000 (RSLC) inlet system, and electrospray (ESI) and atmospheric pressure chemical ionization (APCI) sources.

All titrations with different anions in the form of tetra-*n*-butylammonium ($[n\text{-}Bu_4N]^+$ or TBA) salts were carried out using ^{1}H NMR spectroscopy on a Bruker Avance 400 MHz spectrometer at room temperature (293 K) unless otherwise noted. 0.5 mL of receptor solutions (~0.0298 M) were

prepared in NMR tubes and aliquots of concentrated salt solutions (0.2 mL, 7-10 eq) in screw-cap scintillation vials were prepared and added using micro-syringes. The titration started with 5 μL of the salt's solution corresponding to 0.2 eq of the salt relative to host. Subsequent titrations were double checked and corroborated by integrating the $[n\text{-Bu}_4\text{N}]^+$ protons relative to the host's protons. To determine the exact host:guest equivalence, relative integration of proton "e" (for host) and the methylene highlighted in $[\text{N}(\boldsymbol{CH_2}\text{CH}_2\text{CH}_2\text{CH}_3)_4]^+$ was carried out. Following the integration of these protons shows a 1:1 stoichiometry for all examined anions especially those with a strong binding constant (e.g., TBAMeSO$_3$ into **6**, see Figure S58, or TBAMeSO$_3$ into **4**, see Figure S64). The titration was stopped when the ^{1}H resonance of protons "a", "b_{in}", and "b_{out}" did not show any further shift. The ^{1}H NMR binding constant have been determined using Bindfit online software.[2, 3] NMR 1:1 fitting method with Nelder–Mead algorithm has been used for calculating the binding constants using non-linear regression method. The excel input files were prepared as follows: the first row has the headers, the first two columns are the host and guest concentrations, and the following three columns represents the proton resonances (in ppm) for protons "a", "b_{in}", and "b_{out}". The calculated errors are based on so-called "asymptotic standard error" at the 95% confidence interval level.

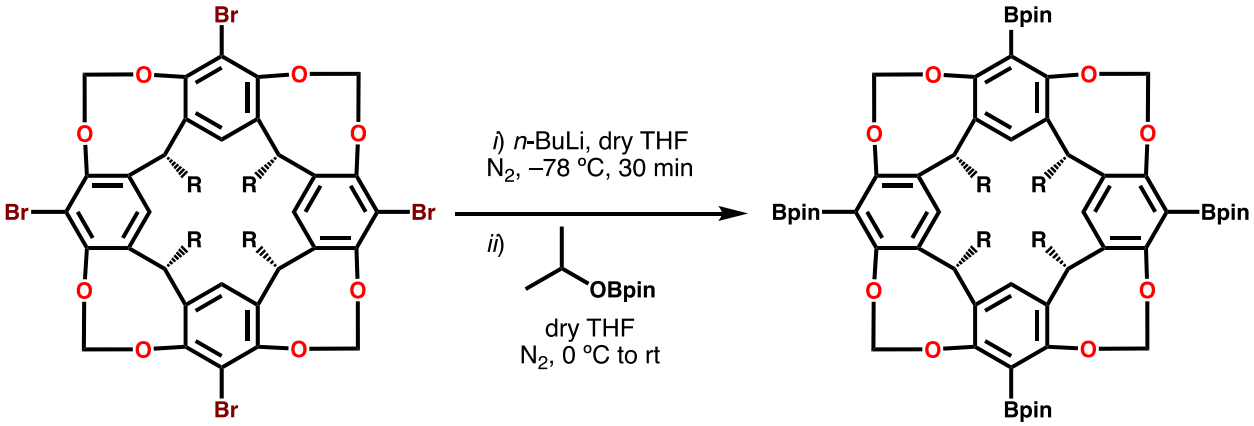
The titration of **7** with $[n\text{-Bu}_4\text{N}][\text{PF}_6]$ (Figure S43), **6** with $[n\text{-Bu}_4\text{N}][p\text{TsO}]$ (Figure S59-S60), and **8** with $[n\text{-Bu}_4\text{N}][\text{MeSO}_3]$ (Figure S67) have shown a slow exchange on the ^{1}H NMR time scale (Table S4). In these cases, we used the ^{1}H NMR single-point method to determine the binding constant (K_a) at different concentrations using eq. 1, where I(HG) and I(H) are the integrals of a specific proton in the host-guest adduct (HG) and free host (H), respectively, and c(H) and c(G) are the initial molar concentrations of host and guest, respectively.[4]

$$K_a = \frac{I(\text{HG})}{I(\text{H})\left(c(\text{G}) - \frac{I(\text{HG})}{I(\text{H}) + I(\text{HG})}\, c(\text{H})\right)} \qquad eq.1$$

Single crystal data for **1** – **8**, and adducts $[n\text{-Bu}_4\text{N}][\text{MeSO}_3 \subset \text{host}]$, for host = **4** and **6** – **8**, were collected on a Bruker X8 Prospector Ultra diffractometer equipped with an APEX II CCD detector and an IμS microfocus Cu Kα X-ray source (λ = 1.54178 Å). Temperature was maintained using an Oxford

Cryosystem nitrogen flow apparatus. Single crystals suitable for X-ray structure analysis were coated with Paratone N-oil and mounted on MiTeGen Kapton loops (polyimide). Raw data was integrated and corrected for Lorentz and polarization effects using Bruker APEX3.[5] Absorption corrections were applied using SADABS.[6] Space group assignments were determined by examination of systematic absences, E-statistics, and successive refinement of the structures. The program PLATON[7, 8] was employed to confirm the absence of higher symmetry for all crystals. The positions of the heavy atoms were determined using intrinsic phasing methods using the program SHELXT[9] and SHELXL[10] with Olex2[11] interface. Successive cycles of least-square refinement followed by difference Fourier syntheses revealed the positions of the remaining non-hydrogen atoms. Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were added in idealized positions. Crystallographic data for **1** – **8**, and adducts [*n*-Bu_4N][$MeSO_3$⊂host], for host = **4** and **6** – **8**,·are given in Table S1.

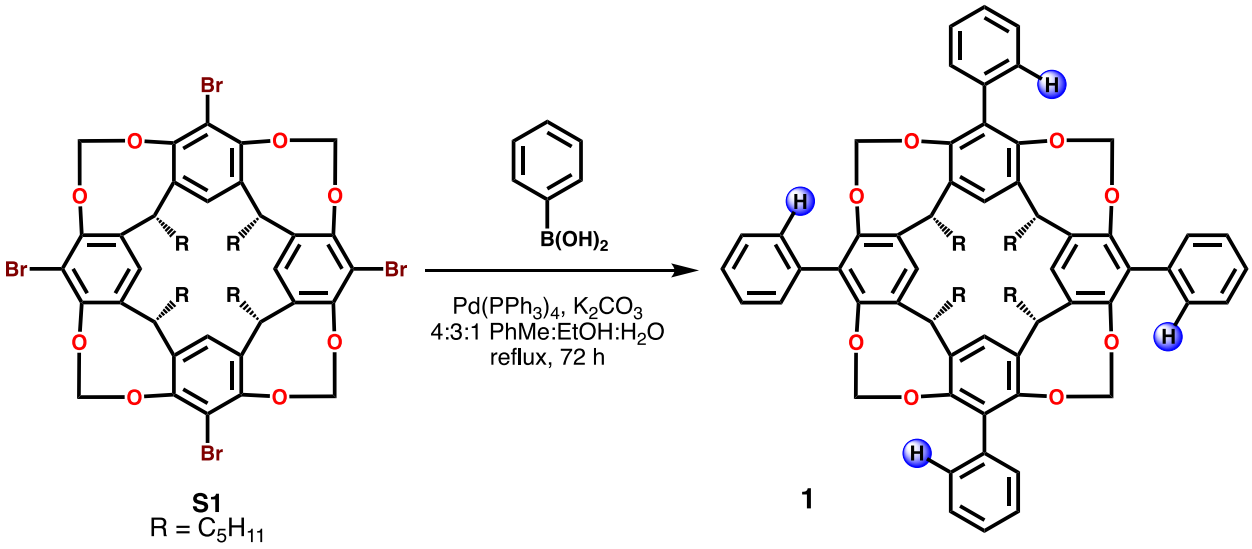
Synthetic details. Compound **S1** was prepared according to literature procedures in large quantities (>30 g).[1]



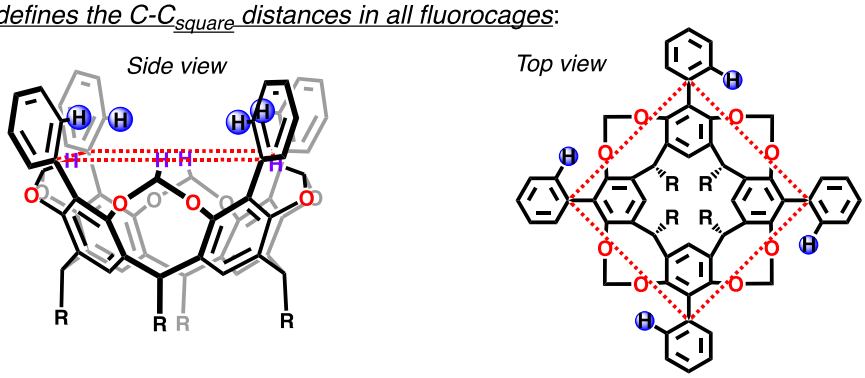
S1
R = C_5H_{11}

S2

Compound **S2**. The synthesis of **S2** has been reported in the literature.[12] However, we have modified the synthetic procedure, as described next, increasing the overall product yield. A 250 mL Schlenk flask was loaded with **S1** (4.0 g, 3.53 mmol), sealed with rubber septum and dried at 80 °C for 4 h using high vacuum. The flask was filled with nitrogen and put under a nitrogen flow by placing a needle (0.7 mm×40 mm) through the rubber septum. Dry tetrahydrofuran (THF, 170 mL) was added through the rubber septum using another needle (0.9 mm× 40 mm). The resulting clear solution was cooled down to –78 °C using a dry ice/acetone bath. After stirring for 10 min at this temperature, *n*-butyllithium (1.6 M in hexanes, 9.24 mL, 14.83 mmol, 4.2 eq) was added dropwise over 5 min, and the mixture was stirred for an additional 0.5 h. The dry ice/acetone bath was replaced with ice/NaCl bath and the white cloudy mixture was stirred vigorously for 20 min. 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (10 mL, 53.74 mmol, 15.2 eq) was added dropwise in 5 min. After 30 min the ice/NaCl bath was removed, and the reaction mixture (clean solution) warmed to room temperature. Around 50 mL deionized water was added, and the mixture stirred vigorously for 20 min. The THF was removed under low pressure and the white solid was washed with copious amount of water and 200 mL of acetone to obtain the pure produce (white solid). Yield: 73% (3.40 g, 2.57 mmol). Spectral characterization is in agreement with previous literature.[1]



Red dotted line defines the C-C$_{square}$ distances in all fluorocages:

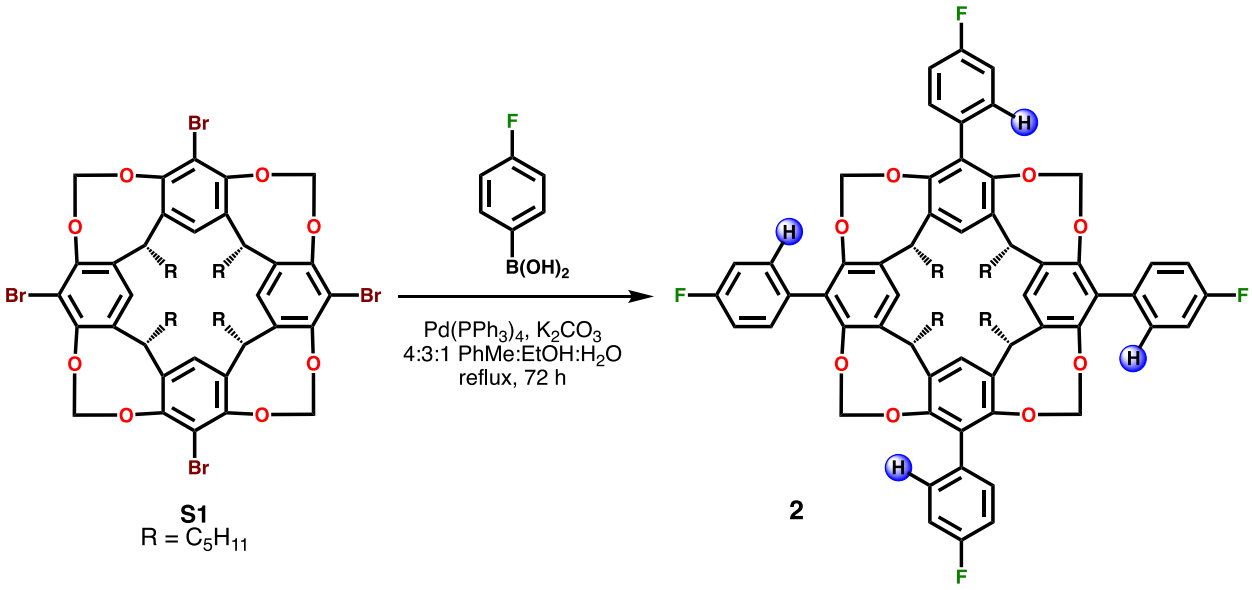


Compound **1**. To a 250 mL Schlenk flask containing **S1** (1.00 g, 0.88 mmol) we added phenylboronic acid (0.53 g, 4.41 mmol, 5 eq), K_2CO_3 (3 g, 21.7 mmol, 24.7 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.32 mmol, 0.36 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for three days after which the solvents were removed under reduced pressure. The crude product was purified by column chromatography using DCM/Hexanes (50-60%, v/v) giving a white solid. Yield: 53% (0.53 g, 0.48 mmol). Melting pint = 258-260 °C. High quality crystals of **1** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34-7.29 (m, 3H), 7.26-7.22 (m, 1H), 7.03 (d, 2H, *J* = 7.2 Hz), 5.20 (d, 1H, *J* = 6.8 Hz), 4.87 (t, 1H, *J* = 7.0 Hz), 4.23 (d, 1H, *J* = 7.0 Hz), 2.37 (q, 2H, *J* = 6.4 Hz), 1.50-1.38 (m, 6H), and 0.96 (t, 3H, *J* = 7.1 Hz).

^{13}C NMR (100 MHz, CDCl3): δ 152.7, 138.5, 134.2, 130.0, 129.5, 128.0, 127.2, 120.0, 100.7, 37.3, 32.2, 30.6, 27.8, 22.9, and 14.3 ppm.

$C_{76}H_{80}O_8$, HRMS $[M+H]^+$ calc.: 1121.5926; exp.: 1121.5900.



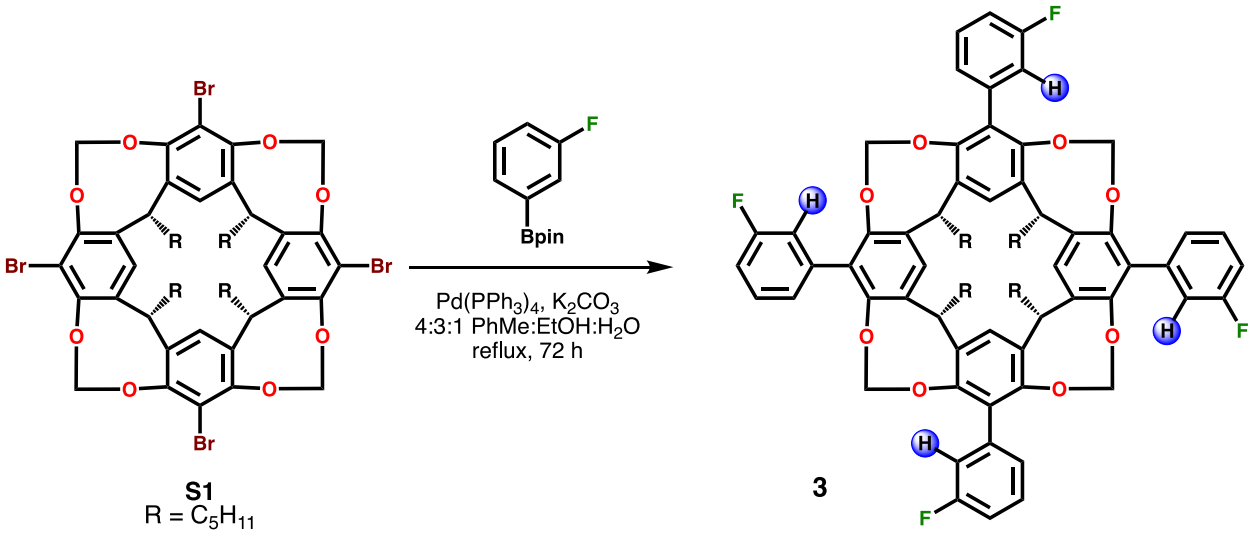
Compound **2**. To a 250 mL Schlenk flask containing **S1** (1.00 g, 0.88 mmol) we added 4-fluorophenylboronic acid (0.68 g, 4.84 mmol, 5.5 eq), K_2CO_3 (3 g, 21.7 mmol, 24.7 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.32 mmol, 0.36 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for three days after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (40-50%, v/v) giving a white solid. Yield: 46% (0.48 g, 0.40 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **2** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.31 (s, 1H), 7.05-6.98 (m, 4H), 5.25 (d, 1H, *J* = 6.8 Hz), 4.83 (t, 1H, *J* = 8.0 Hz), 4.19 (d, 1H, *J* = 7.0 Hz), 2.33 (q, 2H, *J* = 6.6 Hz), 1.49-1.35 (m, 6H), and 0.95 (t, 3H, *J* = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.3, 160.8, 152.7, 138.5, 131.6, 131.6, 129.8, 129.8, 128.5, 120.1, 115.2, 115.0, 100.6, 32.2, 30.5, 27.8, 22.9, and 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –114.91 ppm.

$C_{76}H_{76}O_8F_4$, HRMS $[M+H]^+$ calc.: 1193.5549; exp.: 1193.5532.



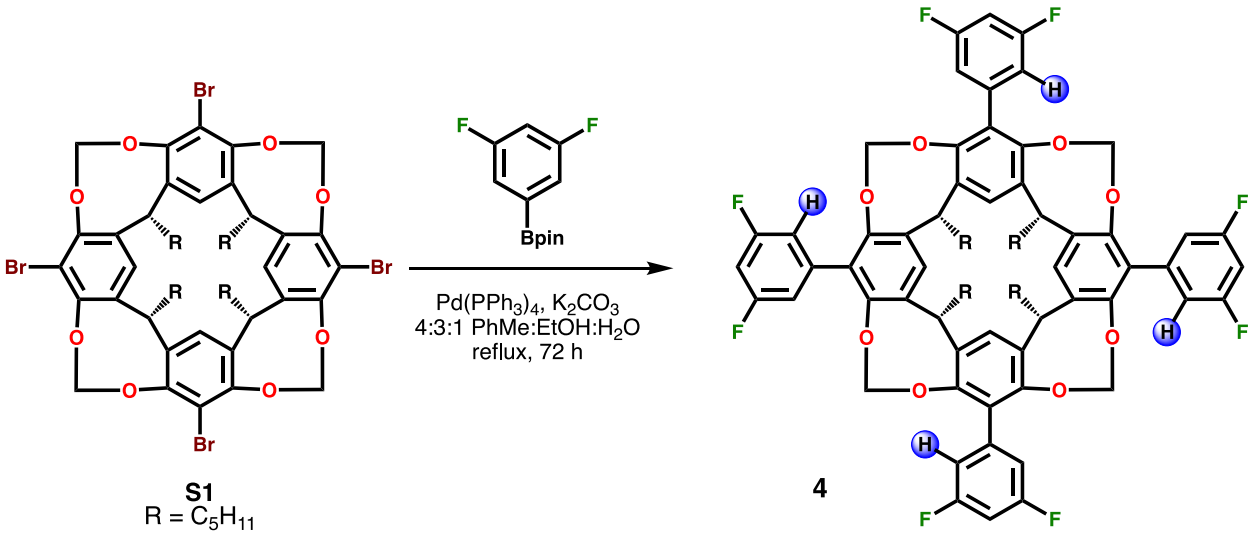
Compound **3**. To a 250 mL Schlenk flask containing **S1** (1.00 g, 0.88 mmol) we added 3-fluorophenylboronic acid pinacol ester (1.17 g, 5.28 mmol, 6 eq), K_2CO_3 (3 g, 21.7 mmol, 24.7 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.32 mmol, 0.36 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for three days after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (50%, v/v) giving a white solid. Yield: 38% (0.40 g, 0.33 mmol). Melting pint = 249-251 °C. High quality crystals of **3** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (s, 1H), 7.30 (m, 1H), 6.99 (dt, 1H, , J = 2.1 Hz and J = 8.4 Hz), 6.80 (t, 2H, J = 7.7 Hz), 5.26 (d, 1H, J = 6.9 Hz), 4.85 (t, 1H, J = 8.1 Hz), 4.20 (d, 1H, J = 7.0 Hz), 2.35 (q, 2H, J = 6.5 Hz), 1.50-1.36 (m, 6H), and 0.94 (t, 3H, J = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 161.3, 152.6, 138.5, 136.3, 136.2, 129.6, 129.5, 128.5, 125.6, 120.4, 117.2, 117.0, 114.5, 114.5, 100.6, 37.2, 32.2, 30.5, 27.8, 22.9, and 14.3.

^{19}F NMR (376 MHz, $CDCl_3$): δ –113.45 ppm.

$C_{76}H_{76}O_8F_4$, HRMS $[M+H]^+$ calc.: 1193.5549; exp.: 1193.5528.



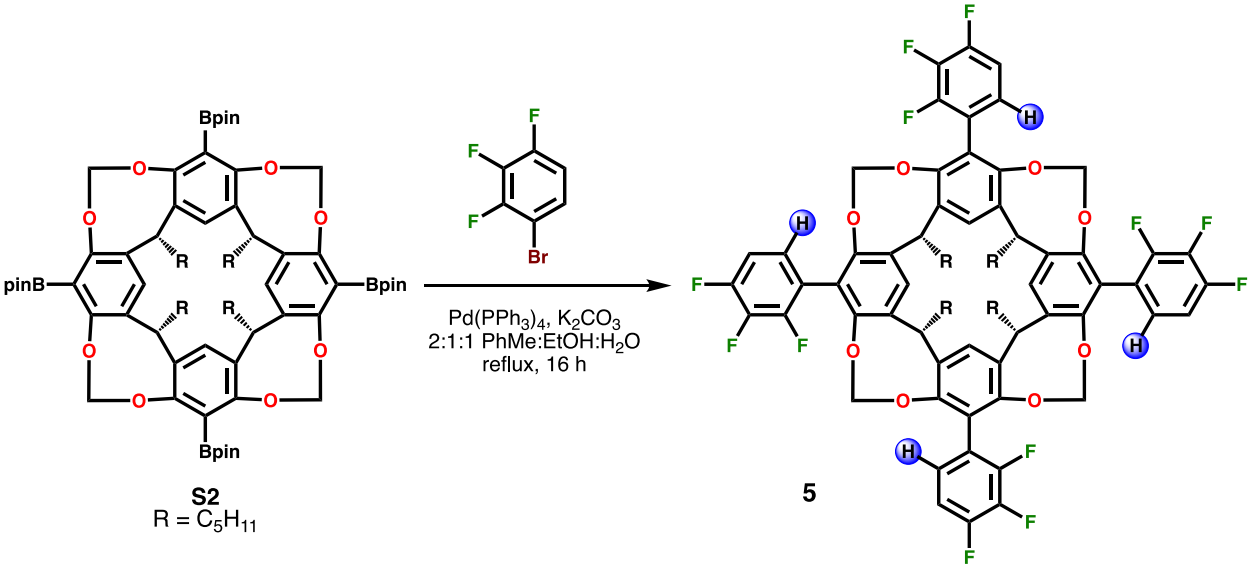
Compound **4**. To a 250 mL Schlenk flask containing **S1** (1.00 g, 0.88 mmol) we added 3,5-difluorophenylboronic acid pinacol ester (1.27 g, 5.28 mmol, 6 eq), K_2CO_3 (3 g, 21.7 mmol, 24.7 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.32 mmol, 0.36 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for three days after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (50%, v/v) giving a white solid. Yield: 42% (0.47 g, 0.37 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **4** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.34 (s, 1H), 6.68 (b, 1H), 6.56 (d, 2H, *J* = 7.8 Hz), 5.30 (d, 1H, *J* = 6.8 Hz), 4.83 (t, 1H, *J* = 8.1 Hz), 4.13 (d, 1H, *J* = 7.0 Hz), 2.33 (q, 2H, *J* = 6.5 Hz), 1.49-1.36 (m, 6H), and 0.95 (t, 3H, *J* = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 163.7, 161.4, 161.3, 152.4, 138.7, 137.3, 137.2, 137.1, 127.8, 120.8, 113.1, 112.9, 103.1, 103.0, 102.8, 100.6, 37.1, 32.2, 30.4, 27.8, 22.9, and 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –110.27 ppm.

$C_{76}H_{72}O_8F_8$, HRMS $[M+H]^+$ calc.: 1265.5172; exp.: 1265.5130.



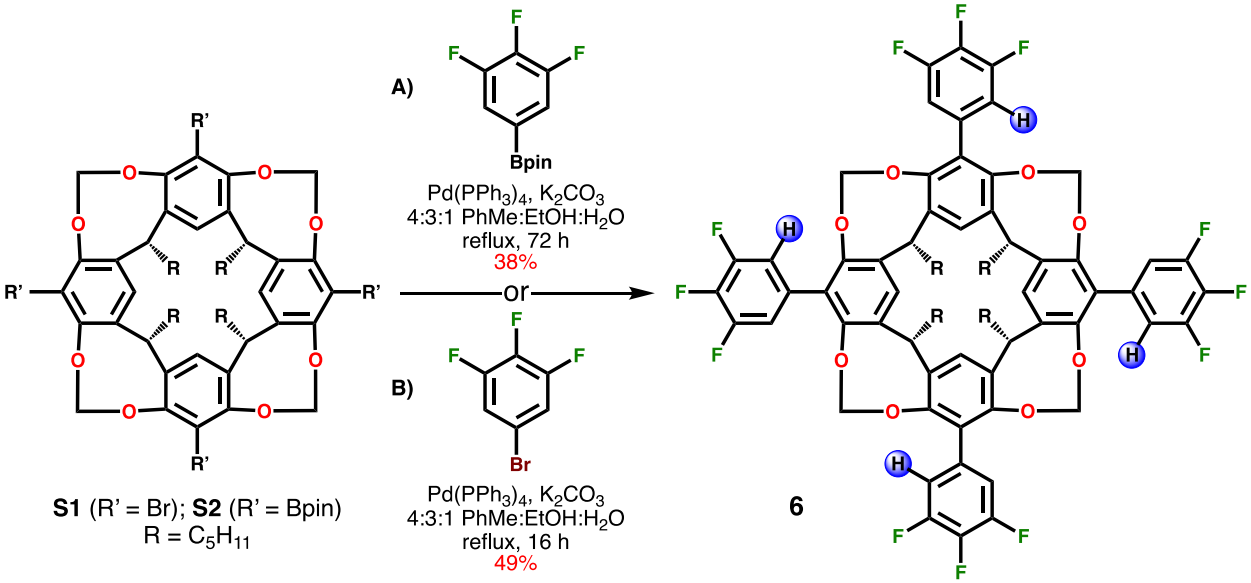
Compound **5**. To a 250 mL Schlenk flask containing **S2** (0.5 g, 0.38 mmol) we added 1-bromo-2,3,4-trifluorobenzene (0.4 g, 1.9 mmol, 5 eq), K_2CO_3 (1.5 g, 10.8 mmol, 28.4 eq), and a mixed solvent of toluene, ethanol, and water (40/20/20, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.2 g of $Pd(PPh_3)_4$ (0.16 mmol, 0.47 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~0.12 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for 16 h after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (50%, v/v) giving a white solid. Yield: 43% (0.22 g, 0.16 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **5** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (s, 1H), 6.90 (b, 1H), 6.52 (b, 0.4), 5.21 (b, 1H), 4.81 (b, 1H), 4.13 (b, 1H), 2.34 (b, 2H), 1.45 (b, 6H), and 0.95 (t, 3H, J = 6.9 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 37.1, 32.2, 30.4, 27.7, 22.8, 14.3, and several multiplets in 100-160 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –159.05 to –160.57 (m), and –136.09 to –131.40 (m) ppm.

$C_{76}H_{68}O_8F_{12}$, HRMS $[M+H]^+$ calc.: 1337.4795; exp.: 1337.4810.



Compound **6** (**Method A**). To a 250 mL Schlenk flask containing **S1** (1.00 g, 0.88 mmol) we added 3,4,5-trifluorophenylboronic acid pinacol ester (1.83 g, 7.04 mmol, 8 eq), K_2CO_3 (3 g, 21.7 mmol, 24.7 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.32 mmol, 0.36 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for three days after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (50%, v/v) giving a white solid. Yield: 38% (0.45 g, 0.34 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **6** were grown by slow evaporation of a DCM/MeCN solution.

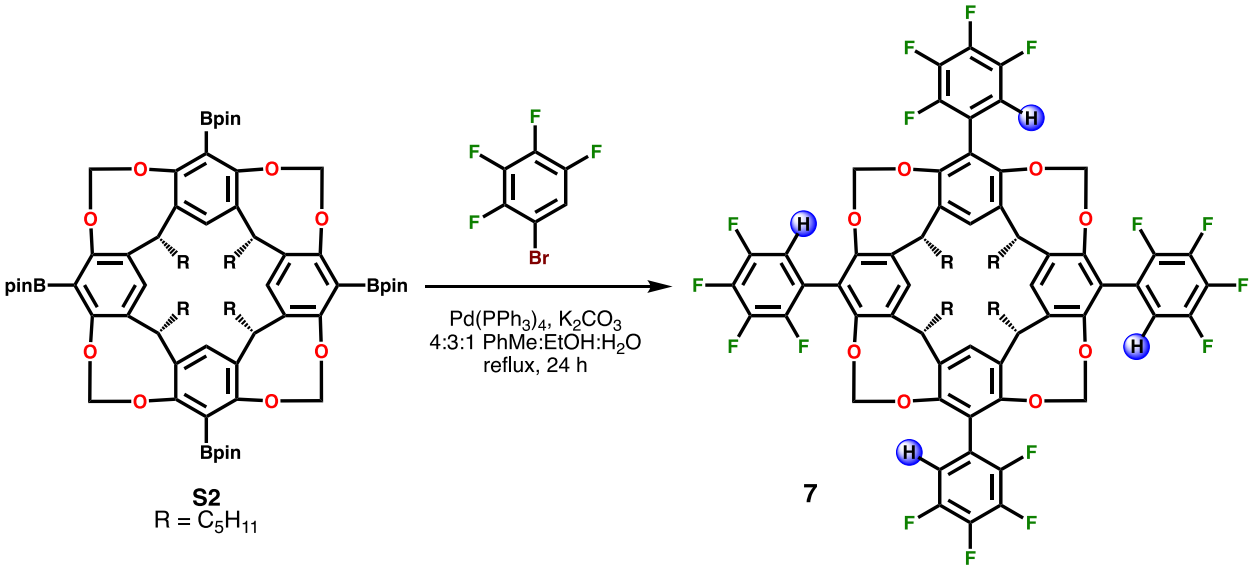
Compound **6 (Method B)**. To a 250 mL Schlenk flask containing **S2** (1.5 g, 1.14 mmol) we added 1-bromo-3,4,5-trifluorobenzene (1.92 g, 9.1 mmol, 8 eq), K_2CO_3 (3 g, 21.7 mmol, 19 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.5 g of $Pd(PPh_3)_4$ (0.43 mmol, 0.38 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~9 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for 16 h after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/ Hexanes (50%, v/v) giving a white solid. Yield: 49% (0.74 g, 0.55 mmol).

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.35 (s, 1H), 6.61 (b, 1H), 5.35 (d, 1H, J = 6.6 Hz), 4.85 (t, 1H, , J = 8.0 Hz), 4.08 (d, 1H, J = 7.0 Hz), 2.34 (q, 2H, J = 6.4 Hz), 1.50-1.39 (m, 6H), and 0.97 (t, 3H, J = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 151.6, 149.9, 139.7, 138.9, 138.0, 130.1, 127.3, 121.0, 114.3, 100.5, 37.2, 32.1, 30.3, 27.8, 22.9, and 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –135.46 (d), and –162.93 (t).

$C_{76}H_{68}O_8F_{12}$, HRMS $[M+H]^+$ calc.: 1337.4795; exp.: 1337.4752.



Compound **7**. To a 250 mL Schlenk flask containing **S2** (0.5 g, 0.37 mmol) we added 1-bromo-2,3,4,5-tetrafluorobenzene (0.52 g, 2.27 mmol, 6 eq), K_2CO_3 (1.5 g, 10.8 mmol, 29 eq), and a

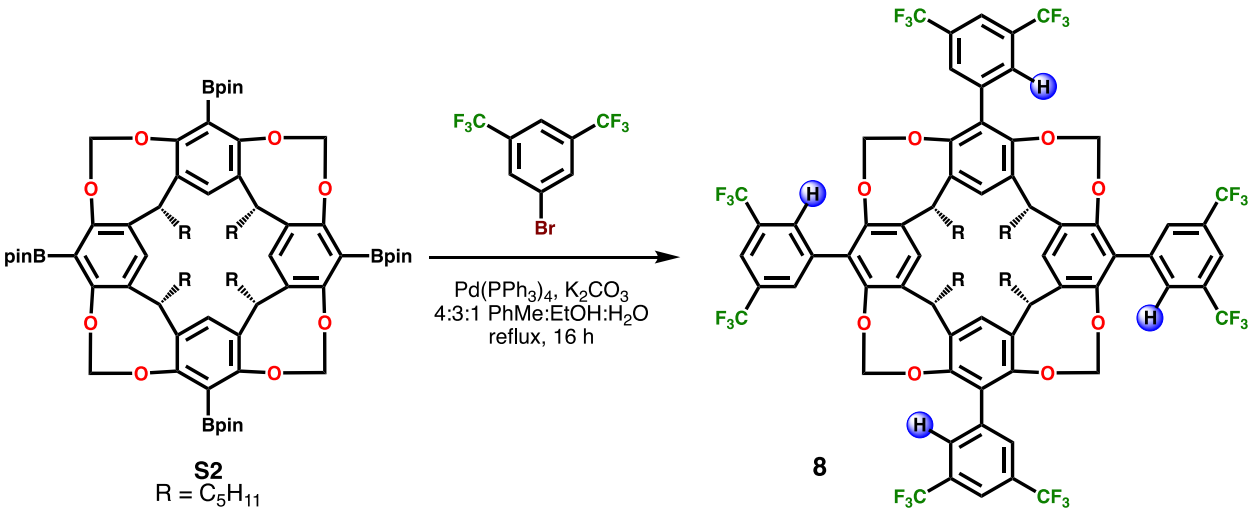
mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for 15 min while stirring vigorously at room temperature. To this mixture, 0.2 g of $Pd(PPh_3)_4$ (0.17 mmol, 0.46 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~11 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for 24 h after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (50%, v/v) giving a white solid. Yield: 53% (0.28 g, 0.20 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **7** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.28 (s, 1H), 6.71 (b, 0.72H), 6.39 (b, 0.3), 5.19 (b, 1H), 4.71 (b, 1H), 4.06 (b, 1H), 2.24 (b, 2H), 1.32 (b, 6H), and 0.85 (t, 3H, J = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$) δ 37.1, 32.2, 30.3, 27.7, 22.8, 14.3, and several multiplets in 100-160 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –156.01 to –154.65 (m) and –140.86 to –136.03 (m) ppm.

$C_{76}H_{64}O_8F_{16}$, HRMS $[M+H]^+$ calc.: 1409.4419; exp.: 1409.4417.



Compound **8**. To a 250 mL Schlenk flask containing **S2** (1.0 g, 0.75 mmol) we added 1-bromo-3,5-bis(trifluoromethyl)benzene (1.32 g, 4.5 mmol, 6 eq), K_2CO_3 (3 g, 21.7 mmol, 28.9 eq), and a mixed solvent of toluene, ethanol, and water (40/30/10, mL/mL/mL). The reaction mixture was degassed for

15 min while stirring vigorously at room temperature. To this mixture, 0.4 g of $Pd(PPh_3)_4$ (0.34 mmol, 0.46 eq) was added. This amount of catalyst forms 4 C-C bonds, thus representing ~11 mol% for each bond formation. The solution was degassed again for an additional 15 min while gradually increasing the temperature to reflux. The reaction mixture was left at reflux and under N_2 atmosphere for 16 h after which the solvents were removed under reduced pressure. The crude product was further purified by column chromatography using DCM/Hexanes (20%, v/v) giving a white solid. Yield: 46% (0.58 g, 0.35 mmol). Melting pint = >260 °C (exceeded measurable range). High quality crystals of **8** were grown by slow evaporation of a DCM/MeCN solution.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.83 (s, 1H), 7.53 (s, 2H), 7.44 (s, 1H), 5.33 (d, 1H, *J* = 6.8 Hz), 4.88 (t, 1H, *J* = 8.0 Hz), 4.29 (d, 1H, *J* = 6.9 Hz), 2.38 (q, 2H, *J* = 6.6 Hz), 1.52-1.38 (m, 6H), and 0.98 (t, 3H, *J* = 7.1 Hz).

^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 139.0, 135.7, 132.1, 131.8, 131.4, 131.1, 130.4, 127.3, 126.7, 124.6, 121.9, 121.6, 121.4, 119.2, 100.6, 37.4, 32.2, 30.5, 27.8, 22.9, and 14.3 ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ –62.94 ppm.

$C_{92}H_{108}N_4O_{20}$, HRMS $[M+H]^+$ calc.: 1825.7423; exp.: multiple attempts were carried out, however none of them was successful.

Isolated host-guest adducts

Compound [*n*-Bu_4N][$MeSO_3$⊂**4**]

15 mg of compound **4** in 0.5 mL of $CDCl_3$ were titrated with [*n*-Bu_4N][$MeSO_3$] up to ~1.1 eq. This solution was transferred to a 20 mL vial. The NMR tube was rinsed with 5-7 mL of DCM, which was combined with the initial solution. Additionally, around 4-5 mL of MeCN were added to the latter solution. The vial was left aside for slow solvent evaporation. Colorless crystals were formed within 12-16 hours.

Compound [*n*-Bu_4N][$MeSO_3$⊂**6**]

15 mg of compound **6** in 0.5 mL of $CDCl_3$ were titrated with [*n*-Bu_4N][$MeSO_3$] up to ~1.1 eq. This solution was transferred to a 20 mL vial. The NMR tube was rinsed with 5-7 mL of DCM, which was combined with the initial solution. Additionally, around 4-5 mL of MeCN were added to the latter solution. The vial was left aside for slow solvent evaporation. Colorless crystals were formed within 12-16 hours.

Compound [*n*-Bu_4N][$MeSO_3$⊂**7**].

15 mg of compound **7** in 0.5 mL of $CDCl_3$ were titrated with [*n*-Bu_4N][$MeSO_3$] up to ~1.2 eq. This solution was transferred to a 20 mL vial. The NMR tube was rinsed with 5-7 mL of DCM, which was combined with the initial solution. Additionally, around 4-5 mL of MeCN were added to the latter solution. The vial was left aside for slow solvent evaporation. Colorless crystals were formed within 12-16 hours.

Compound [*n*-Bu_4N][$MeSO_3$⊂**8**].

15 mg of compound **8** in 0.5 mL of $CDCl_3$ were titrated with [*n*-Bu_4N][$MeSO_3$] up to ~4.2 eq. This solution was transferred to a 20 mL vial. The NMR tube was rinsed with 5-7 mL of DCM, which was combined with the initial solution. Additionally, around 4-5 mL of MeCN were added to the latter solution. The vial was left aside for slow solvent evaporation. Colorless crystals were formed within 12-16 hours.

Computational details. All calculations were carried out using Gaussian 16 software package.[13] The M06-2X[14] functional was used for all optimizations and subsequent studies. The frequency calculations were carried out for all optimized structures to ensure the absence of any imaginary frequencies for the ground state molecules. The intrinsic reaction coordinate (IRC) calculation is carried out, in addition to the presence of one imaginary frequency, for the transition state structures. The double-zeta quality basis set (6-31+G(d,p)) was used for all calculations. For the sake of accuracy, the single point energies were calculated using 6-311++G(3df,2p) basis set. The implicit solvation effects were included using the CPCM solvation model with standard parameters of chloroform ($CHCl_3$) and dimethyl sulfoxide (DMSO).[15, 16] This method [M062X/6-311++G(3df,2p)+CPCM(solvent)//M062X/6-31+G(d,p)] showed reliable results in the previous study.[17] The quantitative charge distributions are calculated using Hirshfeld method at 6-31+G(d,p) level.[18] This method showed the lowest basis set dependency for population analysis.[19]

Table S1. Crystallographic data for compounds **1** – **8**, and $[MeSO_3]^-$ adducts with **4** and **6** – **8**.

	1	**2**	**3**	**4**
CCDC Number	2104071	2104070	2104074	2104072
Chemical formula	$C_{76}H_{80}O_8$ $\cdot 3(C_2H_3N)$	$C_{76}H_{76}F_4O_8$ $\cdot 3(C_2H_3N)$	$C_{76}H_{76}F_4O_8$ $\cdot 3(C_2H_3N)$	$C_{76}H_{72}F_8O_8$ $\cdot 2(C_2H_3N)$ $\cdot 2(CH_2Cl_2)$
Formula weight	1244.56	1316.52	1316.52	1517.29
Space group	*P–1*	*P–1*	*P–1*	*C2/c*
***a* (Å)**	11.9327(3)	11.969 (4)	11.9504(3)	33.1351(6)
***b* (Å)**	12.8148(3)	12.961(3)	12.9188(3)	12.8854(2)
***c* (Å)**	24.0608(5)	24.112(4)	24.0391(7)	23.6066(7)
***α* (deg)**	100.145(1)	101.319(7)	99.832(1)	90
***β* (deg)**	96.381(1)	91.758(13)	96.529(1)	131.764(1)
***γ* (deg)**	102.831(1)	101.826(14)	101.954(1	90
***V* (Å^3)**	3487.76(14)	3580.1(14)	3534.42(16)	7517.9(3)
Z	2	2	2	4
μ (mm^{-1})	0.60	0.69	0.70	2.08
T (K)	220	150	220	230
***R*1[a] (*wR*2[b])**	0.154 (0.505)	0.119 (0.382)	0.098 (0.282)	0.133 (0.448)
Reflections	10814	12398	10927	7100
Radiation type	Cu *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*

[a]$R1 = [\Sigma w(F_o - F_c)^2/\Sigma wF_o^2]^{1/2}$; [b]$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}]$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2,0) + 2(F_c^2)]/3$

Table S1. *Continued…*

	5	**6**	**7**	**8**
CCDC Number	2104075	2104076	2104073	2104069
Chemical formula	$C_{76}H_{68}F_{12}O_8$ $\cdot 4(C_2H_3N)$	$C_{75}H_{66}F_{12}O_8$ $\cdot C_{76}H_{68}F_{12}O_8$ $\cdot 2(C_2H_3N)$	$C_{68}H_{48}F_{16}O_8$	$C_{84}H_{72}F_{24}O_8$ $\cdot 3(C_2H_3N)$
Formula weight	1501.52	2742.68	1297.06	1788.11
Space group	*P–1*	*P2₁/c*	*Fddd*	*P2₁/c*
***a* (Å)**	12.0029(7)	22.7987(9)	28.0557(13)	21.8730(5)
***b* (Å)**	12.9090(7)	33.3050(13)	31.8586(13)	15.4168(3)
***c* (Å)**	25.4812(14)	21.4220(8)	36.4490(12)	27.7277(6)
***α* (deg)**	78.324(3)	90	90	90
***β* (deg)**	77.909(3)	94.928(2)	90	113.23
***γ* (deg)**	79.550(3)	90	90	90
***V* (Å^3)**	3740.7(4)	16205.8(11)	32579(2)	8592.1(3)
Z	2	4	16	4
μ (mm^{-1})	0.89	0.77	0.81	1.07
T (K)	210	200	220	210
***R*1[a] (*wR*2[b])**	0.160 (0.495)	0.207 (0.575)	0.252 (0.658)	0.188 (0.489)
Reflections	11581	25677	5085	8191
Radiation type	Cu *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*

[a]$R1 = [\Sigma w(F_o - F_c)^2/\Sigma wF_o^2]^{1/2}$; [b]$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}]$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2,0) + 2(F_c^2)]/3$

Table S1. *Continued…*

	[*n*-Bu$_4$N][MeSO$_3$@**4**]	[*n*-Bu$_4$N][MeSO$_3$@**6**]	[*n*-Bu$_4$N][MeSO$_3$@**7**]	[*n*-Bu$_4$N][MeSO$_3$@**8**]
CCDC Number	2104080	2104078	2104077	2104079
Chemical formula	$CH_3SO_3 \cdot C_{75}H_{70}F_8O_8 \cdot C_2H_3N \cdot C_{16}H_{36}N$	$CH_3SO_3 \cdot C_{76}H_{68}F_{12}O_8 \cdot C_{16}H_{36}N$	$CH_3SO_3 \cdot C_{82.11}H_{77.75}F_{16}N_{0.38}O_8 \cdot C_2H_3N \cdot 0.62(C_{16}H_{36}N)$	$2(CH_3SO_3 \cdot C_{84}H_{72}F_{24}O_8) \cdot C_{15}H_{34}N \cdot C_{12}H_{19}N$
Formula weight	1629.91	1674.85	1787.87	3926.72
Space group	*P2$_1$2$_1$2$_1$*	*P2$_1$/n*	*P2$_1$*	*P-1*
***a* (Å)**	23.0191(11)	12.5311(2)	12.7581(10)	18.7373(19)
***b* (Å)**	22.9578(11)	20.5937(3)	22.867(2)	23.963(2)
***c* (Å)**	32.8882(19)	32.9760(5)	16.3241(14)	25.256(3)
***α* (deg)**	90	90	90	82.849(5)
***β* (deg)**	90	94.627(1)	94.056(6)	74.062(6)
***γ* (deg)**	90	90	90	78.107(5)
***V* (Å^3)**	17380.4(15)	8482.1(2)	4750.5(7)	10641.9(19)
Z	8	4	2	2
μ (mm^{-1})	0.97	1.08	1.06	1.10
T (K)	150	220	110	110
***R*1[a] (*wR*2[b])**	0.133 (0.379)	0.081 (0.246)	0.174 (0.493)	0.313 (0.668)
Reflections	23869	12068	14968	26546
Radiation type	Cu *Kα*	Cu *Kα*	Cu *Kα*	Cu *Kα*

[a]$R1 = [\Sigma w(F_o - F_c)^2/\Sigma wF_o^2]^{1/2}$; [b]$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma w(F_o^2)^2]^{1/2}]$, $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where $P = [\max(F_o^2,0) + 2(F_c^2)]/3$

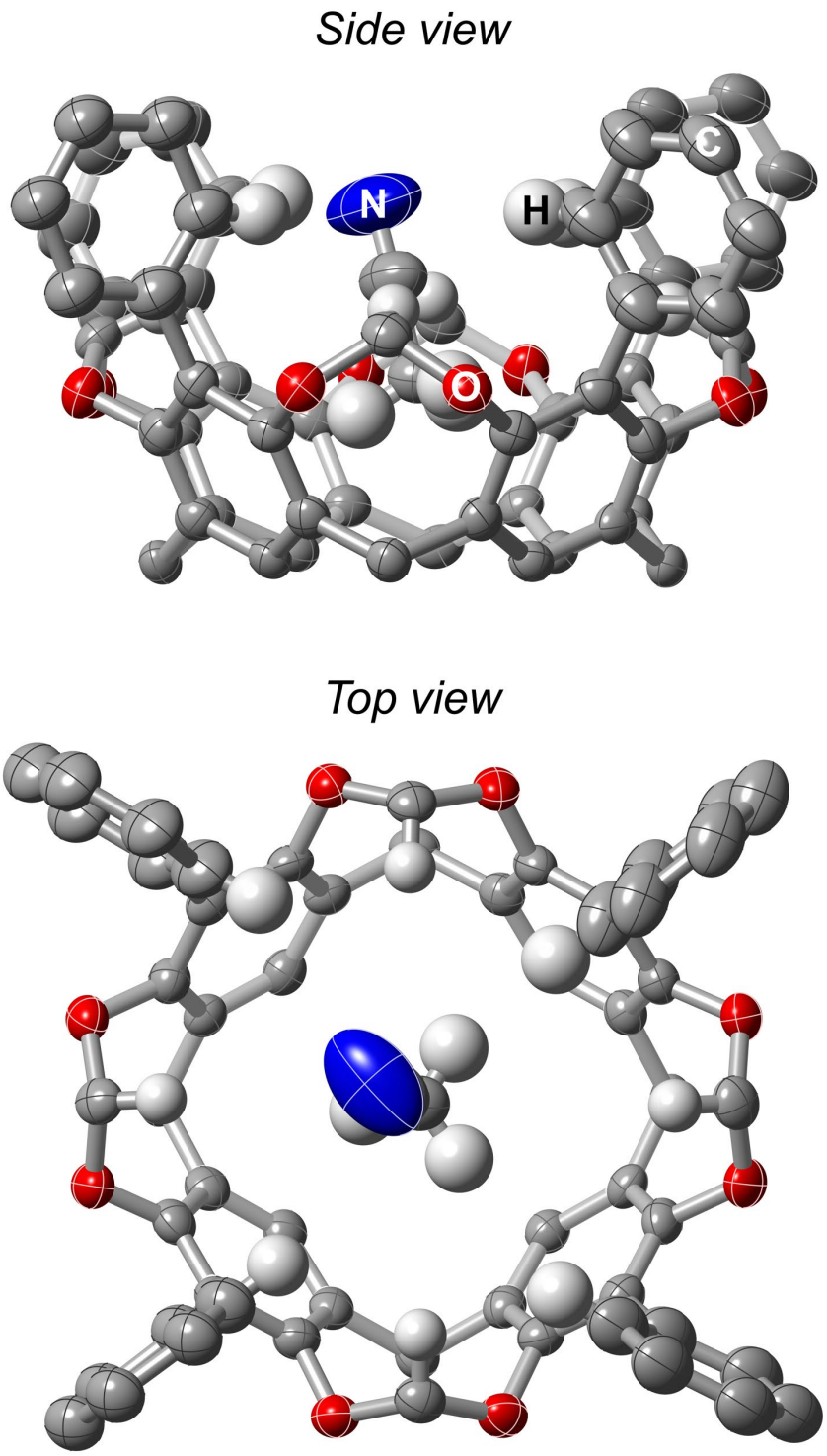


Figure S1. Molecular crystal structure of **1** obtained at 220 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

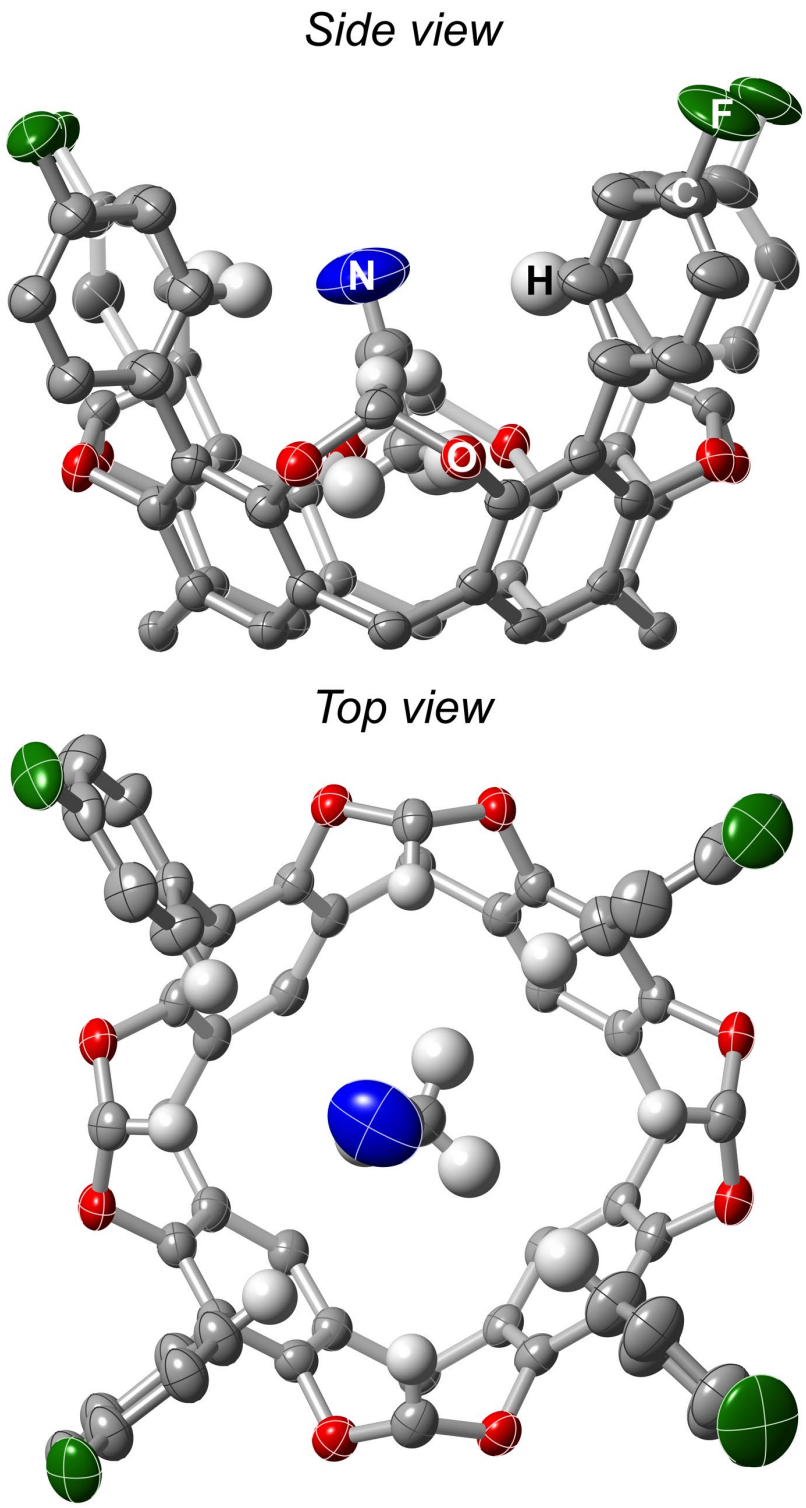


Figure S2. Molecular crystal structure of **2** obtained at 150 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

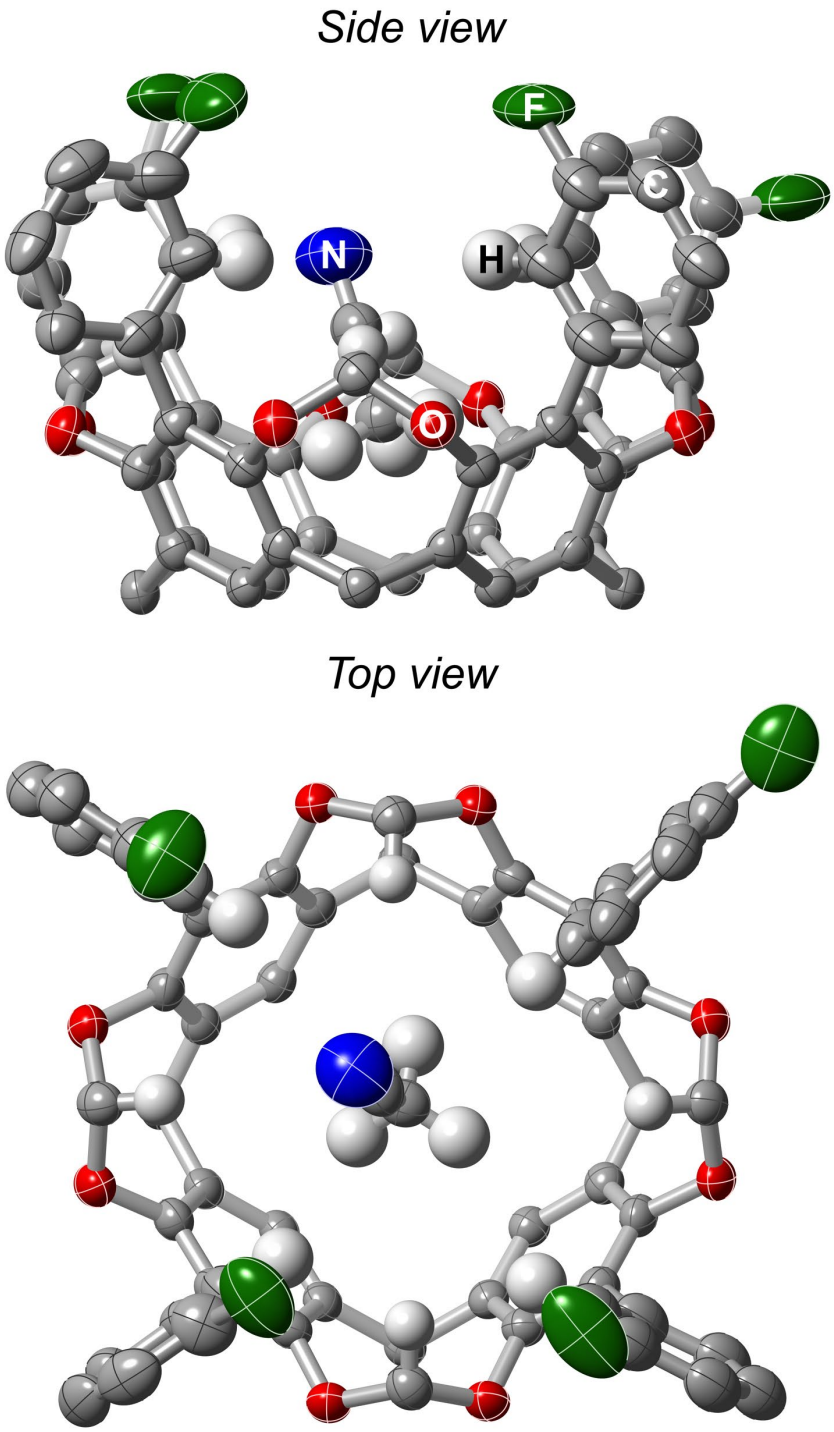


Figure S3. Molecular crystal structure of **3** obtained at 220 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

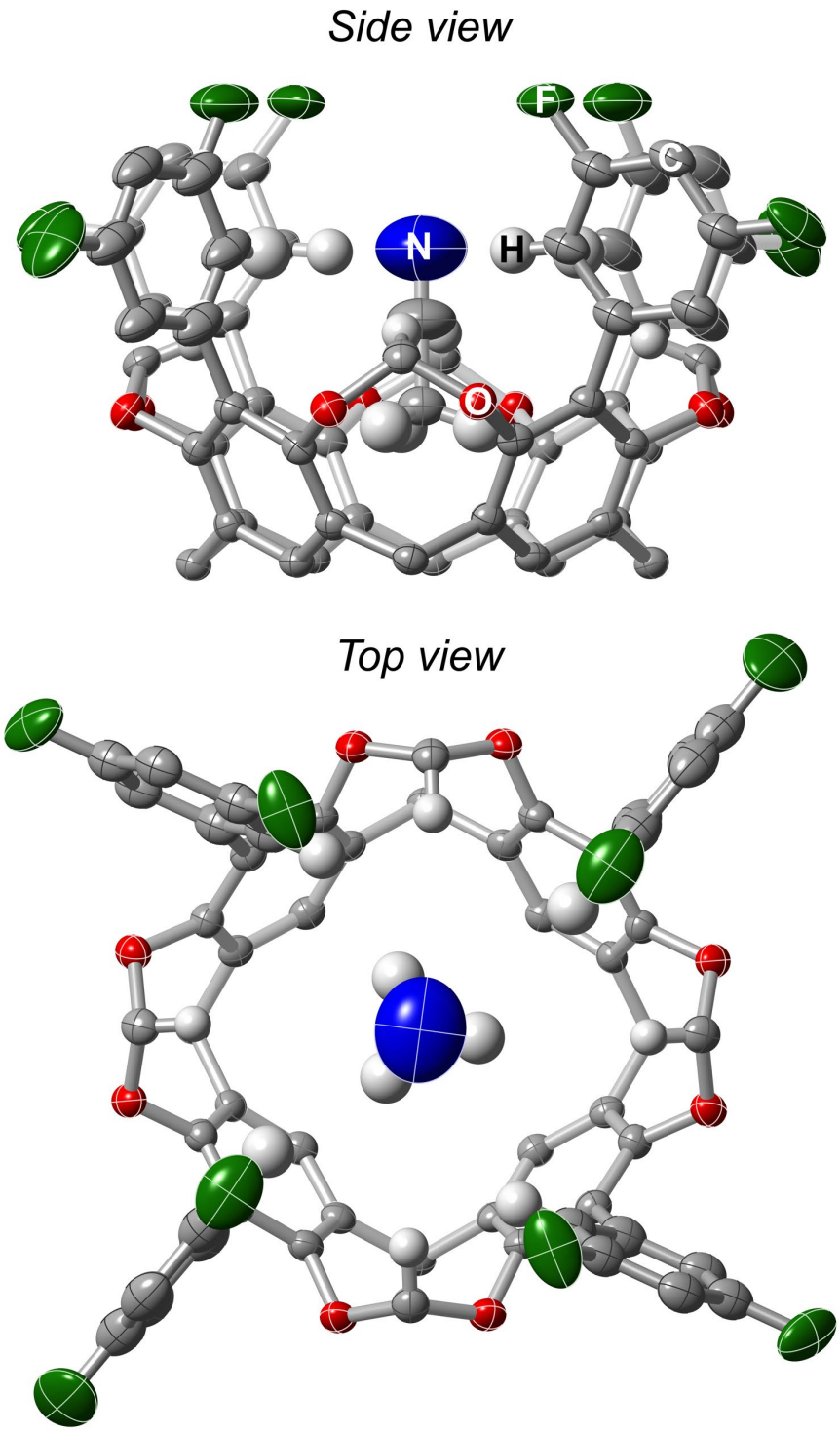


Figure S4. Molecular crystal structure of **4** obtained at 230 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

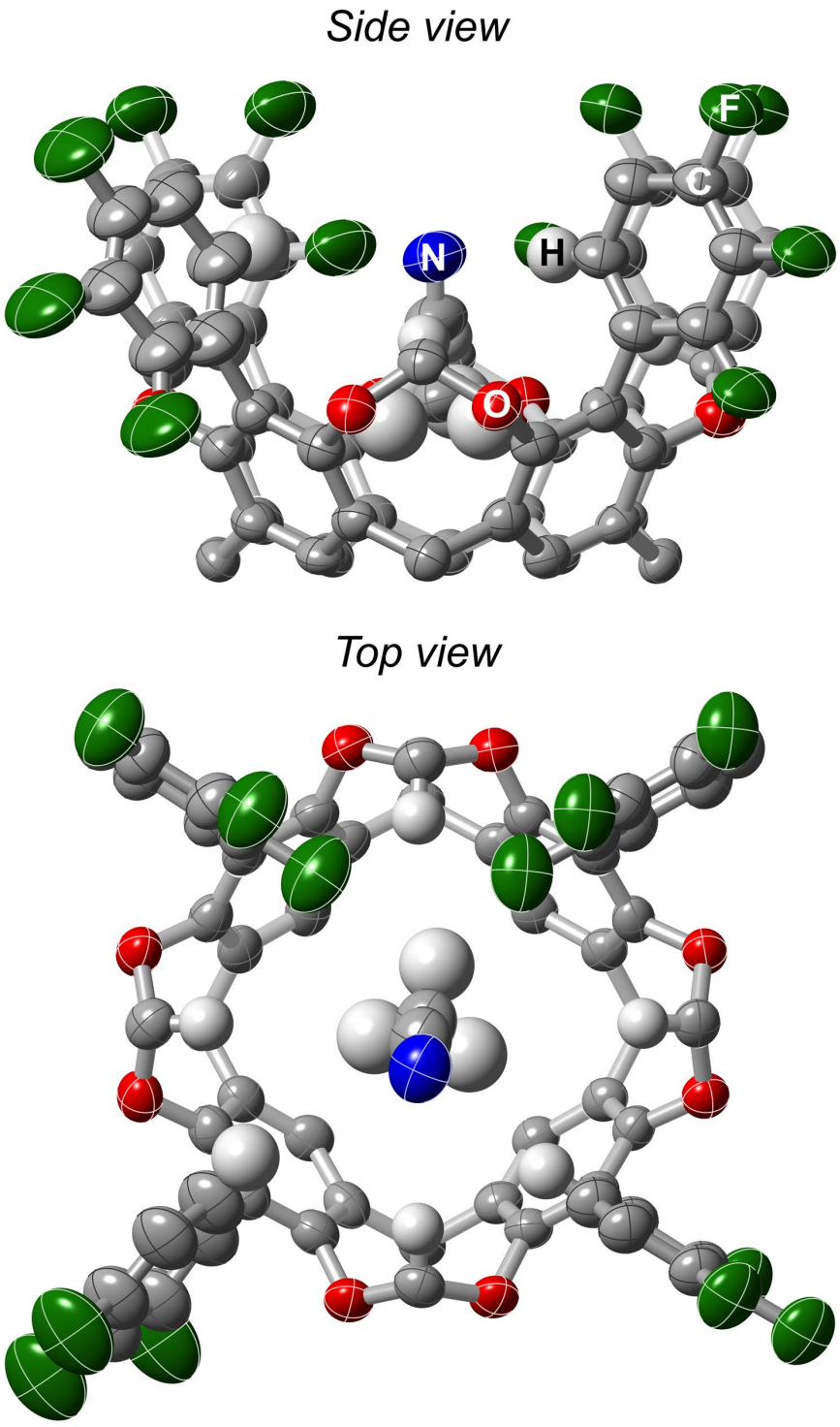


Figure S5. Molecular crystal structure of **5** obtained at 210 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

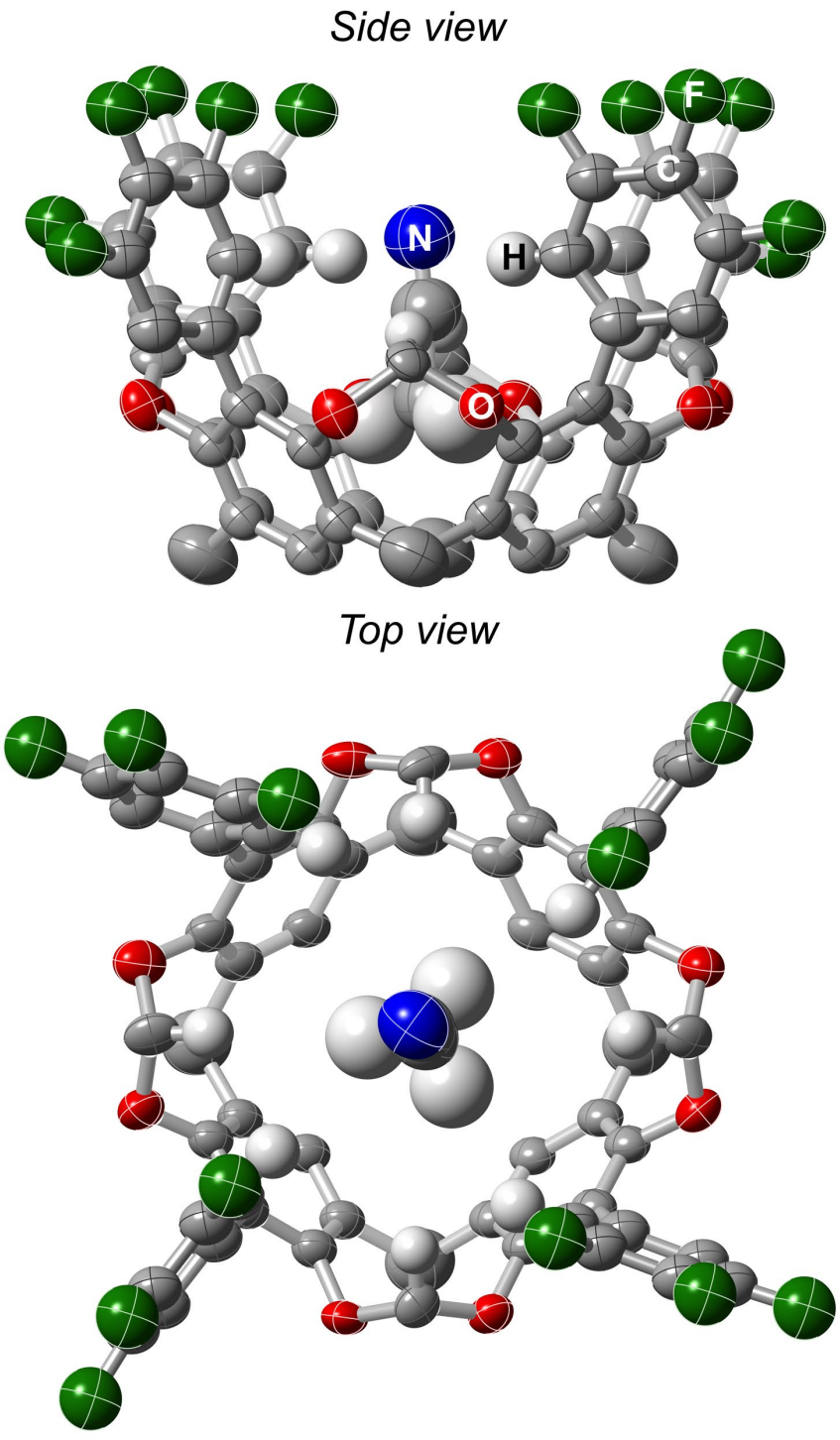


Figure S6. Molecular crystal structure of **6** obtained at 200 K. Thermal ellipsoids are set at 30% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

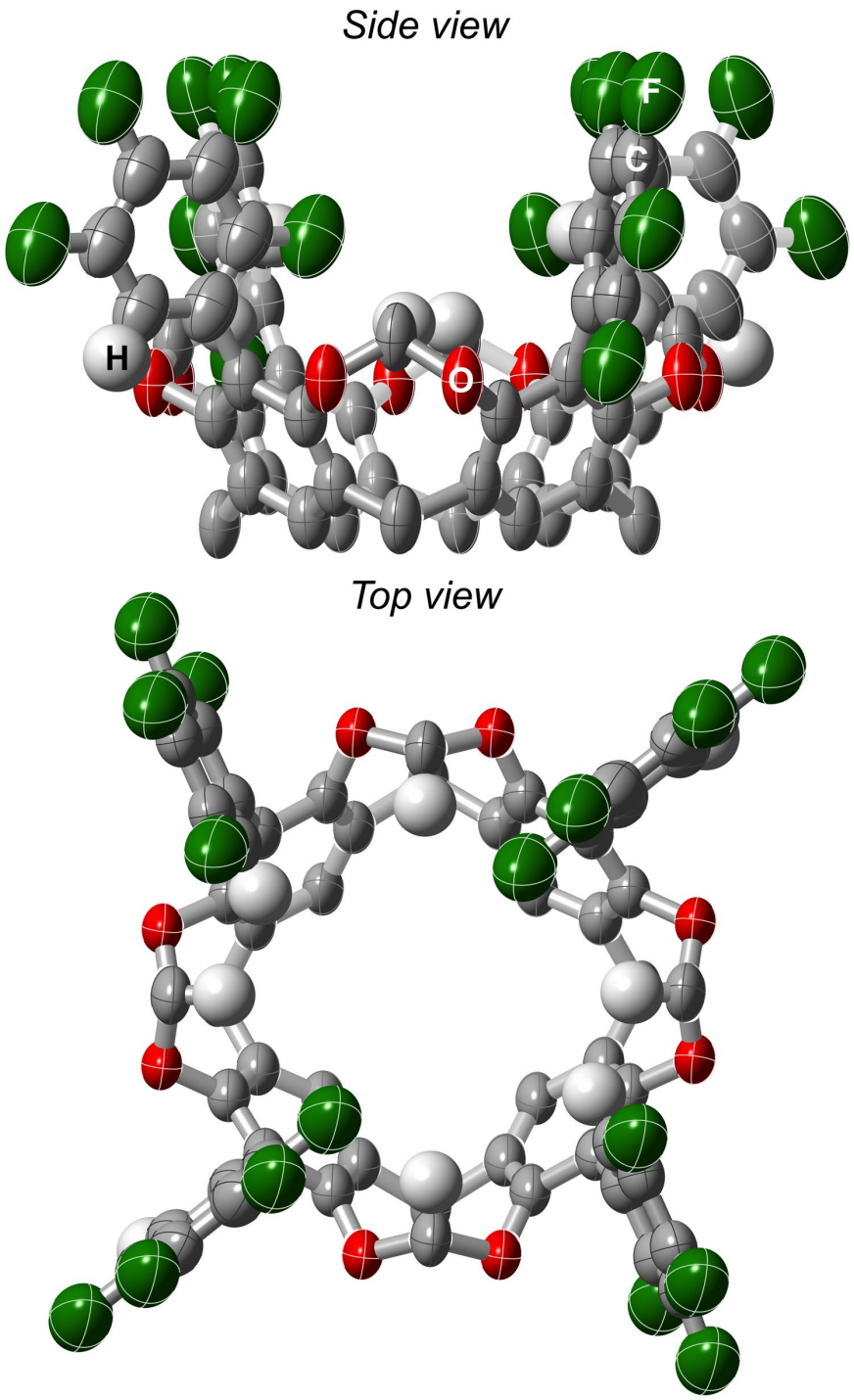


Figure S7. Molecular crystal structure of **7** obtained at 220 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

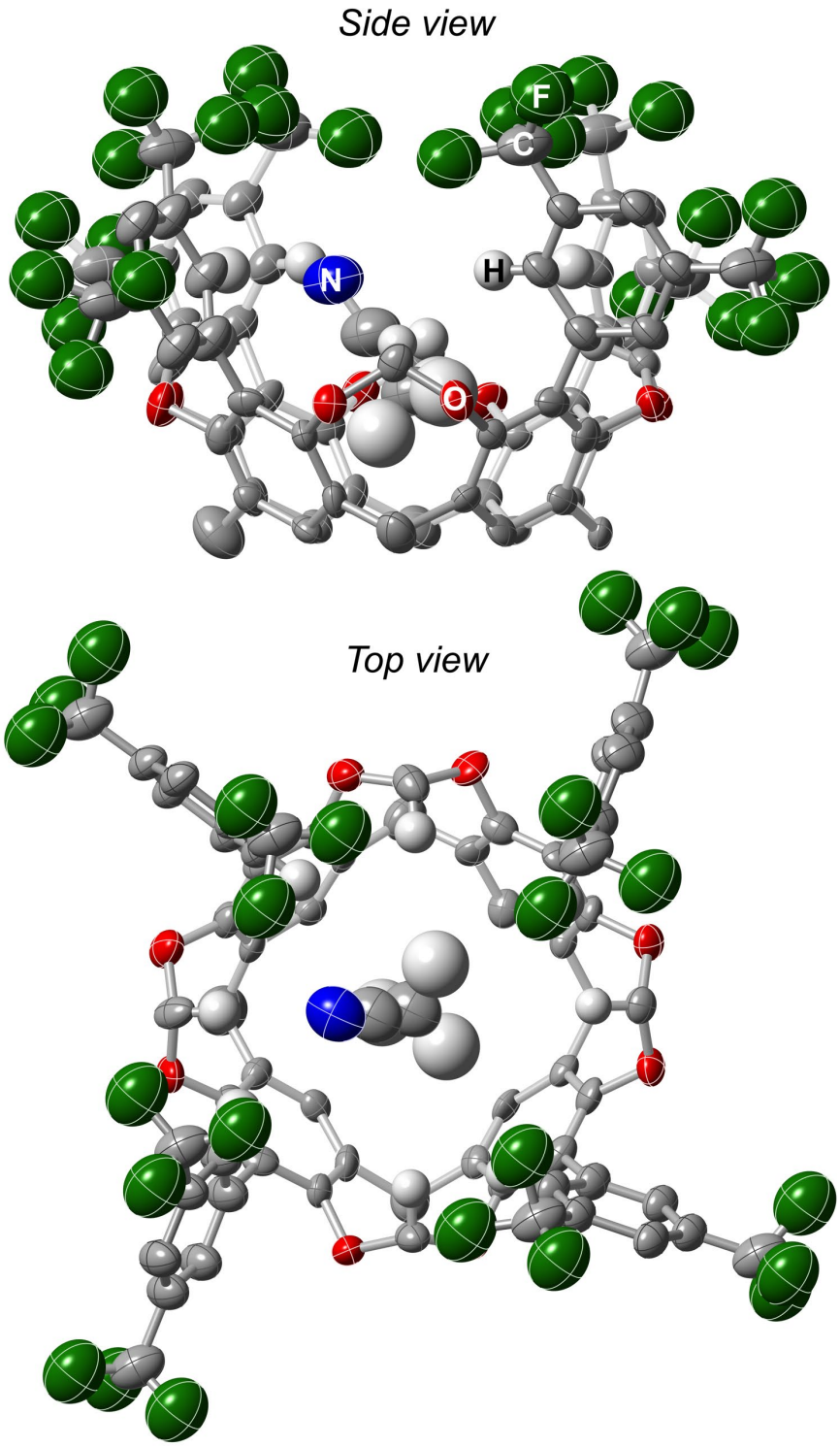
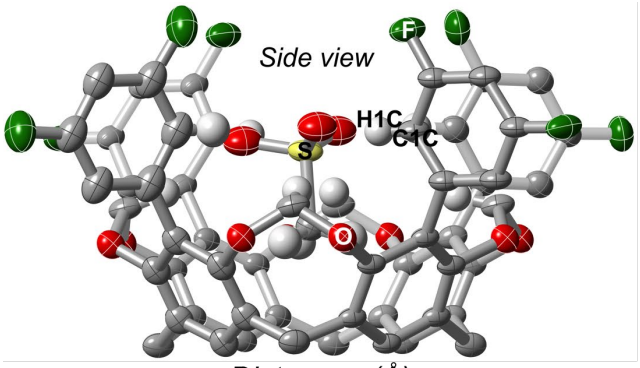
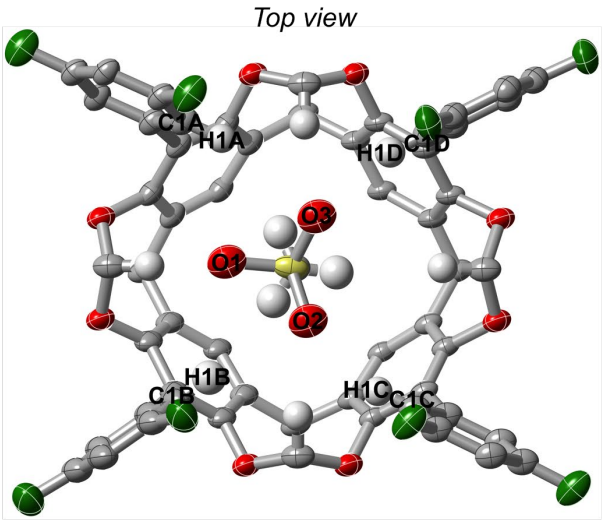


Figure S8. Molecular crystal structure of **8** obtained at 210 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity.

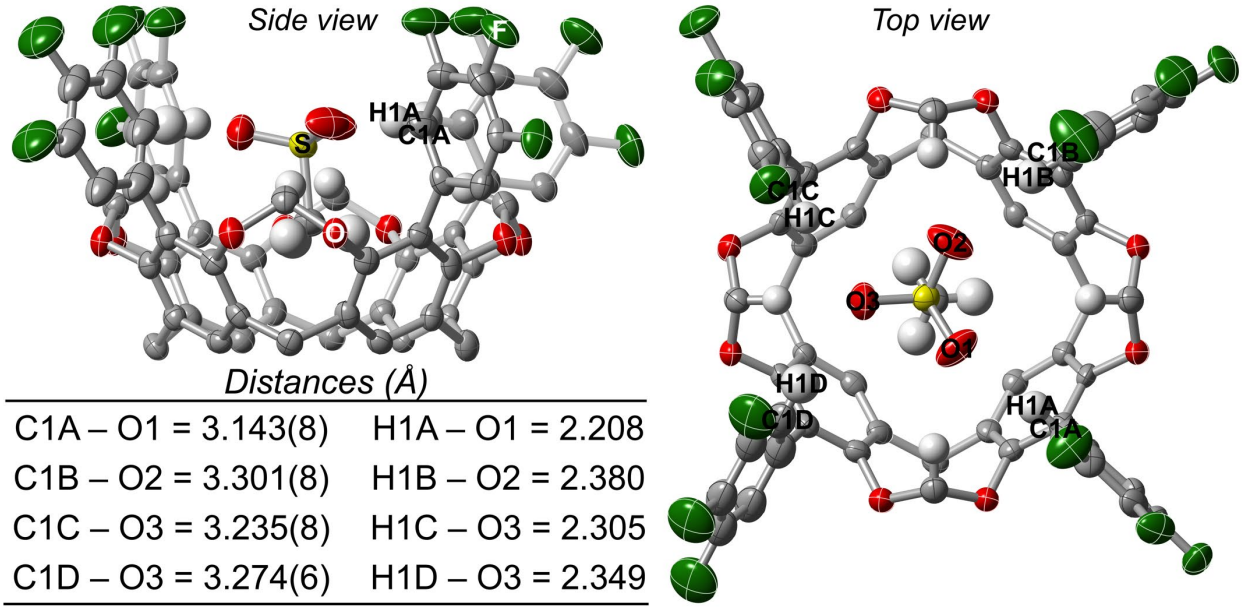




Distances (Å)

C1A – O1 = 3.39(2)	H1A – O1 = 2.86
C1B – O1 = 3.44(2)	H1B – O2 = 2.64
C1C – O2 = 3.20(2)	H1C – O3 = 2.29
C1D – O3 = 3.18(1)	H1D – O3 = 2.25
C1E – O4 = 3.24(2)	H1E – O4 = 2.36
C1F – O5 = 3.44(2)	H1F – O5 = 2.77
C1G – O5 = 3.43(2)	H1G – O5 = 2.87
C1H – O6 = 3.15(1)	H1H – O6 = 2.20

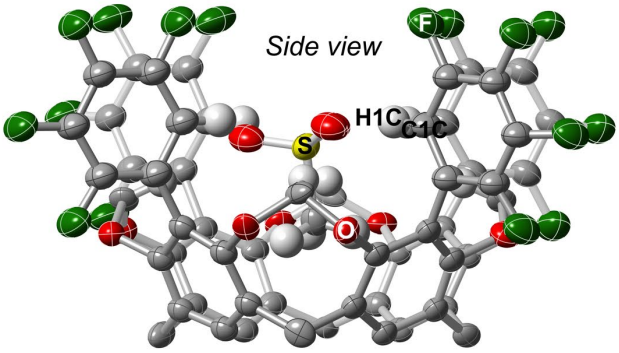
Figure S9. Molecular crystal structure of $[MeSO_3 \subset \mathbf{4}]^-$ obtained at 150 K. Thermal ellipsoids are set at 30% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity. The asymmetric unit contains two unique $[MeSO_3 \subset \mathbf{4}]^-$ moieties. Distances: d_{avg} (C–O) = 3.31(4) Å, and d_{avg} (H–O) = 2.5(1) Å.

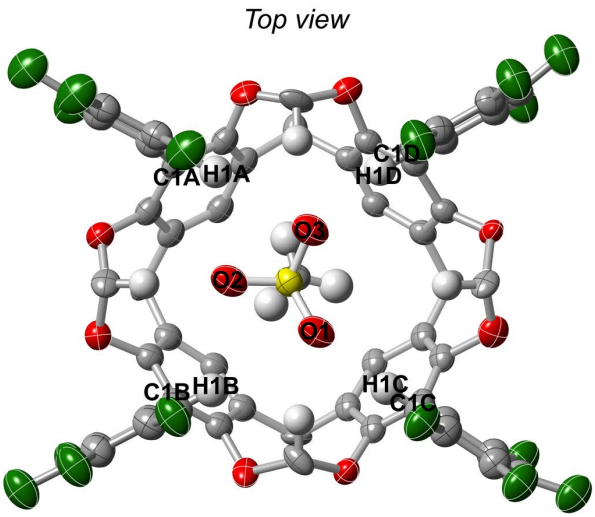


Distances (Å)

C1A – O1 = 3.143(8)	H1A – O1 = 2.208
C1B – O2 = 3.301(8)	H1B – O2 = 2.380
C1C – O3 = 3.235(8)	H1C – O3 = 2.305
C1D – O3 = 3.274(6)	H1D – O3 = 2.349

Figure S10. Molecular crystal structure of $[MeSO_3 \subset \mathbf{6}]^-$ obtained at 220 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity. Distances: d_{avg} (C–O) = 3.24(3) Å, and d_{avg} (H–O) = 2.31(4) Å.

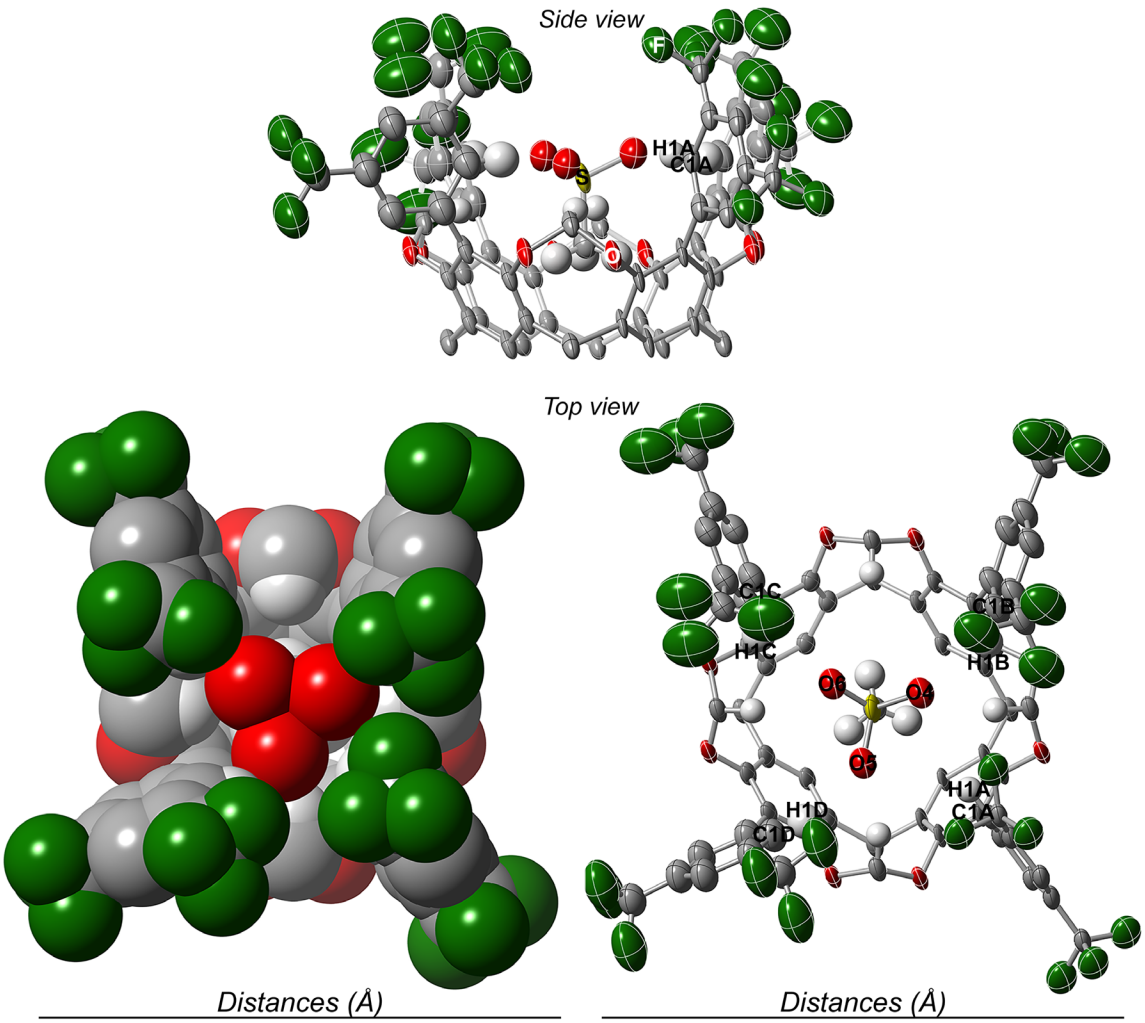




Distances (Å)

C1A – O2 = 3.25(3)	H1A – O2 = 2.61
C1B – O2 = 3.30(3)	H1B – O2 = 2.66
C1C – O1 = 3.08(3)	H1C – O1 = 2.13
C1D – O3 = 3.11(3)	H1D – O3 = 2.18
C1A – O3X = 2.87(5)	H1A – O3X = 1.97
C1B – O1X = 3.14(5)	H1B – O1X = 2.20
C1C – O1X = 3.58(5)	H1C – O1X = 2.63
C1D – O2X = 3.10(4)	H1D – O2X = 2.41

Figure S11. Molecular crystal structure of $[MeSO_3 \subset \mathbf{7}]^-$ obtained at 110 K. Thermal ellipsoids are set at 30% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity. $[MeSO_3]^-$ is disordered around two positions, where the second position is labeled with an "X" at the end of the atom's name. Distances: d_{avg} (C–O) = 3.18(7) Å, and d_{avg} (H–O) = 2.35(9) Å.



Distances (Å)		Distances (Å)	
C1A – O5 = 3.78(4)	H1A – O4 = 2.95	C1E – O1 = 3.23(4)	H1E – O1 = 2.30
C1B – O4 = 3.11(4)	H1B – O4 = 2.29	C1F – O1 = 3.53(4)	H1F – O1 = 2.63
C1C – O6 = 3.21(4)	H1C – O6 = 2.40	C1G – O2 = 3.45(4)	H1G – O2 = 2.95
C1D – O5 = 3.14(3)	H1D – O5 = 2.24	C1H – O3 = 3.13(4)	H1H – O3 = 2.42
C1A – O5M = 3.17(5)	H1A – O5M = 2.24	C1E – O3M = 3.71(4)	H1E – O3M = 2.91
C1B – O5M = 3.71(4)	H1B – O5M = 2.81	C1F – O1M = 3.10(4)	H1F – O1M = 2.27
C1C – O4M = 3.49(5)	H1C – O4M = 2.91	C1G – O2M = 3.06(3)	H1G – O2M = 2.27
C1D – O6M = 3.43(3)	H1D – O6M = 2.76	C1H – O3M = 3.14(3)	H1H – O3M = 2.24

Figure S12. Molecular crystal structure of $[MeSO_3 \subset \mathbf{8}]^-$ obtained at 110 K. Thermal ellipsoids are set at 50% probability level. Hydrogen atoms are omitted for clarity, except those in the binding cavity. The asymmetric unit contains two unique $[MeSO_3 \subset \mathbf{8}]^-$ moieties, and in each of them the anion $[MeSO_3]^-$ is disordered around two positions, where the second position is labeled with an an "M" at the end of the atom's name. Distances: d_{avg} (C–O) = 3.34(6) Å, and d_{avg} (H–O) = 2.54(7) Å. Left top view is the sphere packing model using van der Waals radii.

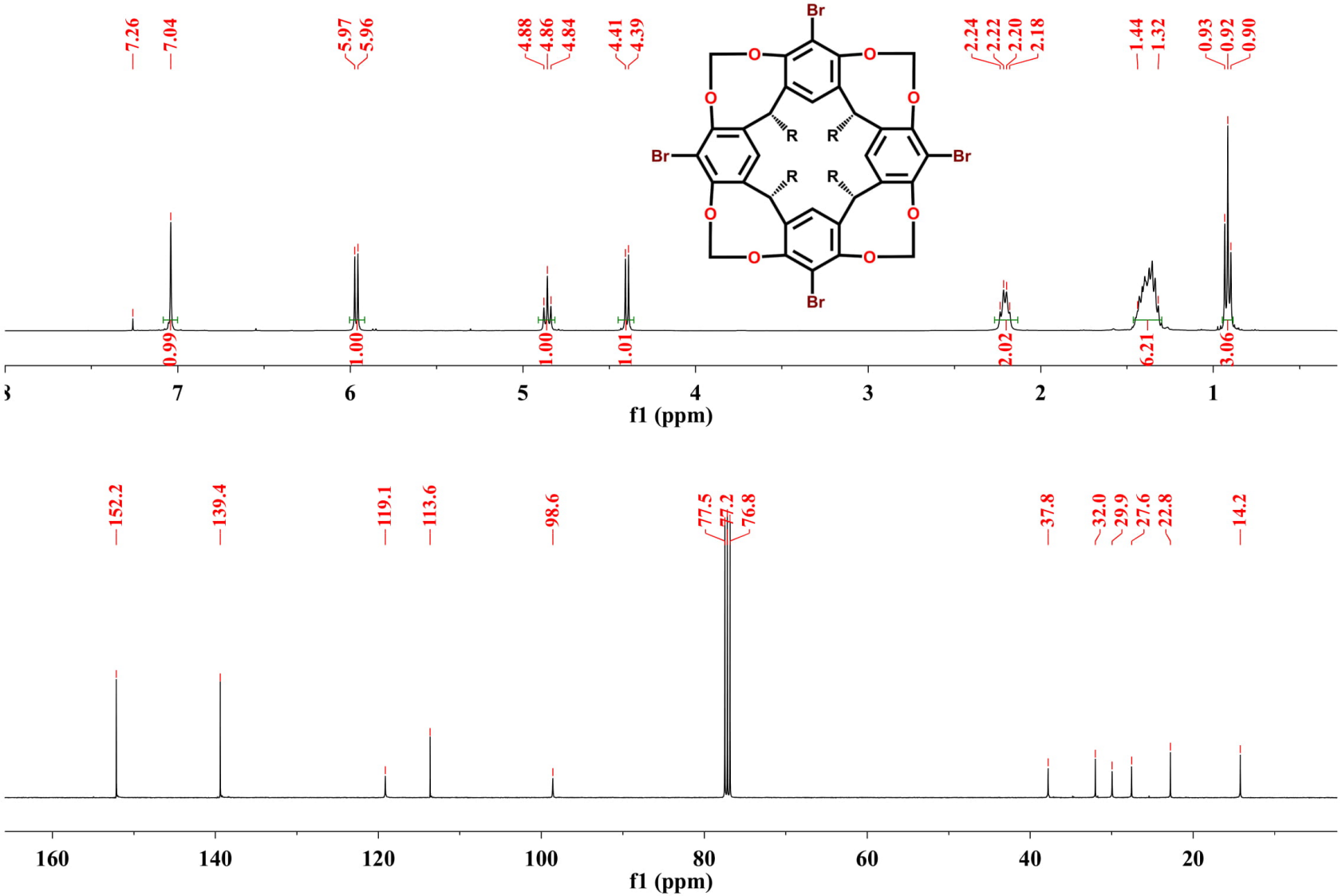


Figure S13. ^{1}H and ^{13}C NMR spectra of **S1**. Data collected in $CDCl_3$ at 20 °C.

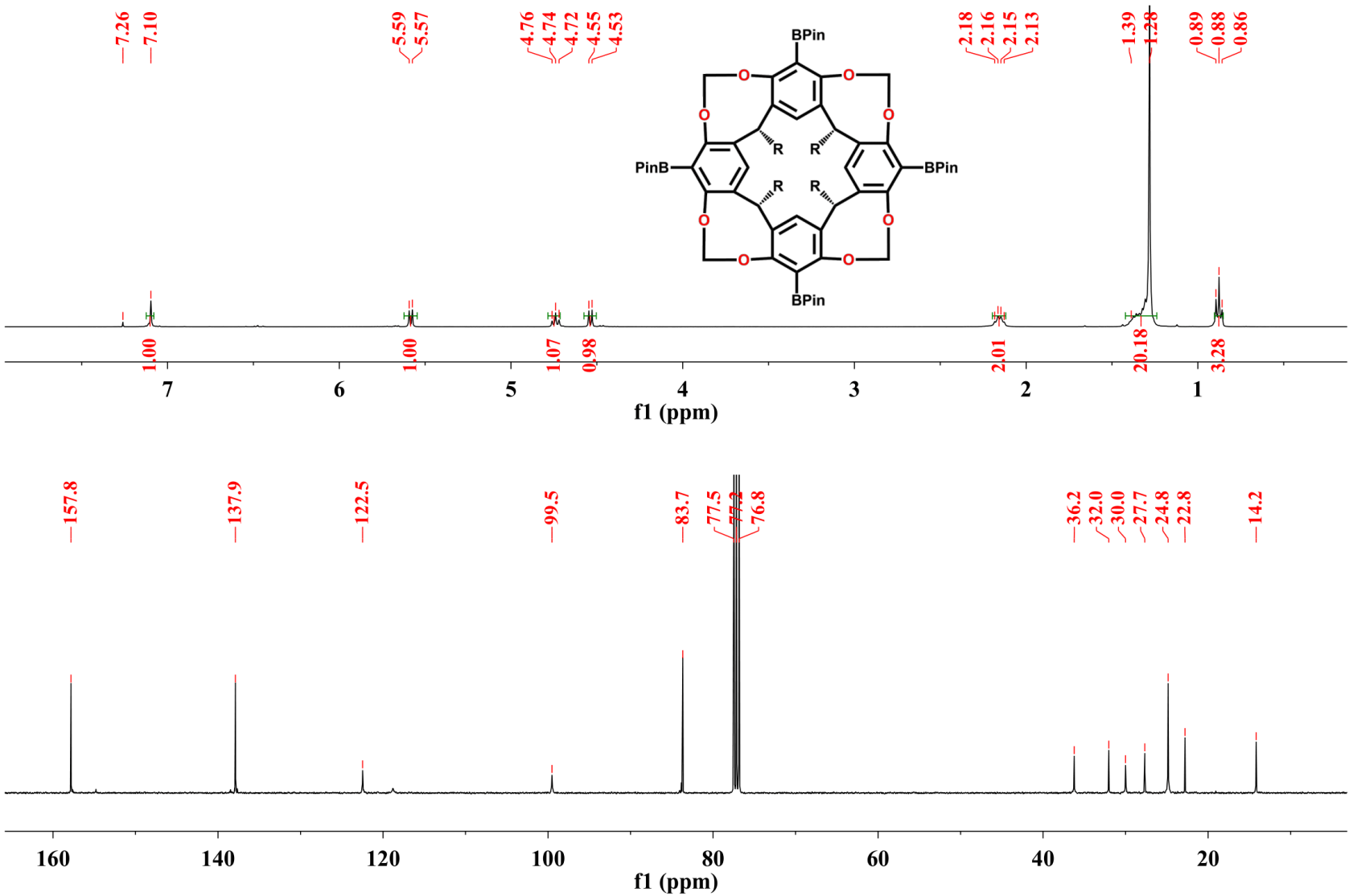


Figure S14. ^{1}H and ^{13}C NMR spectra of **S2**. Data collected in $CDCl_3$ at 20 °C.

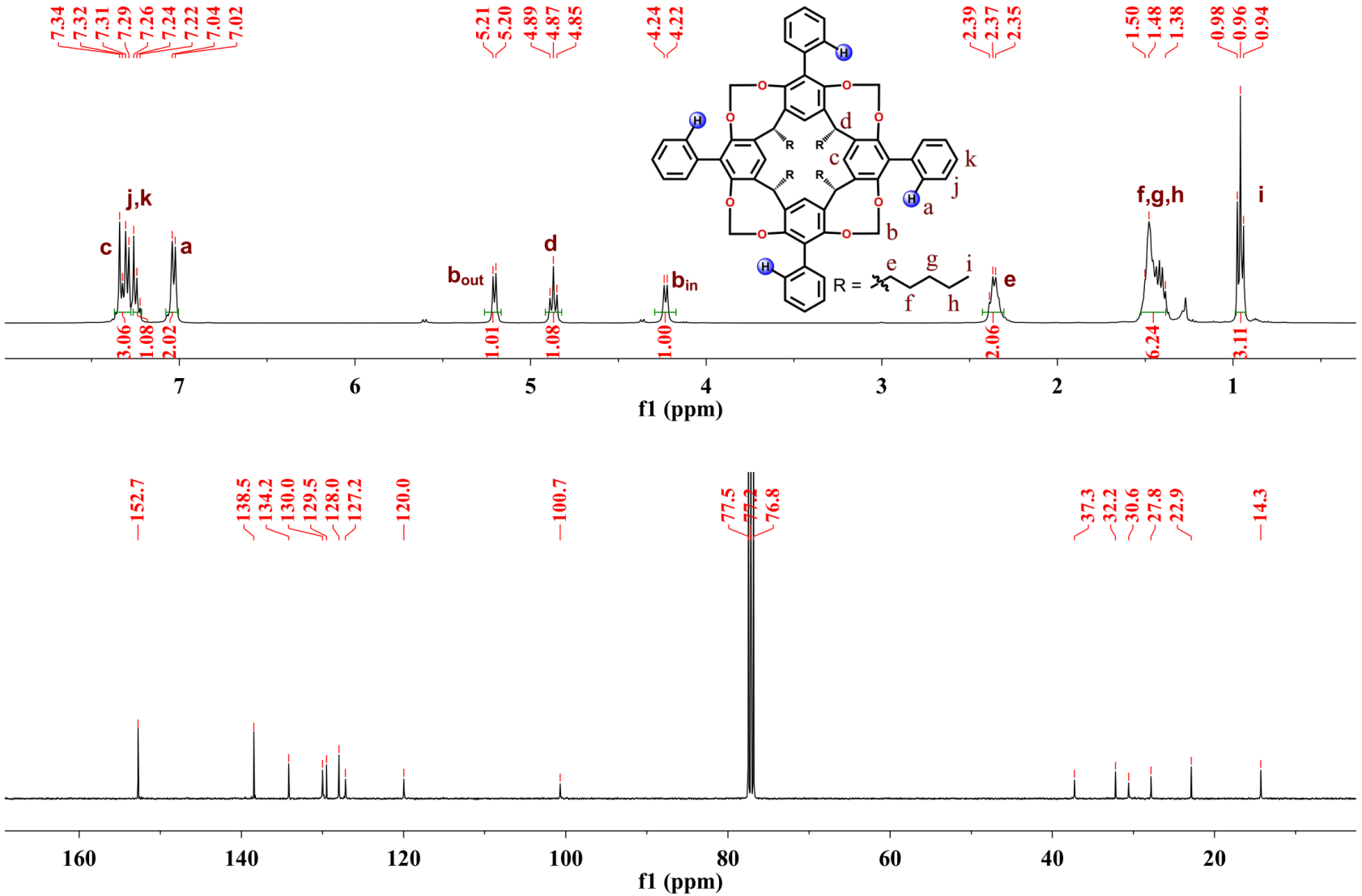


Figure S15. ^{1}H and ^{13}C NMR spectra of **1**. Data collected in $CDCl_3$ at 20 °C.

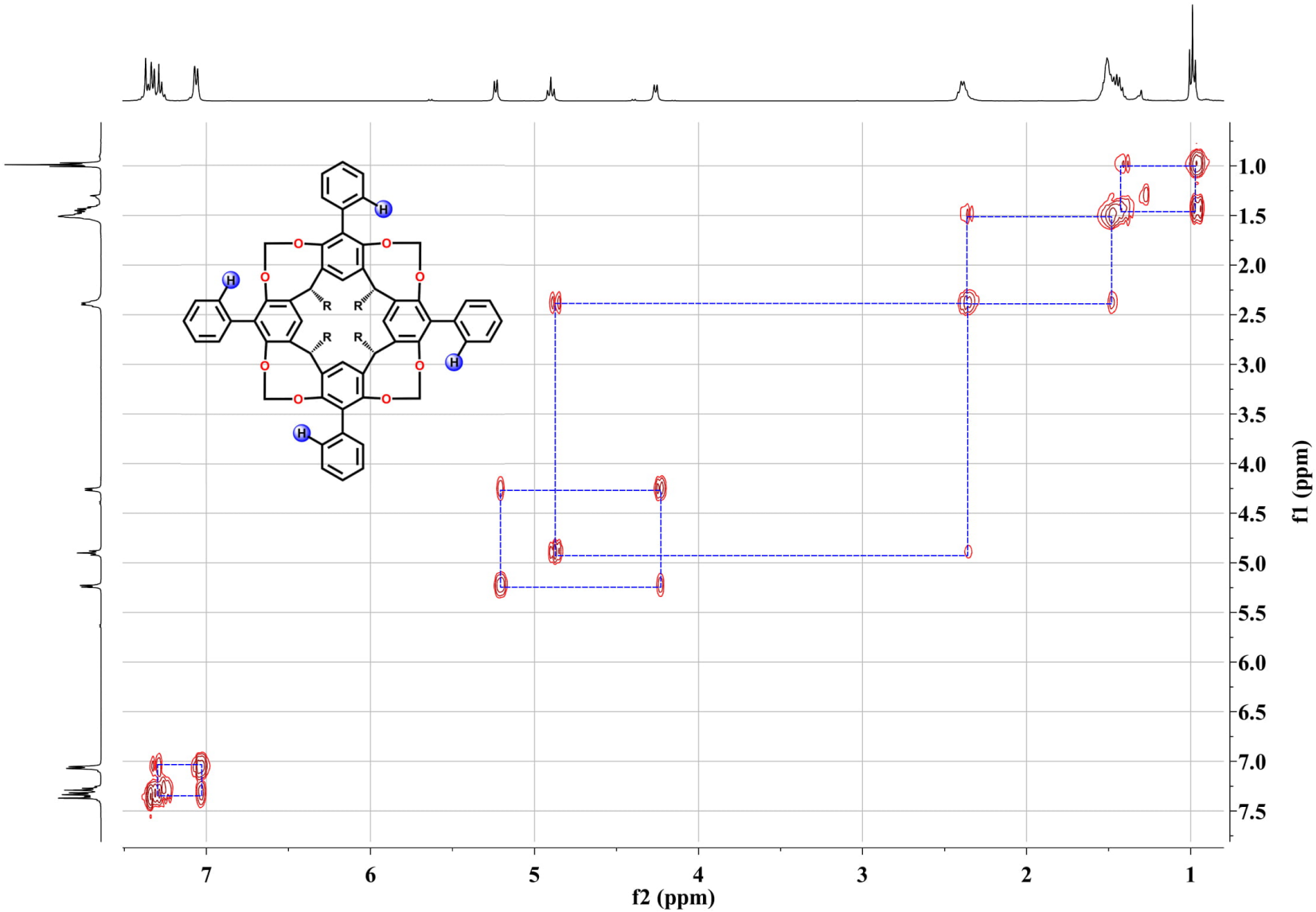


Figure S16. COSY NMR spectrum of **1**. Data collected in $CDCl_3$ at 20 °C.

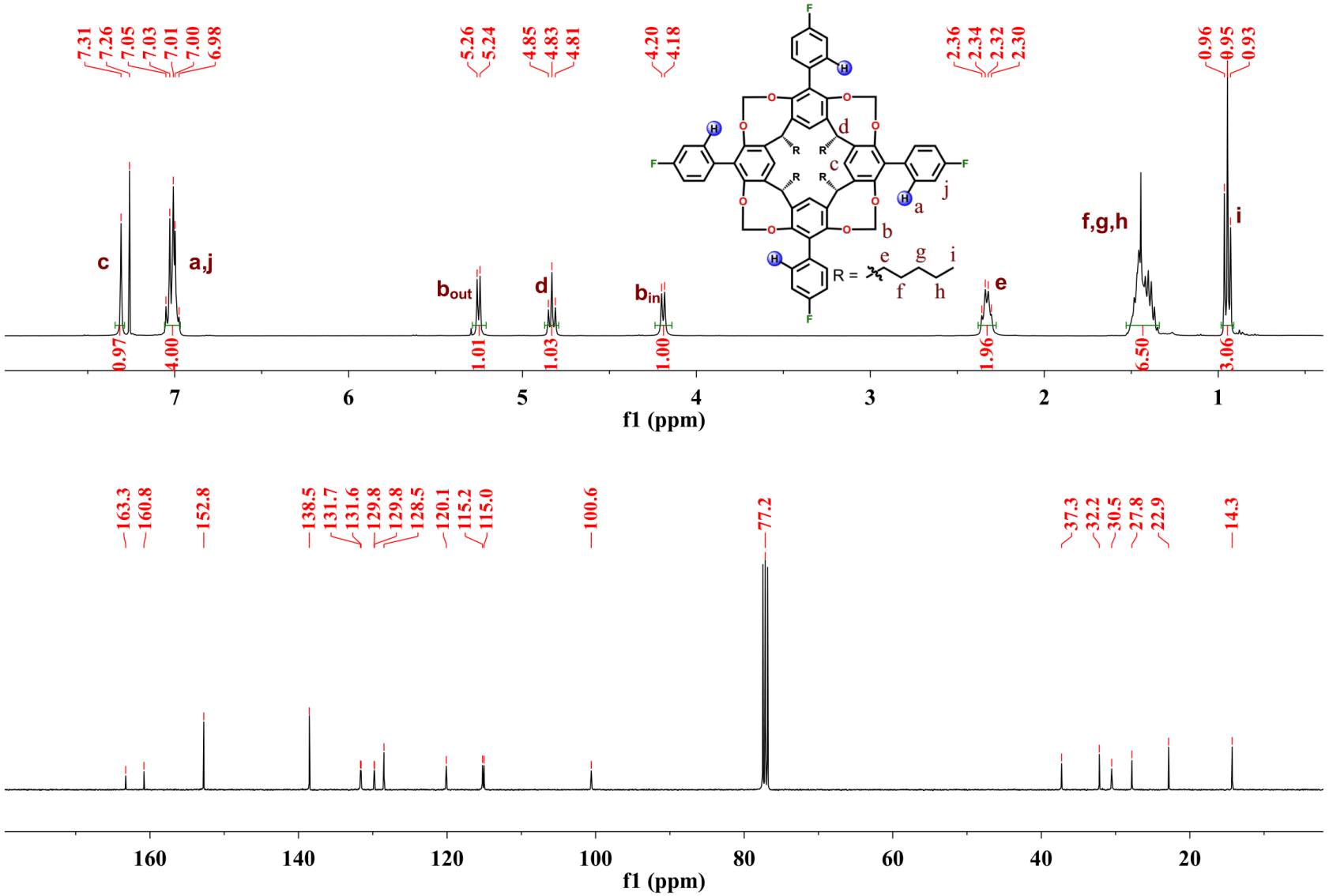


Figure S17. ^{1}H and ^{13}C NMR spectra of **2**. Data collected in $CDCl_3$ at 20 °C.

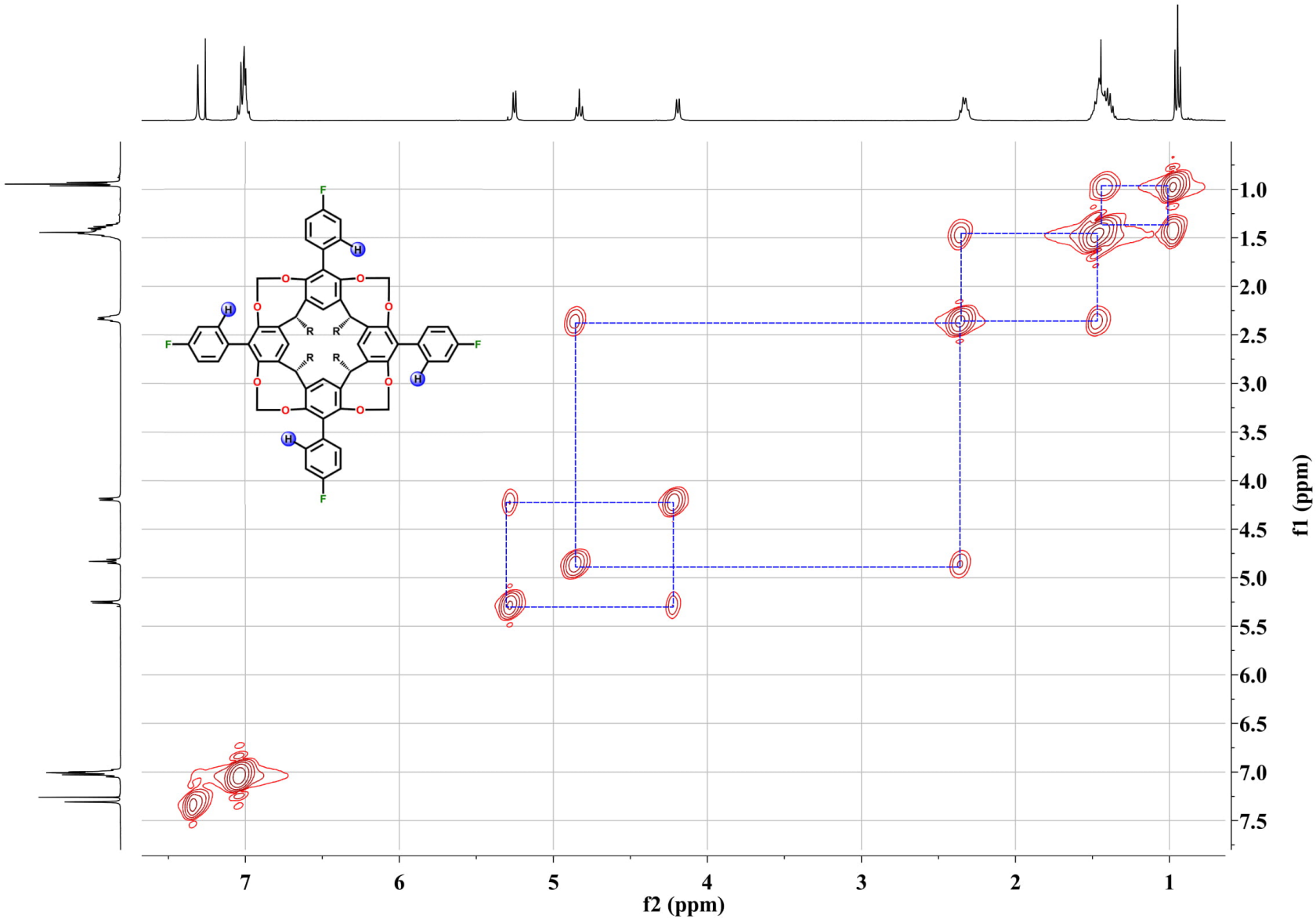


Figure S18. COSY NMR spectrum of **2**. Data collected in $CDCl_3$ at 20 °C.

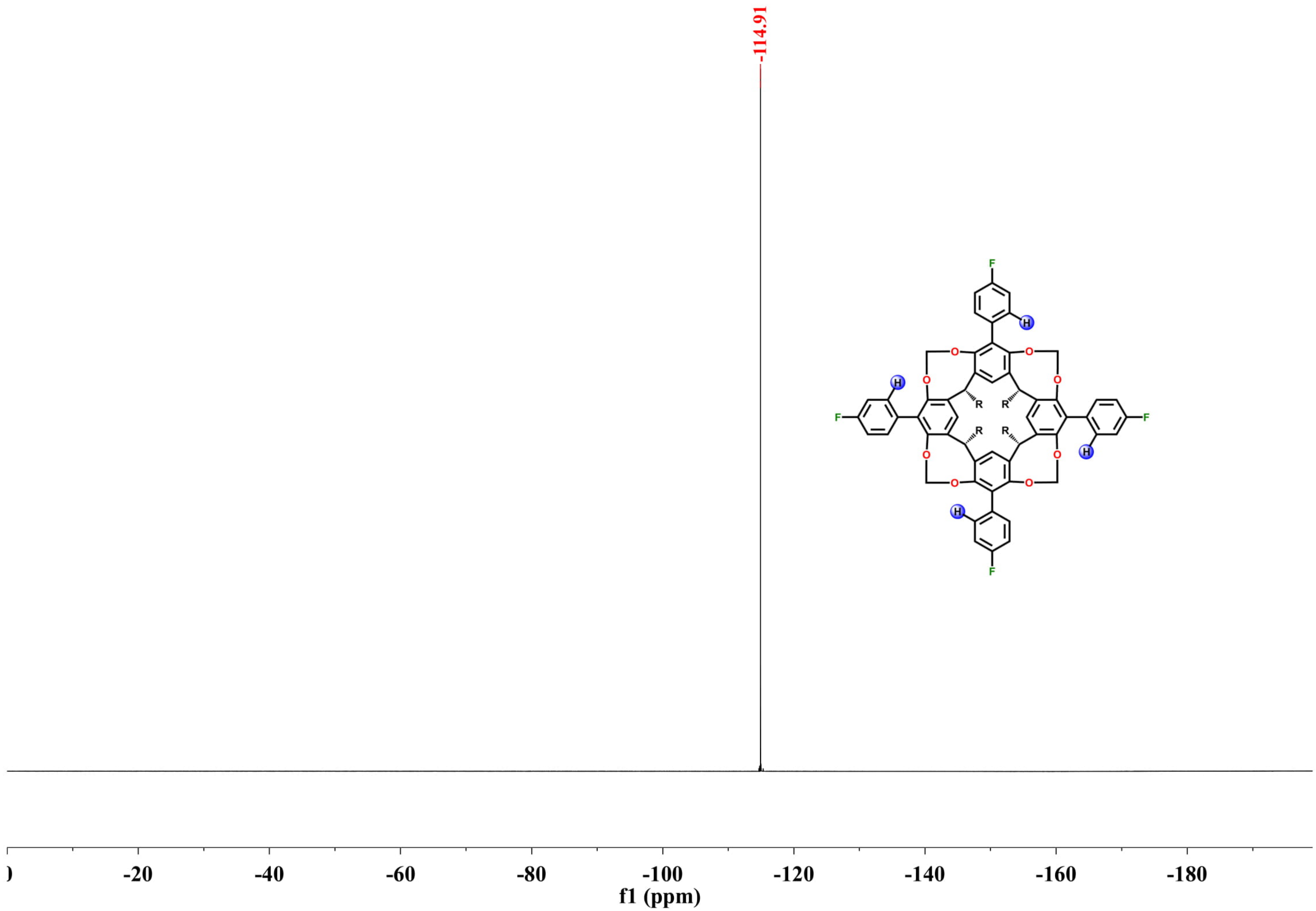


Figure S19. ^{19}F NMR spectrum of **2**. Data collected in $CDCl_3$ at 20 °C.

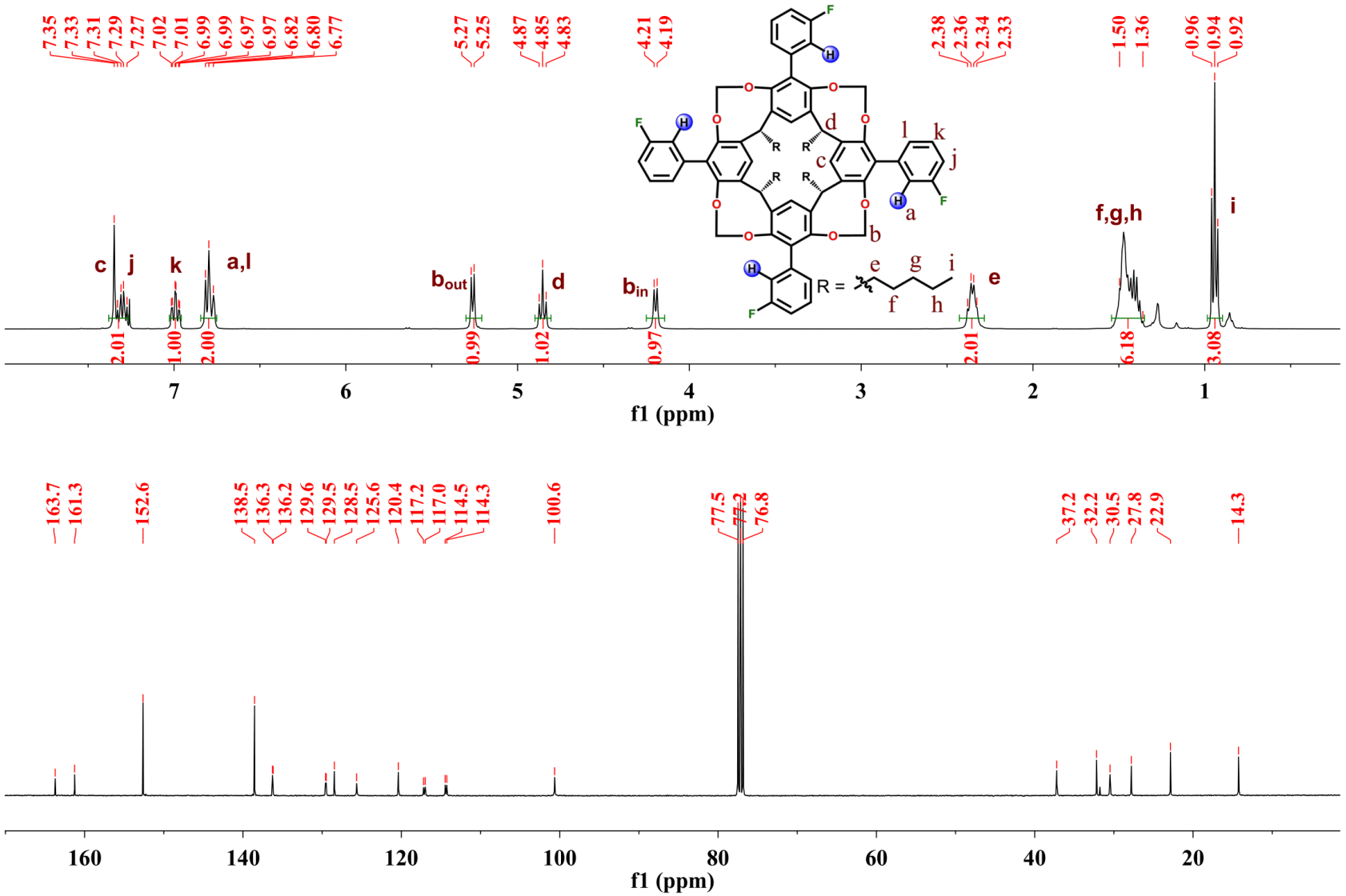


Figure S20. ^{1}H and ^{13}C NMR spectra of **3**. Data collected in $CDCl_3$ at 20 °C.

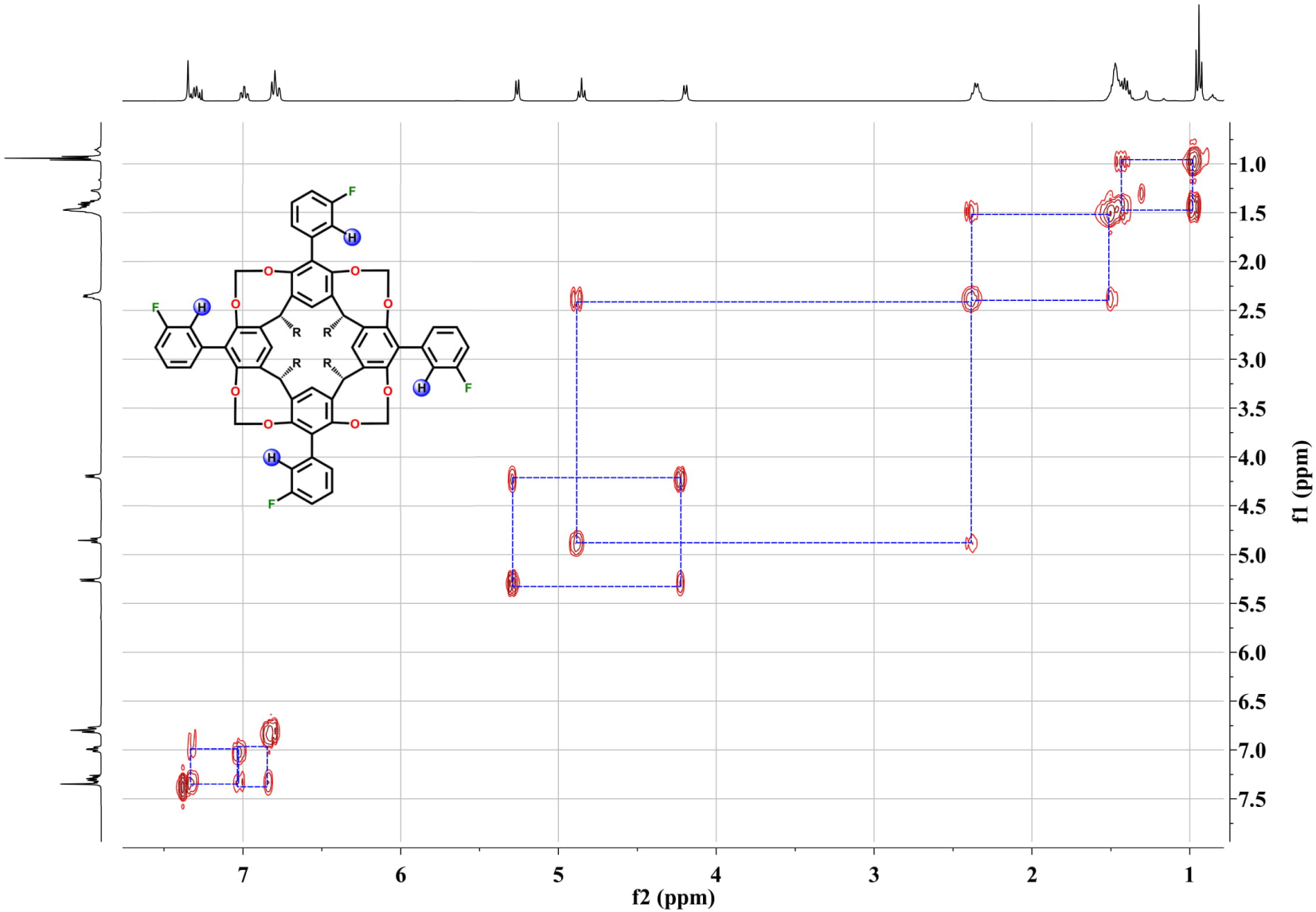


Figure S21. COSY NMR spectrum of **3**. Data collected in $CDCl_3$ at 20 °C.

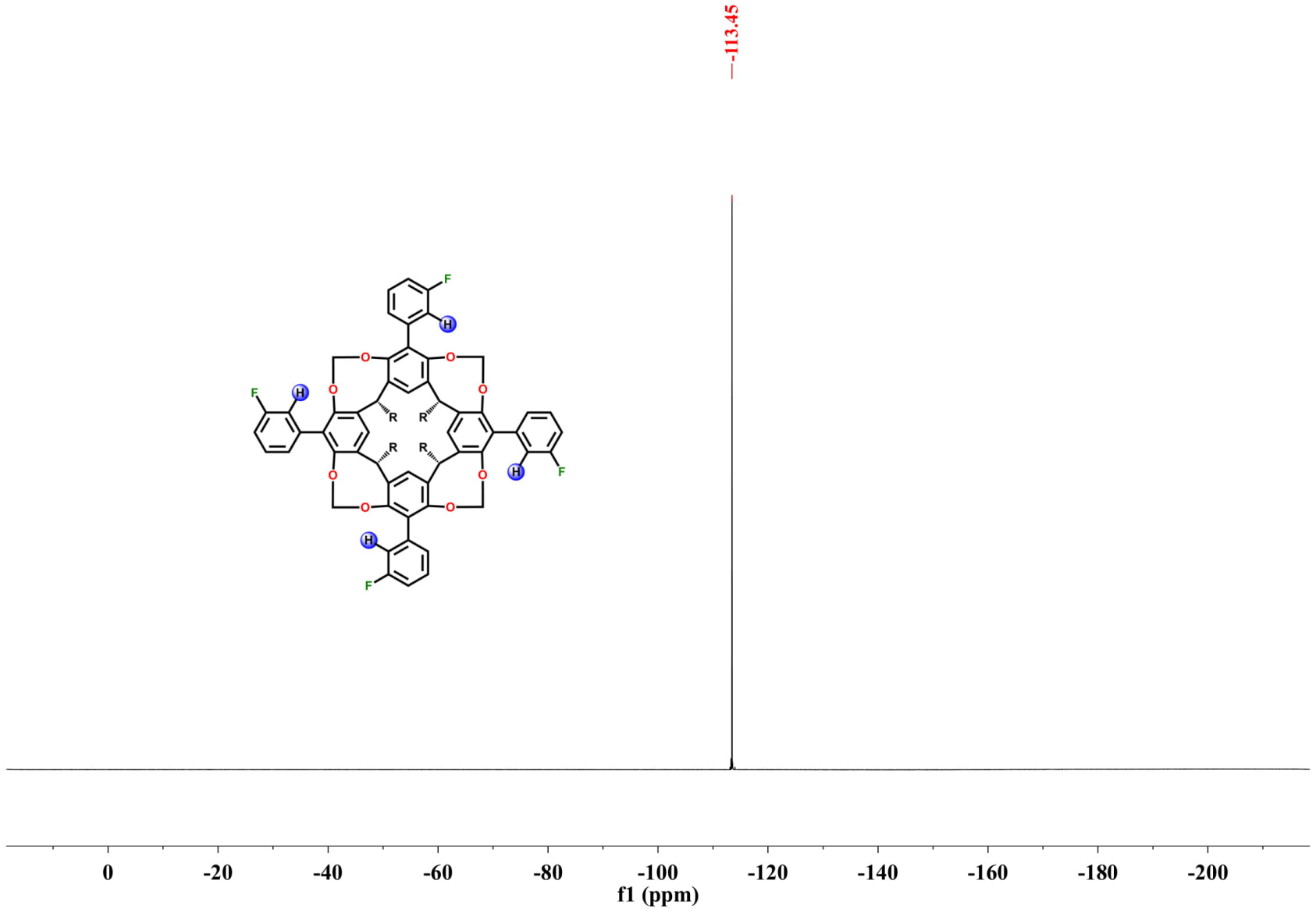


Figure S22. ^{19}F NMR spectrum of **3**. Data collected in $CDCl_3$ at 20 °C.

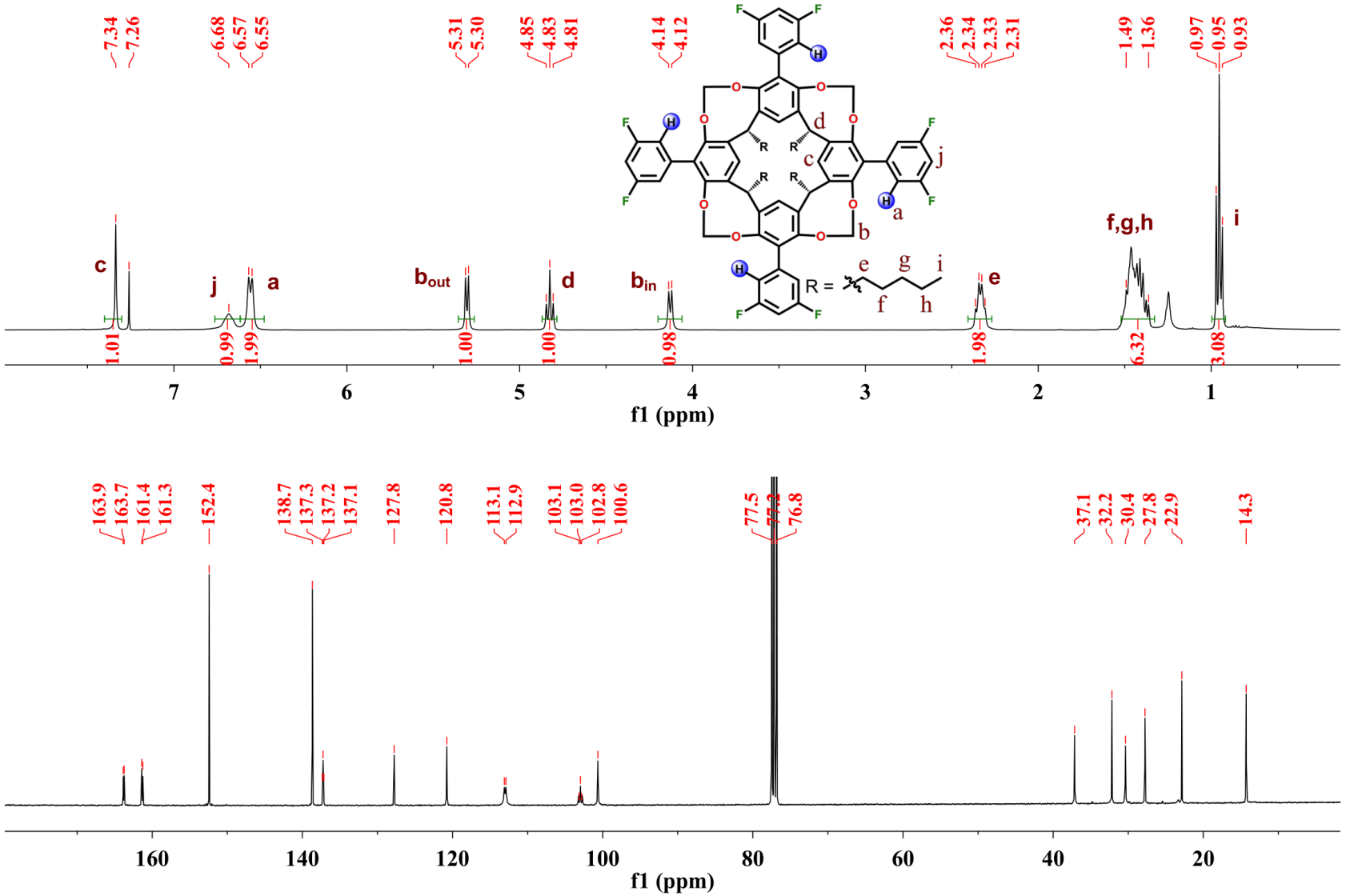


Figure S23. ^{1}H and ^{13}C NMR spectra of **4**. Data collected in $CDCl_3$ at 20 °C.

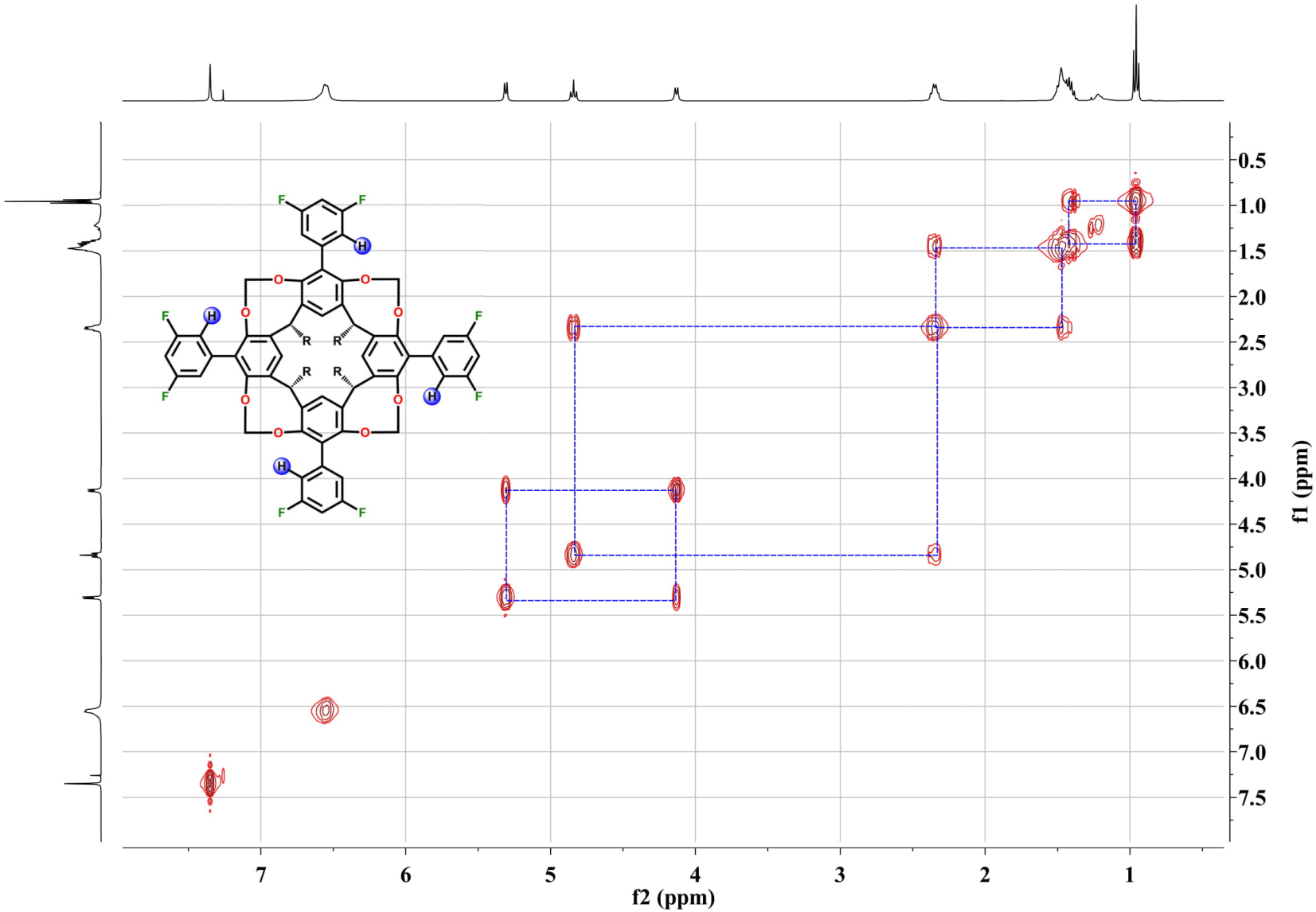


Figure S24. COSY NMR spectrum of **4**. Data collected in $CDCl_3$ at 20 °C.

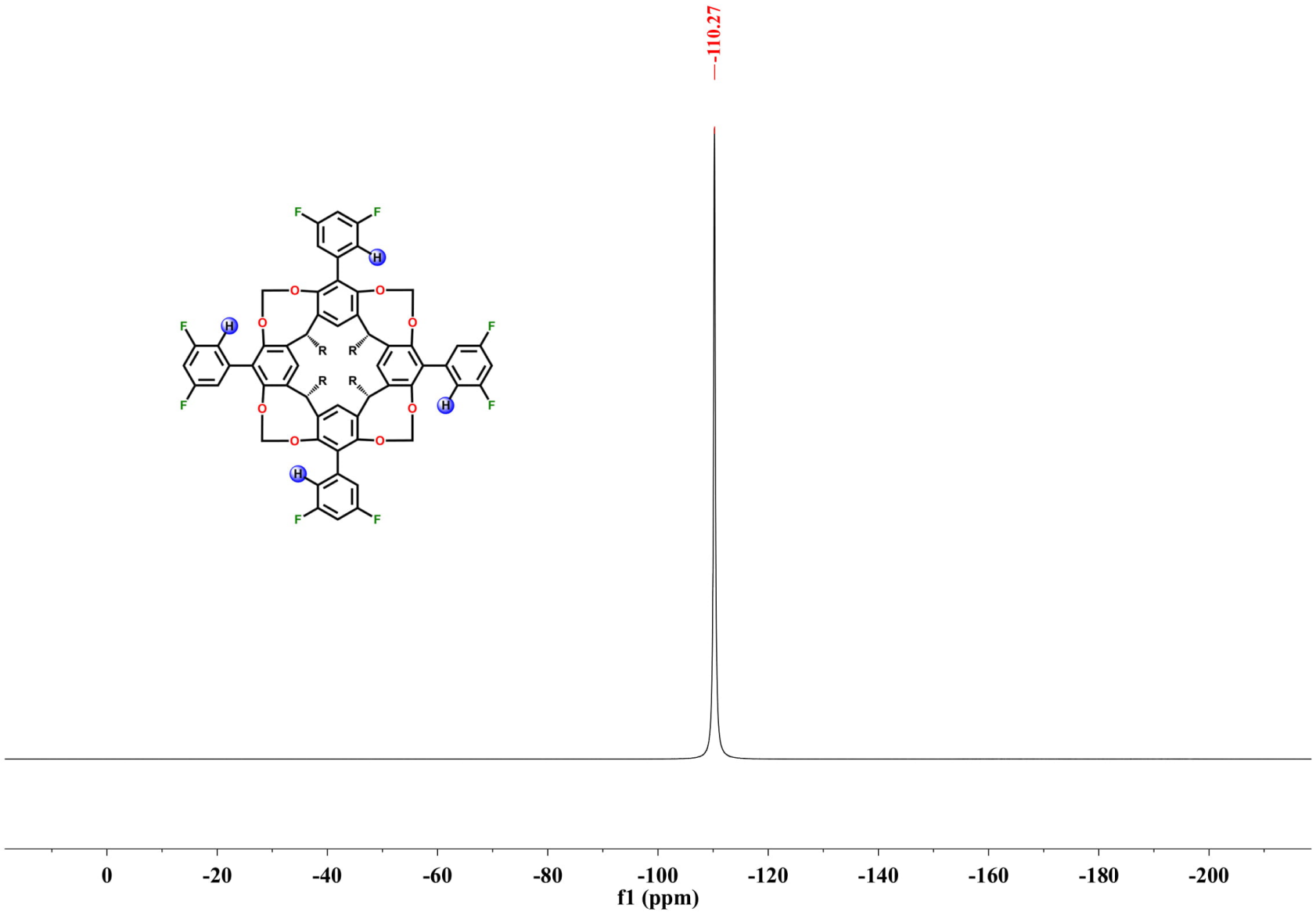


Figure S25. ^{19}F NMR spectrum of **4**. Data collected in $CDCl_3$ at 20 °C.

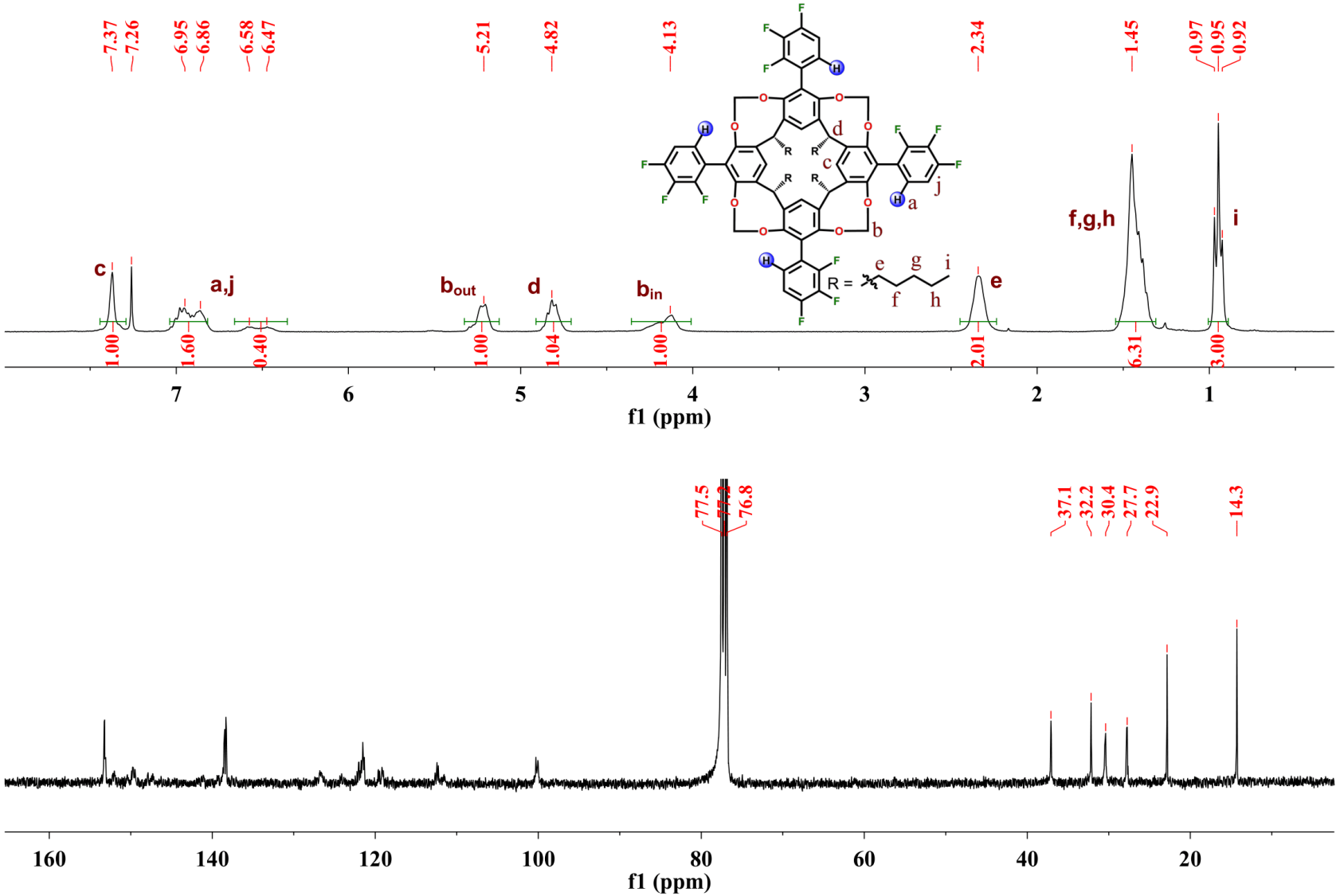


Figure S26. ^{1}H and ^{13}C NMR spectra of **5**. Data collected in $CDCl_3$ at 20 °C.

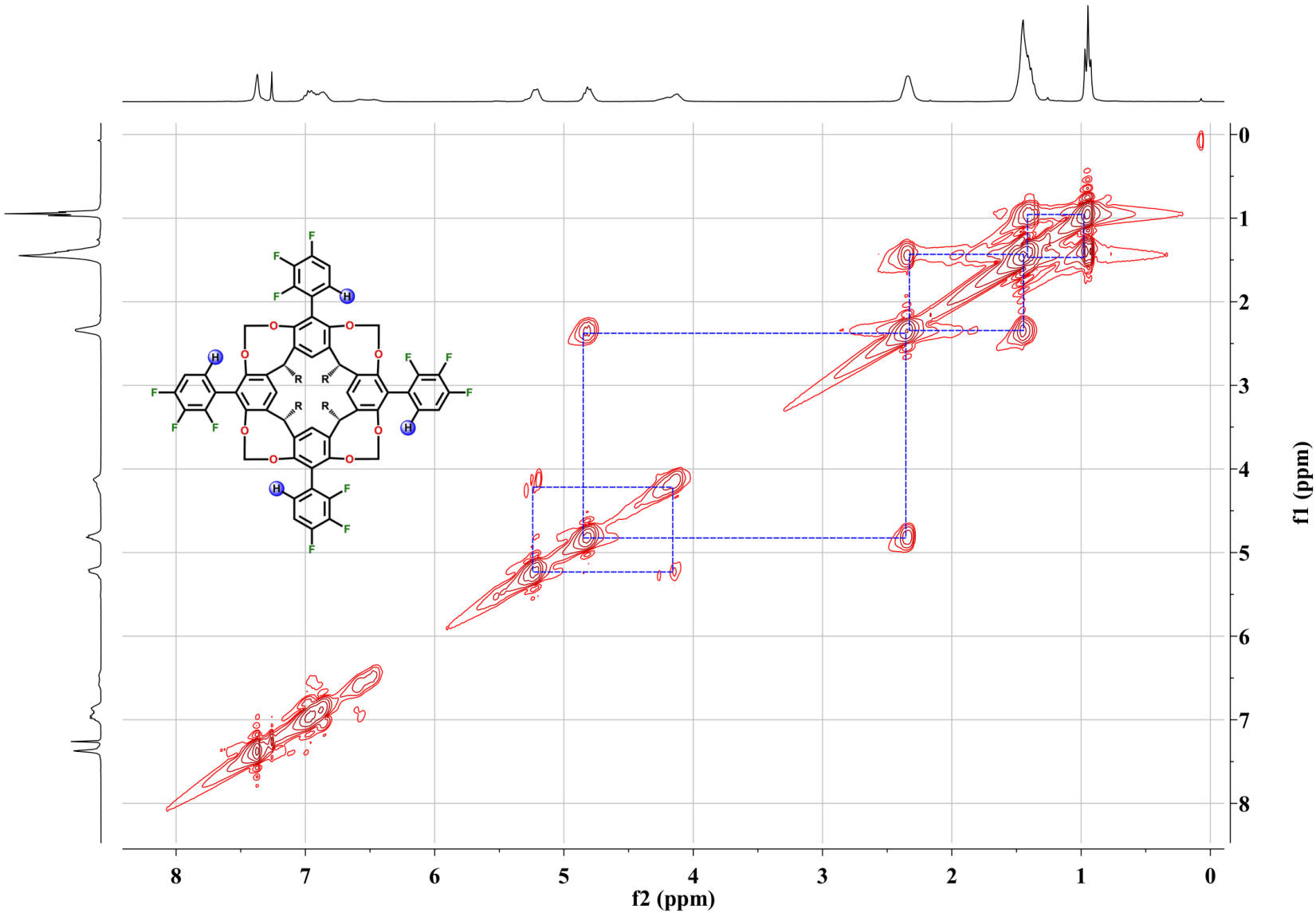


Figure S27. COSY NMR spectrum of **5**. Data collected in $CDCl_3$ at 20 °C.

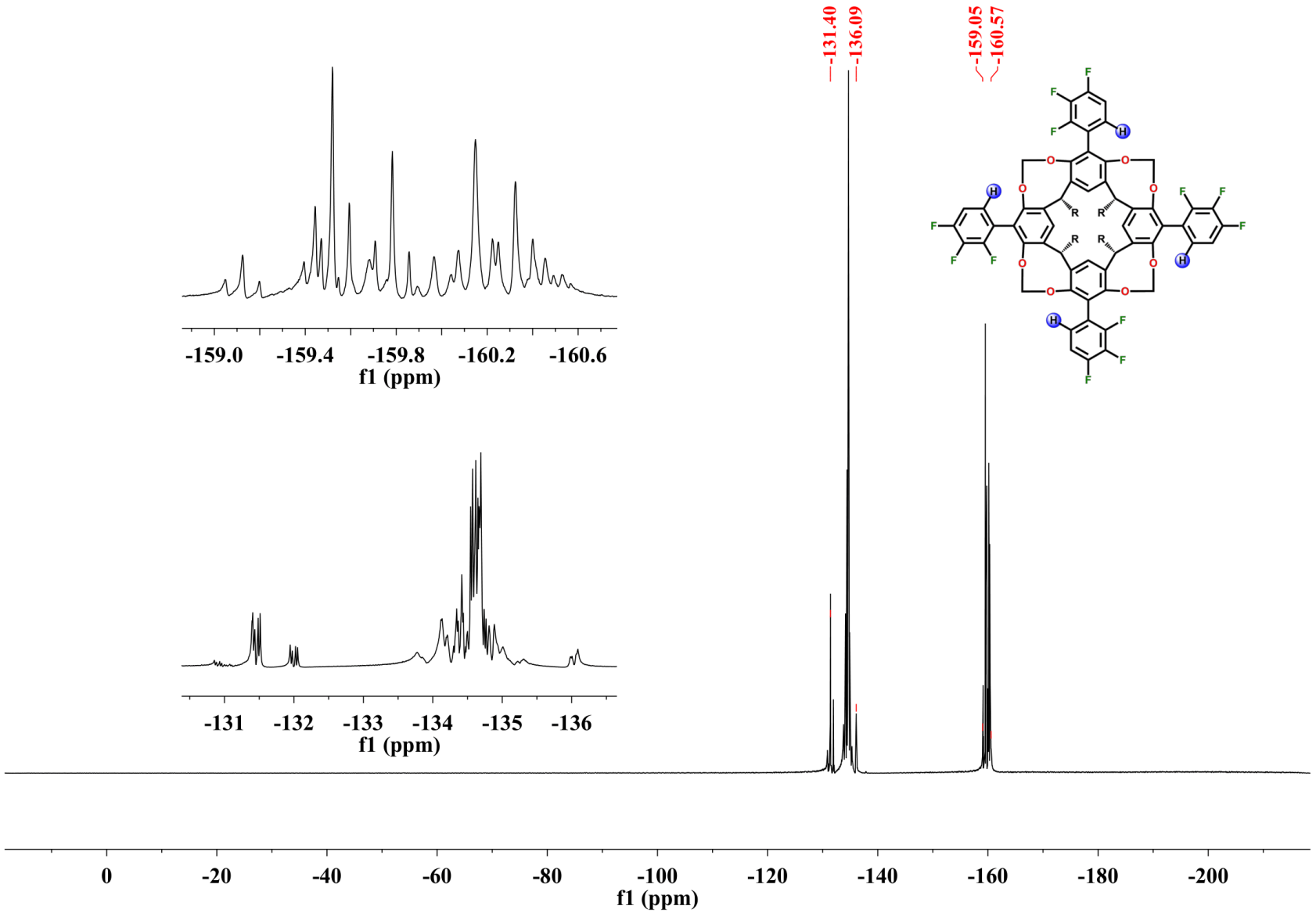


Figure 28. ^{19}F NMR spectrum of **5**. Data collected in $CDCl_3$ at 20 °C.

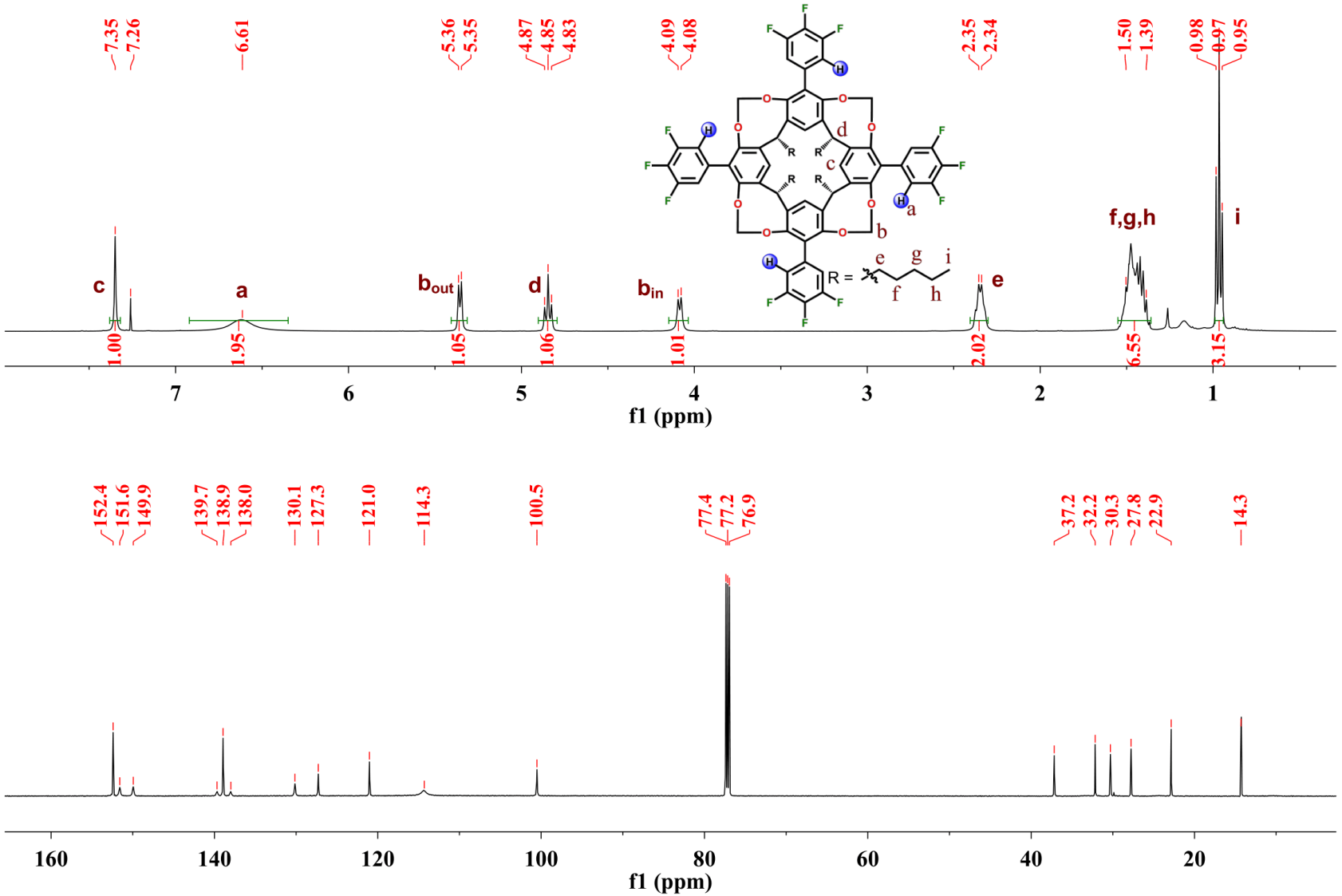


Figure S29. ^{1}H and ^{13}C NMR spectra of **6**. Data collected in $CDCl_3$ at 20 °C.

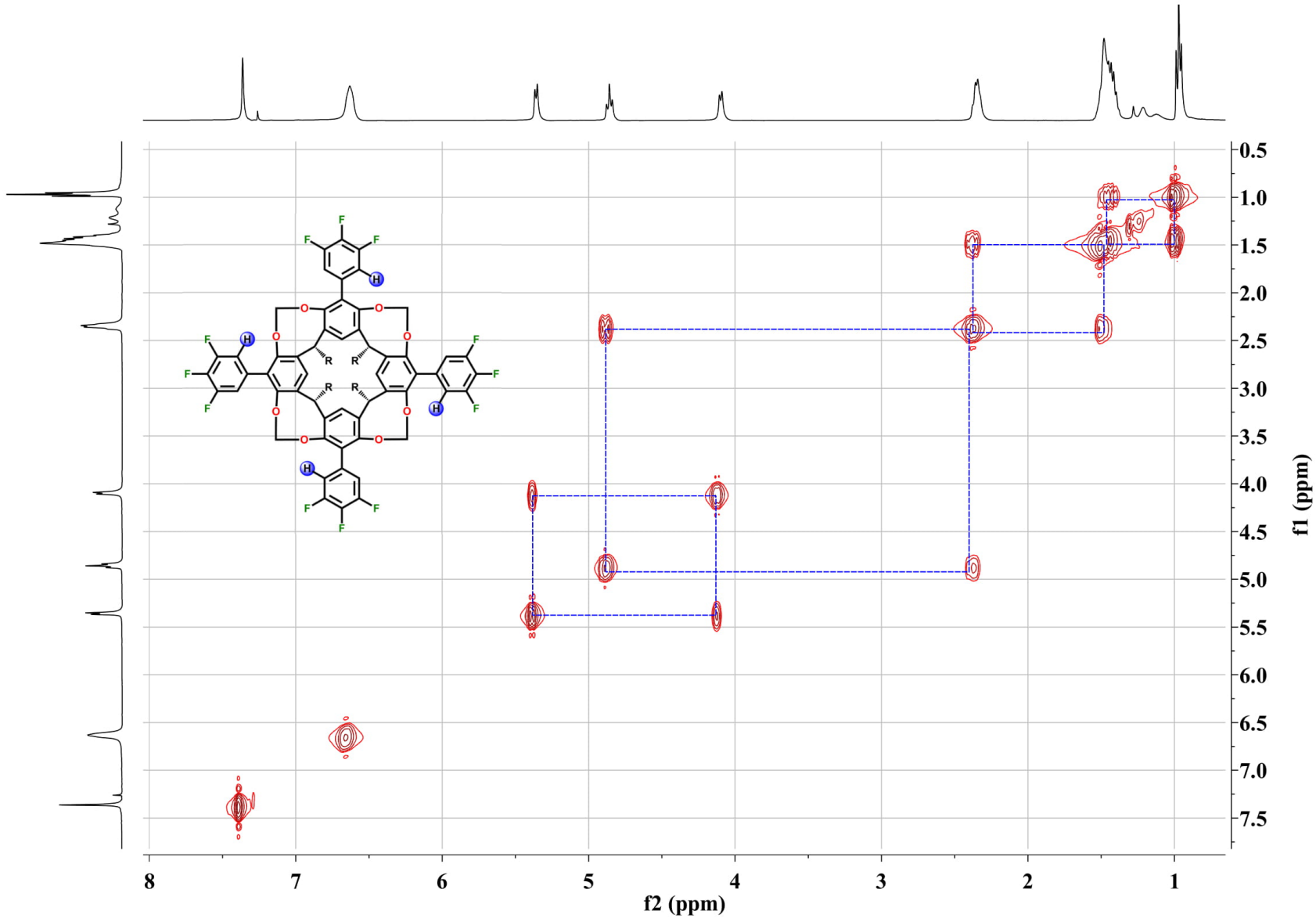


Figure S30. COSY NMR spectrum of **6**. Data collected in $CDCl_3$ at 20 °C.

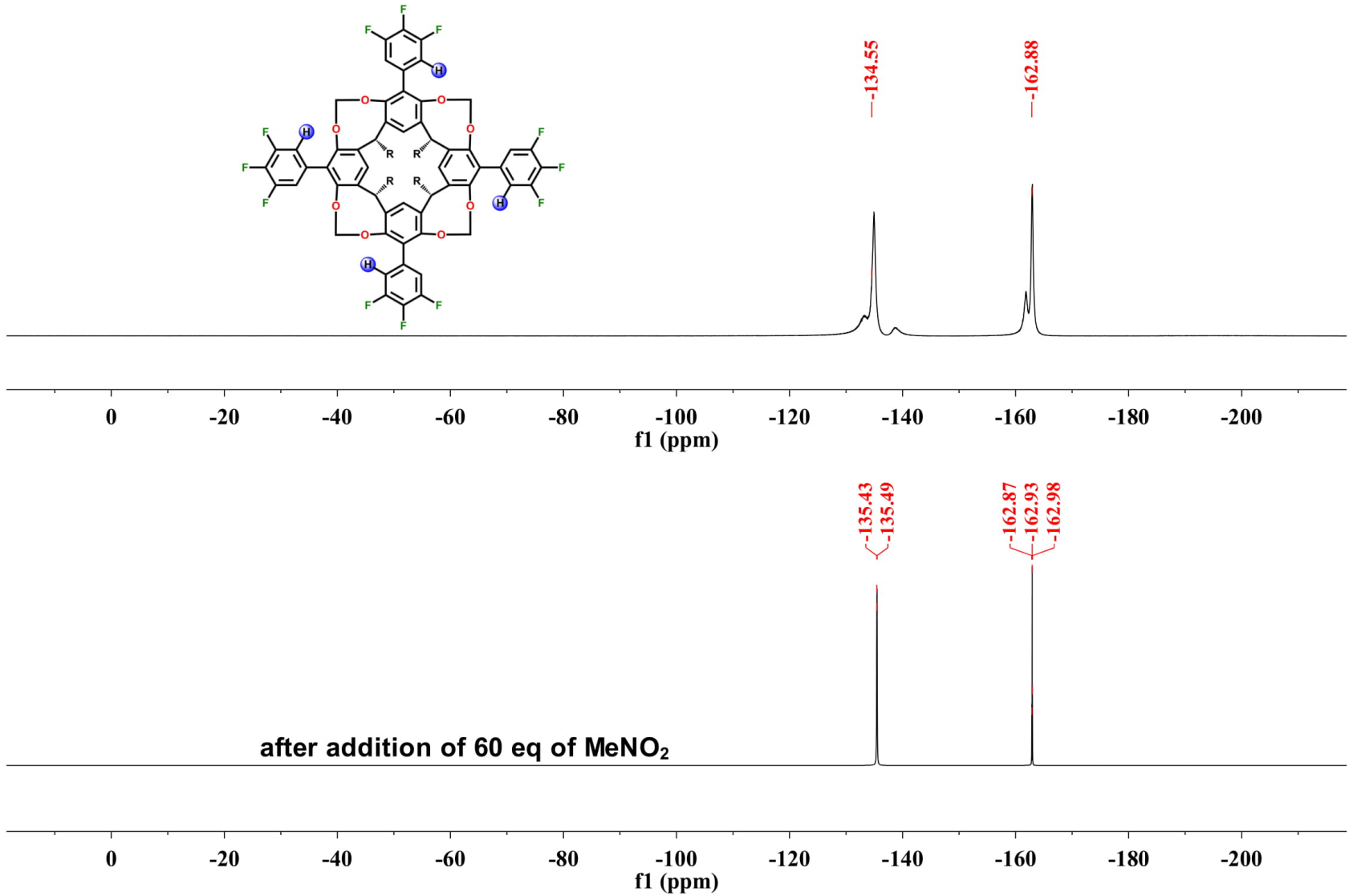


Figure S31. ^{19}F NMR spectra of **6**. Data collected in $CDCl_3$ at 20 °C.

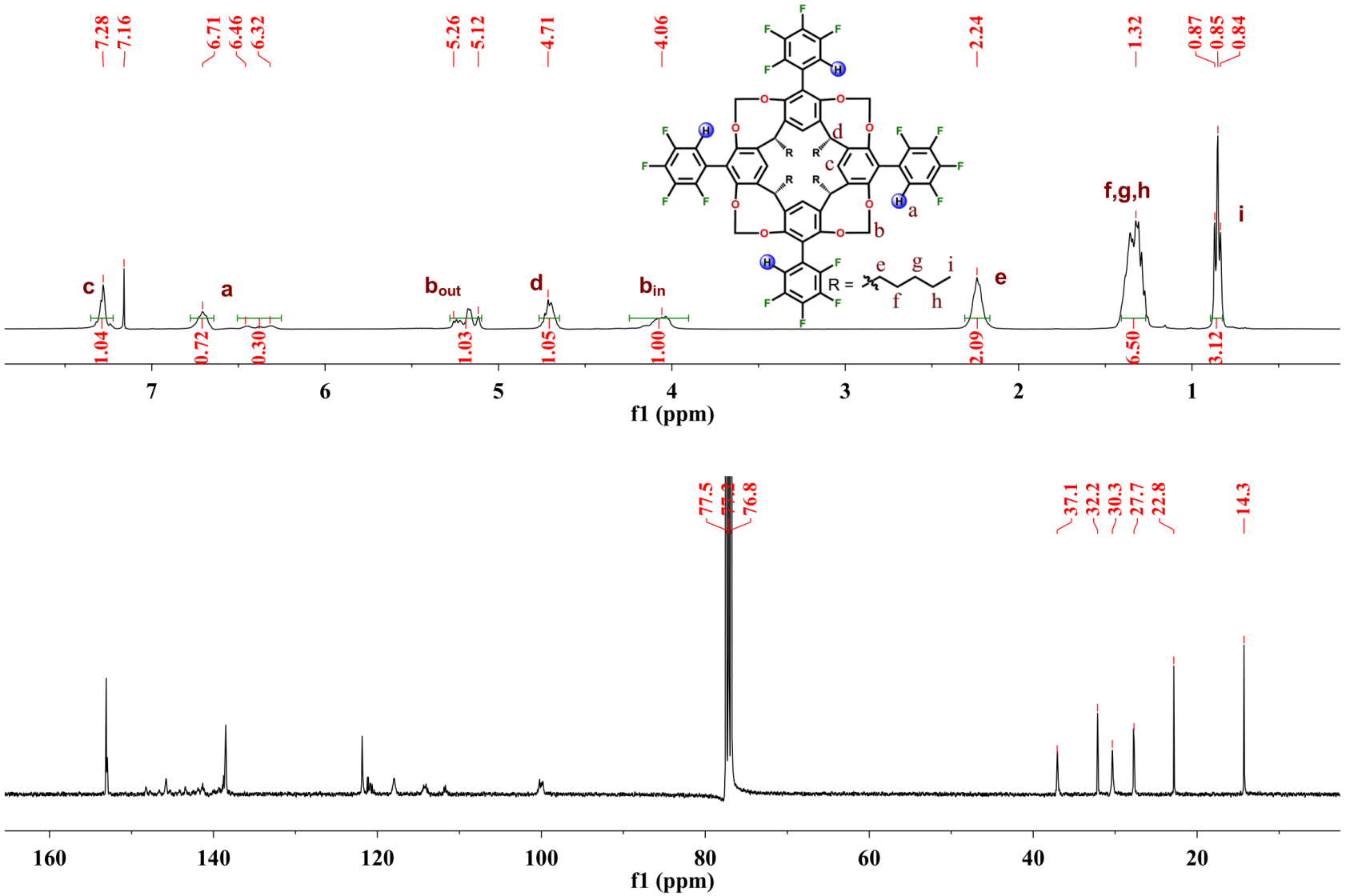


Figure S32. ^{1}H and ^{13}C NMR spectra of **7**. Data collected in $CDCl_3$ at 20 °C.

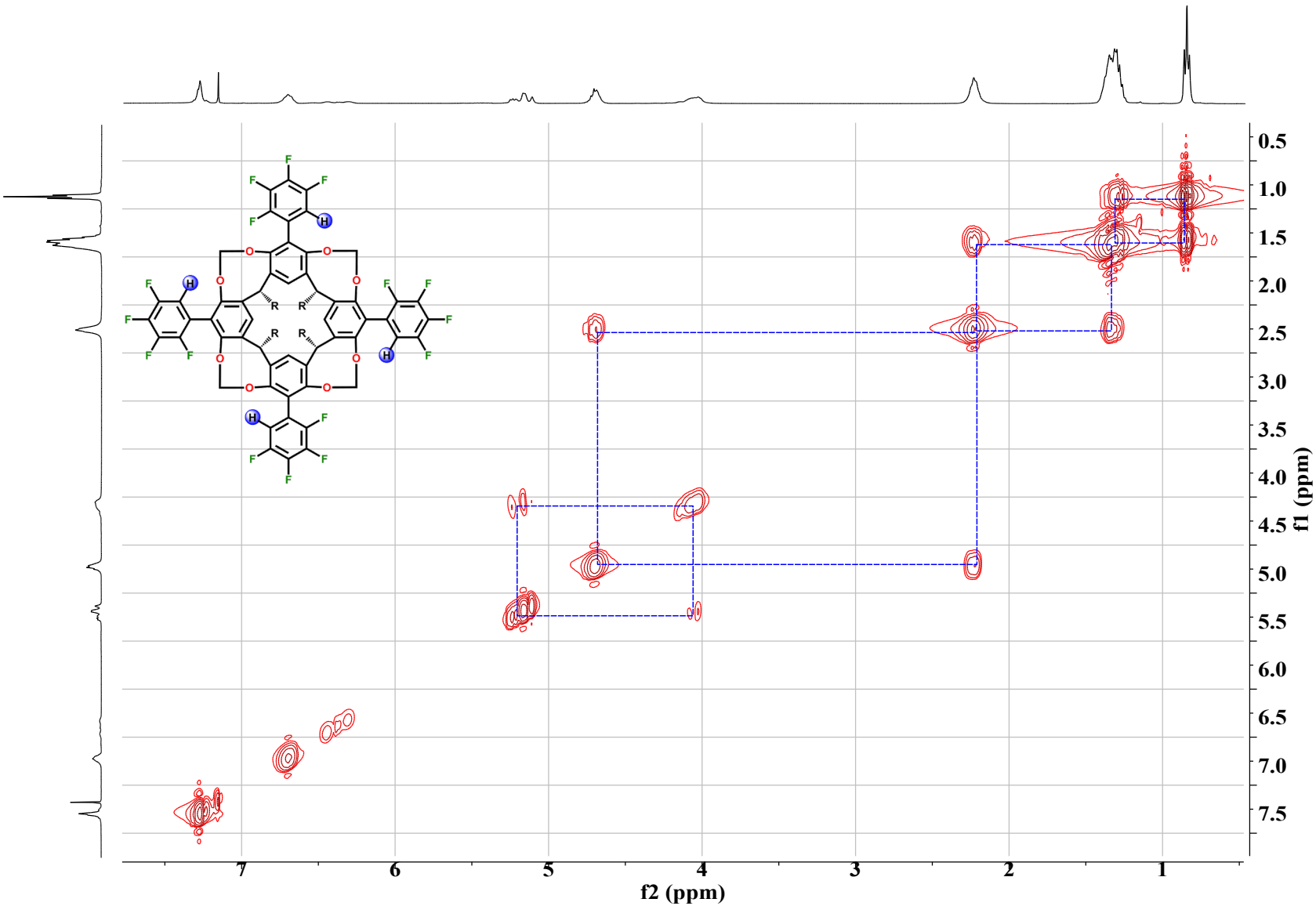


Figure S33. COSY NMR spectrum of **7**. Data collected in $CDCl_3$ at 20 °C.

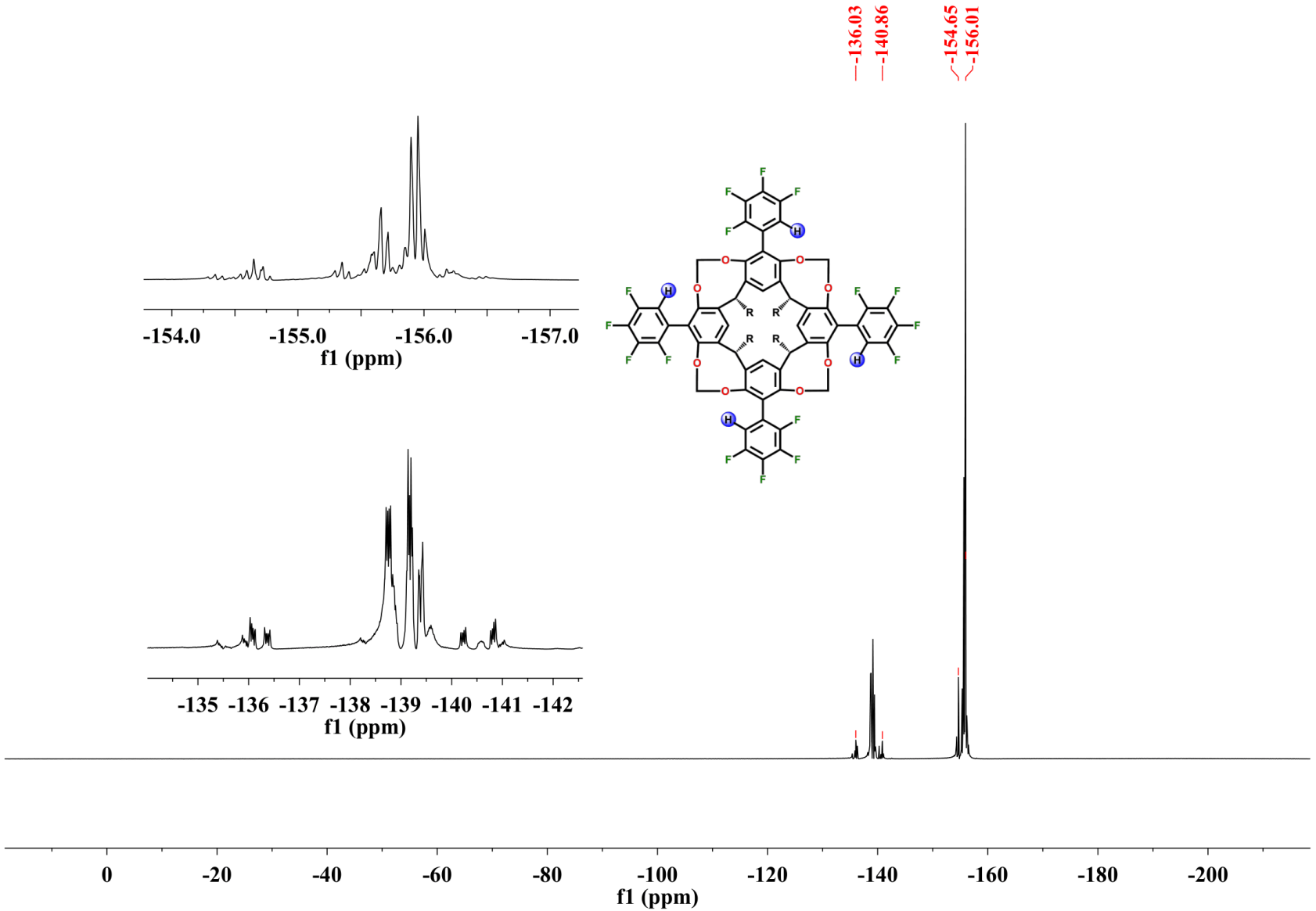


Figure S34. ^{19}F NMR spectrum of **7**. Data collected in $CDCl_3$ at 20 °C.

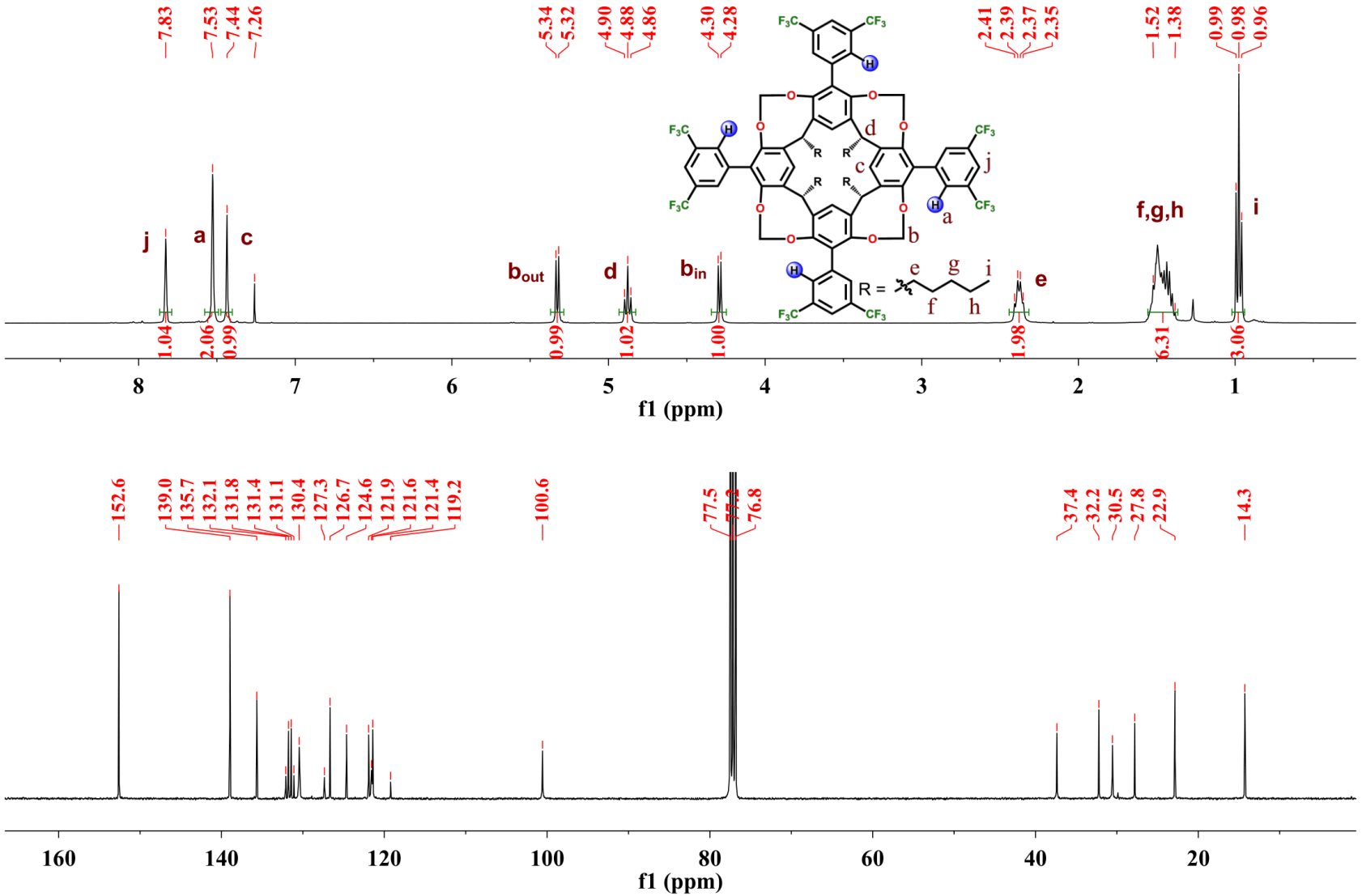


Figure S35. ^{1}H and ^{13}C NMR spectra of **8**. Data collected in $CDCl_3$ at 20 °C.

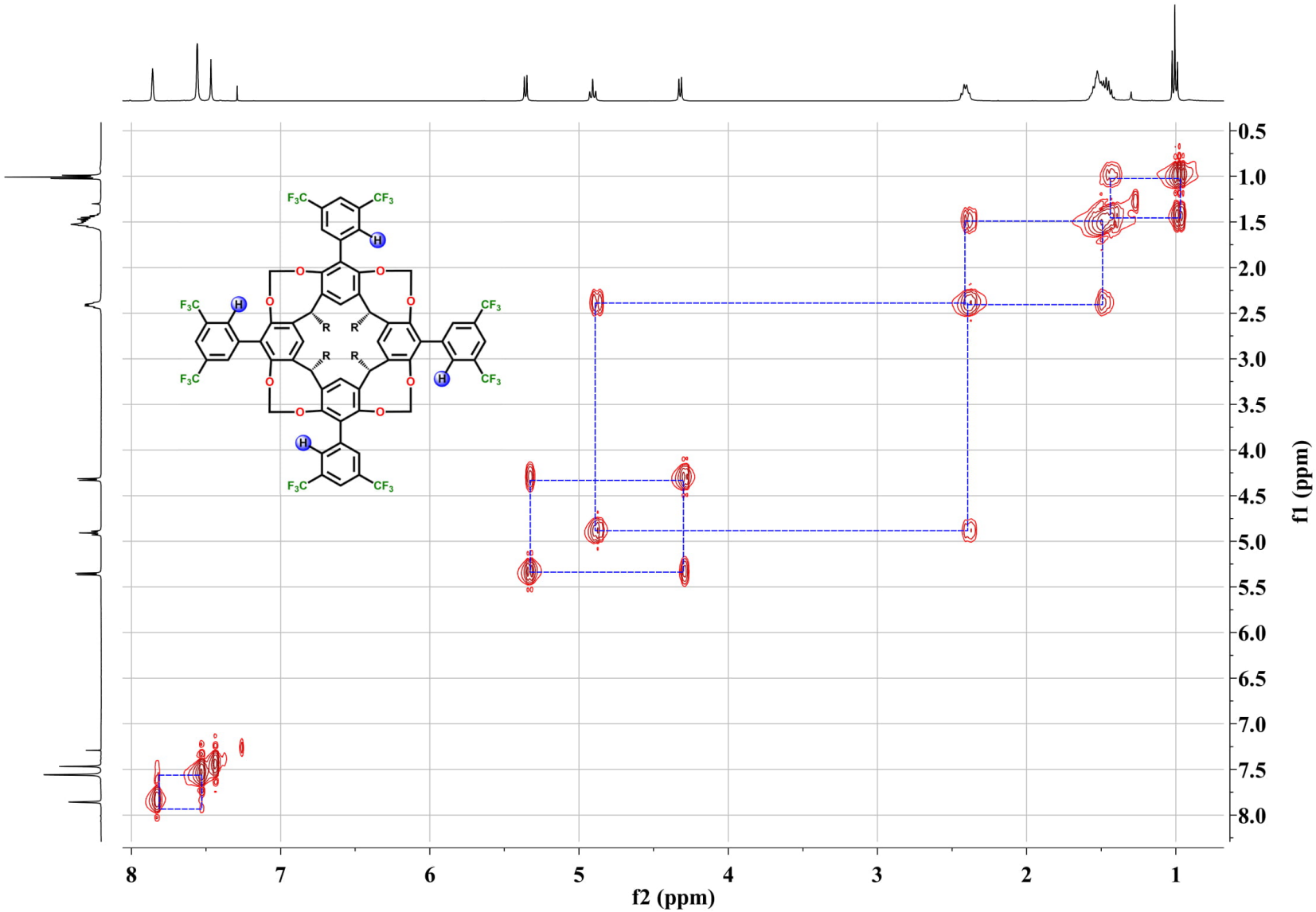


Figure S36. COSY NMR spectrum of **8**. Data collected in $CDCl_3$ at 20 °C.

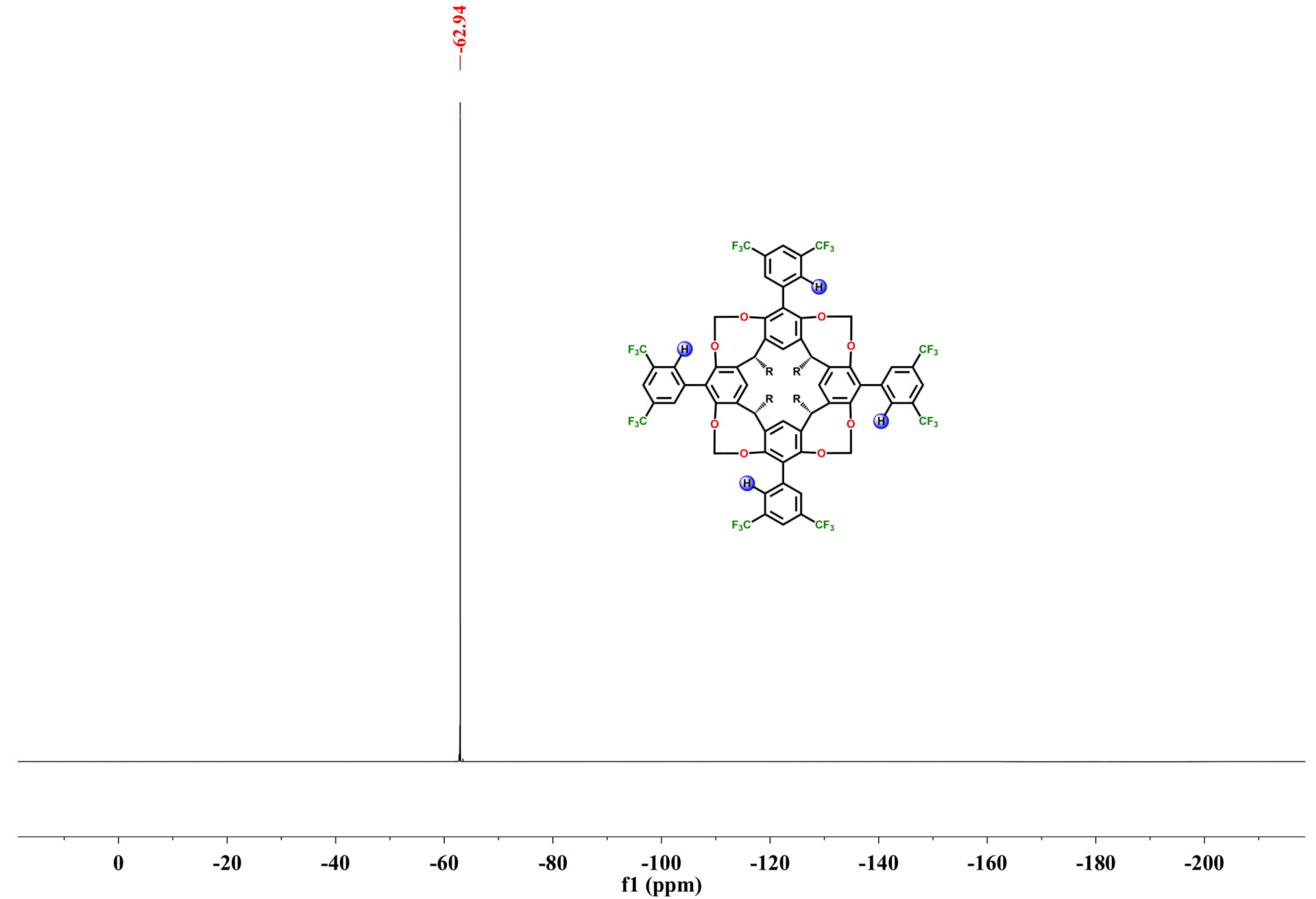


Figure S37. ^{19}F NMR spectrum of **8**. Data collected in $CDCl_3$ at 20 °C.

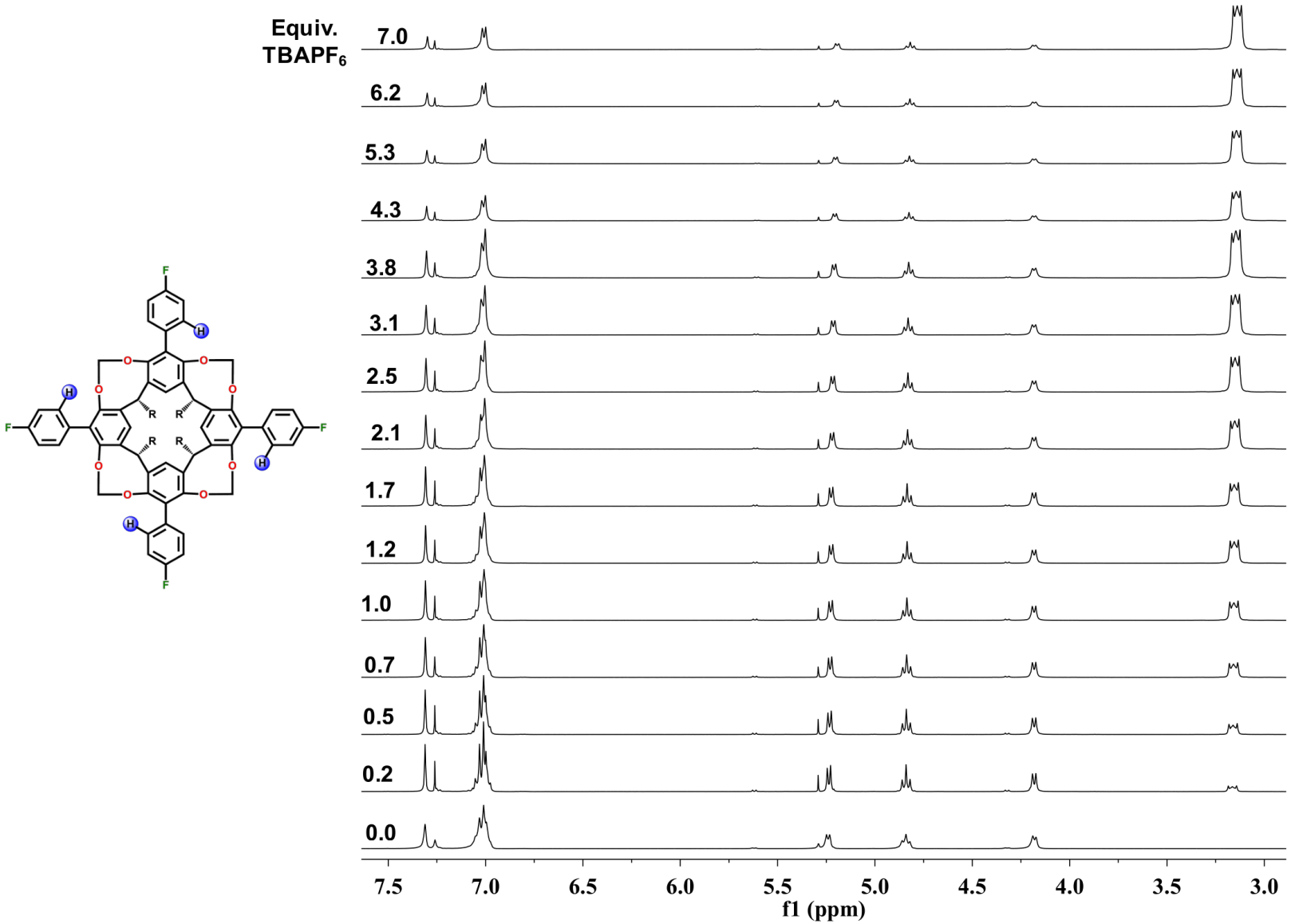


Figure S38. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **2** in CDCl$_3$ at 20 °C.

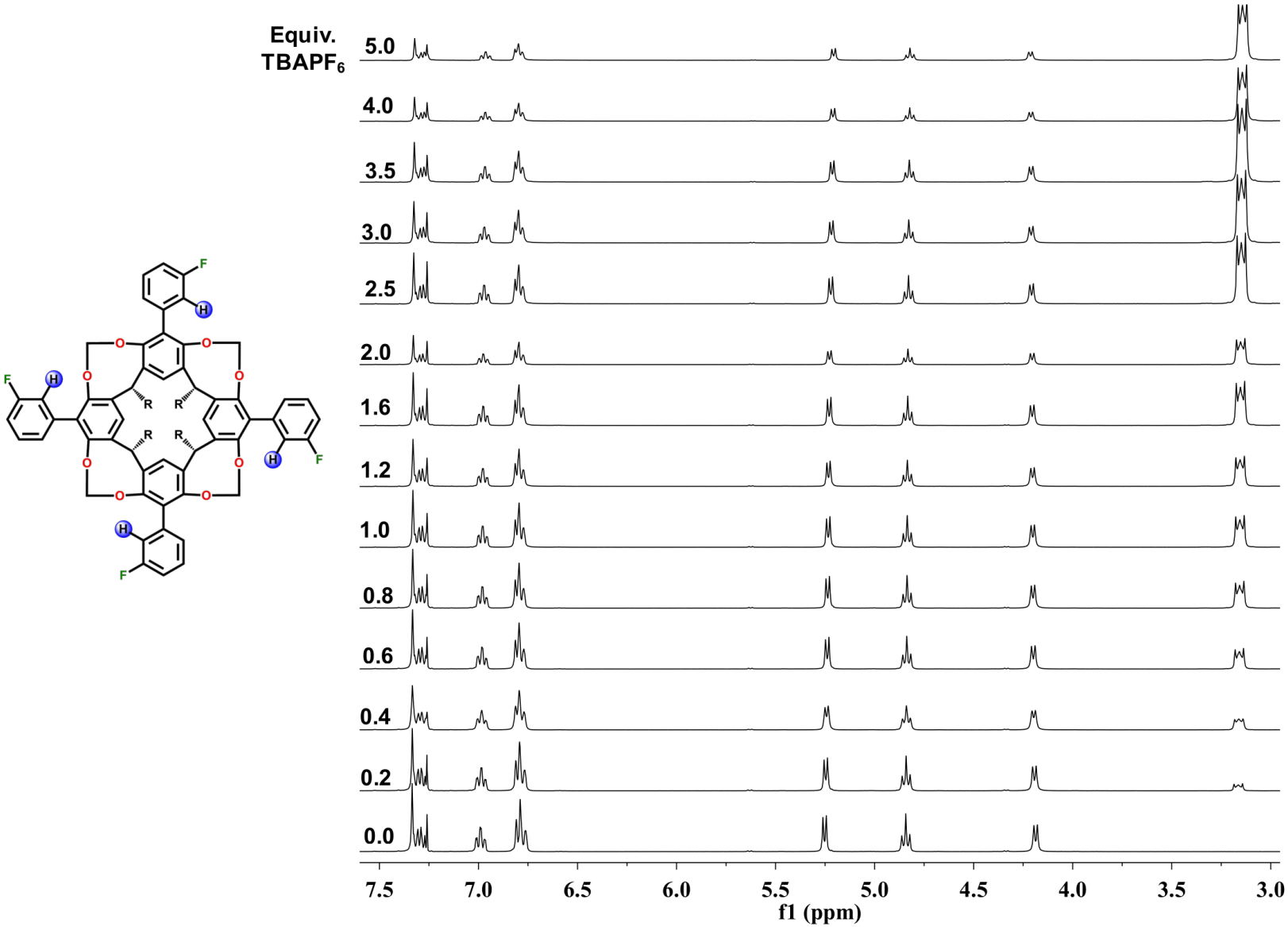


Figure S39. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **3** in CDCl$_3$ at 20 °C.

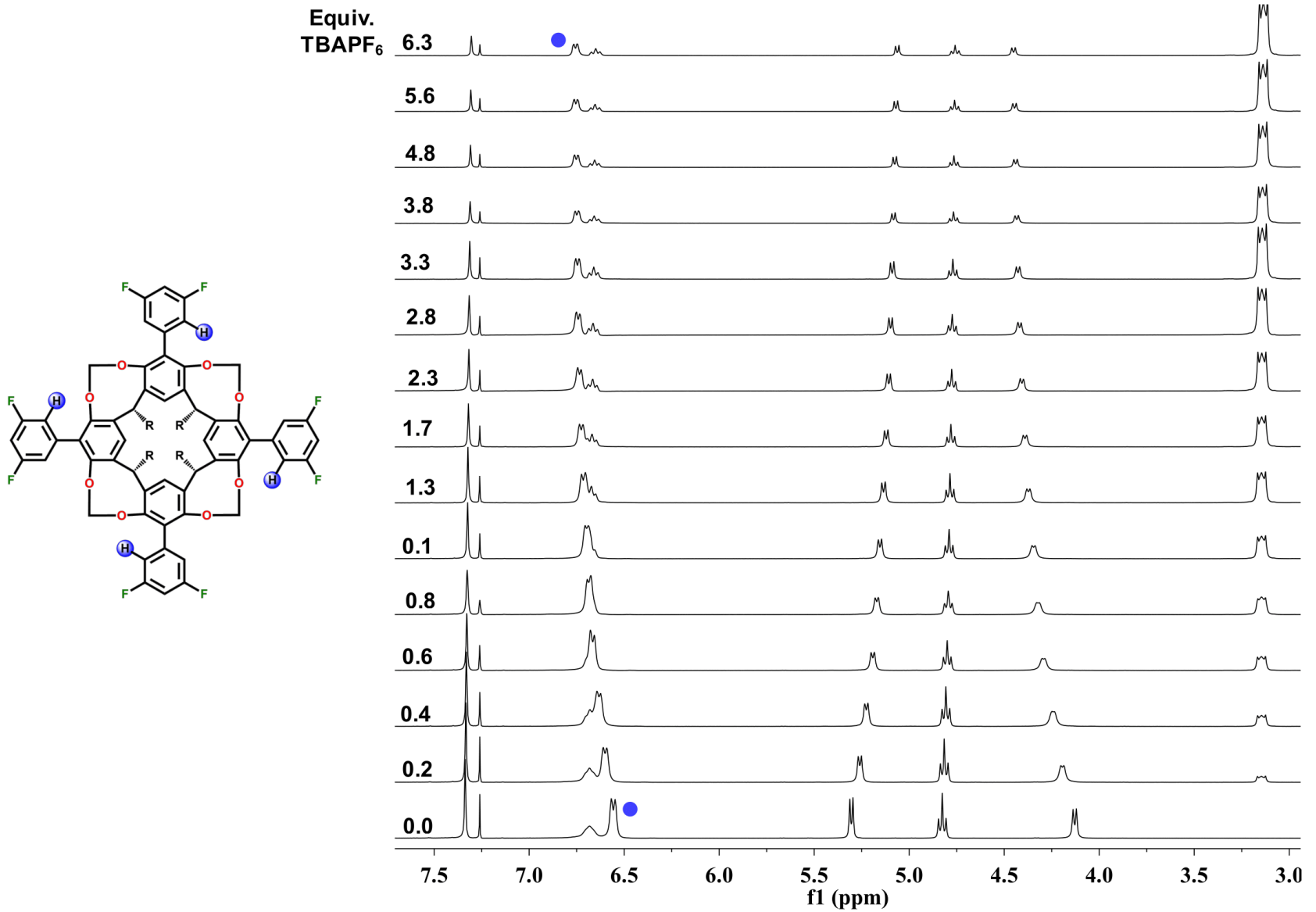


Figure S40. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **4** in CDCl$_3$ at 20 °C.

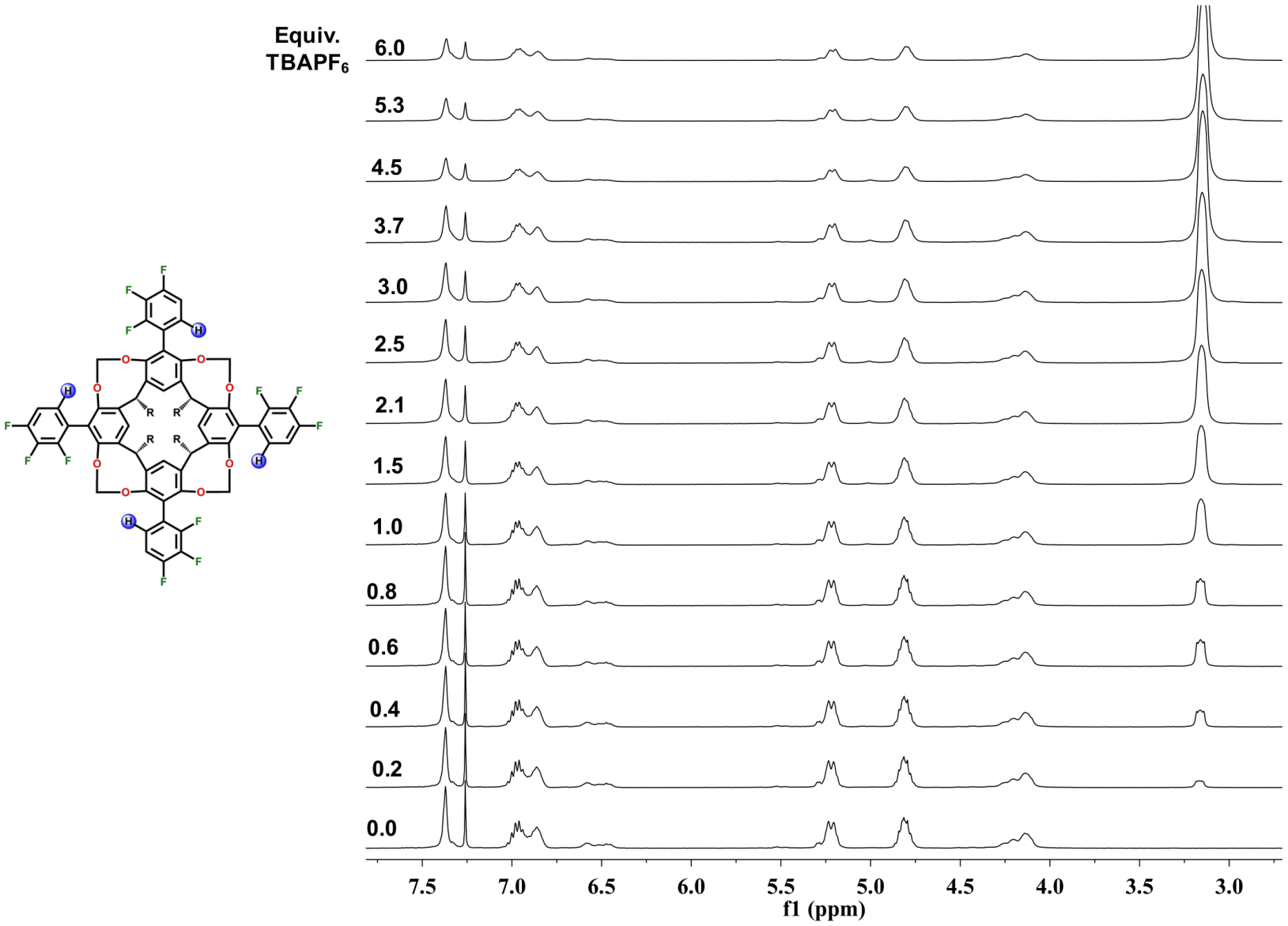


Figure S41. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **5** in CDCl$_3$ at 20 °C.

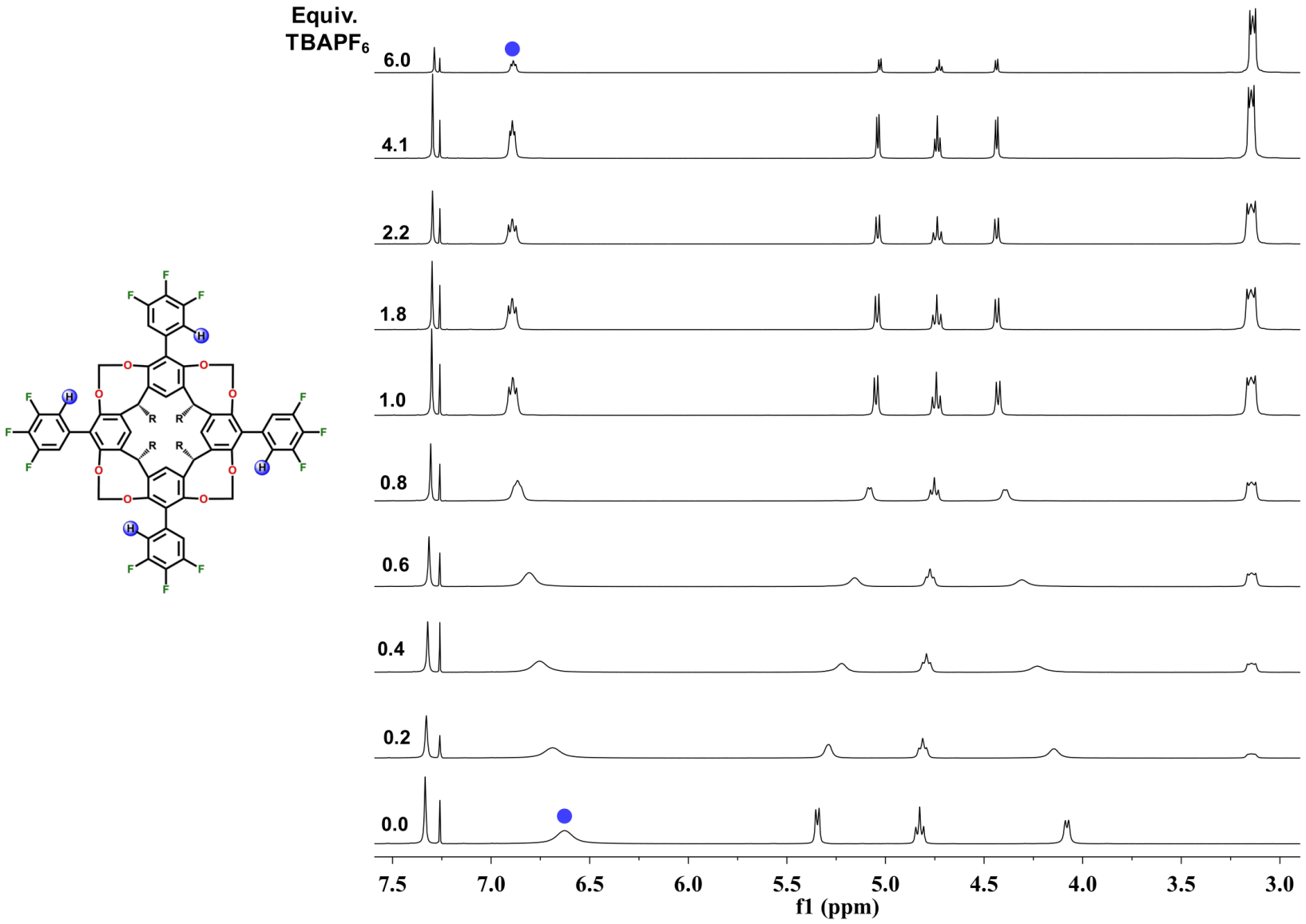


Figure S42. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **6** in CDCl$_3$ at 20 °C.

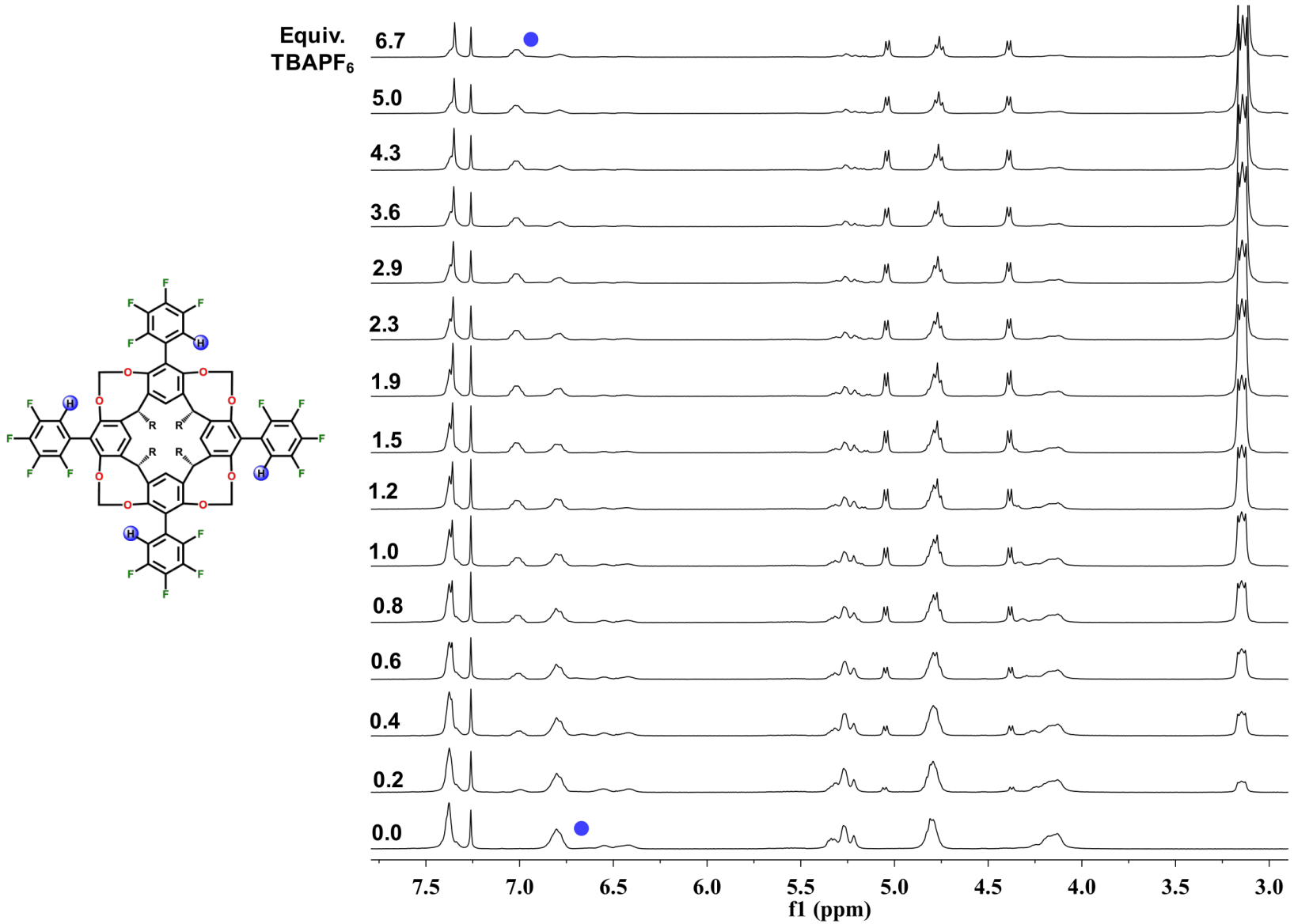


Figure S43. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **7** in CDCl$_3$ at 20 °C.

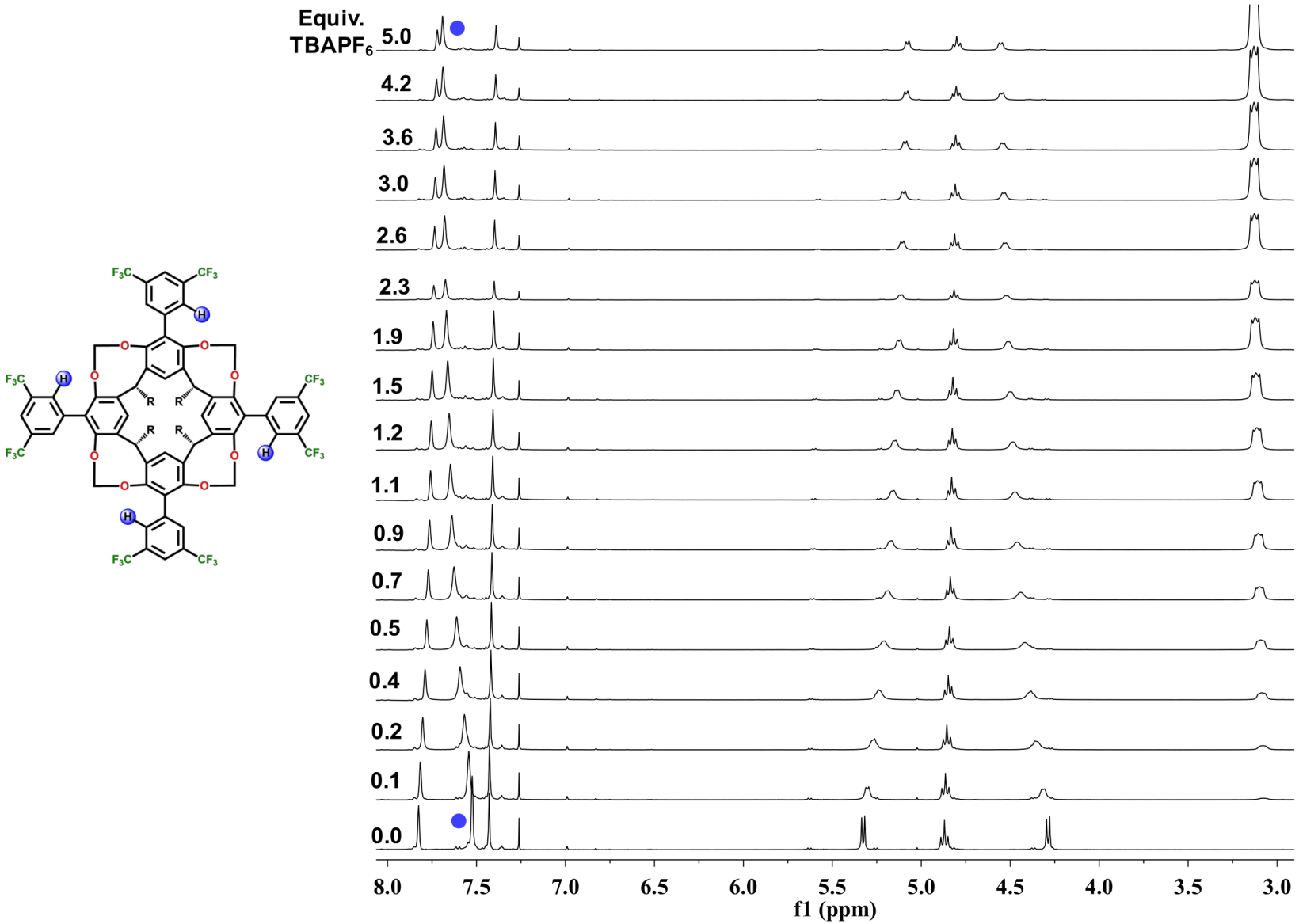


Figure S44. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][PF$_6$] added to **8** in CDCl$_3$ at 20 °C.

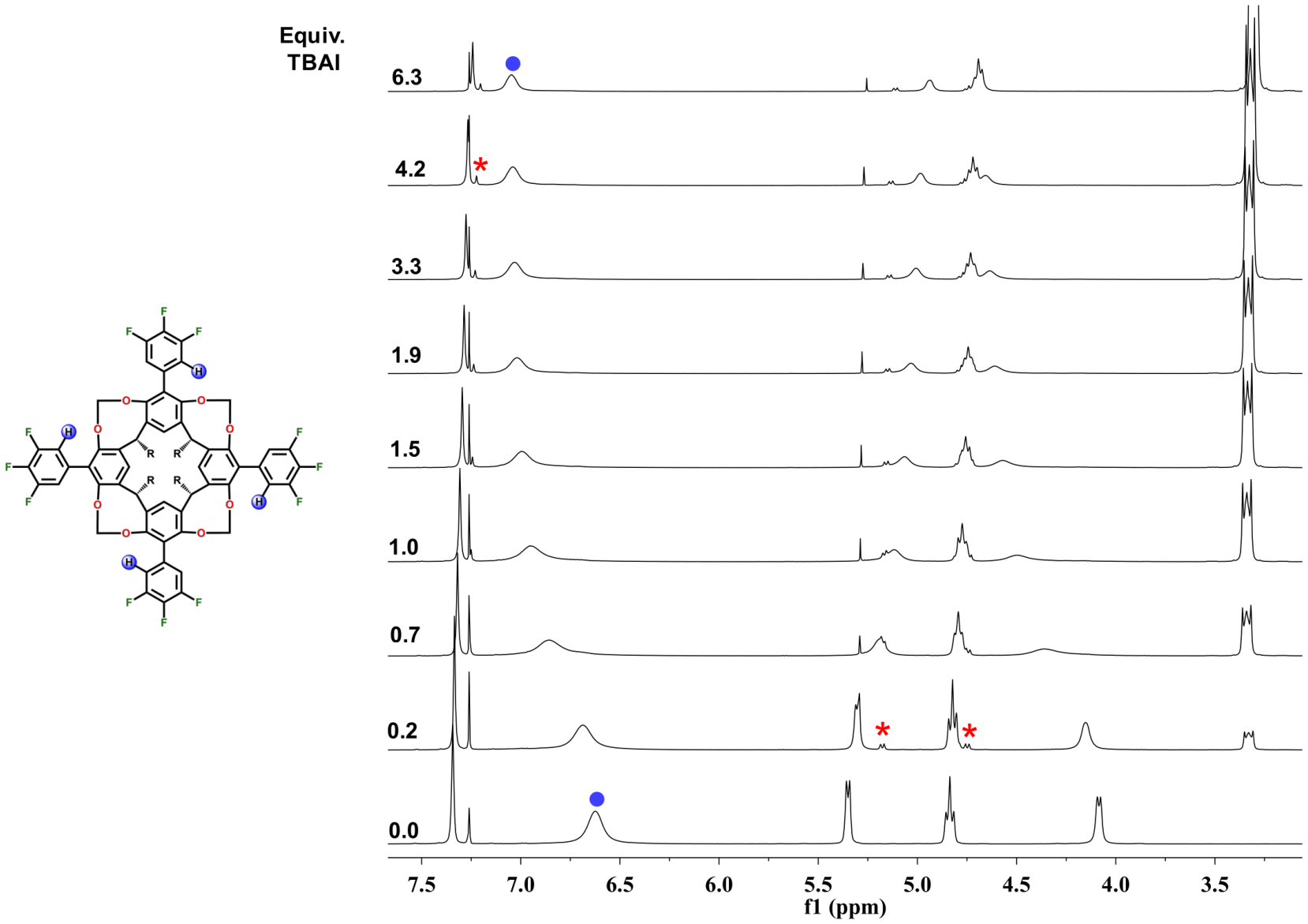


Figure S45. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][I] added to **6** in $CDCl_3$ at 20 °C (asterisk sign shows impurities from [*n*-Bu$_4$N][I]).

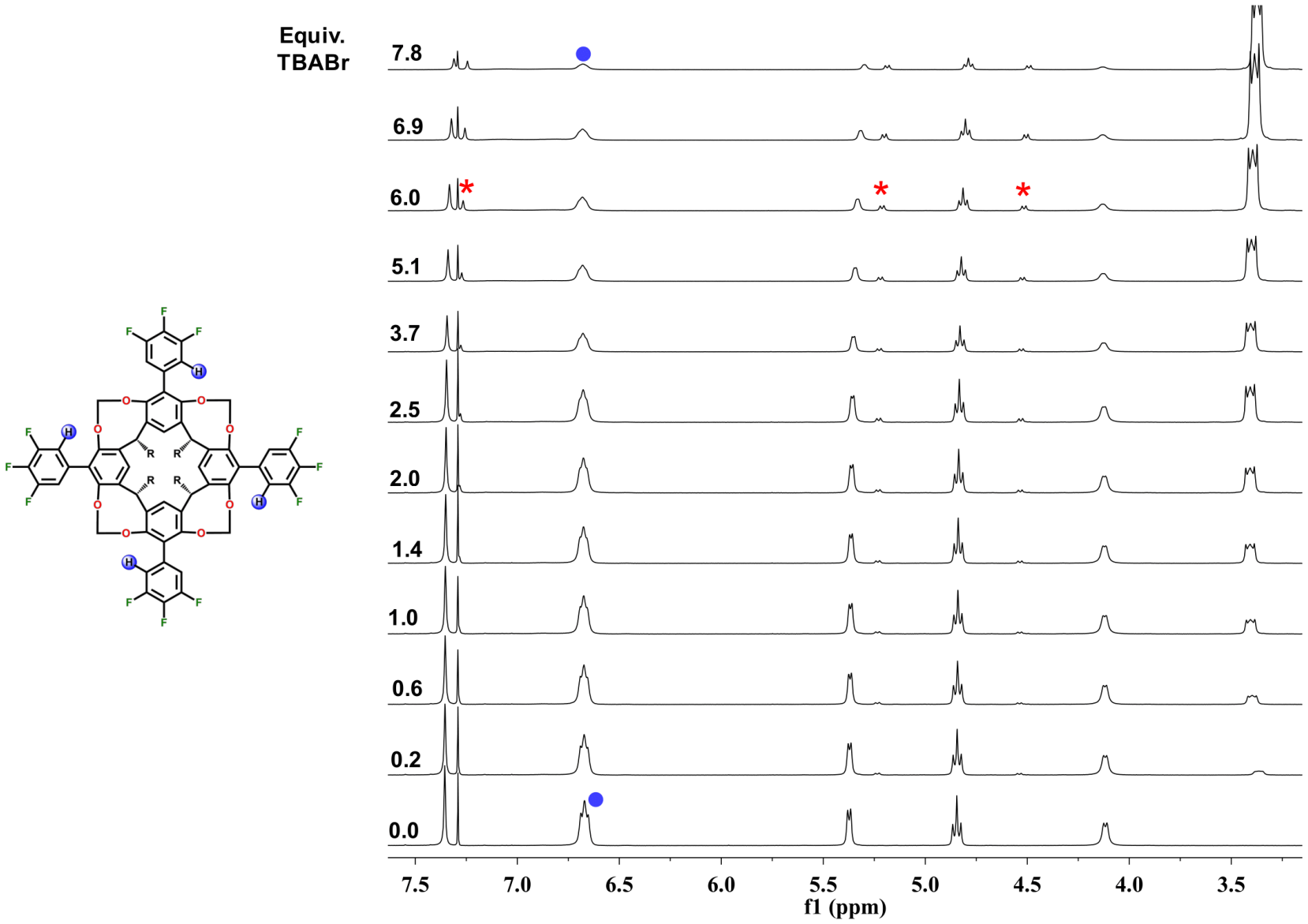


Figure S46. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][Br] added to **6** in $CDCl_3$ at 20 °C (asterisk sign shows impurities from [*n*-Bu$_4$N][Br]).

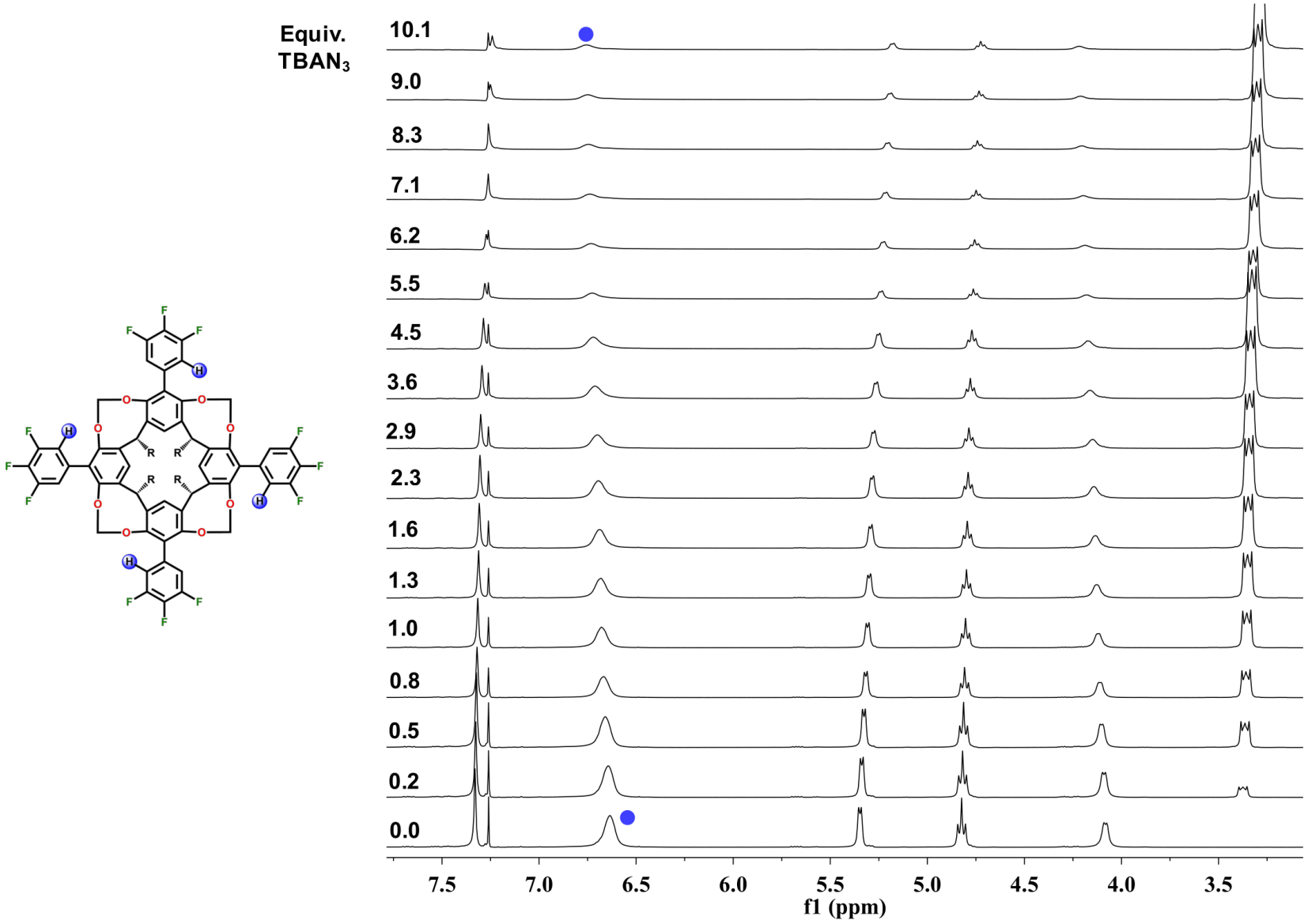


Figure S47. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][N$_3$] added to **6** in CDCl$_3$ at 20 °C.

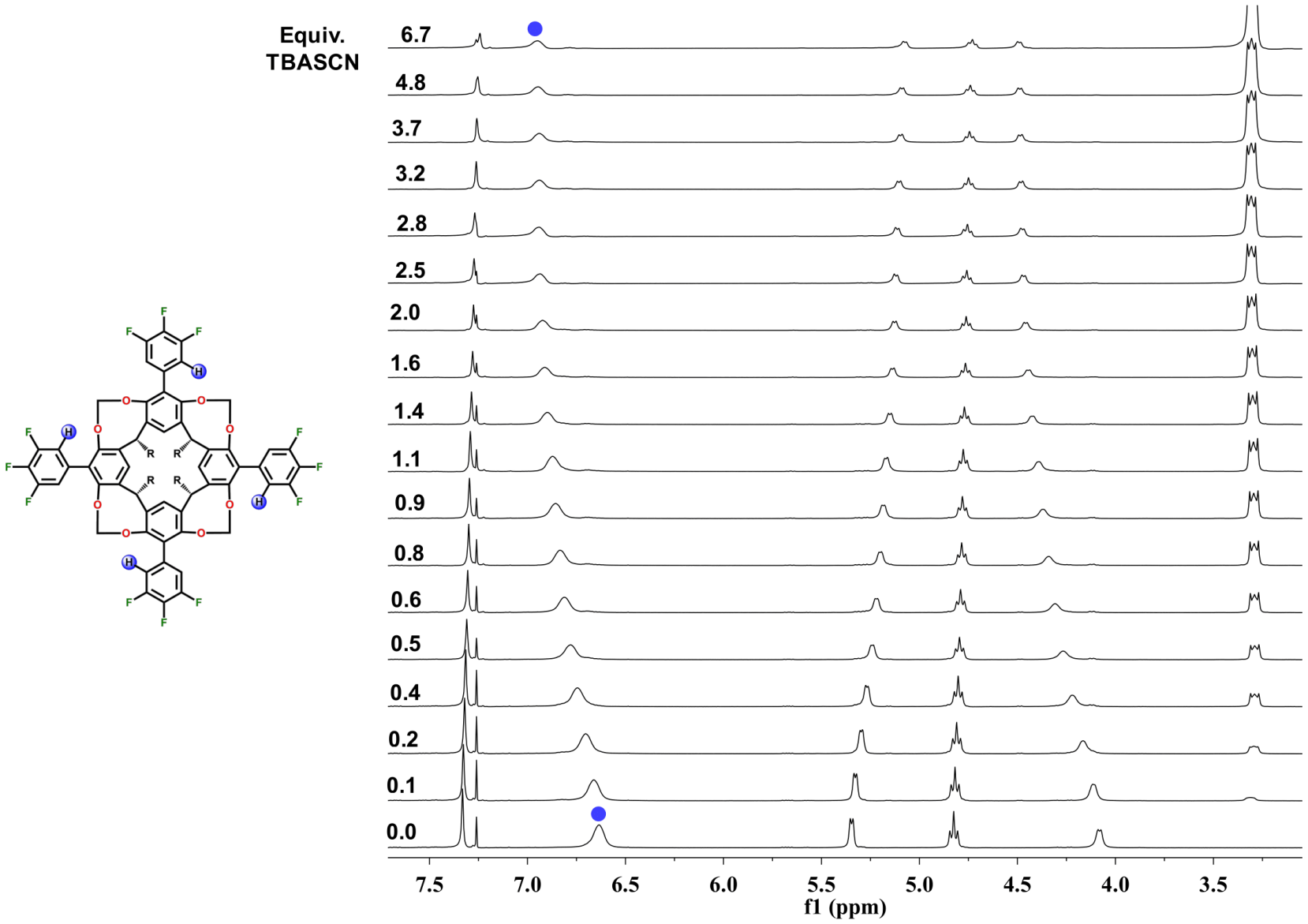


Figure S48. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][SCN] added to **6** in $CDCl_3$ at 20 °C.

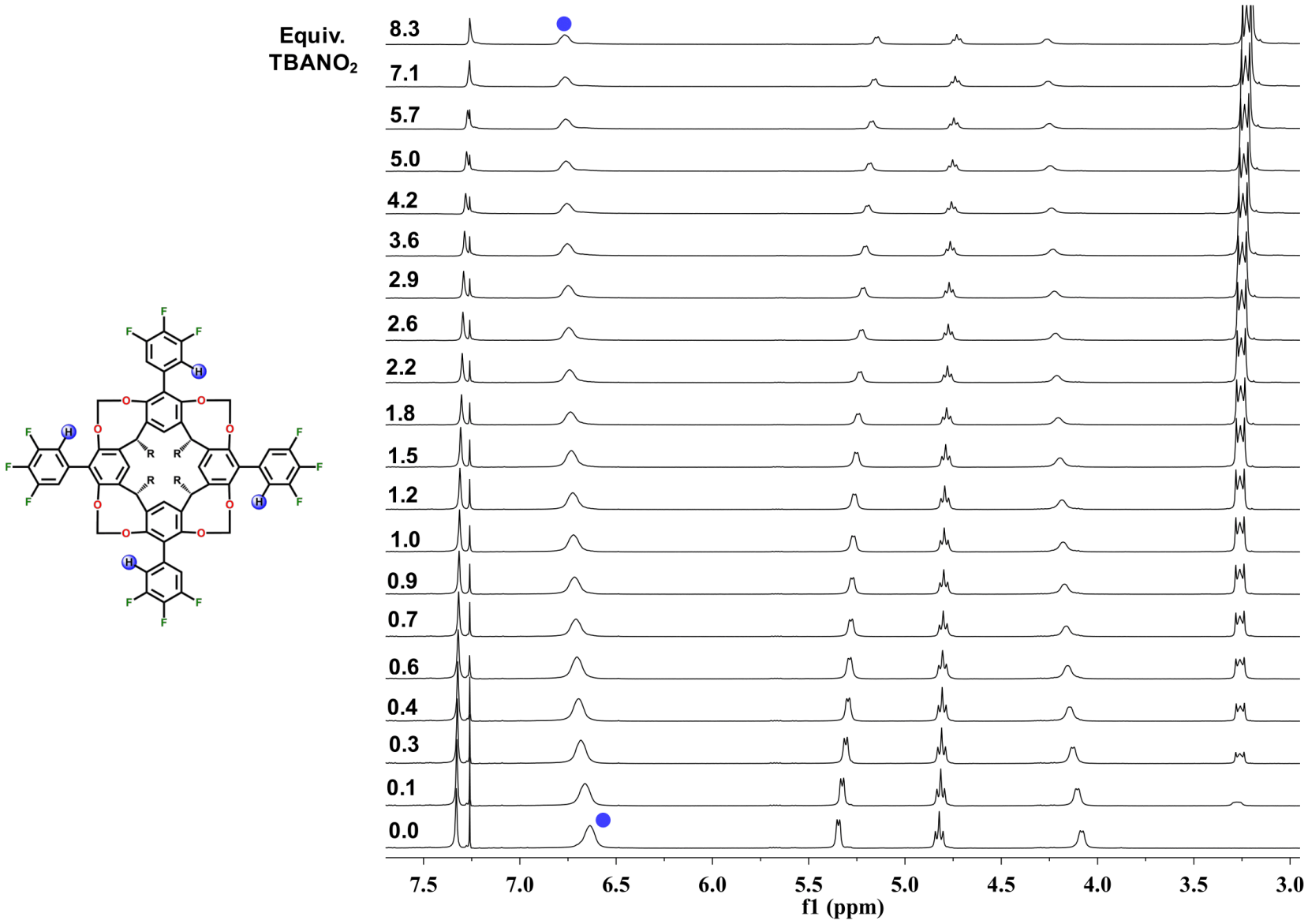


Figure S49. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][NO$_2$] added to **6** in CDCl$_3$ at 20 °C.

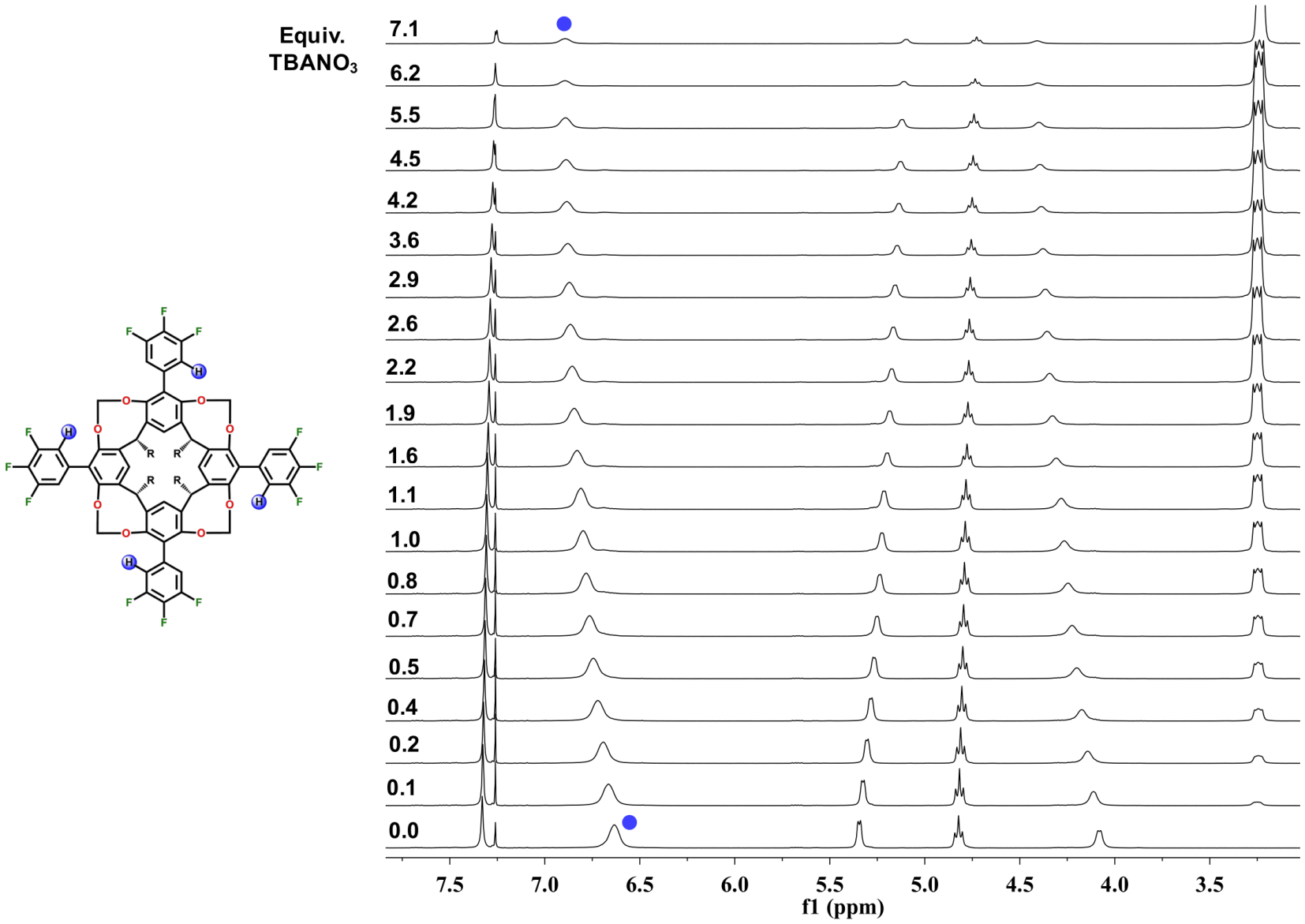


Figure S50. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][NO$_3$] added to **6** in CDCl$_3$ at 20 °C.

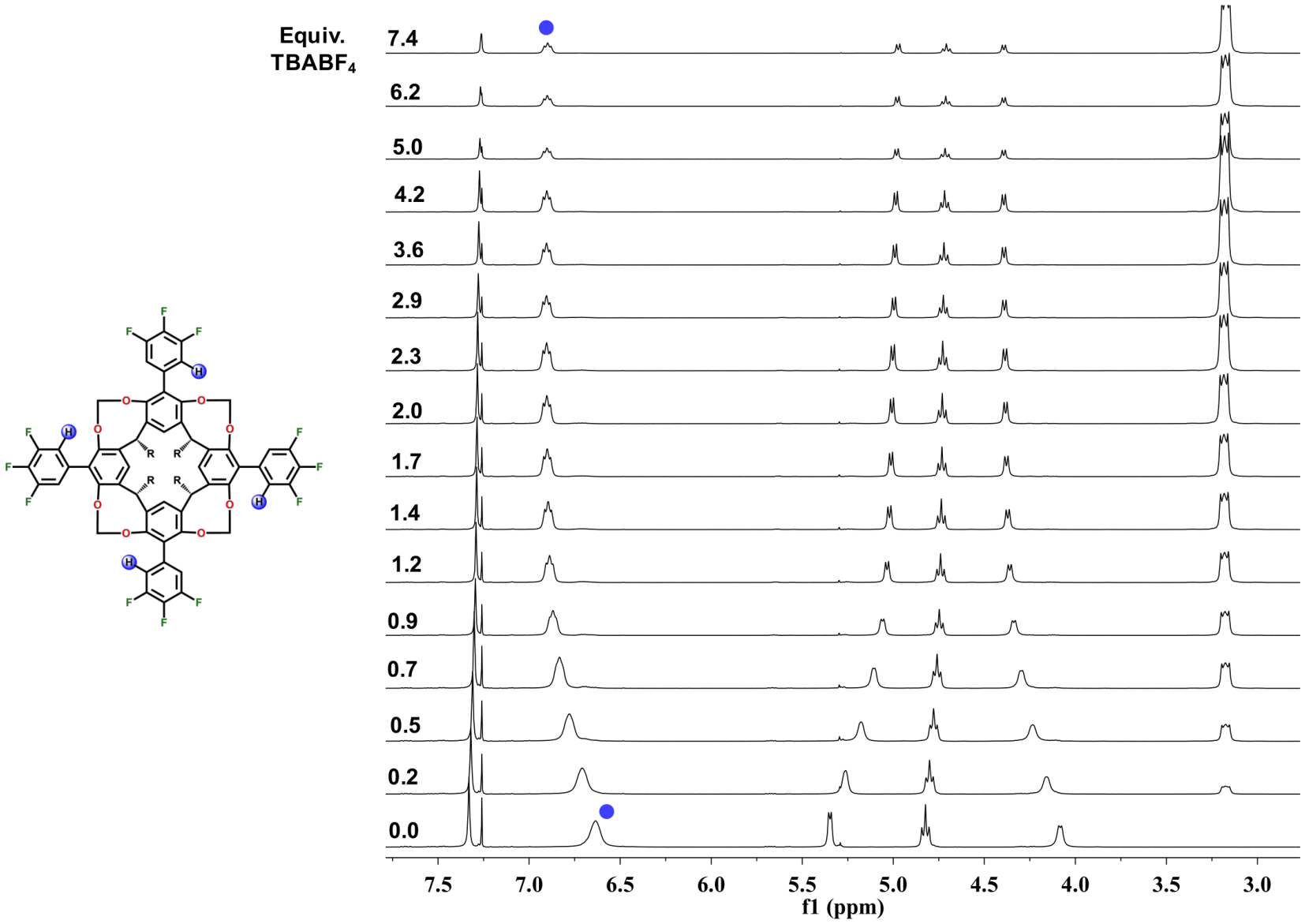


Figure S51. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][BF$_4$] added to **6** in CDCl$_3$ at 20 °C.

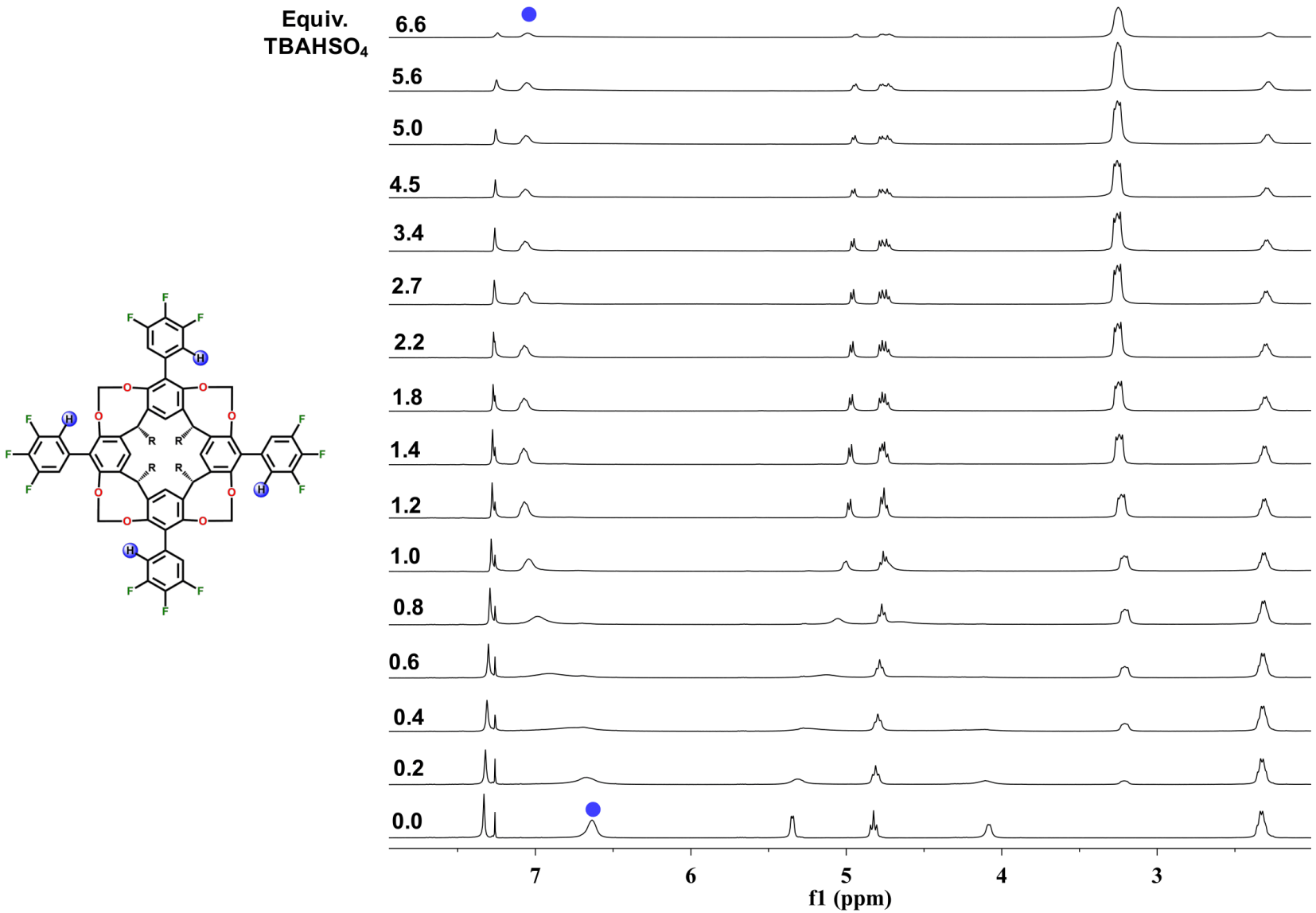


Figure S52. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][HSO$_4$] added to **6** in CDCl$_3$ at 20 °C. Poor data fitting due to broadness, $4 \times 10^4 <$ Ka $< 1 \times 10^5$ M^{-1}.

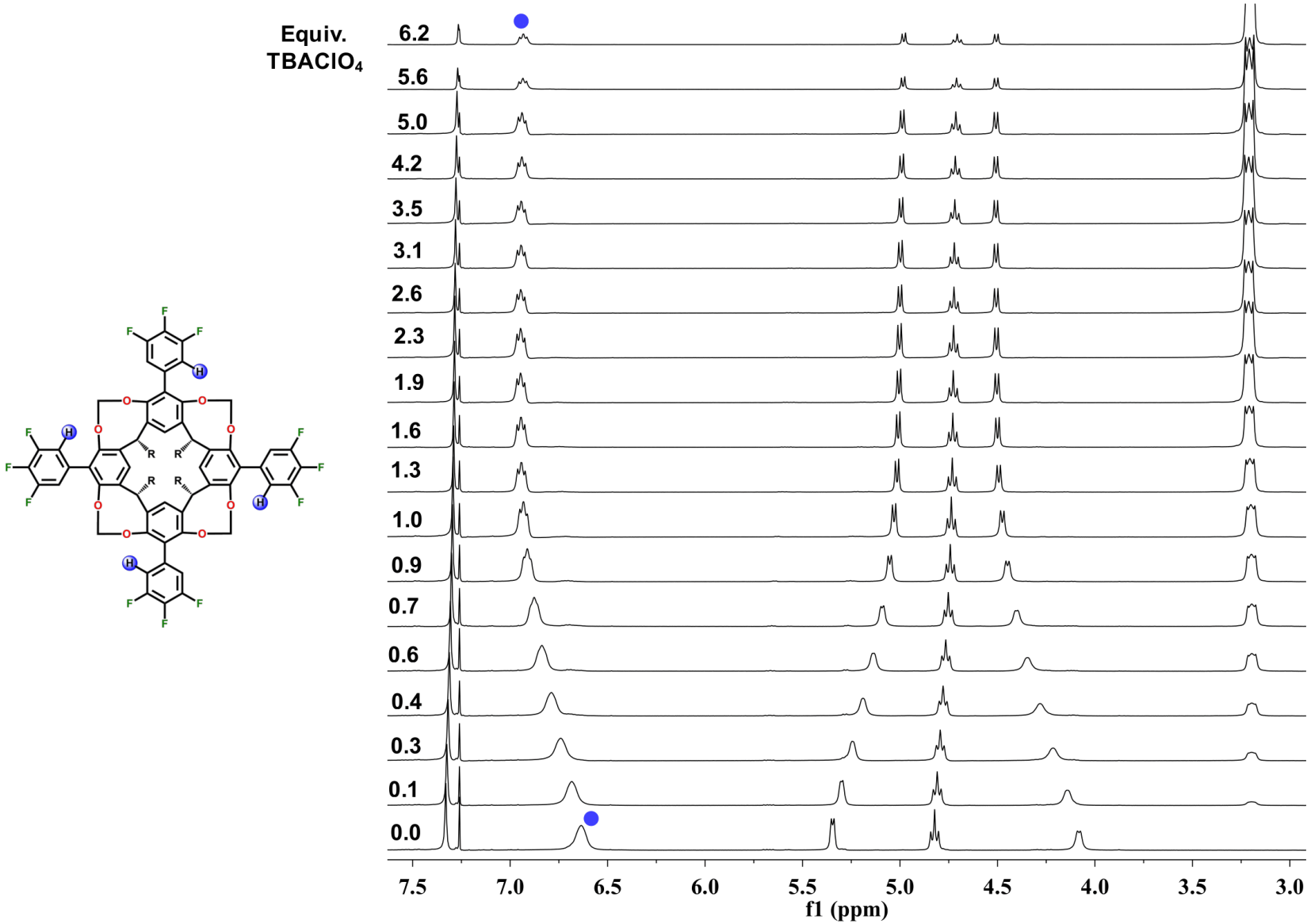


Figure S53. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][ClO$_4$] added to **6** in CDCl$_3$ at 20 °C.

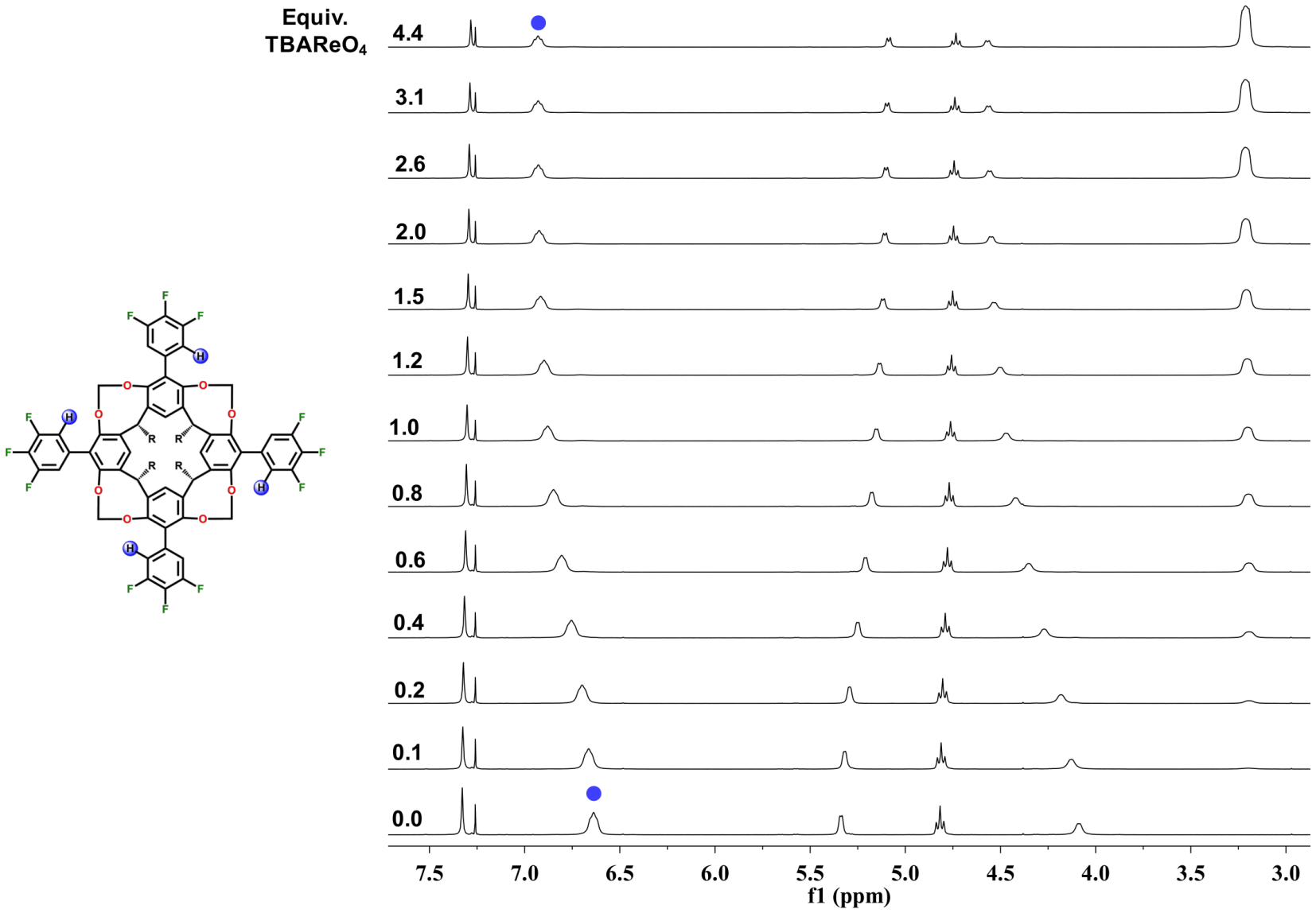


Figure S54. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][ReO$_4$] added to **6** in CDCl$_3$ at 20 °C.

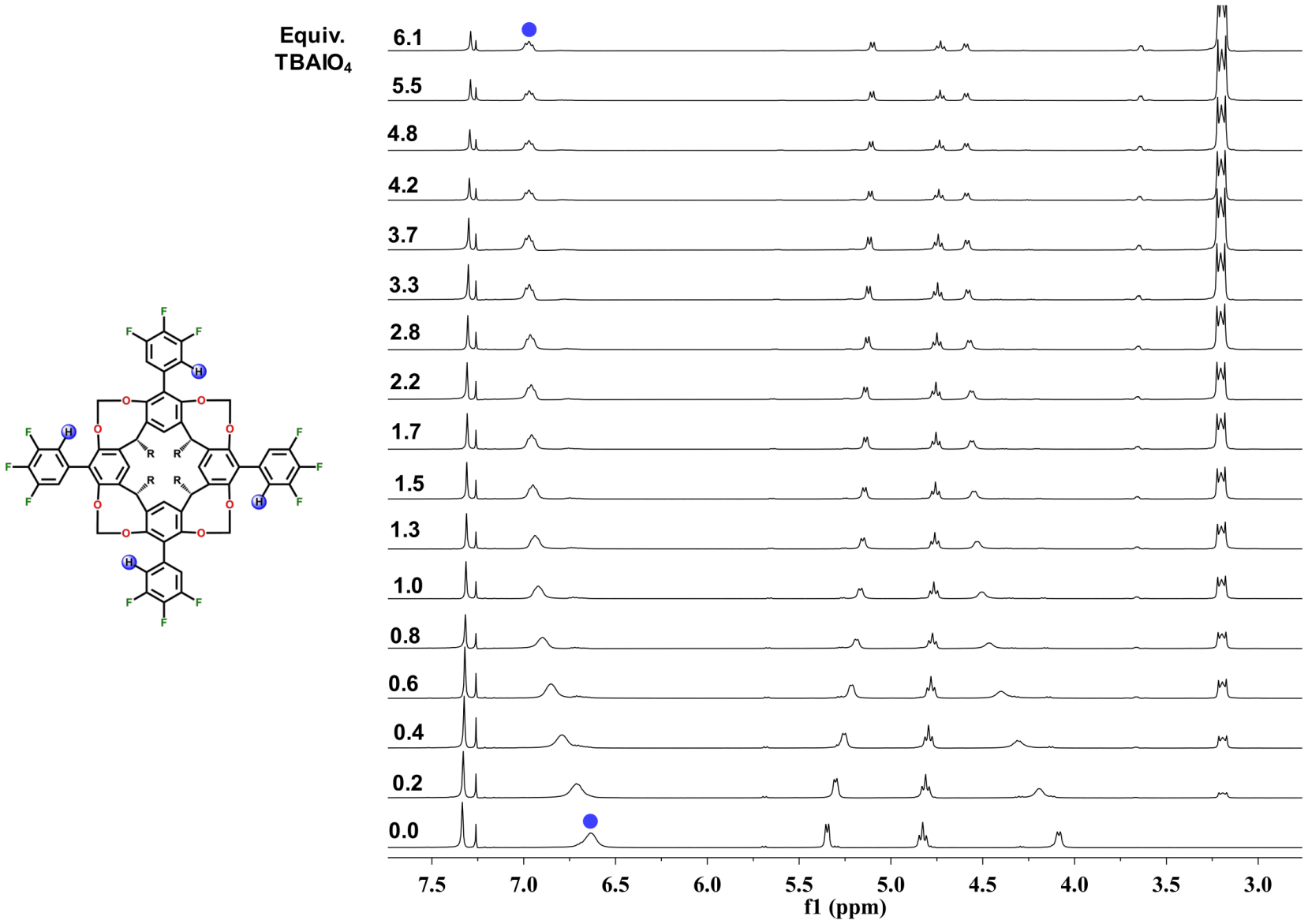


Figure S55. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][IO$_4$] added to **6** in CDCl$_3$ at 20 °C.

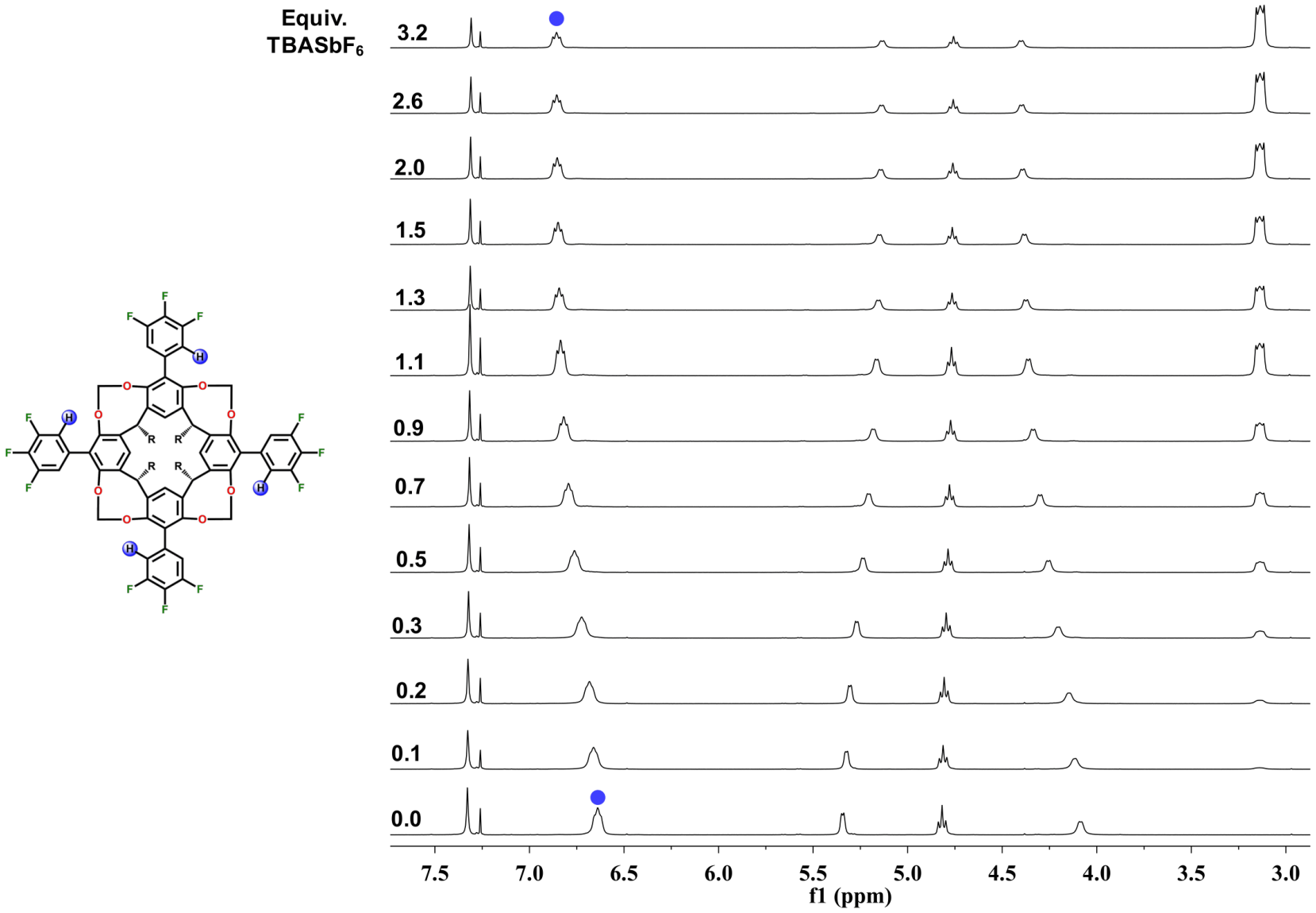


Figure S56. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][SbF$_6$] added to **6** in CDCl$_3$ at 20 °C.

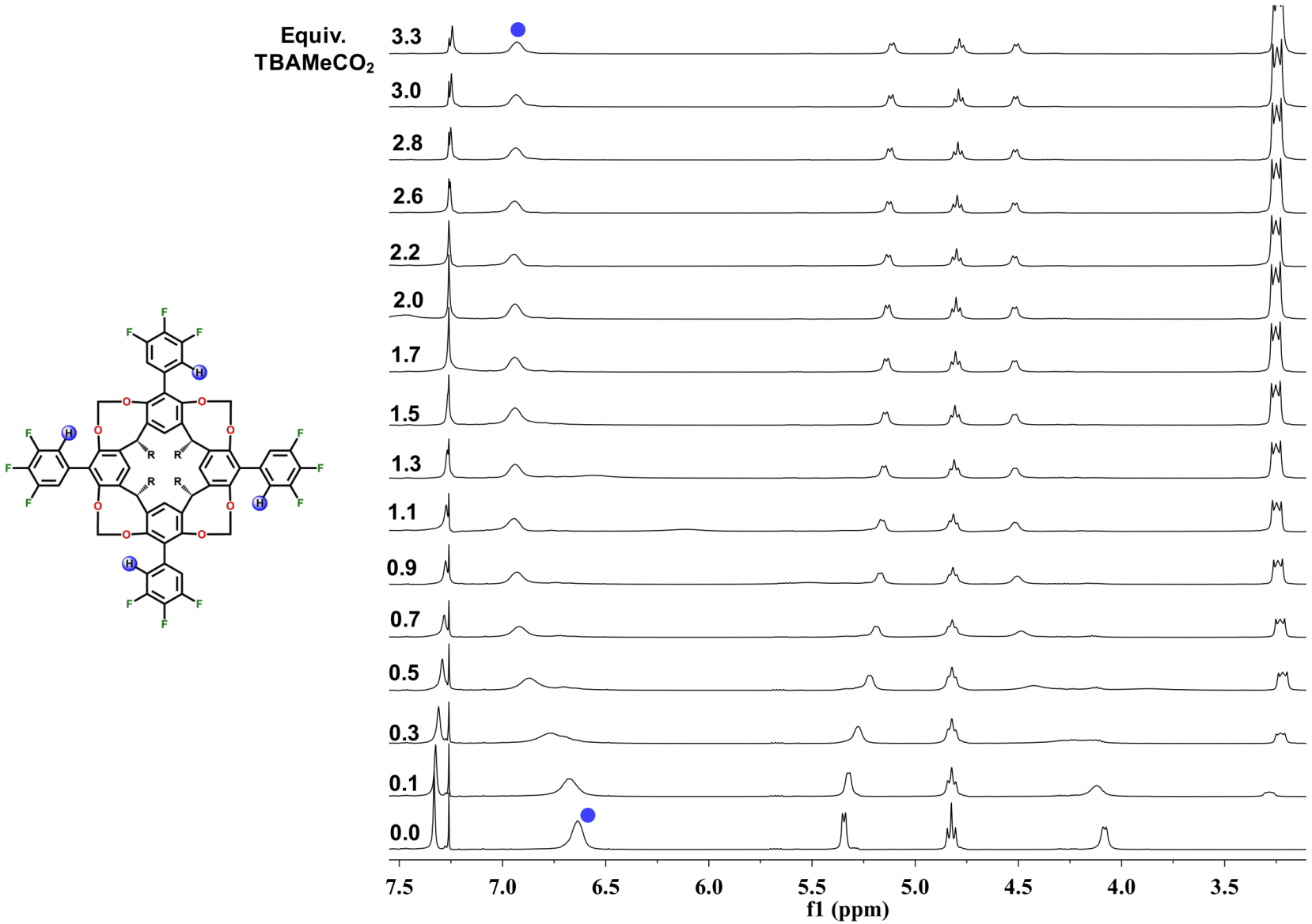


Figure S57. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeCO$_2$] added to **6** in CDCl$_3$ at 20 °C.

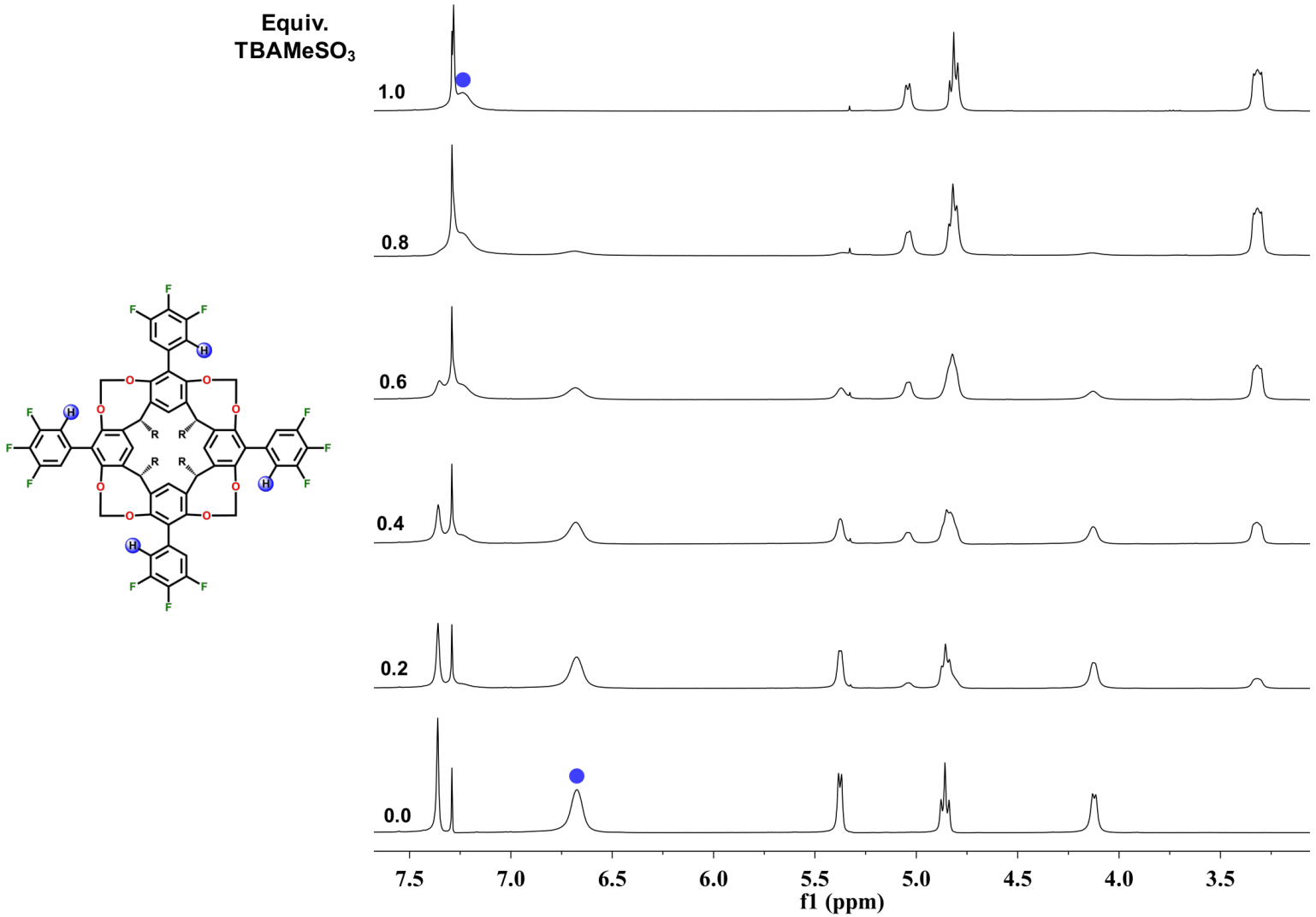


Figure S58. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **6** in CDCl$_3$ at 20 °C.

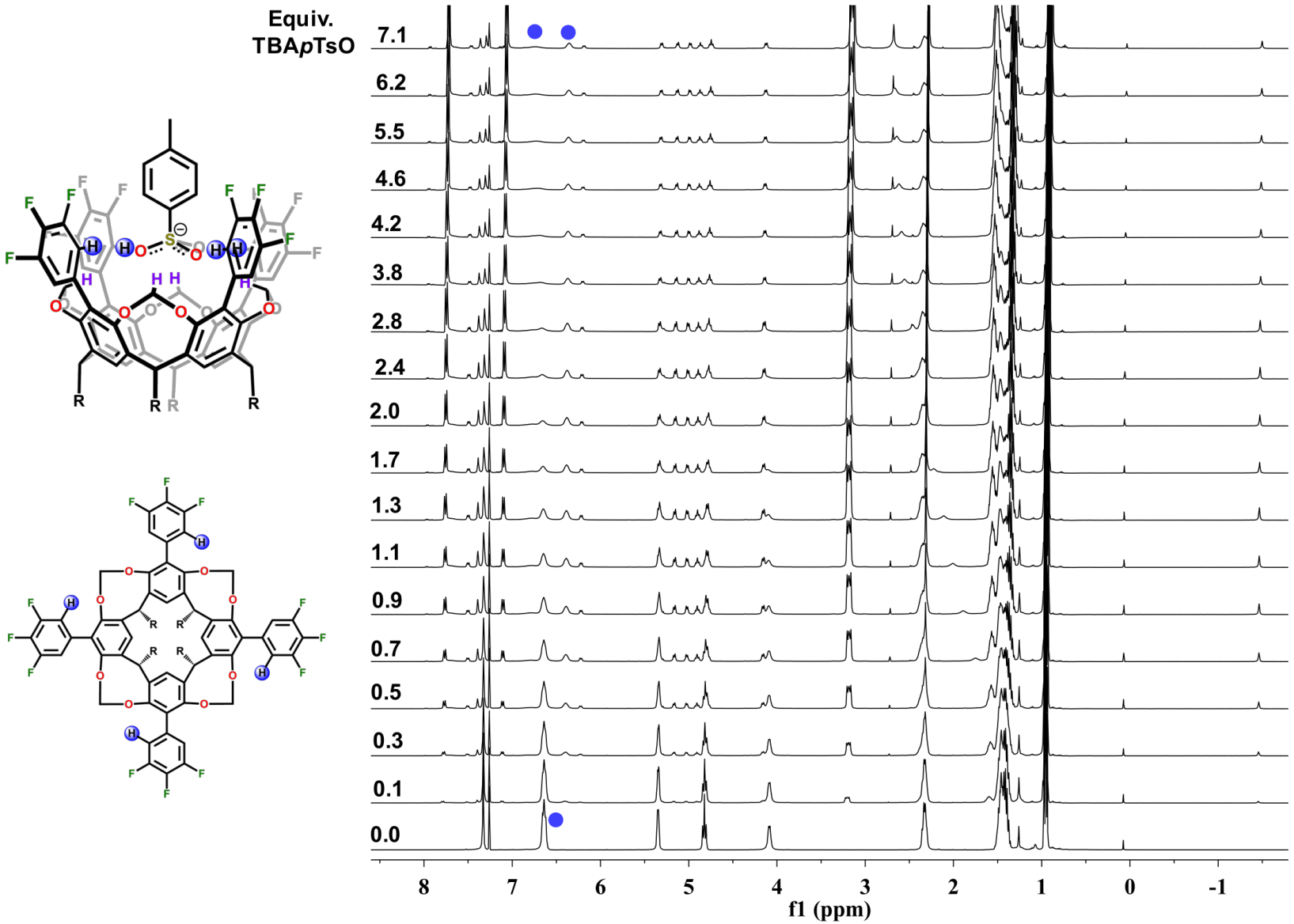


Figure S59. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][*p*TsO] added to **6** in $CDCl_3$ at 20 °C.

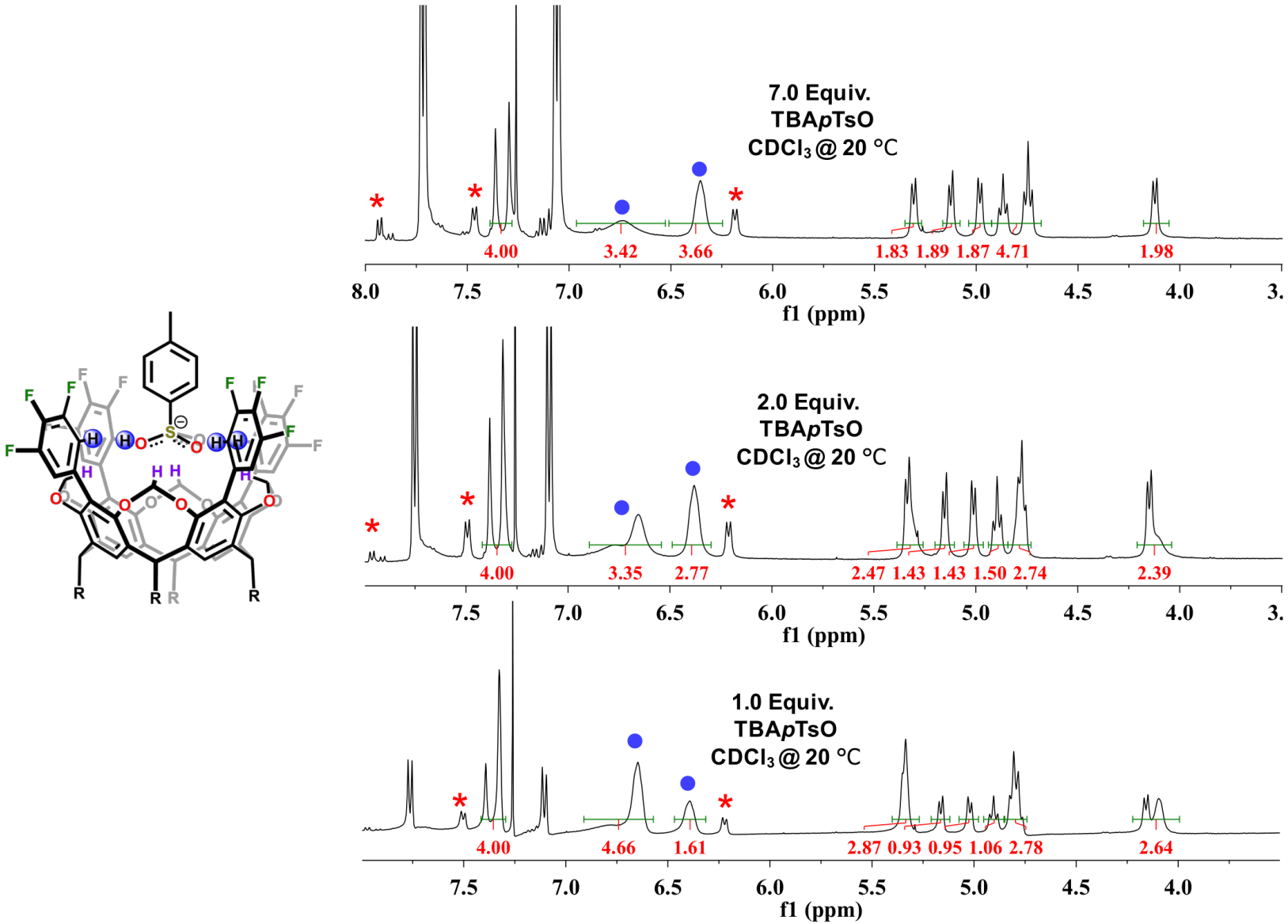


Figure S60. Zoomed-in ^{1}H NMR titration spectra of [*n*-Bu$_4$N][*p*TsO] added to **6** in $CDCl_3$ at 20 °C (asterisk sign shows impurities from [*n*-Bu$_4$N][*p*TsO]).

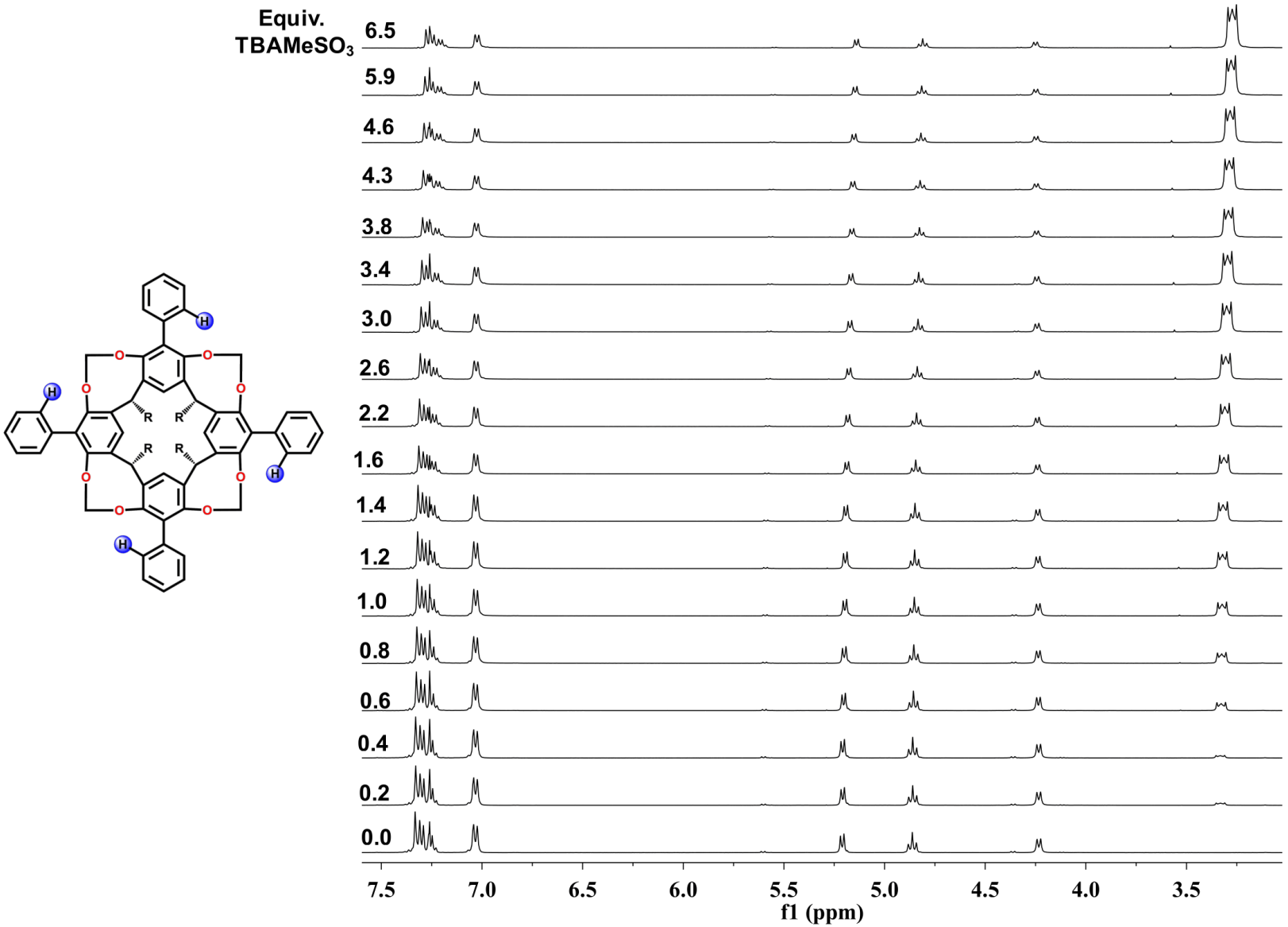


Figure S61. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **1** in CDCl$_3$ at 20 °C.

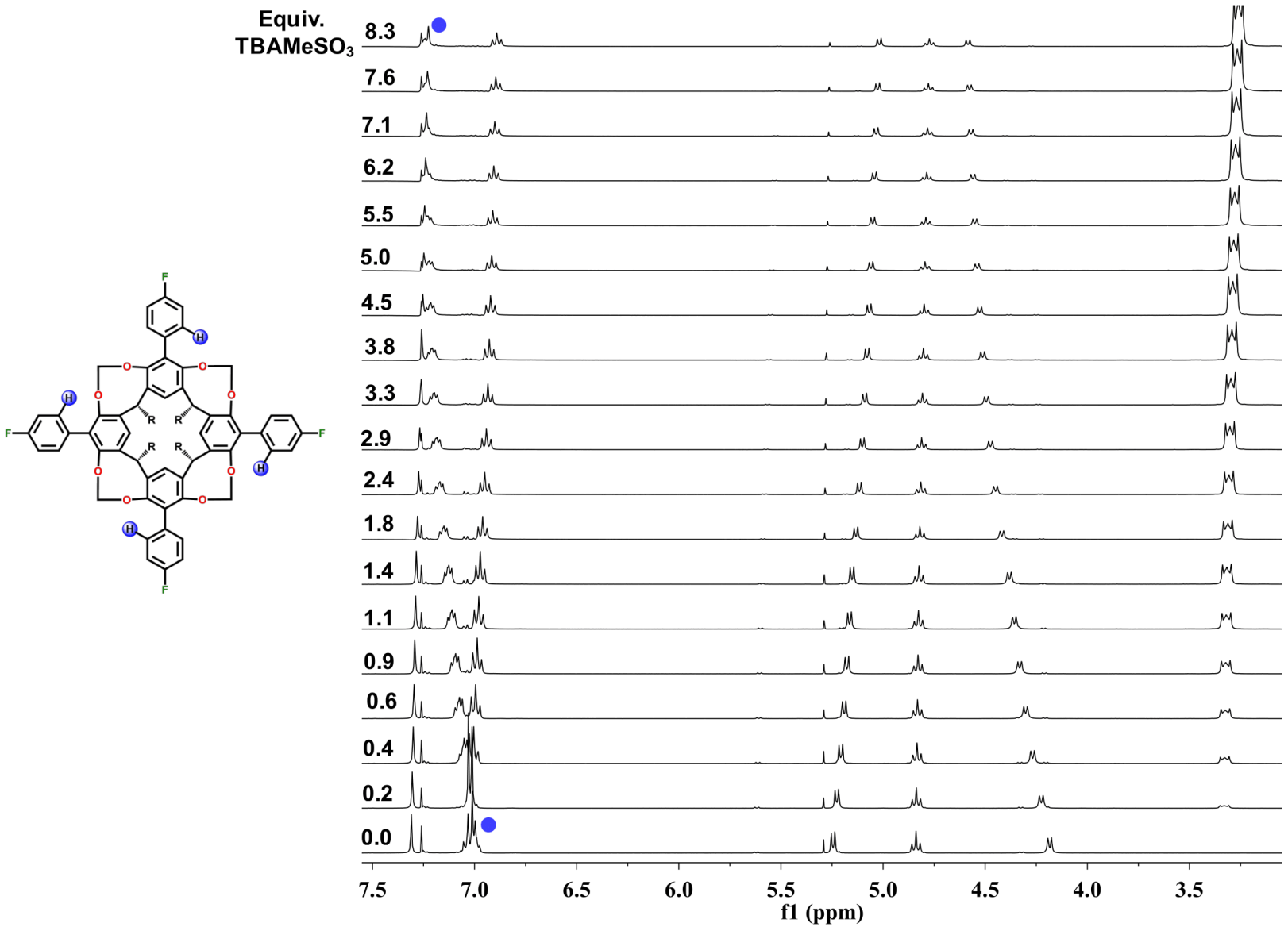


Figure S62. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **2** in CDCl$_3$ at 20 °C.

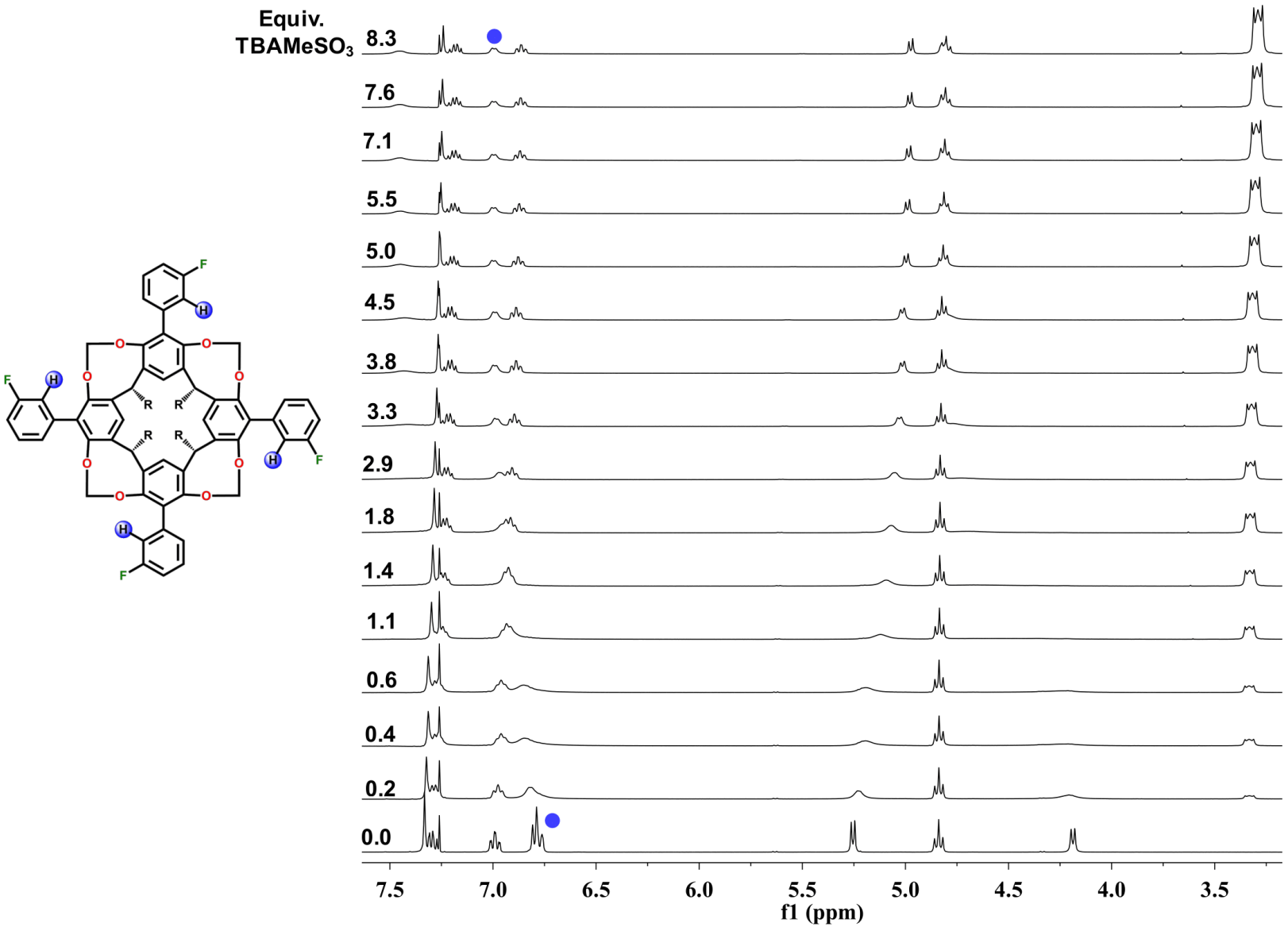


Figure S63. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **3** in CDCl$_3$ at 20 °C.

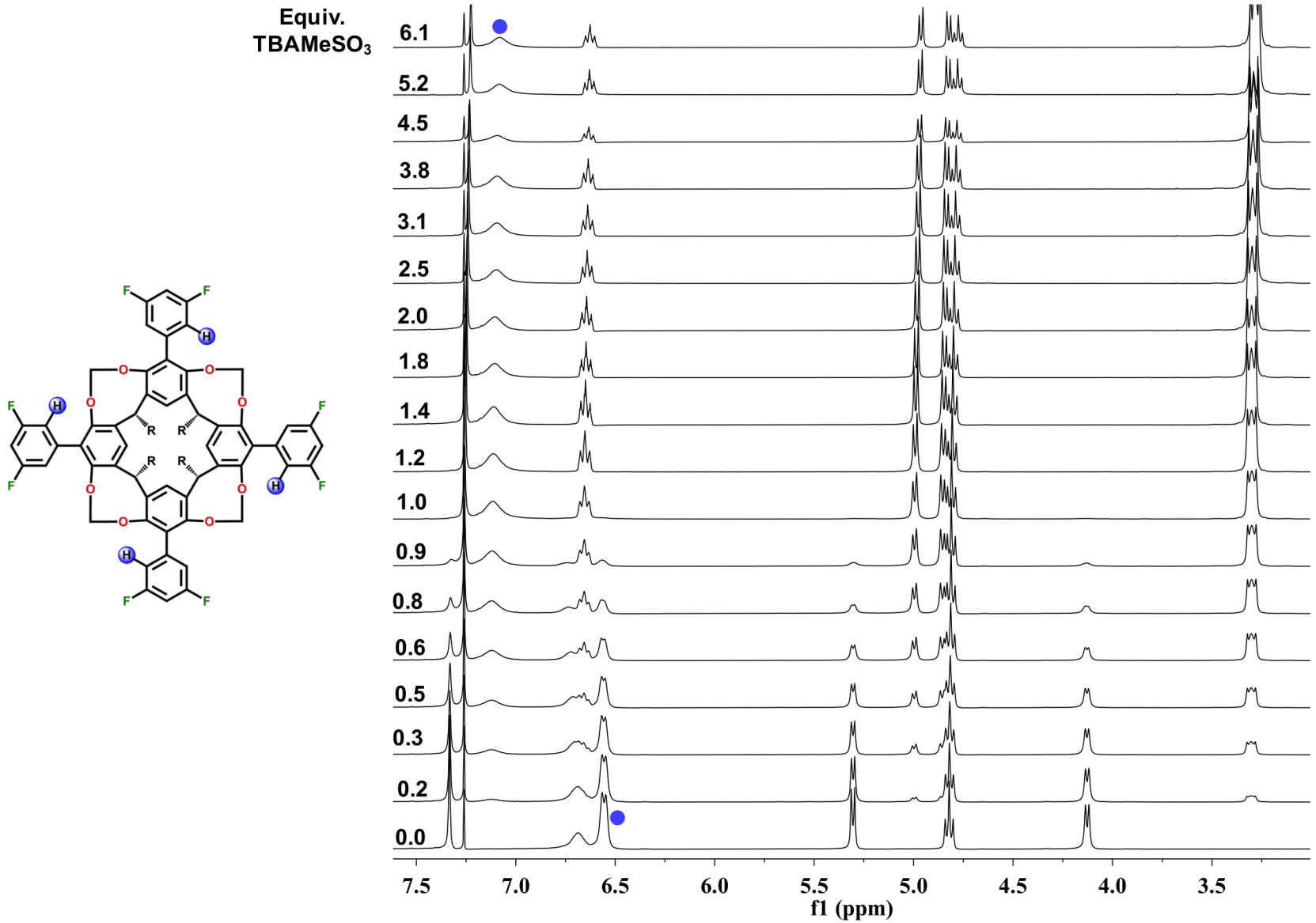


Figure S64. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **4** in CDCl$_3$ at 20 °C.

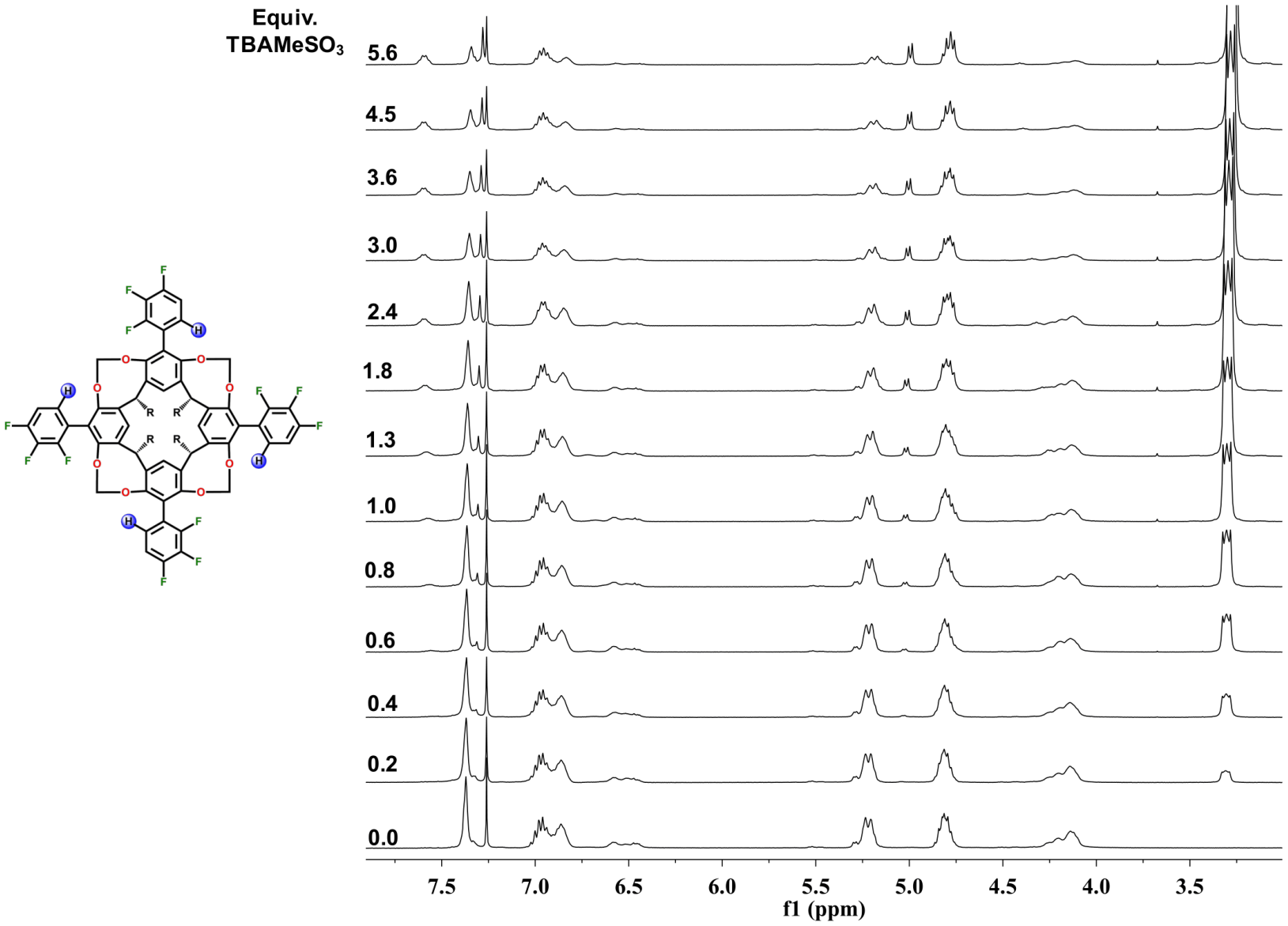


Figure S65. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **5** in CDCl$_3$ at 20 °C.

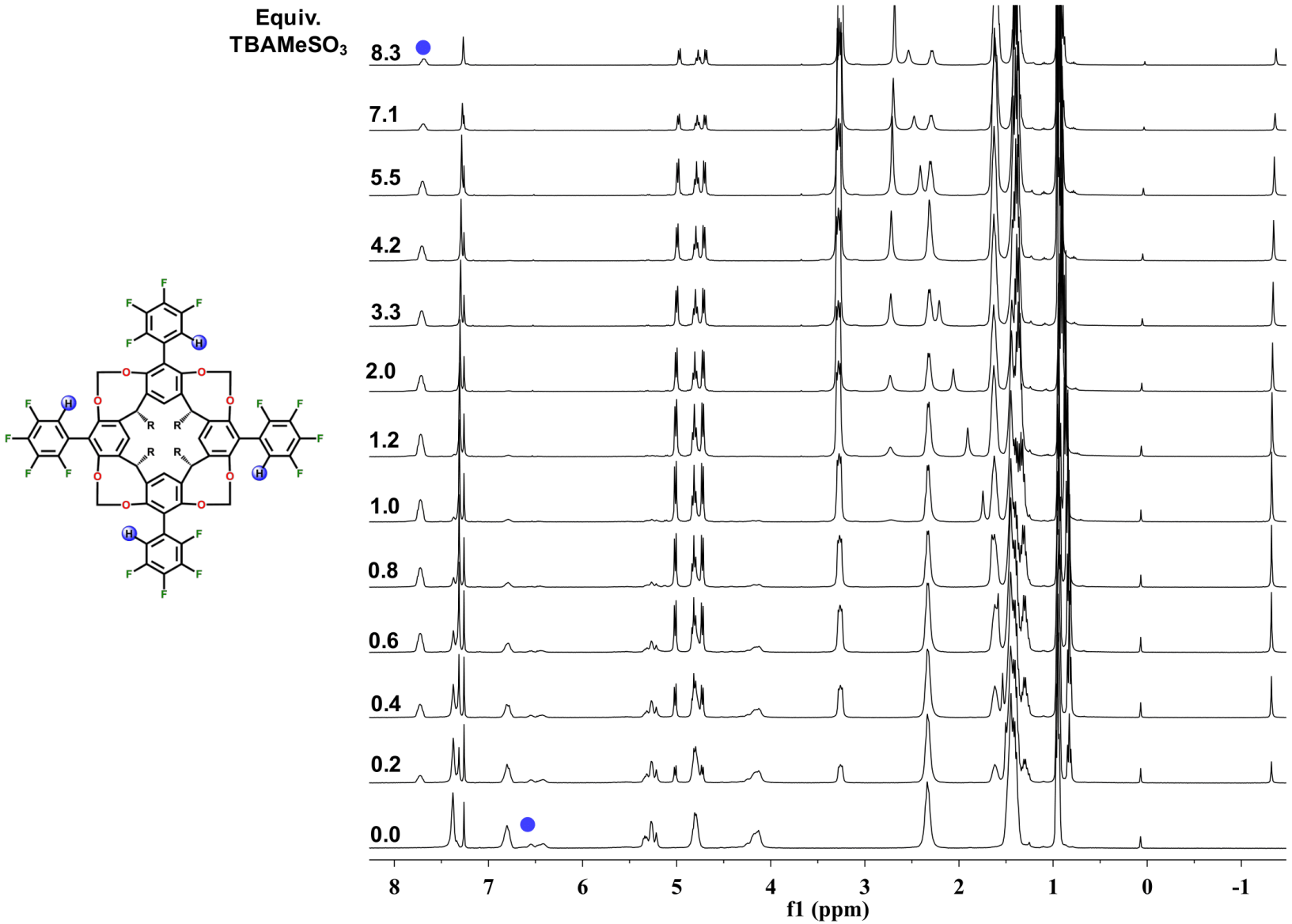


Figure S66. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **7** in CDCl$_3$ at 20 °C.

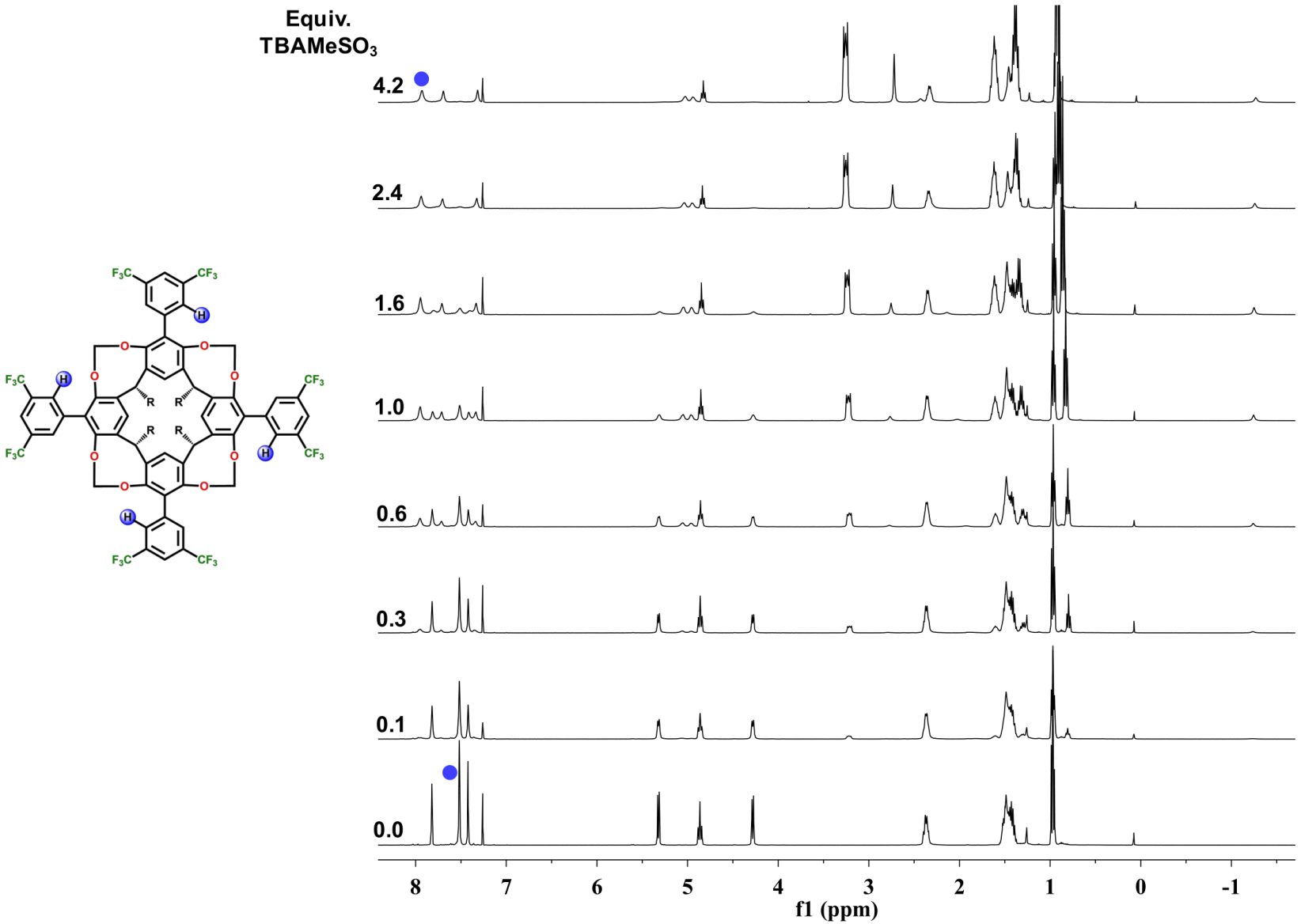


Figure S67. ^{1}H NMR titration spectra of [*n*-Bu$_4$N][MeSO$_3$] added to **8** in CDCl$_3$ at 20 °C.

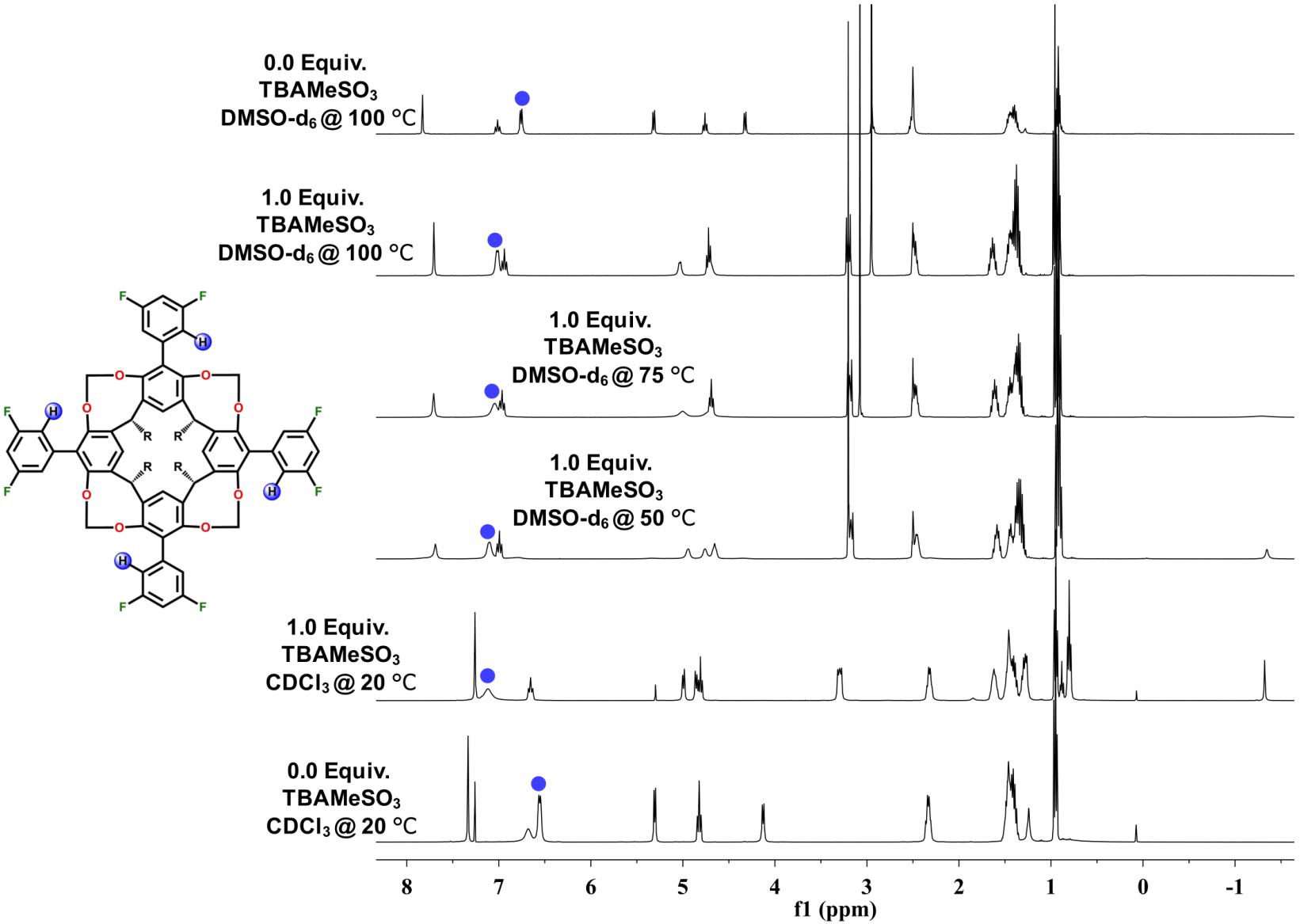


Figure S68. ^{1}H NMR spectra of 1eq [*n*-Bu$_4$N][MeSO$_3$] added to **4** in CDCl$_3$ and DMSO-*d*$_6$.

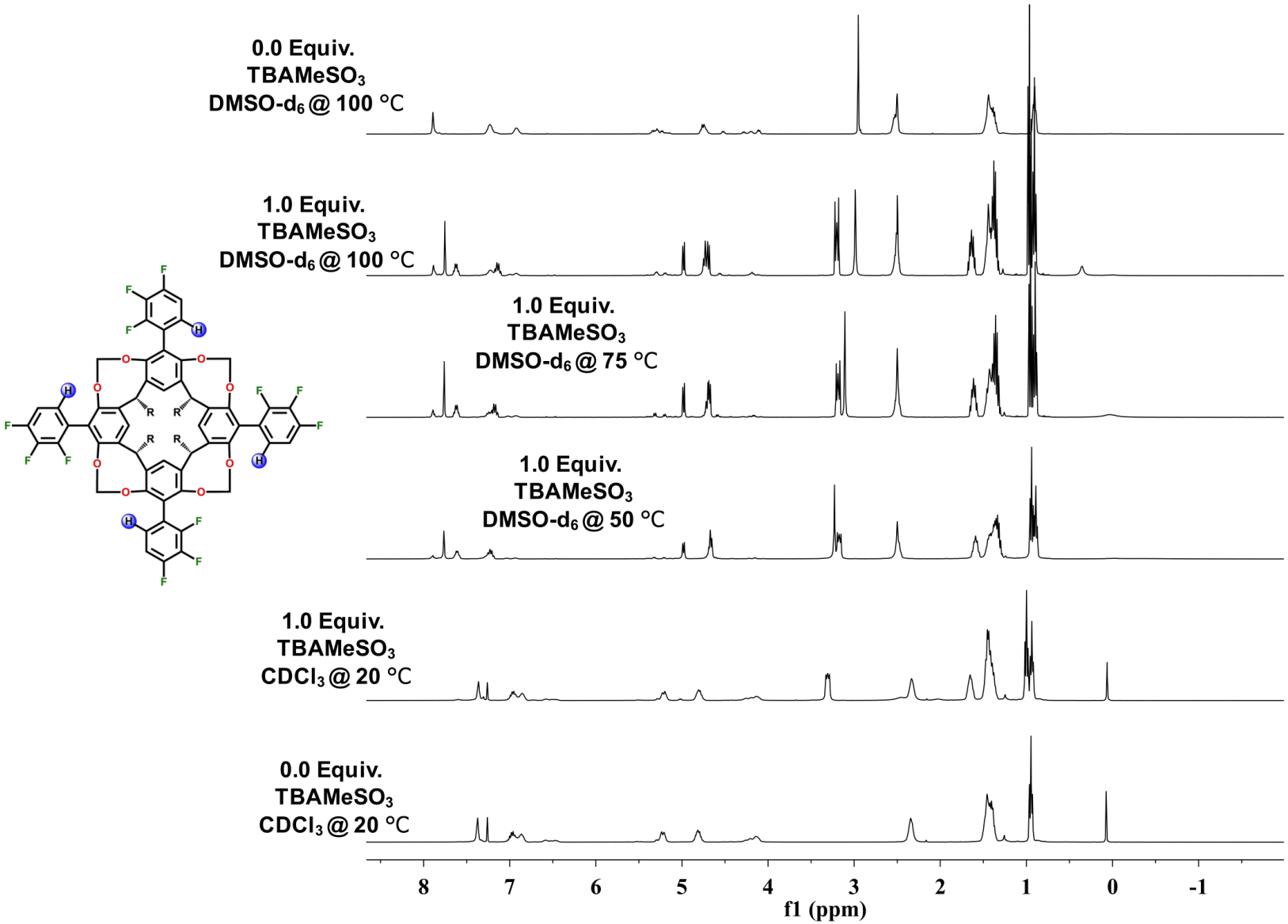


Figure S69. ^{1}H NMR spectra of 1eq [*n*-Bu$_4$N][MeSO$_3$] added to **5** in CDCl$_3$ and DMSO-*d*$_6$.

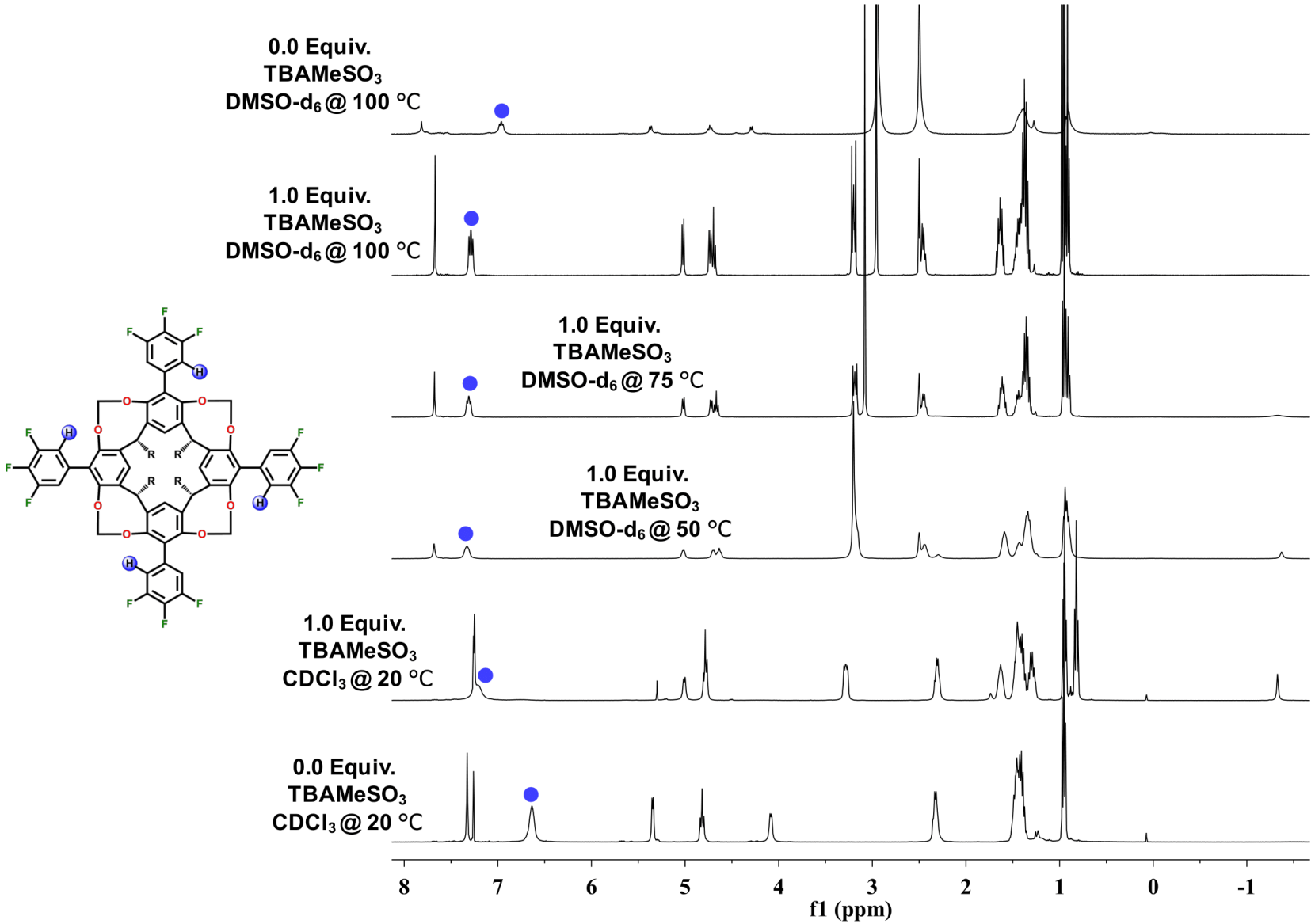


Figure S70. ^{1}H NMR spectra of 1eq [*n*-Bu$_4$N][MeSO$_3$] added to **6** in CDCl$_3$ and DMSO-*d*$_6$.

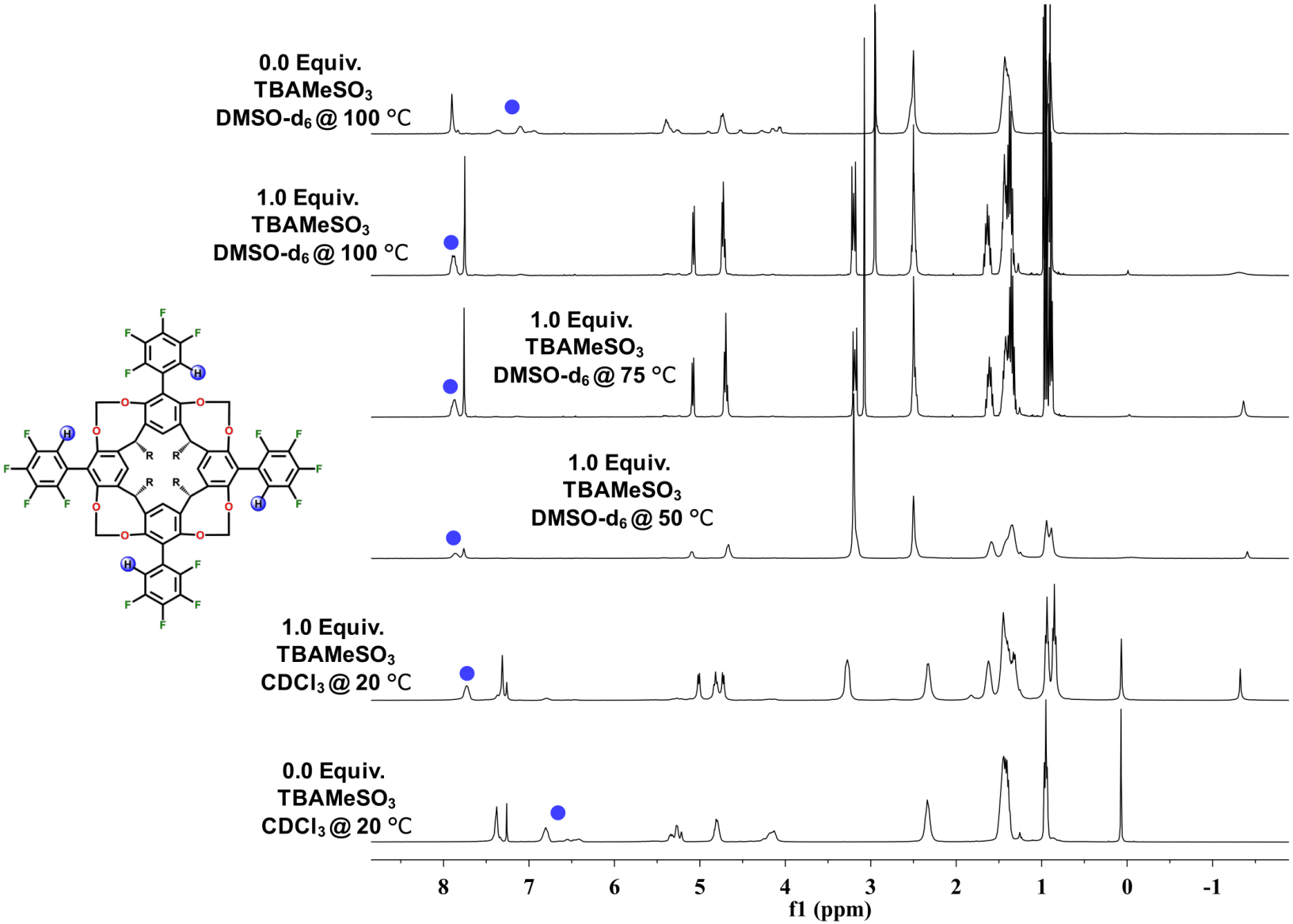
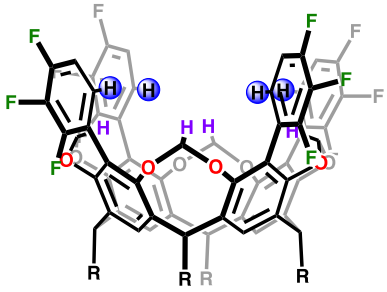
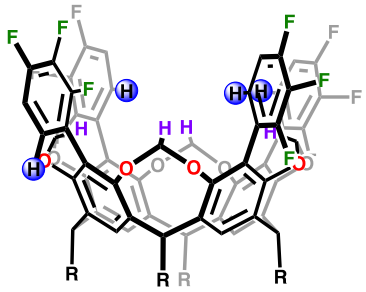


Figure S71. ^{1}H NMR spectra of 1eq [*n*-Bu$_4$N][MeSO$_3$] added to **7** in CDCl$_3$ and DMSO-*d*$_6$.

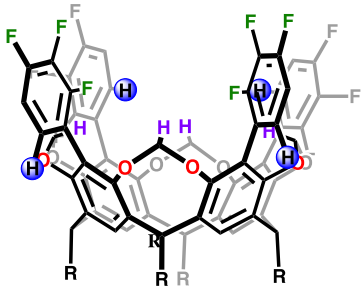
Table S2. DFT calculated conformational energies of the six possible rotamers of **5** at the M062X/6-311++G(3df,2p)+CPCM(solvent)//M062X/6-31+G(d,p) level of theory, where solvent = $CHCl_3$ or DMSO. Provided in this table are the relative energy (ΔE+ZPE), enthalpy (ΔH), and Gibbs free energy (ΔG) for these rotamers.



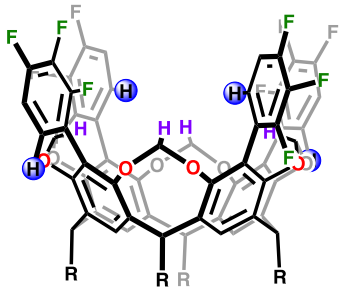
5



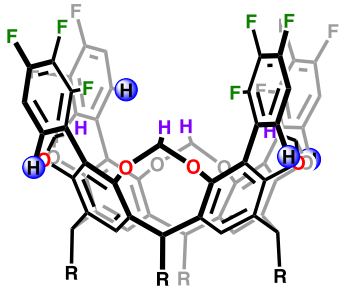
5-1in



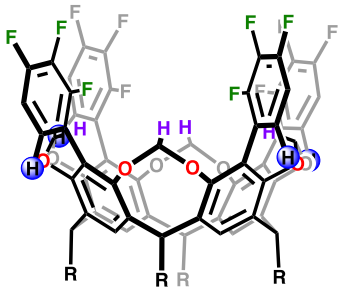
5-2*syn*-in



5-2*anti*-in



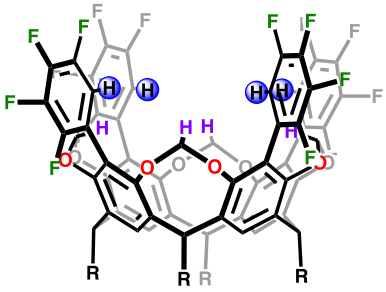
5-3in



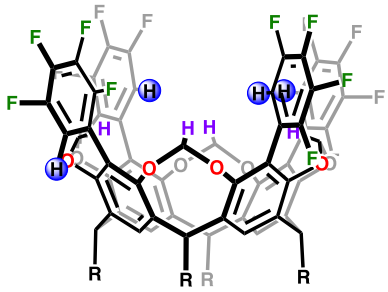
5-4in

Conformational energies in kcal/mol						
			$CHCl_3$			
	5	**5-1in**	**5-2*syn*-in**	**5-2*anti*-in**	**5-3in**	**5-4in**
ΔE+ZPE	0.0	–0.6	–0.7	–0.8	–0.6	–0.1
ΔH	0.0	–0.5	–0.7	–0.8	–0.6	–0.2
ΔG	0.0	–1.8	–0.5	–0.7	–1.1	0.2
			DMSO			
ΔE+ZPE	0.0	0.0	0.4	0.4	0.7	1.3
ΔH	0.0	0.1	0.3	0.3	0.7	1.3
ΔG	0.0	–1.2	0.5	0.5	0.2	1.6

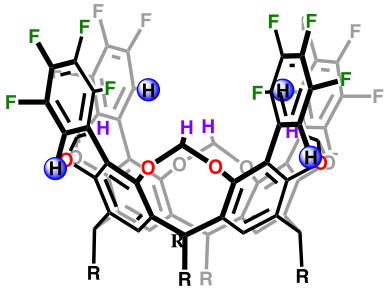
Table S3. DFT calculated conformational energies of the six possible rotamers of **7** at the M062X/6-311++G(3df,2p)+CPCM(solvent)//M062X/6-31+G(d,p) level of theory, where solvent = $CHCl_3$ or DMSO. Provided in this table are the relative energy (ΔE+ZPE), enthalpy (ΔH), and Gibbs free energy (ΔG) for these rotamers.



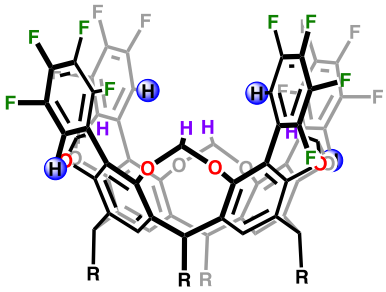
7



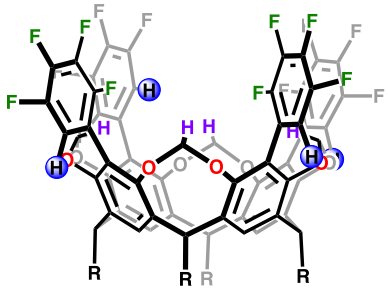
7-1in



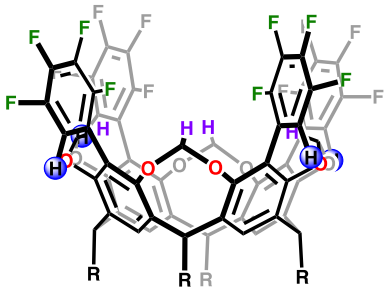
7-2*syn*-in



7-2*anti*-in



7-3in



7-4in

Conformational energies in kcal/mol						
			$CHCl_3$			
	7	**7-1in**	**7-2*syn*-in**	**7-2*anti*-in**	**7-3in**	**7-4in**
ΔE+ZPE	0.0	–0.6	–0.6	–0.7	–0.6	–0.3
ΔH	0.0	–0.5	–0.7	–0.6	–0.7	–0.4
ΔG	0.0	–1.9	–0.3	–2.0	–0.8	–0.4
			DMSO			
ΔE+ZPE	0.0	–0.1	0.2	0.2	0.5	1.0
ΔH	0.0	0.0	0.1	0.2	0.4	0.9
ΔG	0.0	–1.4	0.5	–1.2	0.3	0.9

Table S4. K_as calculated from the slow exchange (Eq. 1) between [*n*-Bu$_4$N][PF$_6$] and **7**, [*n*-Bu$_4$N][*p*TsO] and **6**, and [*n*-Bu$_4$N][MeSO$_3$] and **8** in CDCl$_3$ at 20 °C (Figure S43, S59-S60, and S67).

No. Eq.	*I(HG)*	*I(H)*	*c(H)*	*c(G)*	K_a (M^{-1})	K_a (average, M^{-1})
[*n*-Bu$_4$N][PF$_6$] and **7**						
1.0	0.17	0.38	0.0281	0.0267	1929	$1.64(11) \times 10^3$
1.2	0.15	0.28	0.0275	0.0327	1706	
1.5	0.14	0.22	0.0270	0.0405	1496	
1.9	0.12	0.15	0.0260	0.0489	1416	
[*n*-Bu$_4$N][*p*TsO] and **6**						
0.9	0.68	1.32	0.0294	0.0259	1992	$1.88(4) \times 10^3$
1.2	0.30	0.37	0.0285	0.0339	1873	
1.4	0.28	0.27	0.0282	0.0403	1791	
1.8	0.24	0.16	0.0276	0.0491	1844	
[*n*-Bu$_4$N][MeSO$_3$] and **8**						
0.6	0.28	0.56	0.0291	0.0163	3163	$2.5(2) \times 10^3$
1.0	1.00	0.96	0.0287	0.0287	2479	
1.7	0.19	0.10	0.0285	0.0476	2138	
2.4	0.13	0.04	0.0281	0.0674	2243	

Table S5. DFT calculated rotational barriers of biaryl bonds for hosts **1** – **7** at the M062X/6-311++G(3df,2p)+CPCM(solvent)//M062X/6-31+G(d,p) level of theory, where solvent = $CHCl_3$ or DMSO. Provided in this table are the relative energy (ΔE+ZPE), enthalpy (ΔH), and Gibbs free energy (ΔG) for the rotation of one of the aromatic flanking units around the biaryl bond.

	Rotational barrier in kcal/mol $CHCl_3$							
	1	**2**	**3**	**4**	**5**[a]	**6**	**7**[b]	**8**
ΔE+ZPE	11.0	10.5	10.6	10.2	20.6	9.5	19.9	10.2
ΔH	10.3	9.8	9.9	9.4	19.9	8.8	19.2	9.5
ΔG	12.6	12.5	13.1	13.1	22.7	12.6	22.6	12.9
	DMSO							
ΔE+ZPE	11.2	10.7	11.0	10.4	20.6	9.8	20.0	10.4
ΔH	10.5	10.0	10.2	9.6	19.9	9.0	19.2	9.6
ΔG	12.8	12.7	13.4	13.3	22.8	12.8	22.6	13.0

[a]Data for host **5** was calculated starting from the rotamer **5-4in**. [b]Data for host **7** was calculated starting from the rotamer **7-4in.**

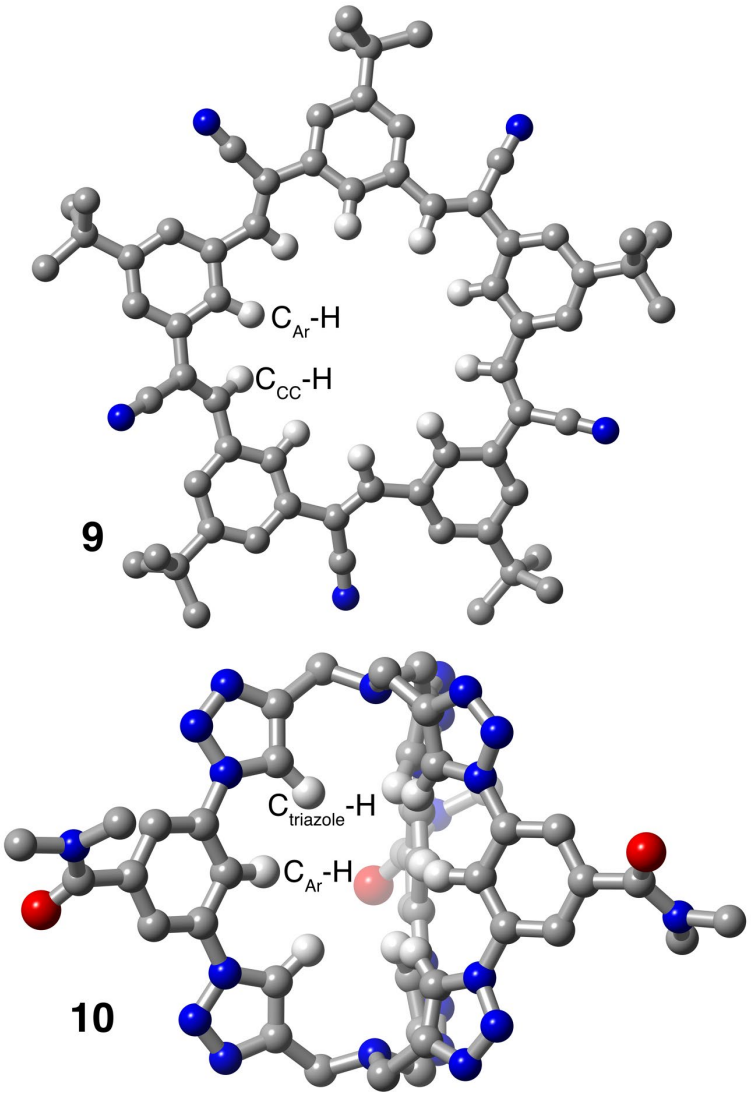


Figure S72. DFT optimized molecular structures for **9** and **10** used for the computation of Hirshfeld charges (HCs). Hydrogen atoms are omitted for clarity, except those within the anion binding cavity. Hirshfeld charges for **9**: C_{Ar}-H = 0.039, and C_{CC}-H = 0.049. Hirshfeld charges for **10**: C_{Ar}-H = 0.042, and $C_{triazole}$-H = 0.053. Note: **10** has been optimized [M062X/6-31+G(d,p)] with Cl as reported by Flood et al.,[20] then the Cl anion has been removed and single point calculations been used for the reported charges; this procedure is used to prevent the huge conformational changes upon the optimization.

Cartesian coordinates of all DFT optimized molecules

1

Zero-point correction= 0.947545 (Hartree/Particle)
Thermal correction to Energy= 1.000611
Thermal correction to Enthalpy= 1.001556
Thermal correction to Gibbs Free Energy= 0.860943
Sum of electronic and zero-point Energies= -2915.100334
Sum of electronic and thermal Energies= -2915.047267
Sum of electronic and thermal Enthalpies= -2915.046323
Sum of electronic and thermal Free Energies= -2915.186935

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O	-1.15664100	4.60623200	4.15235500
O	-4.62610800	1.33972000	4.18972800
O	-4.61889000	-1.01002800	4.14638200
O	-1.35490600	-4.47744900	4.32785600
O	0.99533800	-4.47344400	4.30664900
O	4.46215400	-1.20517100	4.41170400
O	4.45660800	1.14304700	4.30980500
C	2.78950900	2.84259100	4.25223000
C	1.71258400	3.48593300	4.87429000
C	0.05650200	4.42576600	3.46127800
C	-1.74072700	3.51358400	4.75813100
C	-2.85574800	2.93796400	4.13326200
C	-3.50474200	1.88150400	4.78386000
C	-4.43110500	0.17957700	3.41739800
C	-3.53234900	-1.57427700	4.78127700
C	-2.95171000	-2.70933600	4.19858400
C	-1.90168600	-3.33708500	4.87978300
C	-0.18721200	-4.30839200	3.56079600
C	1.55467900	-3.36688400	4.91058100
C	2.69596000	-2.80669300	4.32006600
C	3.31684900	-1.73368500	4.97113000
C	4.29935100	-0.06457700	3.60352100
C	3.34488800	1.72187300	4.88519900
C	1.77024100	1.92241000	6.68030500
C	1.17847300	3.03471200	6.08336300
C	-0.06374400	3.71055000	6.64393100
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C	-1.95815700	1.99820400	6.60162000
C	-3.06487700	1.38705300	6.01386100
C	-3.74604200	0.16378700	6.60865100
C	-3.09699600	-1.08125300	6.01818100
C	-2.03398600	-1.73156900	6.64462200
C	-1.41831100	-2.85725800	6.09920500
C	-0.20100900	-3.51849200	6.72753900
C	1.04966400	-2.88979500	6.12711200
C	1.69396600	-1.80599000	6.72343900
C	2.82520000	-1.20920500	6.16857500
C	3.48126100	0.02839700	6.76167000
C	2.85821100	1.25821800	6.11432700
C	3.32435400	3.35101800	2.95848300
C	3.19031600	2.60329900	1.78494100
C	3.68888300	3.08343900	0.57490800
C	4.32581100	4.32150200	0.52592700
C	4.45480400	5.07816600	1.69041000
C	3.95455700	4.59768100	2.89770000
C	-0.10964000	3.73017600	8.17278300
C	-3.78013000	0.16853800	8.13793400
C	-0.21965700	-3.50101100	8.25703200
H	0.08668400	5.21357200	2.70871900
H	-3.42909100	0.20036400	2.96972500
H	-5.21126800	0.18484600	2.65633600
H	-0.20267300	-3.32129200	3.08095900
H	-0.18613600	-5.11272800	2.82531500
H	5.11056600	-0.08779500	2.87601800
H	3.31687100	-0.09754000	3.11516300
H	1.36766800	1.55818600	7.62042900
H	-0.04037400	4.74829900	6.29686300
H	-1.60275200	1.62659500	7.55774200
H	-4.78050300	0.17551600	6.25127200
H	-1.67103800	-1.34488700	7.59189500
H	-0.21003500	-4.56440900	6.40522400
H	1.29805700	-1.41090600	7.65389600
H	4.52993700	0.00853700	6.44894000
H	2.67780700	1.64550900	1.81682700
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H	-2.78533500	0.17135600	8.59107800
H	-4.30635300	-0.71771200	8.50242000
H	-0.22584000	-2.49148500	8.67632300
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C	-4.05938500	-4.49786000	2.84009400
C	-3.24978800	-2.53048000	1.71146300
C	-4.50901400	-5.00837800	1.62526600
H	-4.18906000	-5.06655700	3.75595600
C	-3.69775800	-3.04066600	0.49393900
H	-2.73877400	-1.57182100	1.74095800
C	-4.33203700	-4.28023500	0.44895800
C	3.25028100	-3.33320300	3.04188000
C	4.50019800	-3.95967700	3.02218900
C	2.54426100	-3.19523400	1.84325900
C	5.02475100	-4.45241900	1.83031900
H	5.05873800	-4.05528500	3.94843300
C	3.06857500	-3.68630200	0.64858700
H	1.58437300	-2.68569300	1.84358500
C	4.30947400	-4.31953200	0.64037100
C	-3.35360600	3.43144000	2.81909300
C	-4.60063000	4.05746900	2.72879900
C	-2.59632700	3.26238900	1.65630500
C	-5.07205300	4.51949300	1.50286300
H	-5.19897000	4.17686100	3.62699500
C	-3.06734500	3.72276600	0.42764000
H	-1.63835500	2.75222400	1.71145900
C	-4.30579100	4.35599000	0.34906600
C	3.45034300	0.06082500	8.29072100
H	3.96063900	-0.81950400	8.69042100
H	3.96073900	0.95613600	8.65558100
H	2.43715600	0.06821300	8.70109000
H	0.76737200	4.25326600	8.56312600
H	-4.30623600	1.05826100	8.49397400
H	-1.11296000	-4.01441500	8.62253000
H	4.04726200	5.18849000	3.80399400
H	0.09245700	3.42834500	3.00437000
H	-1.00789900	4.25253600	8.51262600

H	4.71643900	4.69696100	-0.41461400
H	4.71917200	-4.70433900	-0.28819500
H	-4.68335200	-4.67898700	-0.49748500
H	-4.67409400	4.71690300	-0.60607200
H	-2.46728400	3.58394200	-0.46641800
H	3.57698200	2.49082400	-0.32785200
H	2.50802400	-3.57153100	-0.27407800
H	-3.54860100	-2.47017800	-0.41764300
H	5.99451300	-4.94024400	1.83036600
H	-4.99771400	-5.97727800	1.59677700
H	-6.04018900	5.00746500	1.44811300
H	4.94553300	6.04593500	1.65853700

2

Zero-point correction= 0.914762 (Hartree/Particle)
Thermal correction to Energy= 0.971125
Thermal correction to Enthalpy= 0.972069
Thermal correction to Gibbs Free Energy= 0.823262
Sum of electronic and zero-point Energies= -3311.979731
Sum of electronic and thermal Energies= -3311.923369
Sum of electronic and thermal Enthalpies= -3311.922425
Sum of electronic and thermal Free Energies= -3312.071231

O	1.01351600	4.60346100	4.18641600
O	-1.33856800	4.62320700	4.21600200
O	-4.61754000	1.16222700	4.10466100
O	-4.64054400	-1.18740700	4.20967100
O	-1.17879600	-4.46830000	4.23564800
O	1.16984900	-4.49011700	4.36865400
O	4.45210300	-1.02901900	4.31720200
O	4.47126900	1.32296000	4.37318900
C	2.71635700	2.93773100	4.24171400
C	1.57045600	3.50911900	4.81476400
C	-0.17393100	4.42810600	3.45087700
C	-1.89307500	3.49697400	4.78993900
C	-2.94937300	2.86307400	4.12265400
C	-3.52910100	1.73758500	4.72656000
C	-4.43724300	-0.04822700	3.40903900
C	-3.52013900	-1.72373500	4.81163400
C	-2.88040000	-2.80092300	4.18410500
C	-1.76041900	-3.36074500	4.81672400
C	0.04006700	-4.31101000	3.54910700
C	1.70136600	-3.35134800	4.93972400
C	2.78674900	-2.73352500	4.30413700
C	3.33910300	-1.59276200	4.90549200
C	4.29951100	0.16665300	3.58988800
C	3.32761400	1.87267700	4.91668300
C	1.69879100	1.98535900	6.66050700
C	1.06044200	3.05838500	6.03940400
C	-0.18621500	3.70636000	6.62763500
C	-1.40760100	3.03778300	6.01585200
C	-2.02659200	1.92571600	6.58445600
C	-3.09285500	1.26764200	5.97226300
C	-3.74732700	0.04013500	6.59247500
C	-3.07270900	-1.19970700	6.02588900
C	-1.96632600	-1.80027800	6.62444700
C	-1.30278300	-2.88528200	6.05266700
C	-0.08251900	-3.51989600	6.70666200
C	1.16370400	-2.86408300	6.13238600
C	1.75797900	-1.73881000	6.70119200
C	2.84988200	-1.09473800	6.12027100
C	3.47842900	0.14576200	6.74125800
C	2.82902900	1.37320900	6.12126500
C	3.29545000	3.45087200	2.97000300
C	2.57849700	3.39681200	1.77130000
C	3.12385700	3.87757300	0.58248100
C	4.40168500	4.41156600	0.61607700
C	5.15029600	4.47476400	1.78174000
C	4.58819800	3.98702700	2.95729000
C	-0.20271100	3.72244100	8.15721500
C	-3.77931200	0.07131800	8.12155500
C	-0.13017600	-3.50268600	8.23558800
H	-0.16966600	5.21388200	2.69524200
H	-3.43391800	-0.08897100	2.96488900
H	-5.21644200	-0.06750100	2.64690100
H	0.08737200	-3.32215600	3.07421300
H	0.06701400	-5.11381200	2.81208600
H	5.10815500	0.17021900	2.85876500
H	3.31429600	0.19733200	3.10610300
H	1.29928300	1.61218500	7.59835300
H	-0.19032900	4.74513000	6.28313200
H	-1.66426100	1.55689900	7.53898700
H	-4.78241100	0.02520900	6.23735100
H	-1.60686300	-1.40789900	7.57060700
H	-0.06431700	-4.56587300	6.38526400
H	1.35510400	-1.34825100	7.63047700
H	4.52761800	0.15349200	6.43012200
H	1.58544500	2.95767400	1.75868100
H	-0.21544100	2.72266000	8.59897600
H	-2.78418200	0.07188100	8.57388800
H	-4.31140700	-0.80601100	8.49862500
H	-0.13478100	-2.49351500	8.65566100
H	0.74261600	-4.02278500	8.63899800
C	-3.40167000	-3.33706600	2.89691200
C	-4.69115800	-3.87728100	2.83426000
C	-2.63109900	-3.30002500	1.73122900
C	-5.19802400	-4.38535300	1.64223700
H	-5.30253400	-3.89604800	3.73085800
C	-3.12055700	-3.80135500	0.52668000
H	-1.63956800	-2.85798500	1.75669000
C	-4.39737200	-4.33849100	0.51081300
C	3.34008200	-3.30058800	3.04394000
C	3.87319200	-4.59466400	3.03510400
C	3.32756000	-2.57086800	1.85181800
C	4.39775100	-5.14584300	1.87027700
H	3.87347500	-5.17448900	3.95259800
C	3.84567600	-3.10510900	0.67370200
H	2.89174100	-1.57642500	1.83527400
C	4.37475700	-4.38487800	0.71116700
C	-3.44268700	3.39465000	2.82256500
C	-3.99355800	4.67920300	2.75422300
C	-3.35316100	2.63814000	1.65054400
C	-4.46147000	5.19483200	1.54952300
H	-4.05256600	5.27966200	3.65645800
C	-3.81358500	3.13662800	0.43340700
H	-2.90197300	1.65084500	1.68190200
C	-4.36328400	4.40800700	0.41171700
C	3.44582900	0.14671000	8.27070700
H	3.95026600	-0.74354300	8.65549000

H	3.96181600	1.03208500	8.65134900
H	2.43248700	0.15509900	8.68054900
H	0.68366600	4.23900500	8.53478900
H	-4.29906600	0.96932200	8.46584300
H	-1.03225000	-4.01066800	8.58673800
H	5.15817800	4.01901400	3.88039400
H	-0.19911100	3.42850400	2.99719700
H	-1.09183900	4.25015300	8.51218100
F	4.88007700	-4.91161300	-0.42191900
F	4.93889400	4.88152100	-0.52724000
F	-4.81349600	4.90057900	-0.75932300
F	-4.88152900	-4.82770100	-0.64803300
H	2.57987200	3.84120600	-0.35468200
H	6.14824500	4.89780600	1.75690000
H	3.84170700	-2.55110300	-0.25826700
H	4.81874300	-6.14473700	1.84877000
H	-2.53447100	-3.77833500	-0.38518200
H	-6.19291700	-4.81154300	1.57880100
H	-3.74977200	2.56169200	-0.48361000
H	-4.89543100	6.18603400	1.48114700

3

Zero-point correction= 0.914428 (Hartree/Particle)
Thermal correction to Energy= 0.970958
Thermal correction to Enthalpy= 0.971902
Thermal correction to Gibbs Free Energy= 0.821206
Sum of electronic and zero-point Energies= -3311.980042
Sum of electronic and thermal Energies= -3311.923512
Sum of electronic and thermal Enthalpies= -3311.922568
Sum of electronic and thermal Free Energies= -3312.073264

O	1.18547500	4.61319600	4.26820700
O	-1.16247100	4.60752700	4.15335200
O	-4.62069800	1.33268600	4.17993800
O	-4.61474000	-1.01768800	4.14576800
O	-1.34702200	-4.47751400	4.32553000
O	1.00338600	-4.47936300	4.31789900
O	4.45652100	-1.20127200	4.40199800
O	4.45360500	1.14809900	4.30768200
C	2.78351100	2.84369300	4.25213100
C	1.70551400	3.48691700	4.87140500
C	0.04886200	4.43043500	3.45853700
C	-1.74244600	3.51279800	4.75842900
C	-2.85361200	2.93244200	4.13248200
C	-3.50191700	1.87351700	4.77869000
C	-4.42833300	0.16899900	3.41196900
C	-3.52737600	-1.57764000	4.78216100
C	-2.94170500	-2.70972800	4.20041800
C	-1.89079100	-3.33724600	4.87935300
C	-0.17430400	-4.31716500	3.56397500
C	1.55810900	-3.36953500	4.91902500
C	2.69376300	-2.80407300	4.32501600
C	3.31433000	-1.72750100	4.96867900
C	4.29547400	-0.05738600	3.59805100
C	3.34202400	1.72482700	4.88440800
C	1.76838000	1.92594200	6.67958400
C	1.17383600	3.03654700	6.08198400
C	-0.06766800	3.71198000	6.64465700
C	-1.29116100	3.06692600	6.00713500
C	-1.96057100	1.99686700	6.60060000
C	-3.06443400	1.38214500	6.01090400
C	-3.74567400	0.15992500	6.60778600
C	-3.09427000	-1.08463300	6.01942700
C	-2.03117100	-1.73445000	6.64633500
C	-1.41186000	-2.85845400	6.10121600
C	-0.19683400	-3.51931800	6.73455400
C	1.05391800	-2.89076000	6.13473300
C	1.69767600	-1.80425600	6.72693400
C	2.82569100	-1.20445900	6.16821800
C	3.48204200	0.03318400	6.76085100
C	2.85668800	1.26189200	6.11396100
C	3.31992900	3.35053400	2.95823000
C	3.16411400	2.61361300	1.77978000
C	3.66723700	3.09394800	0.57159400
C	4.33030900	4.31739900	0.51925000
C	4.46458100	5.03451400	1.69894000
C	3.97435600	4.58399800	2.91352500
C	-0.11249200	3.73078400	8.17345200
C	-3.78122400	0.16717300	8.13693800
C	-0.21862200	-3.49876600	8.26384500
H	0.07765800	5.22267100	2.71077000
H	-3.42754100	0.18670400	2.96109200
H	-5.21114900	0.17227200	2.65381500
H	-0.18312500	-3.33406400	3.07547800
H	-0.17193200	-5.12795500	2.83589200
H	5.10747800	-0.07971500	2.87157000
H	3.31311500	-0.08696100	3.10890400
H	1.36816000	1.56344800	7.62135100
H	-0.04529200	4.74988500	6.29790800
H	-1.60767500	1.62756700	7.55850800
H	-4.77978200	0.17019300	6.24921700
H	-1.67170700	-1.34939100	7.59555700
H	-0.20520100	-4.56582300	6.41398500
H	1.30426700	-1.40955100	7.65860100
H	4.53028000	0.01403400	6.44644600
H	2.63372500	1.66647600	1.80784600
H	-0.12425000	2.73159400	8.61667200
H	-2.78696200	0.16992400	8.59122300
H	-4.30860300	-0.71802200	8.50206200
H	-0.22285900	-2.48847400	8.68129200
H	0.66168800	-4.01444200	8.65644100
C	-3.42181300	-3.24626500	2.89633400
C	-4.08796200	-4.47340600	2.85314700
C	-3.20079300	-2.54325600	1.70770500
C	-4.52435200	-4.95174200	1.62868100
H	-4.26357400	-5.05166700	3.75372100
C	-3.65111700	-3.05094500	0.48984300
H	-2.66116800	-1.60129400	1.73641700
C	-4.32517400	-4.26842000	0.43820900
C	3.23982700	-3.33175500	3.04338200
C	4.45326100	-4.02355400	3.03798200
C	2.55830400	-3.13123900	1.83874100
C	4.94017600	-4.50475100	1.83380500
H	5.01432100	-4.18503100	3.95199800
C	3.07419900	-3.62683900	0.64201900
H	1.62669000	-2.57302400	1.83828700
C	4.27821900	-4.32635200	0.62803400
C	-3.34782100	3.42680500	2.81704700
C	-4.57880500	4.08296300	2.74036900

C	-2.60181600	3.22951500	1.65065700
C	-5.01798100	4.53343200	1.50640200
H	-5.18981900	4.24015400	3.62253300
C	-3.07067600	3.69357100	0.42241200
H	-1.65678500	2.69728900	1.70421300
C	-4.29164400	4.35795000	0.33786400
C	3.45343600	0.06582800	8.28987000
H	3.96393900	-0.81455700	8.68894300
H	3.96528000	0.96066900	8.65359000
H	2.44095600	0.07415400	8.70192500
H	0.76476000	4.25351400	8.56349300
H	-4.30735800	1.05752500	8.49109100
H	-1.11364800	-4.00944000	8.62869600
H	4.09985300	5.18817000	3.80543400
H	0.08277600	3.43538100	2.99606400
H	-1.01011600	4.25362600	8.51395200
F	6.10899500	-5.17501400	1.83421800
F	-5.17005600	-6.13387800	1.59284300
F	-6.20402800	5.16940500	1.43854200
F	5.09895000	6.22276300	1.66204700
H	4.73446100	4.71849000	-0.40317200
H	4.70573100	-4.72572400	-0.28455000
H	-4.68926400	-4.69016600	-0.49165800
H	-4.68385800	4.73223300	-0.60084700
H	-2.48274100	3.53597800	-0.47605600
H	3.54150300	2.51308100	-0.33644900
H	2.53645200	-3.46688900	-0.28695700
H	-3.47524300	-2.49630000	-0.42622400

4

Zero-point correction= 0.881336 (Hartree/Particle)
Thermal correction to Energy= 0.941424
Thermal correction to Enthalpy= 0.942368
Thermal correction to Gibbs Free Energy= 0.782132
Sum of electronic and zero-point Energies= -3708.854771
Sum of electronic and thermal Energies= -3708.794684
Sum of electronic and thermal Enthalpies= -3708.793740
Sum of electronic and thermal Free Energies= -3708.953975

O	1.07093500	4.59443000	4.20574200
O	-1.27906600	4.61348200	4.19256700
O	-4.60976400	1.21750300	4.13047400
O	-4.62939600	-1.13157500	4.19658000
O	-1.23377100	-4.46253600	4.27371500
O	1.11491600	-4.48066900	4.36004000
O	4.44772200	-1.08589600	4.35097800
O	4.46519800	1.26430700	4.35637500
C	2.72828100	2.88935800	4.25299800
C	1.60775900	3.49233200	4.83583700
C	-0.10142700	4.42243100	3.44534700
C	-1.83646100	3.50108100	4.78636600
C	-2.90360200	2.87427300	4.13491300
C	-3.51239100	1.77489600	4.75081200
C	-4.43229500	0.02016200	3.41144300
C	-3.52190000	-1.66860600	4.81774600
C	-2.89040700	-2.75726000	4.20765600
C	-1.79592800	-3.34492100	4.85218900
C	-0.03026800	-4.30965200	3.55928000
C	1.64765600	-3.35327600	4.94822800
C	2.74237300	-2.74353100	4.32694300
C	3.32515700	-1.62801900	4.93899900
C	4.30058900	0.09219900	3.59416000
C	3.33305200	1.81682300	4.91650700
C	1.72709000	1.97150300	6.68085700
C	1.09787600	3.05228300	6.06289700
C	-0.14483100	3.71397100	6.64262700
C	-1.36751600	3.05247200	6.02430100
C	-2.00696600	1.95661800	6.60337400
C	-3.08287200	1.30698400	5.99815500
C	-3.74935400	0.08446200	6.61405400
C	-3.08280900	-1.15822100	6.04262400
C	-1.99150900	-1.77769200	6.65131000
C	-1.33768800	-2.87353400	6.08795100
C	-0.12076000	-3.51890600	6.73633600
C	1.12691800	-2.87256200	6.15295200
C	1.74159200	-1.76126800	6.72947400
C	2.84308900	-1.12762700	6.15409700
C	3.48362200	0.11064600	6.76583400
C	2.84273500	1.33759500	6.13452000
C	3.27571600	3.38038600	2.95695300
C	2.63714700	3.05287200	1.75773600
C	3.16992400	3.52560600	0.56693000
C	4.31158900	4.30836000	0.50956700
C	4.91767200	4.60552400	1.72192800
C	4.43252600	4.16220900	2.94207200
C	-0.16961600	3.73605500	8.17174700
C	-3.78402900	0.11133200	8.14289000
C	-0.16040400	-3.50100500	8.26522300
H	-0.08750900	5.21400600	2.69687800
H	-3.43357900	-0.00581200	2.95575800
H	-5.21816500	0.00873300	2.65695300
H	-0.00001400	-3.32689100	3.07039900
H	-0.01299300	-5.12051700	2.83185000
H	5.11728300	0.08462900	2.87311900
H	3.32175900	0.10537600	3.09669500
H	1.33184100	1.60906400	7.62476400
H	-0.13857300	4.75118500	6.29273800
H	-1.65265000	1.59387900	7.56328800
H	-4.78362800	0.07857700	6.25554400
H	-1.63617400	-1.39097800	7.60143300
H	-0.11242500	-4.56490600	6.41376400
H	1.34662400	-1.37336900	7.66333700
H	4.53234600	0.10762500	6.45217200
H	1.74727500	2.43282400	1.73715200
H	-0.18396500	2.73779700	8.61696500
H	-2.78947900	0.11151700	8.59656100
H	-4.31686100	-0.76649400	8.51756100
H	-0.16412000	-2.49142700	8.68440000
H	0.71408900	-4.02062100	8.66537600
C	-3.38194100	-3.28097200	2.90198100
C	-4.53242100	-4.07091900	2.85768500
C	-2.69684500	-2.97577600	1.72275000
C	-4.96472300	-4.54443100	1.62903700
H	-5.08560200	-4.31327900	3.75762200
C	-3.17788800	-3.47824600	0.52209700
H	-1.81034300	-2.35055200	1.72471600
C	-4.31158900	-4.26989300	0.43594600
C	3.27724400	-3.27929900	3.04342200
C	4.07062800	-4.42826100	3.04555800

C	2.97926600	-2.63686700	1.83861500
C	4.55463000	-4.90203100	1.83642000
H	4.30784200	-4.94864000	3.96620600
C	3.49213000	-3.15825400	0.65940600
H	2.35199600	-1.75245100	1.80482500
C	4.28739300	-4.29198100	0.61910000
C	-3.38208900	3.37571900	2.81570400
C	-4.16844900	4.52777700	2.75249500
C	-3.03749500	2.69857800	1.64268900
C	-4.59891700	4.96954400	1.51143100
H	-4.44057500	5.07505800	3.64752800
C	-3.49789800	3.18886600	0.42897000
H	-2.41362600	1.81129200	1.65957300
C	-4.28457500	4.32439900	0.32378900
C	3.45260700	0.12357800	8.29498200
H	3.95769400	-0.76373900	8.68544200
H	3.96875600	1.01150400	8.66922200
H	2.43947000	0.13398700	8.70537100
H	0.71501100	4.25399900	8.55131600
H	-4.30439800	1.00857600	8.48799700
H	-1.06066600	-4.00916300	8.62051300
H	4.95039300	4.42126000	3.85824700
H	-0.11186900	3.42720800	2.98148400
H	-1.06005900	4.26532400	8.52085200
F	5.32075300	-6.00622400	1.83573100
F	3.20346600	-2.53803500	-0.49811000
F	-2.51664600	-3.18266800	-0.61069300
F	-6.07035900	-5.30710900	1.58381600
F	-3.16448400	2.53510900	-0.69768300
F	-5.35789100	6.07681600	1.44793600
F	2.55317000	3.20884300	-0.58512500
F	6.02946200	5.36038400	1.70494300
H	4.71108000	4.66689500	-0.43088100
H	4.67746000	-4.68265700	-0.31245300
H	-4.67036100	-4.65174600	-0.51171700
H	-4.63327300	4.69046800	-0.63381000

6

Zero-point correction= 0.849572 (Hartree/Particle)
Thermal correction to Energy= 0.913411
Thermal correction to Enthalpy= 0.914356
Thermal correction to Gibbs Free Energy= 0.746236
Sum of electronic and zero-point Energies= -4105.672526
Sum of electronic and thermal Energies= -4105.608687
Sum of electronic and thermal Enthalpies= -4105.607743
Sum of electronic and thermal Free Energies= -4105.775862

O	1.05214600	4.60872200	4.19838000
O	-1.29955300	4.62976900	4.20580100
O	-4.60278400	1.19951800	4.10832300
O	-4.63377300	-1.15126500	4.19831100
O	-1.21237300	-4.46546200	4.25148400
O	1.13758500	-4.49456600	4.36456800
O	4.44219200	-1.06240700	4.31304400
O	4.46477600	1.29069300	4.34376000
C	2.72384400	2.91561400	4.24143700
C	1.59471600	3.50627500	4.82308600
C	-0.12778800	4.44361700	3.44834200
C	-1.85365500	3.50824400	4.78646400
C	-2.91557800	2.87874600	4.12626100
C	-3.50977200	1.76305200	4.73116600
C	-4.43019600	-0.00720800	3.40397300
C	-3.52142100	-1.68984900	4.81052600
C	-2.88839800	-2.77565700	4.19401400
C	-1.77963600	-3.35017300	4.82989600
C	0.00109800	-4.32033700	3.55249400
C	1.67118400	-3.35999100	4.93932300
C	2.76082000	-2.74825100	4.30788600
C	3.32740500	-1.61476400	4.90654100
C	4.29104800	0.12594400	3.57299100
C	3.33153400	1.84271700	4.90330100
C	1.72036300	1.97836400	6.66313900
C	1.08688200	3.05843400	6.04870400
C	-0.15586200	3.71361600	6.63600900
C	-1.37751500	3.05104900	6.01757500
C	-2.00824800	1.94644000	6.58849900
C	-3.07867000	1.29332400	5.97792200
C	-3.74306200	0.07093900	6.59679700
C	-3.07539300	-1.17194000	6.02851100
C	-1.97726600	-1.78380900	6.63160000
C	-1.32048500	-2.87581200	6.06495000
C	-0.10400600	-3.51794300	6.71785800
C	1.14328800	-2.87053500	6.13612300
C	1.74972100	-1.75096900	6.70415400
C	2.84496400	-1.11342900	6.12181800
C	3.48459500	0.12380700	6.73719600
C	2.83978400	1.35286600	6.11547900
C	3.28380200	3.42215700	2.95767200
C	2.60885300	3.20002500	1.75476100
C	3.14480200	3.68193600	0.57027600
C	4.34390300	4.38058200	0.55420100
C	5.00809700	4.58625100	1.75810100
C	4.49646700	4.11569800	2.95550800
C	-0.17641500	3.72700200	8.16534000
C	-3.77688300	0.10084000	8.12571600
C	-0.14672100	-3.49634500	8.24669500
H	-0.11799300	5.24044700	2.70514600
H	-3.42950400	-0.04667000	2.95335900
H	-5.21394700	-0.02021500	2.64690400
H	0.04584200	-3.33746100	3.06475500
H	0.02021300	-5.13218400	2.82580300
H	5.09994800	0.12228000	2.84271900
H	3.30590400	0.15047600	3.08823800
H	1.32590100	1.61020200	7.60511400
H	-0.15363800	4.75284000	6.29248800
H	-1.65269700	1.58041300	7.54661500
H	-4.77769600	0.06327000	6.23977600
H	-1.61945400	-1.39501800	7.57986100
H	-0.09352900	-4.56478800	6.39862500
H	1.35413700	-1.36001200	7.63640500
H	4.53239700	0.12414600	6.42084100
H	1.67763400	2.64502500	1.71739000
H	-0.18989700	2.72648800	8.60541800
H	-2.78243300	0.09764000	8.57950800
H	-4.31306700	-0.77437800	8.50154600
H	-0.14715200	-2.48608700	8.66415200
H	0.72520500	-4.01844500	8.64906200
C	-3.40421000	-3.31277400	2.90445600
C	-4.64665700	-3.95106600	2.86725400

C	-2.66059100	-3.17438300	1.72970500
C	-5.11850900	-4.45137200	1.66572300
H	-5.25151100	-4.06052600	3.76024700
C	-3.15786500	-3.68407100	0.54021700
H	-1.70482600	-2.66204500	1.71649600
C	-4.38572600	-4.32909000	0.49052700
C	3.31251100	-3.31463000	3.04610400
C	3.93634800	-4.56499800	3.06534100
C	3.20437000	-2.61277400	1.84284800
C	4.45256300	-5.08600900	1.89127200
H	4.02265000	-5.13813800	3.98148900
C	3.72935900	-3.15891600	0.68181200
H	2.70414100	-1.65231900	1.78514200
C	4.36028700	-4.39509400	0.68839500
C	-3.40802500	3.40548800	2.82334600
C	-4.04580900	4.64780900	2.77444500
C	-3.22796100	2.67210600	1.64781700
C	-4.50421000	5.12962800	1.56019600
H	-4.18688500	5.24505800	3.66811600
C	-3.69631000	3.17915400	0.44553300
H	-2.71440900	1.71690300	1.64436000
C	-4.34034800	4.40698900	0.38380000
C	3.45894600	0.12880300	8.26662700
H	3.96330700	-0.76154700	8.65094200
H	3.97909600	1.01344400	8.64294200
H	2.44755900	0.14028400	8.68117000
H	0.70899000	4.24304300	8.54555300
H	-4.29405800	1.00030600	8.46970100
H	-1.04912300	-4.00081300	8.60167300
H	5.04757900	4.29154600	3.87236200
H	-0.14591500	3.45098000	2.97891700
H	-1.06583900	4.25454800	8.51944800
F	4.86154100	-4.91011100	-0.43255300
F	4.84946600	4.83976100	-0.58885900
F	-4.78660100	4.88478100	-0.77620200
F	-4.85410300	-4.81528500	-0.65719800
F	5.05784000	-6.27769700	1.88667300
F	3.63304300	-2.50032000	-0.47830200
F	-2.45897400	-3.55847800	-0.59317900
F	-6.30206300	-5.06952900	1.60675600
F	-3.53046400	2.49004700	-0.68866200
F	-5.12096500	6.31331500	1.48974000
F	2.51256500	3.47695300	-0.59018400
F	6.16430300	5.25593200	1.73128800

8

Zero-point correction= 0.986861 (Hartree/Particle)
Thermal correction to Energy= 1.069577
Thermal correction to Enthalpy= 1.070521
Thermal correction to Gibbs Free Energy= 0.850042
Sum of electronic and zero-point Energies= -5610.694871
Sum of electronic and thermal Energies= -5610.612155
Sum of electronic and thermal Enthalpies= -5610.611211
Sum of electronic and thermal Free Energies= -5610.831689

O	0.78983700	4.62422700	4.13196400
O	-1.56186000	4.53556800	4.16697300
O	-4.65993600	0.91608500	4.06359400
O	-4.57310300	-1.43287500	4.17967000
O	-0.95152000	-4.53075200	4.20878900
O	1.39650400	-4.44247500	4.34478800
O	4.49766000	-0.82432500	4.28132500
O	4.40628000	1.52693700	4.33305500
C	2.57207700	3.04667300	4.20406300
C	1.39734600	3.56364900	4.76949100
C	-0.39061800	4.39333800	3.39895500
C	-2.05744900	3.38752200	4.74978900
C	-3.08087600	2.69822600	4.08777300
C	-3.60400000	1.54406600	4.68885400
C	-4.42456200	-0.28874600	3.37295200
C	-3.42951000	-1.90827700	4.78753200
C	-2.73426400	-2.95248200	4.16516400
C	-1.58500300	-3.45479900	4.79306800
C	0.26036400	-4.31910600	3.52275900
C	1.86760100	-3.27974400	4.91876800
C	2.91905300	-2.60731900	4.28379400
C	3.41614300	-1.43758800	4.87674500
C	4.29130000	0.36215100	3.55069800
C	3.23867400	2.01735700	4.88031400
C	1.60625400	2.05886700	6.62288900
C	0.91298300	3.09512100	5.99758800
C	-0.36254100	3.68458300	6.58535000
C	-1.54957600	2.95499000	5.97581400
C	-2.11499500	1.81561200	6.54678200
C	-3.14644900	1.10184500	5.93679300
C	-3.74148000	-0.15280000	6.56274400
C	-3.00732300	-1.35974100	5.99947500
C	-1.87279600	-1.90538700	6.59846100
C	-1.15377100	-2.95614500	6.02905600
C	0.09469700	-3.53042700	6.68600600
C	1.30757500	-2.81614100	6.11014000
C	1.84852900	-1.66221000	6.67544800
C	2.90553500	-0.96376100	6.09209000
C	3.47385700	0.30684600	6.71046400
C	2.76480500	1.49873400	6.08637500
C	3.12086000	3.58163200	2.92936500
C	2.38946300	3.51084400	1.74733200
C	2.90675300	4.03089500	0.56062500
C	4.16189200	4.61860700	0.52864400
C	4.90005200	4.67370000	1.71211600
C	4.39547200	4.16236000	2.89987300
C	-0.37918500	3.70483800	8.11477200
C	-3.77393800	-0.11755000	8.09162500
C	0.04519100	-3.51218900	8.21473500
H	-0.42335100	5.17616200	2.64105800
H	-3.42017300	-0.28632200	2.92895600
H	-5.20185800	-0.34705700	2.61092900
H	0.26355300	-3.32970200	3.04630000
H	0.32481900	-5.12080200	2.78695100
H	5.09971200	0.40153700	2.82049200
H	3.30627400	0.34708900	3.06543800
H	1.22849000	1.67330900	7.56470400
H	-0.41718300	4.72077600	6.23718100
H	-1.73742200	1.47010900	7.50410100
H	-4.77481300	-0.21892300	6.20818900
H	-1.53549900	-1.49618800	7.54561900
H	0.16333600	-4.57501700	6.36652800
H	1.43033200	-1.29234100	7.60639000
H	4.52133400	0.36471900	6.39843600

H	1.41305400	3.03568700	1.73824100
H	-0.34429600	2.70715900	8.56006900
H	-2.77978100	-0.06776000	8.54337900
H	-4.26360300	-1.01766000	8.47199700
H	-0.00791400	-2.50359300	8.63285600
H	0.94125300	-3.98956500	8.61950500
C	-3.22584300	-3.51665500	2.87974200
C	-4.49854400	-4.09717000	2.80442700
C	-2.44040800	-3.47359600	1.73141000
C	-4.94816700	-4.63565900	1.60649300
H	-5.12883000	-4.12877700	3.68683300
C	-2.90240800	-4.02121100	0.53449400
H	-1.46400600	-2.99908800	1.75652700
C	-4.15564700	-4.60888800	0.45773100
C	3.49732900	-3.14400300	3.02290100
C	4.08460200	-4.41629700	3.00244700
C	3.46187800	-2.40331700	1.84555900
C	4.63634100	-4.90854500	1.82826200
H	4.10936500	-5.01250800	3.90825400
C	4.02270000	-2.90866400	0.67187500
H	2.98269500	-1.42895400	1.82882200
C	4.61667300	-4.16052900	0.64934800
C	-3.60312500	3.20096600	2.78898700
C	-4.18897000	4.47099800	2.70817800
C	-3.51592200	2.42865200	1.63448100
C	-4.68962100	4.93049900	1.49783700
H	-4.25409800	5.09117700	3.59583700
C	-4.02584300	2.90067200	0.42466100
H	-3.03637300	1.45483200	1.66517200
C	-4.61885200	4.15084600	0.34198300
C	3.44158200	0.31036800	8.23977600
H	3.98943700	-0.55272600	8.62661900
H	3.91433500	1.22053500	8.61760400
H	2.42923900	0.27040300	8.65022400
H	0.48126900	4.26473800	8.49008200
H	-4.33631900	0.75532700	8.43298700
H	-0.83134600	-4.06242200	8.56637500
H	4.98396800	4.21524000	3.80967700
H	-0.37221100	3.39214700	2.94803800
H	-1.29196000	4.19126300	8.46818000
H	5.05623600	-4.55036700	-0.26281500
H	-4.51107700	-5.03957400	-0.47232100
H	-5.02018800	4.51409900	-0.59821600
H	4.56013200	5.02764900	-0.39381800
C	3.95715100	-2.05414000	-0.56437800
C	5.25616700	-6.27974100	1.78793400
C	-2.00045400	-3.94859000	-0.66721800
C	-6.32844500	-5.22891500	1.51151100
C	-3.90515100	2.01367300	-0.78428200
C	-5.29339600	6.30570700	1.39605800
C	2.06232800	3.92869100	-0.68009400
C	6.28197500	5.26899400	1.66714200
F	4.59885100	-2.60600000	-1.60157900
F	2.68588000	-1.83515000	-0.94380400
F	4.50508200	-0.84233600	-0.34706600
F	4.51908500	-7.12922700	1.04924800
F	5.38032900	-6.81869000	3.00891000
F	6.48006300	-6.24937200	1.23269400
F	-1.77099400	-2.67532200	-1.03351700
F	-2.50915200	-4.58824900	-1.72748700
F	-0.79623200	-4.49352700	-0.40454800
F	-6.32881600	-6.36668100	0.79697000
F	-6.84474400	-5.50810400	2.71718700
F	-7.18228500	-4.38746200	0.89947300
F	-2.61859200	1.80761100	-1.11650000
F	-4.52195100	2.52494300	-1.85682900
F	-4.43880000	0.79854000	-0.55063200
F	-6.43250900	6.29252300	0.68338500
F	-4.46002900	7.16193500	0.77655500
F	-5.57490600	6.82722600	2.59877300
F	6.74827100	5.56206500	2.88967700
F	7.16156500	4.42347300	1.09886100
F	6.30903700	6.39932900	0.94125500
F	0.85013200	4.48587700	-0.49070600
F	1.84343800	2.64663400	-1.02147500
F	2.62465100	4.53627200	-1.73218800

5

Zero-point correction= 0.850443 (Hartree/Particle)
Thermal correction to Energy= 0.914012
Thermal correction to Enthalpy= 0.914956
Thermal correction to Gibbs Free Energy= 0.751106
Sum of electronic and zero-point Energies= -4105.670708
Sum of electronic and thermal Energies= -4105.607140
Sum of electronic and thermal Enthalpies= -4105.606195
Sum of electronic and thermal Free Energies= -4105.770045

O	1.16942300	4.55931500	4.20349400
O	-1.18325400	4.53081500	4.10125200
O	-4.66064000	1.28572700	4.20799100
O	-4.70556700	-1.06313100	4.23708200
O	-1.30505100	-4.39468300	4.17382900
O	1.05450500	-4.43634200	4.22021000
O	4.53672200	-1.18950800	4.40961900
O	4.50502800	1.16369000	4.31576100
C	2.80523200	2.83063300	4.23517000
C	1.70349300	3.45473700	4.83227100
C	0.02766800	4.34500800	3.40885800
C	-1.75932500	3.44673100	4.72819800
C	-2.88092700	2.86127100	4.12701900
C	-3.52532800	1.80920200	4.78841700
C	-4.52858100	0.09976800	3.46198100
C	-3.58695200	-1.61138500	4.82564800
C	-2.97929600	-2.69687100	4.18348400
C	-1.86646200	-3.29415700	4.78739200
C	-0.10798100	-4.20253000	3.46205100
C	1.62643000	-3.35482500	4.85620300
C	2.78317600	-2.79642500	4.29832900
C	3.38887800	-1.72091800	4.95838700
C	4.37845400	-0.04490200	3.60623300
C	3.37634100	1.72362400	4.87557900
C	1.77835500	1.90898200	6.65060600
C	1.17072600	3.00674200	6.04145200
C	-0.07492300	3.67646800	6.59995400
C	-1.29685400	3.01577400	5.97722000
C	-1.96319400	1.95518900	6.59011400
C	-3.07487300	1.33355800	6.02213200
C	-3.74829600	0.12236700	6.65056100
C	-3.11272400	-1.12045200	6.04459900

C	-2.01081200	-1.75654400	6.61604500
C	-1.37692900	-2.84528800	6.01829400
C	-0.16009200	-3.52169800	6.63175400
C	1.09859900	-2.88318200	6.06307600
C	1.73398600	-1.80518100	6.67856700
C	2.87383800	-1.20241700	6.14723100
C	3.51176400	0.03654600	6.75564200
C	2.88071600	1.25706900	6.09965800
C	3.35912100	3.36774800	2.96584700
C	3.33615100	2.65407600	1.76459900
C	3.85581200	3.18456600	0.58611100
C	4.40593200	4.45549400	0.61094300
C	4.44038200	5.19527900	1.78601700
C	3.91651600	4.64488500	2.94878100
C	-0.11204900	3.71406800	8.12869000
C	-3.73602300	0.13518600	8.17953800
C	-0.18734300	-3.55058600	8.16127700
H	0.04627800	5.11765200	2.64014700
H	-3.55206200	0.07462100	2.95844400
H	-5.35065600	0.10641900	2.74704300
H	-0.08228800	-3.18263200	3.05458000
H	-0.10510500	-4.95561500	2.67287600
H	5.20701700	-0.05600900	2.89808800
H	3.40619700	-0.08753900	3.09642400
H	1.37714600	1.54843200	7.59262600
H	-0.06180700	4.71061000	6.24138300
H	-1.60443200	1.60205600	7.55178800
H	-4.79232400	0.13537000	6.32248100
H	-1.63128000	-1.38928400	7.56449400
H	-0.16962500	-4.55851700	6.28085000
H	1.32209500	-1.41720900	7.60509700
H	4.56494700	0.02799600	6.45819000
H	2.88559000	1.66716600	1.75062700
H	-0.11319300	2.72063200	8.58483300
H	-2.72818400	0.12110900	8.60285700
H	-4.26732100	-0.73987900	8.56249100
H	-0.17890800	-2.55480300	8.61189800
H	0.68511300	-4.09063400	8.53789700
C	-3.53725000	-3.20530000	2.90411900
C	-4.81052000	-3.77113400	2.88941300
C	-2.84682800	-3.12971600	1.69161600
C	-5.37902200	-4.25417500	1.71773300
C	-3.39596400	-3.60692800	0.50378000
H	-1.86454300	-2.66877400	1.67718500
C	-4.66193700	-4.16818900	0.53119100
C	3.38513600	-3.33018900	3.04983400
C	4.65679100	-3.89892700	3.09234400
C	2.74050100	-3.27651300	1.81096400
C	5.26776500	-4.40324900	1.95134300
C	3.33245800	-3.77579900	0.65322200
H	1.75924500	-2.81726900	1.75129900
C	4.59585900	-4.33743200	0.73749800
C	-3.41024800	3.35392200	2.82953200
C	-4.67048200	3.94620800	2.78216400
C	-2.70094900	3.23983900	1.63081900
C	-5.20890700	4.41696500	1.59133600
C	-3.21971700	3.70471300	0.42465600
H	-1.72733800	2.76094400	1.64279100
C	-4.47404100	4.29218400	0.41921400
C	3.45811200	0.06348300	8.28389100
H	3.97345400	-0.81184800	8.68740000
H	3.95350000	0.96294900	8.65843400
H	2.43930500	0.05796000	8.68006000
H	0.76262700	4.24943500	8.50678400
H	-4.23619500	1.03474800	8.54738200
H	-1.08990600	-4.06136400	8.50652200
H	0.06717400	3.33678000	2.97411300
H	-1.01217100	4.23396100	8.46670200
F	5.19997500	-4.82709600	-0.34998000
F	4.91450900	5.00200500	-0.49838300
F	-5.00900300	4.75157100	-0.71699400
F	-5.22546300	-4.63812100	-0.58651300
F	6.48125900	-4.94661100	2.02338100
F	-6.59522900	-4.79613000	1.73433400
F	-6.41366300	4.98451500	1.57613900
F	4.97228800	6.41605400	1.80051900
F	5.32089200	-3.98667300	4.24431300
F	3.97313400	5.37361300	4.06326100
F	-5.51741700	-3.87532600	4.01436700
F	-5.39304700	4.08995200	3.89285800
H	3.83994300	2.63562800	-0.34810900
H	2.83764500	-3.73538000	-0.31004500
H	-2.86693900	-3.54779000	-0.44012000
H	-2.67475600	3.61763700	-0.50796100

5-1in

Zero-point correction= 0.850324 (Hartree/Particle)
Thermal correction to Energy= 0.914083
Thermal correction to Enthalpy= 0.915028
Thermal correction to Gibbs Free Energy= 0.749086
Sum of electronic and zero-point Energies= -4105.674684
Sum of electronic and thermal Energies= -4105.610925
Sum of electronic and thermal Enthalpies= -4105.609980
Sum of electronic and thermal Free Energies= -4105.775922

O	1.14566100	4.58792000	4.21995600
O	-1.20481600	4.55409100	4.11815000
O	-4.63082500	1.25691100	4.18318100
O	-4.62831300	-1.09081500	4.20615000
O	-1.23390800	-4.41791400	4.23938900
O	1.11345600	-4.49885300	4.36014500
O	4.50480400	-1.16404600	4.40049400
O	4.47257700	1.18765400	4.31364700
C	2.76937700	2.84991200	4.23875100
C	1.67780900	3.48078300	4.84507000
C	0.00522900	4.37942400	3.42179800
C	-1.77063100	3.46101100	4.73864500
C	-2.87667100	2.85980600	4.12594400
C	-3.51279000	1.79851500	4.77958000
C	-4.46093800	0.07604000	3.43595300
C	-3.51394200	-1.62151300	4.81824800
C	-2.88001900	-2.69994200	4.19169500
C	-1.78818100	-3.30116300	4.82846900
C	-0.01760800	-4.27789000	3.54862100
C	1.66690900	-3.39262800	4.96773400
C	2.78815200	-2.81027200	4.37045300
C	3.37938100	-1.70330100	4.98556700
C	4.32249000	-0.01663500	3.60267000
C	3.35030400	1.75112900	4.88239600

C	1.76626000	1.94009900	6.66824200
C	1.15337900	3.03546800	6.05955400
C	-0.09541000	3.69995000	6.61809500
C	-1.31144400	3.03262400	5.98995600
C	-1.97023100	1.96338300	6.59605300
C	-3.06925500	1.32839300	6.01776700
C	-3.73463800	0.10913100	6.63974800
C	-3.07416400	-1.12821200	6.04926700
C	-1.98423600	-1.75934000	6.64882100
C	-1.33285000	-2.84968600	6.07263200
C	-0.13256100	-3.52076400	6.72677200
C	1.13556300	-2.89817500	6.16211300
C	1.75824000	-1.79233500	6.74174700
C	2.87865400	-1.17868500	6.18059100
C	3.51145200	0.07447700	6.76709400
C	2.86675900	1.28864100	6.11209400
C	3.29397000	3.35815000	2.94502000
C	3.19101100	2.63415000	1.75373300
C	3.68162200	3.13308900	0.54903400
C	4.28203700	4.38122400	0.53791100
C	4.39399000	5.13047200	1.70236900
C	3.89762100	4.61221900	2.89166600
C	-0.13670100	3.73436500	8.14663200
C	-3.74709400	0.12940400	8.16864500
C	-0.18535800	-3.51233600	8.25551400
H	0.02200600	5.16061900	2.66190100
H	-3.47521600	0.07228400	2.95027900
H	-5.26975400	0.06743300	2.70609300
H	0.04918800	-3.28297100	3.08866600
H	-0.00995500	-5.07111900	2.80102300
H	5.13007900	-0.02982300	2.87053300
H	3.33602200	-0.05638700	3.12393700
H	1.37074800	1.58135200	7.61345000
H	-0.08650900	4.73459400	6.26085400
H	-1.61416200	1.61208800	7.55946500
H	-4.77346600	0.10665300	6.29498800
H	-1.63224900	-1.38962400	7.60680600
H	-0.14226800	-4.56497300	6.39818100
H	1.34861900	-1.38714300	7.66207200
H	4.56077500	0.07176300	6.45534200
H	2.70054300	1.66589100	1.76834700
H	-0.13516800	2.73988300	8.60056600
H	-2.74593200	0.13466600	8.60780700
H	-4.26963300	-0.75261400	8.54783700
H	-0.16659600	-2.50590500	8.68167300
H	0.67202400	-4.05703000	8.65929500
C	-3.38067200	-3.19678100	2.88402900
C	-4.62491100	-3.81808000	2.81239100
C	-2.65549700	-3.05215200	1.69802700
C	-5.13281000	-4.29156500	1.60938200
C	-3.14415300	-3.51900800	0.47974000
H	-1.69526900	-2.54687800	1.72925600
C	-4.38285100	-4.13800100	0.45014500
C	3.32582000	-3.34581100	3.09076800
C	4.24543400	-4.39680100	3.04612900
C	2.90914400	-2.80196400	1.88149200
C	4.73399600	-4.88486200	1.83764500
C	3.38130400	-3.26979300	0.66178700
C	4.29582400	-4.31389300	0.65295000
C	-3.39677800	3.34193200	2.82042800
C	-4.64952100	3.94822100	2.76193100
C	-2.68675400	3.20034700	1.62516900
C	-5.17961400	4.40880600	1.56356600
C	-3.19754000	3.65420900	0.41121200
H	-1.72025100	2.70739600	1.64575500
C	-4.44390200	4.25796700	0.39494000
C	3.47885100	0.11555700	8.29583400
H	4.00150900	-0.75442600	8.70178600
H	3.97662600	1.02013900	8.65454700
H	2.46542700	0.11187500	8.70548600
H	0.73469200	4.27255200	8.52839700
H	-4.26790300	1.02234200	8.52376400
H	-1.10143600	-3.99954000	8.59929900
H	0.04734000	3.37658000	2.97547500
H	-1.03994500	4.24970100	8.48330500
F	4.74186300	-4.75517900	-0.52761400
F	4.76597600	4.89751600	-0.59687800
F	-4.97117800	4.70790100	-0.74874900
F	-4.88918000	-4.60074000	-0.69798100
F	2.95750200	-2.72200200	-0.47851100
F	-6.32325100	-4.88787700	1.56995400
F	-6.37764200	4.99038400	1.53740500
F	4.97258900	6.33000300	1.68094800
F	4.02457400	5.34925700	3.99532300
F	-5.36177200	-3.98518600	3.91087200
F	-5.37362700	4.11312100	3.86908500
F	2.01817700	-1.79280700	1.85796400
H	4.57781100	-4.83456500	3.98098300
H	3.60375400	2.57647500	-0.37757900
H	5.44767900	-5.69930900	1.79525800
H	-2.58768100	-3.40787000	-0.44352500
H	-2.65243600	3.54525000	-0.51902500

5-2*syn*-in

Zero-point correction= 0.850945 (Hartree/Particle)
Thermal correction to Energy= 0.914422
Thermal correction to Enthalpy= 0.915366
Thermal correction to Gibbs Free Energy= 0.751829
Sum of electronic and zero-point Energies= -4105.676668
Sum of electronic and thermal Energies= -4105.613192
Sum of electronic and thermal Enthalpies= -4105.612247
Sum of electronic and thermal Free Energies= -4105.775784

O	1.09194200	4.40541900	3.99259800
O	-1.27087800	4.43392700	4.00754100
O	-4.79138500	1.23715400	4.29388900
O	-4.79016400	-1.11015100	4.32241600
O	-1.26505700	-4.30787800	4.11276500
O	1.09788500	-4.27573900	4.09625800
O	4.62619300	-1.10018400	4.50292000
O	4.62437700	1.24528400	4.47476200
C	2.84345600	2.81086500	4.22258000
C	1.65954500	3.37846900	4.71452000
C	-0.10081100	4.12703000	3.28778600
C	-1.87035100	3.39364200	4.68386400
C	-3.01464500	2.80912300	4.12900900
C	-3.64045900	1.77198800	4.83056900
C	-4.66902100	0.05424700	3.53985800
C	-3.63859800	-1.63045900	4.87191000

C	-3.01173200	-2.68363600	4.19566200
C	-1.86633600	-3.25277000	4.76404700
C	-0.09568100	-4.01578300	3.38570900
C	1.66427300	-3.23120500	4.79348700
C	2.84766300	-2.67417700	4.28831600
C	3.44658100	-1.62296500	4.99231300
C	4.53949400	0.06320300	3.71362000
C	3.44403800	1.77789200	4.95158400
C	1.74802400	1.93962600	6.62624200
C	1.11855100	2.97960100	5.94155200
C	-0.12923900	3.66459700	6.48002600
C	-1.36967300	2.98410600	5.92280800
C	-2.01770300	1.93767000	6.57820400
C	-3.14798600	1.31031200	6.05437200
C	-3.78747200	0.09323000	6.70793900
C	-3.14629500	-1.13838600	6.08390200
C	-2.01480200	-1.75110500	6.62234500
C	-1.36566300	-2.81237100	5.99238300
C	-0.12407300	-3.47738600	6.56539100
C	1.12259400	-2.80354200	6.01051900
C	1.75039700	-1.74641100	6.67000600
C	2.90155300	-1.13148100	6.18211400
C	3.51270700	0.09992500	6.83562300
C	2.89987100	1.31461800	6.15304800
C	3.48988100	3.32217100	2.98516400
C	2.87839100	3.19424900	1.74391500
C	3.46286500	3.67732600	0.58005700
C	4.69984000	4.30091400	0.65796800
C	5.35025300	4.43733800	1.87468500
C	4.74186400	3.94594100	3.02496300
C	-0.14098500	3.78177300	8.00605300
C	-3.72956200	0.11164900	8.23560000
C	-0.13537600	-3.55832800	8.09376600
H	-0.09344200	4.79388000	2.42471500
H	-3.71517100	0.04814500	2.99418000
H	-5.52121400	0.04560800	2.86119300
H	-0.10802000	-2.97001100	3.06270000
H	-0.08743400	-4.70236200	2.53826700
H	5.42170700	0.05623700	3.07434800
H	3.61069200	0.05545900	3.12613600
H	1.32059200	1.60332800	7.56566500
H	-0.12395400	4.68010100	6.07091800
H	-1.62533700	1.59573300	7.53109200
H	-4.84047200	0.08887900	6.41020000
H	-1.62242100	-1.38528200	7.56633200
H	-0.11729600	-4.50231500	6.18055500
H	1.32222200	-1.38820300	7.60096400
H	4.57809800	0.09767800	6.58593100
H	-0.15864200	2.81340700	8.51284300
H	-2.70915600	0.11697400	8.62810600
H	-4.23322300	-0.77138900	8.63726500
H	-0.15434600	-2.57827700	8.57749000
H	0.75607300	-4.08385700	8.44612900
C	-3.57050600	-3.17925900	2.91187600
C	-4.83251500	-3.76934500	2.89422000
C	-2.88745600	-3.06852800	1.69725000
C	-5.39837400	-4.24119500	1.71682000
C	-3.43471000	-3.53450200	0.50423600
H	-1.91291300	-2.59123000	1.68339500
C	-4.68986700	-4.11971000	0.52826500
C	3.49630300	-3.21476900	3.06459300
C	4.75171600	-3.83045100	3.12096100
C	2.88442000	-3.12327500	1.82031400
C	5.36302400	-4.34900700	1.98424500
C	3.47174200	-3.63411600	0.66979800
C	4.71206800	-4.24861400	0.76430100
C	-3.57355100	3.27217900	2.83318100
C	-4.83635300	3.85987700	2.80040500
C	-2.88988300	3.13212400	1.62192900
C	-5.40242200	4.30138900	1.61139600
C	-3.43733000	3.56738900	0.41746400
H	-1.91472000	2.65589800	1.62032600
C	-4.69329000	4.15128200	0.42647800
C	3.38507700	0.11784600	8.35909200
H	3.87133200	-0.76424500	8.78382100
H	3.86963800	1.01065600	8.76282700
H	2.34807600	0.12090100	8.70466300
H	0.74961700	4.31681800	8.34601300
H	-4.23428400	1.00351000	8.61587700
H	-1.01949100	-4.10729700	8.42788400
H	-0.11120200	3.07404600	2.98905800
H	-1.02598600	4.33719400	8.32690400
F	5.26559100	-4.73656800	-0.35076800
F	5.25060000	4.76222100	-0.46971800
F	-5.25545200	4.58323700	-0.70758800
F	-5.25170900	-4.58069100	-0.59448400
F	2.85031300	-3.52690300	-0.50541200
F	-6.60430100	-4.80760800	1.73029700
F	-6.60916900	4.86619300	1.61022200
F	2.84200300	3.53538000	-0.59174700
F	1.69755800	-2.50916400	1.68614000
H	5.25136100	-3.89804200	4.08113200
H	5.24108600	4.04210200	3.98291200
F	1.69464300	2.57063600	1.62665200
F	-5.53452300	4.02837500	3.92379500
F	-5.53008900	-3.91088200	4.02171800
H	6.31703500	4.92616000	1.90221600
H	6.33246700	-4.83160100	2.02483600
H	-2.90994300	-3.44874100	-0.44002100
H	-2.91209900	3.45888300	-0.52419200

5-2*anti*-in

Zero-point correction= 0.850988 (Hartree/Particle)
Thermal correction to Energy= 0.914468
Thermal correction to Enthalpy= 0.915412
Thermal correction to Gibbs Free Energy= 0.751786
Sum of electronic and zero-point Energies= -4105.676999
Sum of electronic and thermal Energies= -4105.613519
Sum of electronic and thermal Enthalpies= -4105.612575
Sum of electronic and thermal Free Energies= -4105.776201

O	1.10532100	4.77896200	4.37916800
O	-1.24014800	4.78582900	4.33438200
O	-4.40773700	1.25295800	3.92882500
O	-4.44822900	-1.10787800	4.00774100
O	-1.27706300	-4.63742600	4.43376300
O	1.06854900	-4.64599200	4.47954600
O	4.25007000	-1.11977200	4.11699900
O	4.28917100	1.24264600	4.15018300

C	2.67186600	2.99428600	4.24265200
C	1.61699200	3.61772900	4.91890800
C	-0.05141000	4.67254500	3.58548100
C	-1.78054100	3.62354500	4.84239400
C	-2.80601700	3.00229100	4.12047800
C	-3.38464200	1.83777600	4.64337100
C	-4.12871200	0.04147000	3.25916500
C	-3.41818800	-1.69111100	4.71240600
C	-2.83577200	-2.85578200	4.19879800
C	-1.80805300	-3.46469300	4.92806100
C	-0.09048700	-4.54902900	3.68314100
C	1.59007600	-3.47254400	4.98185000
C	2.64372000	-2.86766300	4.28663500
C	3.20086400	-1.69033800	4.80469700
C	3.99632800	0.07834500	3.41372300
C	3.23371900	1.84098600	4.80254700
C	1.72025000	1.97472100	6.65219100
C	1.11427000	3.11327700	6.12127900
C	-0.12297900	3.74730900	6.74150800
C	-1.33236300	3.11604700	6.06578300
C	-1.96665000	1.98116000	6.56733200
C	-3.00110900	1.33365100	5.89054300
C	-3.69622200	0.10372200	6.45620300
C	-3.01653600	-1.15458700	5.93907000
C	-1.97751000	-1.78617500	6.62148900
C	-1.35188100	-2.93506700	6.13804600
C	-0.13941300	-3.55530000	6.81804900
C	1.09474600	-2.93803900	6.17508000
C	1.70923900	-1.79176600	6.67526400
C	2.76929900	-1.15904200	6.02472200
C	3.44334800	0.08225300	6.59116200
C	2.78467900	1.32973000	6.02356100
C	3.17524400	3.56332700	2.96641700
C	3.06427900	2.89291100	1.74475500
C	3.53561000	3.45009600	0.55846700
C	4.12621800	4.70240200	0.59650800
C	4.24781400	5.39844400	1.79239700
C	3.77063800	4.82287300	2.96287200
C	-0.15725900	3.66837400	8.26794200
C	-3.82716500	0.13332000	7.98087300
C	-0.16246500	-3.44382200	8.34264800
H	-0.03633900	5.53472100	2.91959600
H	-3.07313700	0.01743700	2.97041000
H	-4.78793000	0.02754900	2.39028500
H	-0.07433700	-3.61573700	3.10304200
H	-0.08108200	-5.42581200	3.03652300
H	4.68637700	0.07488000	2.56905100
H	2.95191700	0.09667700	3.08655000
H	1.34635600	1.57249700	7.58879400
H	-0.11419700	4.80420900	6.45807600
H	-1.64237100	1.58269600	7.52362600
H	-4.70797700	0.10198700	6.03781600
H	-1.64004500	-1.36469800	7.56341000
H	-0.13784600	-4.61797300	6.55694600
H	1.34838100	-1.37218500	7.60917100
H	4.47012600	0.07560900	6.21123500
H	-0.16734700	2.64275200	8.64619000
H	-2.86337100	0.12726800	8.49658800
H	-4.38821200	-0.74094600	8.32086300
H	-0.16546200	-2.41036900	8.69906900
H	0.71736100	-3.93584100	8.76547900
C	-3.29062600	-3.45258500	2.91707200
C	-3.88485600	-4.71269600	2.91851900
C	-3.13409300	-2.80867900	1.68620200
C	-4.31701100	-5.31431000	1.74367200
C	-3.55986500	-3.39225900	0.49537400
C	-4.15069000	-4.64430900	0.53836700
C	3.18409600	-3.50315200	3.05595100
C	3.80385700	-4.75703600	3.09804100
C	3.08559800	-2.88010000	1.81785600
C	4.32001200	-5.35578000	1.95353900
C	3.59372400	-3.45466600	0.65981600
C	4.21275900	-4.69374100	0.74017200
C	-3.29282900	3.60407800	2.85106200
C	-3.92944700	4.84983200	2.83216800
C	-3.12329000	2.95395400	1.63471000
C	-4.39359100	5.41496600	1.64883100
C	-3.57812100	3.49485300	0.43895500
C	-4.21580200	4.72692800	0.45844600
C	3.51696400	0.08348800	8.11995600
H	4.03912200	-0.81133900	8.46865800
H	4.06593300	0.96426700	8.46285500
H	2.53458400	0.10049300	8.59900100
H	0.72213900	4.16542800	8.68546700
H	-4.36238900	1.03444700	8.29148400
H	-1.05742300	-3.93167700	8.73732800
H	-0.04499000	3.72650000	3.02617300
H	-1.05246000	4.16840900	8.64680000
F	4.69826100	-5.23487300	-0.38205300
F	4.59184000	5.27393300	-0.51939800
F	-4.64956700	5.23564600	-0.69955000
F	-4.57320100	-5.24090500	-0.58157100
F	3.47907000	-2.82251900	-0.50925200
F	-4.88768500	-6.51808800	1.77530300
F	-3.39540700	2.83774200	-0.70740200
F	4.81865900	6.60225800	1.81933400
F	2.46635500	-1.69384600	1.69724500
H	3.87588400	-5.26597500	4.05297800
H	-4.05666700	5.37945200	3.76995900
F	-2.48466100	1.77325100	1.57439000
H	-2.65155600	-1.83700500	1.65846200
H	2.58189900	1.92108400	1.71992500
F	-4.06819600	-5.37421900	4.06185000
F	3.91137100	5.50916500	4.09766500
H	3.44910800	2.93536400	-0.39122600
H	4.80503500	-6.32441300	1.98301100
H	-3.43787100	-2.89820700	-0.46136900
H	-4.89142300	6.37736800	1.63053300

5-3in

Zero-point correction= 0.850812 (Hartree/Particle)
Thermal correction to Energy= 0.914412
Thermal correction to Enthalpy= 0.915356
Thermal correction to Gibbs Free Energy= 0.750657
Sum of electronic and zero-point Energies= -4105.677796
Sum of electronic and thermal Energies= -4105.614197
Sum of electronic and thermal Enthalpies= -4105.613252
Sum of electronic and thermal Free Energies= -4105.777952

O	1.02322400	4.43356400	4.01940300
O	-1.33301700	4.49314200	4.09451500
O	-4.75390900	1.18570800	4.23879900
O	-4.77158700	-1.16332700	4.31911400
O	-1.24545500	-4.36254700	4.14179800
O	1.11609500	-4.30423600	4.10880000
O	4.59623500	-1.06959400	4.46255200
O	4.56401400	1.27580400	4.43448100
C	2.77226400	2.83474600	4.21360900
C	1.59142800	3.39483900	4.72325800
C	-0.18725300	4.19640900	3.32853400
C	-1.91697300	3.42780000	4.74466100
C	-3.02728600	2.81748000	4.15461700
C	-3.62668300	1.73561600	4.80898900
C	-4.61798500	-0.01797000	3.51461600
C	-3.62543800	-1.68694600	4.87666100
C	-2.99468100	-2.74180300	4.20880700
C	-1.85092000	-3.30492600	4.78445600
C	-0.08478700	-4.06762400	3.40152200
C	1.67194900	-3.24636100	4.79410200
C	2.84308300	-2.67531200	4.27598100
C	3.43139200	-1.60993200	4.96777600
C	4.47966100	0.09265200	3.67471000
C	3.38629900	1.79910300	4.92789500
C	1.71431300	1.94562700	6.62673900
C	1.07148200	2.98776200	5.95794100
C	-0.16613100	3.66689200	6.52913700
C	-1.41082400	2.99613000	5.97201000
C	-2.04221200	1.91993300	6.59478000
C	-3.14858500	1.27450400	6.04165100
C	-3.78620100	0.05267200	6.68972200
C	-3.13592000	-1.18229300	6.08355400
C	-2.00317400	-1.78632100	6.62944100
C	-1.35135100	-2.85157400	6.00882600
C	-0.10165500	-3.50181100	6.58087900
C	1.13393700	-2.81831000	6.01295100
C	1.75289000	-1.74958500	6.66166800
C	2.89099900	-1.12125200	6.16066300
C	3.49421400	0.11764000	6.80682600
C	2.86136100	1.32727600	6.13425400
C	3.41022300	3.36507300	2.97990900
C	2.78200000	3.27860800	1.74323000
C	3.36177100	3.78282500	0.58553500
C	4.60935200	4.38455500	0.66533700
C	5.27586300	4.47948900	1.87728800
C	4.67256800	3.96794700	3.02127400
C	-0.15897100	3.75281900	8.05702900
C	-3.74946500	0.07718300	8.21827400
C	-0.10404900	-3.57128600	8.10975500
H	-0.18640700	4.90146100	2.49734000
H	-3.65030000	-0.04388400	2.99921800
H	-5.45138400	-0.03077500	2.81277200
H	-0.11187900	-3.02736900	3.06298600
H	-0.07404300	-4.76645900	2.56448600
H	5.34990600	0.09679500	3.01919200
H	3.54034600	0.07297400	3.10483500
H	1.30358300	1.60441100	7.57172300
H	-0.16332200	4.68990600	6.13921700
H	-1.65400500	1.56618200	7.54510500
H	-4.83548900	0.04165400	6.37869300
H	-1.61055100	-1.40903700	7.56895900
H	-0.08698200	-4.52928100	6.20324500
H	1.32801700	-1.39257000	7.59458200
H	4.55665800	0.12774200	6.54493400
H	-0.18491500	2.77451900	8.54399700
H	-2.73463500	0.07729000	8.62486300
H	-4.26328600	-0.80211900	8.61517600
H	-0.13260400	-2.58783700	8.58611200
H	0.79548400	-4.08322300	8.46165700
C	-3.53955500	-3.23664200	2.91827300
C	-4.76784300	-3.89237100	2.89589700
C	-2.87599400	-3.05346100	1.70175000
C	-5.31890000	-4.36324800	1.71132100
C	-3.40944100	-3.51659700	0.50112900
H	-1.93126800	-2.51906400	1.69250600
C	-4.62969500	-4.17137300	0.52057200
C	3.49381900	-3.21724800	3.05387400
C	4.76017900	-3.81013000	3.11139500
C	2.87468400	-3.15076900	1.81154500
C	5.37546300	-4.33121500	1.97807700
C	3.46591100	-3.66501500	0.66435000
C	4.71716100	-4.25657900	0.76024300
C	-3.55554400	3.31460200	2.85586800
C	-4.35505300	4.45749100	2.77042800
C	-3.25109200	2.64902300	1.67411300
C	-4.84217900	4.91462200	1.54957700
C	-3.72577900	3.08351700	0.44269000
C	-4.52289300	4.21877800	0.39408200
C	3.38464500	0.13229200	8.33184300
H	3.88647600	-0.74445200	8.74949300
H	3.86317400	1.03046300	8.73097500
H	2.35184400	0.12228100	8.68973400
H	0.74209900	4.26889700	8.39880900
H	-4.25416200	0.97294700	8.58967400
H	-0.97976300	-4.12837600	8.45250600
H	-0.22895400	3.15892700	2.98142200
H	-1.03305300	4.31307200	8.39900400
F	5.27426800	-4.74810900	-0.35165900
F	5.15511400	4.86654000	-0.45651900
F	-4.97320600	4.62639300	-0.79749200
F	-5.17766200	-4.63250100	-0.60916000
F	2.83766100	-3.58315800	-0.50902100
F	-6.49308700	-4.99360500	1.71924000
F	-3.41587600	2.41980600	-0.67090100
F	2.72685400	3.68187300	-0.58239400
F	1.67725500	-2.55937600	1.67582600
H	5.26522200	-3.85756700	4.06995300
H	5.18420100	4.03075900	3.97543500
H	-4.59408900	4.99228900	3.68315600
F	1.58878400	2.67780400	1.62486100
F	-2.46974400	1.55657300	1.69057100
F	-5.44769300	-4.09521100	4.02574100
H	6.25064400	4.95206500	1.90599400
H	6.35345200	-4.79614300	2.01965200
H	-2.90121700	-3.37327100	-0.44516000
H	-5.46441300	5.79876100	1.47535800

5-4in

Zero-point correction= 0.850958
(Hartree/Particle)
Thermal correction to Energy= 0.914430
Thermal correction to Enthalpy= 0.915374
Thermal correction to Gibbs Free Energy= 0.752073

Sum of electronic and zero-point Energies= -4105.678029
Sum of electronic and thermal Energies= -4105.614558
Sum of electronic and thermal Enthalpies= -4105.613613
Sum of electronic and thermal Free Energies= -4105.776915

O	1.20926400	4.62555600	4.23006100
O	-1.14392600	4.60254600	4.06549000
O	-4.63565600	1.35574500	4.14438400
O	-4.61325400	-1.00166800	4.05825900
O	-1.37040600	-4.49110300	4.28229500
O	0.98775700	-4.47218100	4.21672300
O	4.47518200	-1.22252700	4.36311200
O	4.45620800	1.13241300	4.21893600
C	2.83469300	2.87472200	4.21768800
C	1.74243600	3.50336800	4.82722500
C	0.08833200	4.40383600	3.40254400
C	-1.73843100	3.52812200	4.69181100
C	-2.88455800	2.98007800	4.09791600
C	-3.51968600	1.90804100	4.73572000
C	-4.40572200	0.20785300	3.35707700
C	-3.54568600	-1.57643300	4.71398100
C	-2.99387500	-2.74231500	4.16359200
C	-1.92758100	-3.35610900	4.83139900
C	-0.21532200	-4.28749400	3.49821800
C	1.55727400	-3.38360200	4.84182300
C	2.72803000	-2.85017500	4.28378700
C	3.33585300	-1.76192900	4.92090000
C	4.27747400	-0.09409600	3.53958400
C	3.36303000	1.72200300	4.81679300
C	1.77747300	1.91089200	6.60568000
C	1.19274900	3.03135200	6.01986400
C	-0.05089300	3.70600400	6.57448900
C	-1.27503900	3.06853100	5.93157600
C	-1.94541400	2.00055900	6.52838300
C	-3.06002900	1.39718400	5.95035200
C	-3.74025700	0.17198700	6.53812900
C	-3.09684600	-1.07255500	5.94180800
C	-2.03469300	-1.72327100	6.56997100
C	-1.42698400	-2.85660800	6.03448000
C	-0.20755000	-3.51712200	6.65567800
C	1.04255500	-2.89416400	6.04947000
C	1.68786400	-1.81162400	6.64774000
C	2.82603500	-1.22200000	6.10236200
C	3.48201000	0.01706900	6.68837400
C	2.86422100	1.24659900	6.03668100
C	3.44440700	3.46903900	2.99893300
C	3.43482400	2.80177900	1.78002500
C	4.01100000	3.34523900	0.63831600
C	4.60668600	4.59583400	0.71596600
C	4.62524900	5.30103700	1.90931100
C	4.04311300	4.73332500	3.03765500
C	-0.10309700	3.72180800	8.10347100
C	-3.77143700	0.16948300	8.06777600
C	-0.21891400	-3.49675100	8.18549600
H	0.12509300	5.17071600	2.62907100
H	-3.39293900	0.23849900	2.94316100
H	-5.16364200	0.21942600	2.57405200
H	-0.24155000	-3.28889700	3.05078700
H	-0.22029300	-5.07086000	2.74057900
H	5.06671100	-0.12388100	2.78865100
H	3.28241000	-0.13576800	3.08560300
H	1.36956200	1.53735500	7.53982700
H	-0.02423000	4.74495300	6.23141300
H	-1.58134000	1.62283500	7.47882600
H	-4.77576100	0.18733500	6.18408500
H	-1.66537700	-1.32791200	7.51117700
H	-0.22021200	-4.56393100	6.33650500
H	1.28433900	-1.41107600	7.57256900
H	4.53125400	-0.00614600	6.37789600
H	-0.10916500	2.72204600	8.54545100
H	-2.77620100	0.17736200	8.51979000
H	-4.29184200	-0.72111800	8.42980200
H	-0.23003500	-2.48680500	8.60357300
H	0.66793100	-4.00508400	8.57298300
C	-3.55315900	-3.36521500	2.93494900
C	-4.15326100	-4.62868900	2.97842800
C	-3.49311300	-2.72661800	1.70217500
C	-4.68870200	-5.22289700	1.84066700
C	-4.02217300	-3.29681200	0.55077100
C	-4.62102400	-4.54558800	0.63297800
C	3.36143200	-3.45027100	3.08003300
C	4.62331600	-4.05054900	3.15466600
C	2.73381300	-3.43009000	1.84036300
C	5.22660500	-4.62415800	2.04047000
C	3.31328700	-3.99758400	0.71212000
C	4.56020800	-4.59521200	0.82518700
C	-3.46448100	3.54828300	2.85243500
C	-4.72629700	4.15323000	2.85660700
C	-2.78527800	3.49109300	1.64138200
C	-5.28022800	4.69583700	1.70201100
C	-3.31481500	4.02720700	0.47393900
C	-4.56344900	4.63054700	0.51723000
C	3.44968400	0.05595700	8.21753800
H	3.96526200	-0.81979300	8.62028600
H	3.95486500	0.95528000	8.57957500
H	2.43649200	0.05822100	8.62785000
H	0.76924100	4.24984700	8.49738200
H	-4.30275800	1.05442600	8.42771600
H	-1.10751900	-4.01513500	8.55514700
H	0.13378500	3.39588000	2.97835300
H	-1.00541300	4.23815200	8.44154300
F	5.10572400	-5.13851300	-0.26854100
F	5.15818800	5.10655700	-0.39037500
F	-5.06076100	5.14344900	-0.61353100
F	-5.12733700	-5.08196600	-0.48279000
F	2.67830000	-3.96130400	-0.45927200
F	-3.94840000	-2.65138300	-0.61316300
F	-2.63125700	3.95589700	-0.66814900
F	3.98467400	2.67281500	-0.51224600
F	1.54139300	-2.83547700	1.68930700
H	5.13482100	-4.06119000	4.11095600
H	4.04545800	5.27544200	3.97697500
H	-5.27760400	4.19244500	3.78974500
H	-4.19442300	-5.14880500	3.92922700
F	2.84216000	1.60463700	1.66246500
F	-1.58967600	2.88950400	1.55774600
F	-2.89556800	-1.53224400	1.58109900
H	5.09385800	6.27776900	1.93606300
H	-6.25507400	5.16912800	1.70176400
H	-5.15836000	-6.19902300	1.87088300
H	6.20152500	-5.09413700	2.09488500

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Zero-point correction= 0.817561 (Hartree/Particle)
Thermal correction to Energy= 0.884995
Thermal correction to Enthalpy= 0.885939
Thermal correction to Gibbs Free Energy= 0.713327
Sum of electronic and zero-point Energies= -4502.508735
Sum of electronic and thermal Energies= -4502.441301
Sum of electronic and thermal Enthalpies= -4502.440357
Sum of electronic and thermal Free Energies= -4502.612969

O	1.16516900	4.56292500	4.19909600
O	-1.18821300	4.53220000	4.09700700
O	-4.66304600	1.28526600	4.20359500
O	-4.70796000	-1.06441500	4.23311900
O	-1.30412800	-4.39274200	4.16330100
O	1.05612300	-4.43319400	4.20984800
O	4.53575500	-1.18364000	4.39877500
O	4.50370400	1.17040800	4.30762700
C	2.80427900	2.83737900	4.23249000
C	1.70046500	3.45922200	4.82773800
C	0.02349800	4.34829400	3.40436500
C	-1.76231400	3.44799800	4.72494200
C	-2.88468200	2.86223600	4.12572700
C	-3.52841500	1.80852200	4.78471500
C	-4.53184400	0.09858000	3.45801400
C	-3.58919300	-1.61274000	4.82080300
C	-2.98221000	-2.69920200	4.17976100
C	-1.86578600	-3.29426200	4.77946400
C	-0.10651000	-4.19955600	3.45144500
C	1.62732900	-3.35222900	4.84686800
C	2.78478900	-2.79369400	4.29075100
C	3.38938900	-1.71632800	4.94852800
C	4.37710100	-0.03809100	3.59671800
C	3.37562000	1.72861600	4.86952200
C	1.77680600	1.91093200	6.64395600
C	1.16798200	3.00871600	6.03611500
C	-0.07762700	3.67725300	6.59599500
C	-1.29909600	3.01611100	5.97315700
C	-1.96491500	1.95467900	6.58529500
C	-3.07634100	1.33232800	6.01765800
C	-3.74866600	0.12062600	6.64605300
C	-3.11276900	-1.12125200	6.03860900
C	-2.00978800	-1.75685800	6.60835700
C	-1.37534200	-2.84479400	6.00967100
C	-0.15809900	-3.52079600	6.62248900
C	1.09958000	-2.88083800	6.05364000
C	1.73484500	-1.80280800	6.66922100
C	2.87383900	-1.19877800	6.13762200
C	3.51164500	0.03956800	6.74719300
C	2.87964700	1.26012600	6.09253600
C	3.36619100	3.38298200	2.97030800
C	3.34640400	2.66632700	1.76962700
C	3.87871000	3.21612200	0.61661700
C	4.43865500	4.48798300	0.62212600
C	4.45854900	5.21110100	1.80726700
C	3.92442200	4.65779100	2.96560900
C	-0.11400200	3.71350800	8.12477000
C	-3.73502500	0.13241700	8.17502400
C	-0.18490000	-3.55063800	8.15199000
H	0.04122000	5.12168400	2.63652500
H	-3.55592800	0.07336500	2.95324200
H	-5.35502600	0.10535100	2.74441200
H	-0.08118400	-3.17902500	3.04495500
H	-0.10343300	-4.95179200	2.66162700
H	5.20540200	-0.04826100	2.88841800
H	3.40457300	-0.08012800	3.08718000
H	1.37632100	1.54944000	7.58591600
H	-0.06540200	4.71172500	6.23832600
H	-1.60594200	1.60157700	7.54688500
H	-4.79302300	0.13322800	6.31901300
H	-1.62981600	-1.39004200	7.55678300
H	-0.16698400	-4.55740700	6.27094400
H	1.32370900	-1.41609700	7.59660200
H	4.56470800	0.03177100	6.44929300
H	2.89935600	1.68011400	1.71695700
H	-0.11421100	2.71977500	8.58023800
H	-2.72690500	0.11832600	8.59763200
H	-4.26583700	-0.74299700	8.55772200
H	-0.17670900	-2.55521800	8.60340600
H	0.68782300	-4.09068800	8.52786200
C	-3.54861100	-3.21678900	2.90785500
C	-4.82372700	-3.77420300	2.90353800
C	-2.85056800	-3.15566800	1.69767100
C	-5.39526300	-4.26726900	1.73584900
C	-3.41825300	-3.64719300	0.53533900
H	-1.86546400	-2.70607100	1.64519600
C	-4.69051200	-4.20622900	0.54102500
C	3.39254000	-3.33588000	3.04866200
C	4.66092700	-3.90636000	3.10133500
C	2.74258400	-3.28561100	1.81131200
C	5.27184900	-4.42223300	1.96381000
C	3.34952900	-3.79956300	0.67892200
H	1.76431600	-2.82875800	1.71373700
C	4.61462600	-4.37130700	0.74178300
C	-3.41806900	3.36091000	2.83217500
C	-4.67427000	3.95774400	2.79103500
C	-2.70265100	3.24290700	1.63630100
C	-5.21070000	4.43528100	1.60033700
C	-3.23566300	3.71875300	0.45132200
H	-1.73084400	2.76270600	1.61451400
C	-4.48902500	4.31800900	0.41979500
C	3.45867000	0.06506500	8.27548100
H	3.97447700	-0.81046200	8.67785100
H	3.95427400	0.96414200	8.65056400
H	2.44013100	0.05902100	8.67231800
H	0.76041400	4.24927400	8.50276700
H	-4.23532600	1.03144000	8.54389900
H	-1.08699100	-4.06221100	8.49717200
H	0.06383000	3.34046000	2.96860800
H	-1.01417200	4.23267800	8.46364500
F	5.19584500	-4.86305200	-0.34799700
F	4.94795200	5.01400600	-0.48770800
F	-4.99916900	4.77350400	-0.72062100
F	-5.23404200	-4.67649600	-0.57754700
F	6.48152700	-4.96864700	2.04008200
F	2.73092400	-3.74923100	-0.50608000
F	-2.75360300	-3.58673300	-0.62422300
F	-6.61261600	-4.80157900	1.75695100

F	-2.55476500	3.60436900	-0.69498000
F	-6.41062500	5.00809900	1.58538300
F	3.85846300	2.53365400	-0.53399400
F	4.99275000	6.42852200	1.82823800
F	5.32310300	-3.98627300	4.25579800
F	3.97341900	5.38259900	4.08369100
F	-5.53085400	-3.86245300	4.03035900
F	-5.39599600	4.10021900	3.90296900

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Zero-point correction= 0.817431 (Hartree/Particle)
Thermal correction to Energy= 0.885029
Thermal correction to Enthalpy= 0.885973
Thermal correction to Gibbs Free Energy= 0.711097
Sum of electronic and zero-point Energies= -4502.511902
Sum of electronic and thermal Energies= -4502.444304
Sum of electronic and thermal Enthalpies= -4502.443360
Sum of electronic and thermal Free Energies= -4502.618236

O	1.14394100	4.59160900	4.21012100
O	-1.20751500	4.55225800	4.10566000
O	-4.63272700	1.25429700	4.17442200
O	-4.63380400	-1.09469400	4.20181600
O	-1.23617500	-4.41981000	4.22804500
O	1.11249900	-4.50060900	4.34945900
O	4.50154400	-1.16336100	4.38241800
O	4.47134700	1.18983600	4.29610400
C	2.77479300	2.85943100	4.23078200
C	1.67880200	3.48553800	4.83445300
C	0.00464800	4.38027900	3.41114000
C	-1.77166800	3.45957500	4.72782700
C	-2.87966100	2.85869400	4.11823500
C	-3.51477100	1.79594400	4.77035400
C	-4.46545600	0.07105700	3.42996900
C	-3.51933500	-1.62604600	4.81280800
C	-2.88874800	-2.70799100	4.18876200
C	-1.79073400	-3.30498400	4.81950400
C	-0.01824700	-4.27852000	3.53832600
C	1.66701800	-3.39494500	4.95677800
C	2.78937400	-2.81425700	4.36050900
C	3.37863000	-1.70376200	4.97071600
C	4.31665200	-0.01549200	3.58596900
C	3.35185700	1.75456200	4.86807400
C	1.76569100	1.93913900	6.65270000
C	1.15266600	3.03550500	6.04625600
C	-0.09596800	3.69877700	6.60626300
C	-1.31147900	3.03082800	5.97842300
C	-1.97002000	1.96168200	6.58492800
C	-3.06925400	1.32610300	6.00791500
C	-3.73406900	0.10768100	6.63169300
C	-3.07464200	-1.12980700	6.04064900
C	-1.98292500	-1.75993600	6.63774600
C	-1.33219900	-2.85058800	6.06139500
C	-0.13169700	-3.52110000	6.71548200
C	1.13572700	-2.89839100	6.15006400
C	1.75852500	-1.79186400	6.72812700
C	2.87795800	-1.17813100	6.16517900
C	3.51170800	0.07491800	6.75016600
C	2.86634700	1.28878900	6.09566800
C	3.31820500	3.38948500	2.95385400
C	3.26135000	2.66384400	1.75930600
C	3.77696200	3.19838900	0.59141400
C	4.35432000	4.46245700	0.57594200
C	4.40963500	5.19402700	1.75474600
C	3.89269900	4.65647100	2.92812600
C	-0.13597800	3.73193700	8.13486700
C	-3.74395600	0.12850000	8.16061100
C	-0.18406300	-3.51195300	8.24424600
H	0.02009500	5.16140700	2.65122800
H	-3.48022200	0.06484800	2.94320200
H	-5.27543800	0.06256900	2.70142700
H	0.04905700	-3.28249600	3.08039700
H	-0.01070900	-5.07050500	2.78946800
H	5.12078900	-0.02927400	2.85010100
H	3.32756100	-0.05452000	3.11220600
H	1.37026400	1.57846600	7.59718700
H	-0.08808200	4.73373200	6.24994200
H	-1.61376600	1.61127800	7.54855100
H	-4.77351100	0.10522300	6.28883300
H	-1.62879300	-1.38932700	7.59456300
H	-0.14129200	-4.56551300	6.38756900
H	1.35015900	-1.38646900	7.64890500
H	4.56062300	0.07190200	6.43709500
H	2.79835200	1.68373900	1.72261200
H	-0.13251400	2.73725200	8.58829100
H	-2.74220600	0.13301100	8.59837100
H	-4.26674700	-0.75287200	8.54079300
H	-0.16436300	-2.50546100	8.67020100
H	0.67303700	-4.05721000	8.64768300
C	-3.40816100	-3.22137900	2.89507800
C	-4.66525100	-3.81511400	2.84633100
C	-2.67760700	-3.11781200	1.70686800
C	-5.18859000	-4.30588800	1.65532300
C	-3.19792700	-3.60722100	0.52146900
H	-1.70521200	-2.63774200	1.69051300
C	-4.45221700	-4.20423400	0.48246900
C	3.33147700	-3.35687600	3.08563500
C	4.24676400	-4.41292200	3.06613000
C	2.92407500	-2.81669700	1.87311400
C	4.72615500	-4.89222400	1.86053300
C	3.40418500	-3.29552000	0.65893100
C	4.31412600	-4.34279600	0.65018500
C	-3.40689700	3.34871800	2.81856700
C	-4.66037800	3.95020700	2.76918000
C	-2.68935500	3.21559800	1.62560900
C	-5.19206900	4.41938700	1.57317700
C	-3.21774200	3.68323000	0.43507900
H	-1.72052600	2.72901500	1.61008700
C	-4.46803600	4.28829400	0.39551000
C	3.48138900	0.11681900	8.27895200
H	4.00496600	-0.75280900	8.68431900
H	3.97985100	1.02147100	8.63641100
H	2.46870700	0.11316800	8.69041700
H	0.73492400	4.27121500	8.51604900
H	-4.26364300	1.02183800	8.51624500
H	-1.10014800	-3.99866900	8.58858900
H	0.04960200	3.37725600	2.96519200
H	-1.03948200	4.24597600	8.47270900
F	4.77989200	-4.80965400	-0.50395500

F	4.84781700	4.97341000	-0.54824000
F	-4.97370300	4.73581600	-0.75019400
F	-4.94978600	-4.67269400	-0.65847300
F	5.60161500	-5.90089600	1.82765100
F	2.99508900	-2.75740300	-0.48677400
F	-2.50422400	-3.50877600	-0.61827300
F	-6.38985000	-4.87602200	1.63256700
F	-2.53542200	3.55524700	-0.70872400
F	-6.38968200	4.99703400	1.55006900
F	3.72355600	2.50936400	-0.55384000
F	4.96073800	6.40431800	1.75493300
F	3.97407100	5.38840600	4.03997500
F	-5.40083100	-3.94060900	3.95154700
F	-5.38483000	4.10327900	3.87821900
F	2.03748200	-1.80421700	1.83970000
H	4.58671400	-4.86464100	3.99096700

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Zero-point correction= 0.818052 (Hartree/Particle)
Thermal correction to Energy= 0.885358
Thermal correction to Enthalpy= 0.886303
Thermal correction to Gibbs Free Energy= 0.714323
Sum of electronic and zero-point Energies= -4502.513735
Sum of electronic and thermal Energies= -4502.446428
Sum of electronic and thermal Enthalpies= -4502.445484
Sum of electronic and thermal Free Energies= -4502.617464

O	1.09567200	4.40491300	3.98545500
O	-1.26806200	4.43424100	3.99481200
O	-4.78891600	1.23741500	4.28016200
O	-4.78793500	-1.11107600	4.30922700
O	-1.26272300	-4.30912900	4.10108900
O	1.10109000	-4.27546400	4.08966100
O	4.62893000	-1.10074300	4.50191000
O	4.62756000	1.24564700	4.47402200
C	2.84787000	2.81153000	4.22123800
C	1.66210700	3.37850900	4.70874300
C	-0.09519200	4.12713900	3.27786700
C	-1.86766600	3.39535800	4.67239000
C	-3.01431300	2.81285000	4.11996800
C	-3.63902300	1.77274900	4.81811900
C	-4.66624500	0.05374400	3.52728800
C	-3.63744200	-1.63187400	4.86007000
C	-3.01194500	-2.68833200	4.18768200
C	-1.86406000	-3.25526500	4.75353000
C	-0.09075900	-4.01673600	3.37648300
C	1.66626900	-3.23129200	4.78808500
C	2.85120700	-2.67456600	4.28693900
C	3.44891200	-1.62230300	4.99017400
C	4.54592000	0.06320900	3.71275800
C	3.44684800	1.77726000	4.94955800
C	1.74789500	1.93990300	6.62090400
C	1.11948500	2.97958200	5.93486700
C	-0.12866100	3.66546500	6.47077700
C	-1.36756000	2.98461600	5.91104300
C	-2.01599900	1.93775600	6.56536000
C	-3.14562500	1.30991000	6.04098100
C	-3.78540600	0.09320200	6.69459100
C	-3.14400500	-1.13825500	6.07083900
C	-2.01314200	-1.75134600	6.60990900
C	-1.36372400	-2.81325500	5.98130200
C	-0.12362300	-3.47843100	6.55692900
C	1.12333000	-2.80370300	6.00439600
C	1.75026700	-1.74685000	6.66508000
C	2.90168000	-1.13102500	6.17892200
C	3.51207500	0.09988300	6.83383100
C	2.90011800	1.31404600	6.14973800
C	3.49893800	3.32583600	2.98736100
C	2.89286000	3.20033300	1.74467400
C	3.48686800	3.68702000	0.58542400
C	4.72305500	4.31136600	0.65912400
C	5.34571100	4.43191700	1.89768600
C	4.75140100	3.94812800	3.04776200
C	-0.14365700	3.78320200	7.99671700
C	-3.72799800	0.11181200	8.22227000
C	-0.13814200	-3.55963300	8.08524800
H	-0.08573500	4.79448600	2.41530100
H	-3.71197300	0.04742900	2.98215200
H	-5.51837900	0.04505100	2.84856400
H	-0.10318400	-2.97098400	3.05252900
H	-0.08040900	-4.70417100	2.52985300
H	5.43146600	0.05619100	3.07826800
H	3.61964200	0.05568200	3.12118600
H	1.31975700	1.60482100	7.56041900
H	-0.12235800	4.68083100	6.06135900
H	-1.62443500	1.59616100	7.51865800
H	-4.83836500	0.08883300	6.39672400
H	-1.62140700	-1.38554800	7.55413300
H	-0.11581500	-4.50330400	6.17197700
H	1.32166600	-1.38990400	7.59630400
H	4.57791700	0.09759900	6.58604700
H	-0.16196300	2.81514600	8.50403400
H	-2.70787100	0.11713500	8.61540800
H	-4.23203400	-0.77102500	8.62375800
H	-0.15779700	-2.57978200	8.56930400
H	0.75239700	-4.08555100	8.43910300
C	-3.58210200	-3.19880300	2.91476000
C	-4.84612600	-3.78107200	2.91593600
C	-2.89624000	-3.10824400	1.69885300
C	-5.42010100	-4.26923800	1.74752400
C	-3.46717300	-3.59528200	0.53621300
H	-1.91880600	-2.64188900	1.64178700
C	-4.72864800	-4.17849600	0.54707700
C	3.50310900	-3.21699800	3.06561000
C	4.75789200	-3.83308800	3.14036900
C	2.89598500	-3.12399200	1.82056200
C	5.35347100	-4.34245000	2.00204300
C	3.49125000	-3.63652900	0.67314600
C	4.72981100	-4.25421500	0.76125400
C	-3.58398800	3.28994600	2.83396600
C	-4.84926800	3.86926800	2.81871500
C	-2.89643100	3.16970300	1.62158000
C	-5.42274700	4.32611500	1.63745100
C	-3.46688700	3.62552500	0.44613800
H	-1.91805200	2.70392700	1.57760400
C	-4.72955400	4.20617800	0.44052400
C	3.38165600	0.11792000	8.35700600
H	3.86736500	-0.76398600	8.78257000
H	3.86584100	1.01053100	8.76144500

H	2.34406200	0.12108600	8.70083500
H	0.74600300	4.31878200	8.33806600
H	-4.23299900	1.00361600	8.60215400
H	-1.02283800	-4.10873400	8.41746600
H	-0.10533100	3.07402300	2.97864900
H	-1.02927100	4.33873400	8.31553600
F	5.30771300	-4.74716900	-0.32994400
F	5.29963500	4.78019500	-0.44334000
F	-5.27501200	4.64246300	-0.69125900
F	-5.27449200	-4.64477400	-0.57250800
F	6.54956000	-4.93649300	2.06538300
F	2.88134600	-3.53097700	-0.50489300
F	-2.81705500	-3.50862700	-0.62965100
F	-6.62679000	-4.82830600	1.77364000
F	-2.81510100	3.51019200	-0.71631000
F	-6.63069700	4.88295900	1.64765600
F	2.87802500	3.55061600	-0.58998000
F	6.53950200	5.03184100	1.94719000
F	1.70997500	-2.50955400	1.68117000
H	5.27424000	-3.91426200	4.09004100
H	5.26682500	4.05442400	3.99545000
F	1.70908200	2.57844300	1.61983400
F	-5.54400900	4.01655000	3.94748900
F	-5.53915900	-3.90116800	4.04899800

7-2*anti*-in

Zero-point correction= 0.817635 (Hartree/Particle)
Thermal correction to Energy= 0.885201
Thermal correction to Enthalpy= 0.886145
Thermal correction to Gibbs Free Energy= 0.711264
Sum of electronic and zero-point Energies= -4502.513993
Sum of electronic and thermal Energies= -4502.446428
Sum of electronic and thermal Enthalpies= -4502.445483
Sum of electronic and thermal Free Energies= -4502.620364

O	1.06606300	4.67916200	4.28492000
O	-1.28115700	4.66636700	4.24843200
O	-4.52334500	1.19408200	4.04582400
O	-4.55764800	-1.15905200	4.14214700
O	-1.20326500	-4.52822900	4.29980200
O	1.14557000	-4.57320600	4.40987700
O	4.40240500	-1.10658700	4.25225200
O	4.36731600	1.25187800	4.21967300
C	2.68011600	2.93489700	4.22916300
C	1.59838100	3.55016400	4.86915000
C	-0.09399400	4.52330000	3.50287800
C	-1.82006800	3.52923800	4.81076500
C	-2.86974200	2.89795300	4.13631200
C	-3.45840100	1.76353600	4.70846800
C	-4.31506200	-0.01793300	3.35232600
C	-3.46985900	-1.70426000	4.78720200
C	-2.84075600	-2.80484000	4.19704400
C	-1.75674600	-3.39467800	4.85613500
C	0.00806500	-4.40838400	3.59468500
C	1.67662400	-3.43090500	4.96942800
C	2.76055400	-2.82599000	4.32672300
C	3.32073800	-1.67411200	4.88973400
C	4.16799400	0.06109700	3.49534100
C	3.26858200	1.81613100	4.83011200
C	1.72345100	1.96416200	6.65247600
C	1.09775200	3.07322200	6.08319200
C	-0.14336400	3.71471900	6.68711700
C	-1.35673300	3.05949100	6.04324700
C	-1.98945800	1.94434900	6.59030100
C	-3.04506500	1.28658500	5.95752600
C	-3.71590200	0.06067100	6.56167400
C	-3.04032200	-1.18428200	6.00896400
C	-1.95798700	-1.80345300	6.63418300
C	-1.30526700	-2.90882500	6.08926200
C	-0.09572100	-3.55008700	6.75595000
C	1.15356900	-2.91916400	6.15986800
C	1.75942700	-1.78564400	6.70031200
C	2.84498600	-1.15044900	6.09587700
C	3.48147400	0.10579200	6.67160700
C	2.81134400	1.32606300	6.05777000
C	3.19850800	3.48974000	2.95237900
C	3.11461100	2.78837500	1.74497700
C	3.60930500	3.34475700	0.57826900
C	4.19203800	4.60648200	0.57703100
C	4.27430700	5.31369900	1.76896600
C	3.77853500	4.75439800	2.94118400
C	-0.16738800	3.68661400	8.21576700
C	-3.77978300	0.09045100	8.08979100
C	-0.13736600	-3.49922100	8.28389500
H	-0.08764900	5.35096100	2.79444700
H	-3.29844900	-0.05094000	2.94480700
H	-5.06782200	-0.03266300	2.56439700
H	0.05861700	-3.43738100	3.08360100
H	0.02113900	-5.23829700	2.88862600
H	4.92419100	0.06076300	2.70974600
H	3.15251400	0.03337100	3.08472600
H	1.34950300	1.58342300	7.59783600
H	-0.14279000	4.76222200	6.36987800
H	-1.64738900	1.57173200	7.55076200
H	-4.74372200	0.05069700	6.18485100
H	-1.61067500	-1.40953300	7.58432800
H	-0.09271800	-4.60263500	6.45571600
H	1.36650300	-1.37604600	7.62584000
H	4.52009200	0.11507500	6.32566000
H	-0.16958800	2.67423400	8.62824200
H	-2.79429300	0.08651300	8.56288400
H	-4.32366900	-0.78483400	8.45401600
H	-0.13037000	-2.48106700	8.68168000
H	0.73080200	-4.01985100	8.69614500
C	-3.34043700	-3.33868700	2.90317800
C	-4.56055600	-4.00424100	2.86026000
C	-2.62792100	-3.18002500	1.71032900
C	-5.06472100	-4.51566200	1.66987300
C	-3.12922200	-3.69009700	0.52499300
C	-4.34563000	-4.36114500	0.49199000
C	3.30721100	-3.40837300	3.07187200
C	4.09163800	-4.56581900	3.08991200
C	3.03861800	-2.81715600	1.84473300
C	4.58766600	-5.08697500	1.90908300
C	3.53643000	-3.33750400	0.65513000
C	4.32009400	-4.48178900	0.68495800
C	-3.36503200	3.44850200	2.84647500
C	-4.09692400	4.63950900	2.80122300
C	-3.10116000	2.79536900	1.65018300

C	-4.54918200	5.13175800	1.59098000
C	-3.55526400	3.28695100	0.43118100
C	-4.28804400	4.46422100	0.39837800
C	3.50154100	0.12877300	8.20133800
H	4.03876000	-0.74497300	8.57913200
H	4.01093300	1.02992600	8.55222200
H	2.50303400	0.11978100	8.64600400
H	0.71172500	4.20220900	8.61068800
H	-4.30323200	0.98997500	8.42402100
H	-1.04335800	-3.99013100	8.64841900
H	-0.08206600	3.54983800	2.99296100
H	-1.06293700	4.19437900	8.58314700
F	4.80179500	-4.98823900	-0.44594300
F	4.66543900	5.13836300	-0.54638300
F	-4.72727200	4.94288200	-0.76188700
F	-4.82481400	-4.84947000	-0.64863700
F	5.34114800	-6.19075600	1.91415900
F	3.26185700	-2.74732200	-0.50509100
F	-2.45367900	-3.54141000	-0.61977900
F	-6.23091800	-5.15479300	1.65199800
F	-3.28678200	2.63742400	-0.69891000
F	-5.25284200	6.26700700	1.53614100
F	3.53027800	2.68028300	-0.57988300
F	4.83113900	6.52168200	1.78274700
F	2.26705200	-1.71798100	1.77012600
H	4.31593700	-5.06414600	4.02609200
H	-4.31372000	5.18694000	3.71138800
F	-2.37676900	1.66381600	1.63494300
H	-1.68776200	-2.63935900	1.69020800
H	2.64588600	1.81142100	1.69751200
F	-5.27965400	-4.17625300	3.97077800
F	3.88646400	5.46299200	4.06611900

7-3in

Zero-point correction= 0.817972 (Hartree/Particle)
Thermal correction to Energy= 0.885369
Thermal correction to Enthalpy= 0.886313
Thermal correction to Gibbs Free Energy= 0.713527
Sum of electronic and zero-point Energies= -4502.515275
Sum of electronic and thermal Energies= -4502.447878
Sum of electronic and thermal Enthalpies= -4502.446934
Sum of electronic and thermal Free Energies= -4502.619721

O	1.02724700	4.44143700	4.02581700
O	-1.32984600	4.50144400	4.09522200
O	-4.74595200	1.18976600	4.22084300
O	-4.76450100	-1.16086700	4.29528900
O	-1.23734600	-4.36078800	4.11989500
O	1.12565800	-4.30187500	4.09851300
O	4.60158100	-1.06438800	4.46106200
O	4.56584500	1.28201300	4.43510200
C	2.77398700	2.84018400	4.21887200
C	1.59298900	3.40026000	4.72744500
C	-0.18162400	4.20844200	3.33092900
C	-1.91295500	3.43429500	4.74240700
C	-3.02260200	2.82523900	4.15022600
C	-3.62160400	1.73901700	4.79694300
C	-4.60707300	-0.01254500	3.49506600
C	-3.62138100	-1.68710700	4.85579600
C	-2.99315800	-2.74672500	4.19209000
C	-1.84476300	-3.30543500	4.76407900
C	-0.07160000	-4.06392500	3.38676200
C	1.67957100	-3.24461200	4.78621000
C	2.85167400	-2.67217500	4.27298400
C	3.43731700	-1.60576500	4.96511400
C	4.48589000	0.09896700	3.67451200
C	3.38785000	1.80231800	4.92971800
C	1.71472900	1.94661300	6.62749300
C	1.07214600	2.99011000	5.96060400
C	-0.16610400	3.66800700	6.53163400
C	-1.40883500	2.99833900	5.96897300
C	-2.04102900	1.91954400	6.58646800
C	-3.14523500	1.27442400	6.02870300
C	-3.78373400	0.05045500	6.67105500
C	-3.13144500	-1.18188900	6.06206200
C	-1.99932200	-1.78622700	6.60847600
C	-1.34609500	-2.85075900	5.98828700
C	-0.09917600	-3.50193600	6.56531000
C	1.13827800	-2.81742900	6.00357500
C	1.75528400	-1.74930100	6.65504400
C	2.89385000	-1.11907800	6.15727800
C	3.49533400	0.11891300	6.80658100
C	2.86196900	1.32862400	6.13480500
C	3.41227400	3.37389800	2.98659800
C	2.78678200	3.28552200	1.75018100
C	3.37063800	3.79437900	0.59504400
C	4.61502900	4.40236100	0.66582700
C	5.25668300	4.48537300	1.89767300
C	4.67298100	3.98012500	3.04376700
C	-0.16265400	3.74893600	8.05976000
C	-3.75047000	0.06940400	8.19977200
C	-0.10858700	-3.57312900	8.09408100
H	-0.17854900	4.91843600	2.50402800
H	-3.63715700	-0.03715100	2.98356400
H	-5.43796500	-0.02332200	2.79023400
H	-0.09669800	-3.02225400	3.05129800
H	-0.05710900	-4.76073300	2.54798000
H	5.35881900	0.10510000	3.02271600
H	3.54834700	0.07834500	3.10157600
H	1.30426100	1.60454600	7.57225800
H	-0.16249400	4.69226700	6.14500600
H	-1.65536500	1.56372800	7.53702000
H	-4.83234700	0.03988300	6.35778400
H	-1.60847200	-1.41011500	7.54913000
H	-0.08281900	-4.52903600	6.18677800
H	1.32877400	-1.39430000	7.58796100
H	4.55813100	0.13043300	6.54612900
H	-0.18945000	2.76916200	8.54368400
H	-2.73672400	0.06924400	8.60898000
H	-4.26446700	-0.81171200	8.59224000
H	-0.13754200	-2.59033200	8.57168500
H	0.78851600	-4.08704900	8.44905000
C	-3.55916600	-3.26450000	2.92025600
C	-4.81725800	-3.85913000	2.92500500
C	-2.87740500	-3.16590800	1.70271100
C	-5.38885500	-4.35465300	1.75875400
C	-3.44602900	-3.66055600	0.54201000
H	-1.90747800	-2.68448700	1.64190600
C	-4.70081100	-4.25797500	0.55682800

C	3.50553100	-3.21309900	3.05192700
C	4.76940300	-3.81045300	3.12638800
C	2.89243400	-3.13801700	1.80859600
C	5.36826500	-4.31950600	1.98974500
C	3.49119900	-3.65033700	0.66276600
C	4.73887200	-4.24932500	0.75074500
C	-3.55165300	3.32972700	2.85459300
C	-4.35192000	4.47426300	2.79124300
C	-3.24717100	2.67281400	1.66971700
C	-4.82710100	4.92185200	1.57224500
C	-3.72440700	3.11996300	0.44220400
C	-4.52250500	4.25349200	0.39056700
C	3.38370400	0.13087500	8.33142900
H	3.88629700	-0.74579200	8.74812000
H	3.86096800	1.02872600	8.73258300
H	2.35050900	0.11906500	8.68814500
H	0.73729800	4.26435600	8.40522400
H	-4.25724400	0.96313300	8.57303300
H	-0.98643700	-4.12947900	8.43237700
H	-0.22287400	3.17283100	2.97811000
H	-1.03749800	4.30808200	8.40137700
F	5.31994200	-4.74201300	-0.33904800
F	5.18113200	4.89210800	-0.43333200
F	-4.98404200	4.68965100	-0.77788800
F	-5.24432700	-4.73178800	-0.56094700
F	6.57309700	-4.89599400	2.05312100
F	2.87570300	-3.56275100	-0.51377800
F	-2.80065300	-3.56822100	-0.62571900
F	-6.58996300	-4.92614200	1.78809100
F	-3.41827400	2.46986900	-0.67746600
F	-5.59514100	6.01355600	1.49840900
F	2.74360100	3.69519800	-0.57471700
F	6.45824100	5.07065700	1.94472500
F	1.69734200	-2.54246400	1.66908900
H	5.29021400	-3.87717600	4.07475300
H	5.20312500	4.05680200	3.98617800
H	-4.60517000	5.01973700	3.69309400
F	1.59525100	2.68165600	1.62721600
F	-2.46604900	1.57995000	1.67633900
F	-5.50718600	-3.98252600	4.06014200

7-4in

Zero-point correction= 0.818034 (Hartree/Particle)
Thermal correction to Energy= 0.885408
Thermal correction to Enthalpy= 0.886352
Thermal correction to Gibbs Free Energy= 0.713686
Sum of electronic and zero-point Energies= -4502.516325
Sum of electronic and thermal Energies= -4502.448951
Sum of electronic and thermal Enthalpies= -4502.448007
Sum of electronic and thermal Free Energies= -4502.620673

O	1.20326400	4.62499300	4.23027000
O	-1.15020600	4.60174000	4.07218100
O	-4.63432800	1.35085400	4.14485500
O	-4.61280000	-1.00665400	4.06466400
O	-1.36696900	-4.49004600	4.28226800
O	0.99127700	-4.47052300	4.22009400
O	4.47242300	-1.21742800	4.35994700
O	4.45284900	1.13782400	4.22097600
C	2.82659200	2.87440700	4.22123700
C	1.73469600	3.50368200	4.82970300
C	0.07999500	4.40650100	3.40511900
C	-1.74100000	3.52588900	4.69872700
C	-2.88374700	2.97329300	4.10401200
C	-3.51979100	1.90126000	4.73966000
C	-4.40712600	0.20079500	3.35998200
C	-3.54436900	-1.57855900	4.72065800
C	-2.98884600	-2.74161900	4.16955700
C	-1.92227700	-3.35636900	4.83491600
C	-0.21065000	-4.28843500	3.49953000
C	1.55797500	-3.38105900	4.84534900
C	2.72571000	-2.84358000	4.28619400
C	3.33461300	-1.75533500	4.92127700
C	4.27639200	-0.08708000	3.53868700
C	3.35912400	1.72416500	4.82012200
C	1.77570100	1.91372000	6.61020800
C	1.18801200	3.03273500	6.02418100
C	-0.05499500	3.70674500	6.58129700
C	-1.27868900	3.06775100	5.93913200
C	-1.94898600	1.99916200	6.53512300
C	-3.06181200	1.39299300	5.95608600
C	-3.74153000	0.16803100	6.54518900
C	-3.09656900	-1.07579000	5.94904100
C	-2.03368000	-1.72656800	6.57610200
C	-1.42352500	-2.85824100	6.03936900
C	-0.20387600	-3.51817200	6.66094900
C	1.04495300	-2.89325100	6.05415200
C	1.69051800	-1.81034800	6.65162100
C	2.82674300	-1.21796300	6.10474200
C	3.48248900	0.02077700	6.69185700
C	2.86249100	1.24957500	6.04096700
C	3.43109600	3.46249200	2.99661600
C	3.39482200	2.79697800	1.77879600
C	3.96463300	3.33740500	0.63095400
C	4.58217000	4.57770500	0.69047900
C	4.61348000	5.25902500	1.90313200
C	4.04760200	4.71838300	3.04207800
C	-0.10530500	3.72201300	8.11025900
C	-3.77265100	0.16624200	8.07476000
C	-0.21502600	-3.49811700	8.19069100
H	0.11461100	5.17771200	2.63589400
H	-3.39549600	0.22973600	2.94263200
H	-5.16823200	0.21094300	2.58006100
H	-0.23627600	-3.29109000	3.04890700
H	-0.21453700	-5.07478100	2.74501800
H	5.06829400	-0.11511300	2.79053500
H	3.28243700	-0.12783700	3.08182900
H	1.37042500	1.54164600	7.54605600
H	-0.02960600	4.74578900	6.23827800
H	-1.58670900	1.62346300	7.48703000
H	-4.77703200	0.18237400	6.19096100
H	-1.66596000	-1.33291000	7.51862700
H	-0.21554400	-4.56491400	6.34140100
H	1.28915900	-1.41201800	7.57831900
H	4.53151300	-0.00124200	6.38043300
H	-0.11121600	2.72214700	8.55199000
H	-2.77744300	0.17381900	8.52682500
H	-4.29358700	-0.72386200	8.43700900
H	-0.22620300	-2.48831800	8.60910200

H	0.67182600	-4.00658400	8.57777200
C	-3.54294600	-3.35653900	2.93430200
C	-4.16602800	-4.60903300	2.98208400
C	-3.45124400	-2.71959500	1.70415800
C	-4.68442100	-5.17417400	1.83245200
C	-3.97327600	-3.28461600	0.54553100
C	-4.59806900	-4.52119500	0.60690200
C	3.35217000	-3.43871800	3.07608500
C	4.60592000	-4.05602200	3.15623000
C	2.72530600	-3.39259600	1.83825700
C	5.18204600	-4.61314000	2.03040100
C	3.30137800	-3.95374600	0.70356500
C	4.53909200	-4.57215800	0.79721900
C	-3.45395100	3.53470700	2.85073200
C	-4.70358600	4.16502600	2.85706600
C	-2.77558000	3.44171200	1.64297100
C	-5.22586400	4.68899400	1.68975300
C	-3.29752000	3.96910200	0.46671100
C	-4.53183400	4.60104700	0.48705400
C	3.45125200	0.05854200	8.22099100
H	3.96739600	-0.81723800	8.62273000
H	3.95687900	0.95747300	8.58314700
H	2.43841600	0.06054100	8.63216000
H	0.76740900	4.24989300	8.50332300
H	-4.30383700	1.05130400	8.43436300
H	-1.10324000	-4.01698200	8.56037000
H	0.12429200	3.40038100	2.97595400
H	-1.00692200	4.23869200	8.44943200
F	5.09761700	-5.11229900	-0.28216600
F	5.13061200	5.10227400	-0.40169100
F	-5.03881100	5.10966800	-0.63239300
F	-5.10136600	-5.06904700	-0.49552700
F	6.37712900	-5.20956200	2.09911000
F	2.67314900	-3.89557300	-0.46815600
F	-3.87184000	-2.64699900	-0.61815800
F	-5.28625000	-6.36791100	1.87009000
F	-2.62090800	3.86616400	-0.67458700
F	-6.41661300	5.29779200	1.68766000
F	3.91579400	2.67255600	-0.52080300
F	5.20943000	6.45578300	1.93902100
F	1.53992100	-2.78151700	1.69375100
H	5.13665900	-4.10105400	4.10037600
H	4.08509700	5.27860000	3.96936300
H	-5.27329700	4.24625500	3.77573500
H	-4.24597700	-5.14740400	3.91957400
F	2.78520100	1.60733400	1.66686400
F	-1.59091700	2.81646200	1.57005000
F	-2.83229200	-1.53480000	1.59147400

1-TS

Zero-point correction= 0.948290 (Hartree/Particle)
Thermal correction to Energy= 1.000211
Thermal correction to Enthalpy= 1.001155
Thermal correction to Gibbs Free Energy= 0.864245
Sum of electronic and zero-point Energies= -2915.084862
Sum of electronic and thermal Energies= -2915.032941
Sum of electronic and thermal Enthalpies= -2915.031997
Sum of electronic and thermal Free Energies= -2915.168907

O	1.07975500	4.44876100	4.05424800
O	-1.25922800	4.59932600	4.14655700
O	-4.68478600	1.17070800	4.11884200
O	-4.51342300	-1.16516800	3.98757000
O	-1.17699400	-4.54810000	4.32707700
O	1.17075300	-4.49127800	4.38193600
O	4.55785400	-1.14851600	4.54664600
O	4.52913200	1.19299800	4.46524900
C	2.76180300	2.77437000	4.21367000
C	1.60759900	3.37275500	4.73838400
C	-0.12922300	4.27310100	3.36612000
C	-1.94959500	3.54017300	4.70045900
C	-3.11050100	3.02416700	4.06576300
C	-3.62937100	1.85669300	4.68577800
C	-4.35178700	0.05685500	3.31894600
C	-3.43131200	-1.68977000	4.66438100
C	-2.80919500	-2.81963100	4.11532200
C	-1.76731800	-3.41200400	4.84059600
C	0.01175500	-4.36649400	3.59404900
C	1.68189600	-3.36185500	4.98669200
C	2.82418100	-2.77839200	4.42239000
C	3.40104100	-1.68241900	5.07589500
C	4.43274000	-0.00658300	3.73299500
C	3.35944000	1.74164600	4.94841400
C	1.68228700	1.92635300	6.64332100
C	1.06119200	2.97413700	5.96372100
C	-0.18088900	3.67171000	6.50151400
C	-1.42931400	3.03822200	5.89887100
C	-2.04225400	1.93735700	6.48294900
C	-3.13380500	1.32438900	5.88170900
C	-3.76045600	0.06090700	6.45998300
C	-3.04546900	-1.16267200	5.90265500
C	-1.98822000	-1.77864800	6.57232600
C	-1.33427900	-2.90126100	6.06643800
C	-0.12782700	-3.52946300	6.74753200
C	1.12891200	-2.88318800	6.18084100
C	1.73008000	-1.77834500	6.78257400
C	2.86286900	-1.15996700	6.25573500
C	3.46159600	0.10090500	6.86221300
C	2.82912300	1.29587300	6.16270200
C	3.35303500	3.22556300	2.92410700
C	2.63164100	3.12298200	1.73087400
C	3.18773500	3.54461300	0.52472400
C	4.47595400	4.07497500	0.49894500
C	5.20554500	4.17401500	1.68331200
C	4.64972000	3.74855800	2.88683900
C	-0.22764000	3.73114700	8.03076800
C	-3.82841600	0.07868200	7.98935200
C	-0.20153500	-3.49058900	8.27492600
H	-0.10209300	4.98871600	2.54147400
H	-3.32397500	0.16632200	2.94966500
H	-5.07026700	0.03606900	2.49666500
H	-0.00939500	-3.38968700	3.09390500
H	0.05373100	-5.18453800	2.87519700
H	5.29276200	-0.01912800	3.06429800
H	3.48716300	-0.03689200	3.17522700
H	1.26133600	1.59467800	7.58726600
H	-0.14030000	4.70143100	6.13598300
H	-1.64194000	1.53028900	7.40601900
H	-4.78754500	0.01675600	6.08775800

H	-1.66538200	-1.37135400	7.52538100
H	-0.10507900	-4.57976500	6.44069500
H	1.29766200	-1.38346000	7.69661200
H	4.52313600	0.10578000	6.59631800
H	-0.28520900	2.74619700	8.50118200
H	-2.84659400	0.13600000	8.46625200
H	-4.31828300	-0.82968000	8.35031300
H	-0.24300400	-2.47565600	8.67890300
H	0.67671100	-3.98066100	8.70353500
C	-3.23634900	-3.38702600	2.80698000
C	-3.73458800	-4.69170900	2.73176200
C	-3.13038800	-2.63602500	1.63231200
C	-4.13302800	-5.22650100	1.50954200
C	-3.52537400	-3.17076300	0.40754500
C	-4.03142900	-4.46738500	0.34407200
C	3.42701800	-3.30914400	3.16783100
C	4.66763100	-3.95282900	3.20098300
C	2.77400100	-3.15991000	1.94115800
C	5.23573100	-4.45128900	2.03171700
C	3.34225600	-3.65670300	0.76904800
C	4.57350900	-4.30700900	0.81273800
C	-3.74291300	3.66687900	2.84873200
C	-3.23704500	4.85263200	2.26954500
C	-4.91728000	3.15976100	2.24809300
C	-3.82011600	5.44268800	1.15101600
C	-5.49759300	3.75243300	1.12951400
C	-4.94828200	4.89219000	0.55470400
C	3.35873100	0.15740800	8.38704700
H	3.86248700	-0.70776000	8.82626000
H	3.83843400	1.06661300	8.75914300
H	2.32743600	0.15700300	8.74968400
H	0.66937600	4.22702000	8.41136400
H	-4.40705600	0.94392100	8.32325300
H	-1.09670400	-4.01723900	8.61624500
H	-0.22285800	3.24280700	2.99928000
H	-1.10422100	4.30015000	8.35140800
H	5.18451900	-4.05698700	4.15026000
H	5.21965200	3.81640500	3.80838600
H	-2.39446300	5.35797100	2.70662400
H	-3.80427100	-5.28467100	3.63853800
H	-5.42281600	2.30896700	2.66828900
H	-5.39864700	5.35029300	-0.32011000
H	1.63386200	2.69269400	1.74492900
H	4.91083900	4.40560200	-0.43899200
H	1.82239100	-2.63626600	1.90220700
H	5.01733000	-4.69573300	-0.09834800
H	-2.71850800	-1.63136100	1.67534700
H	-4.34132900	-4.88580000	-0.60831800
H	6.19795000	-4.95225000	2.07197000
H	-4.52229900	-6.23894800	1.46696700
H	6.21121300	4.58255900	1.67013000
H	-3.38142200	6.35384700	0.75558000
H	2.61582200	3.45494400	-0.39368500
H	2.82393600	-3.53199000	-0.17667500
H	-3.43425600	-2.57535400	-0.49568900
H	-6.40031700	3.31201100	0.71700900

2-TS

Zero-point correction= 0.915474 (Hartree/Particle)
Thermal correction to Energy= 0.970727
Thermal correction to Enthalpy= 0.971672
Thermal correction to Gibbs Free Energy= 0.827144
Sum of electronic and zero-point Energies= -3311.964851
Sum of electronic and thermal Energies= -3311.909598
Sum of electronic and thermal Enthalpies= -3311.908654
Sum of electronic and thermal Free Energies= -3312.053181

O	1.08112300	4.44363100	4.04225400
O	-1.25888600	4.59863000	4.13557600
O	-4.69242700	1.18035700	4.11560500
O	-4.52473200	-1.15700900	3.98229500
O	-1.18715800	-4.54298300	4.31015200
O	1.16286700	-4.48208800	4.35437700
O	4.56483500	-1.15064700	4.54647600
O	4.53487500	1.19139400	4.46309400
C	2.76737000	2.77278900	4.20641400
C	1.61009200	3.36901300	4.72806800
C	-0.12919100	4.26708900	3.35696900
C	-1.95100500	3.54251300	4.69451200
C	-3.11679800	3.03187100	4.06512300
C	-3.63468900	1.86339100	4.68332900
C	-4.36200700	0.06591100	3.31576600
C	-3.44220300	-1.68521200	4.65593400
C	-2.82503300	-2.81756200	4.10532600
C	-1.77907600	-3.40855900	4.82657200
C	-0.00120600	-4.35414200	3.57483400
C	1.67809900	-3.35703200	4.96420100
C	2.82906400	-2.77999400	4.40829500
C	3.40399200	-1.68499100	5.06725000
C	4.44426200	-0.00902300	3.73156100
C	3.36254400	1.73878300	4.94217700
C	1.68180400	1.92289200	6.63332700
C	1.06203800	2.97057600	5.95261800
C	-0.17837400	3.67044700	6.49102900
C	-1.42847900	3.03849900	5.89071800
C	-2.04228800	1.93852900	6.47578500
C	-3.13625400	1.32794500	5.87634500
C	-3.76359800	0.06466800	6.45398300
C	-3.05112100	-1.15860400	5.89279600
C	-1.99234900	-1.77552300	6.55898100
C	-1.34081100	-2.89811700	6.05015400
C	-0.13245800	-3.52789400	6.72570400
C	1.12310000	-2.87989100	6.15820100
C	1.72483500	-1.77851900	6.76522300
C	2.86105200	-1.16208200	6.24423700
C	3.45931500	0.09676300	6.85518800
C	2.82923800	1.29227300	6.15470200
C	3.36884200	3.23209600	2.92518000
C	2.64852300	3.17178800	1.72849800
C	3.20784200	3.60263200	0.52762800
C	4.50260100	4.09546500	0.54718700
C	5.25389900	4.16507900	1.71059700
C	4.67801700	3.72593900	2.89875700
C	-0.22336300	3.73143000	8.02030400
C	-3.82803300	0.07984600	7.98352800
C	-0.20242800	-3.49383100	8.25346400
H	-0.10155600	4.97919600	2.52906400
H	-3.33383600	0.17456600	2.94642100
H	-5.08136800	0.04681500	2.49396300

H	-0.02846700	-3.37258800	3.08374000
H	0.03978200	-5.16648500	2.84912900
H	5.30885500	-0.02113700	3.06867100
H	3.50208000	-0.04069000	3.16803100
H	1.25985200	1.59214000	7.57707800
H	-0.13655300	4.69987700	6.12482900
H	-1.64114200	1.53064500	7.39805800
H	-4.79166900	0.02241800	6.08430200
H	-1.66651400	-1.36913800	7.51136000
H	-0.11015900	-4.57735800	6.41620600
H	1.29078100	-1.38574000	7.67929400
H	4.52173900	0.10135100	6.59314800
H	-0.28282500	2.74717900	8.49186800
H	-2.84519400	0.13553000	8.45844200
H	-4.31810400	-0.82853100	8.34399800
H	-0.24569300	-2.48044200	8.66100900
H	0.67786700	-3.98324800	8.67845000
C	-3.26456400	-3.39352100	2.80555200
C	-3.73055000	-4.71154400	2.74064600
C	-3.20693700	-2.64212700	1.62786600
C	-4.14535500	-5.26597500	1.53366400
C	-3.61408200	-3.17934100	0.40866400
C	-4.07978200	-4.48408800	0.39025900
C	3.45187500	-3.32171000	3.16921900
C	4.73544600	-3.87681700	3.21641700
C	2.78272300	-3.27659400	1.94306700
C	5.33530200	-4.39236500	2.07175000
C	3.36660200	-3.78504000	0.78439500
C	4.63353800	-4.33750100	0.87685500
C	-3.75512000	3.68131900	2.85660300
C	-3.25171600	4.87107400	2.28257400
C	-4.93632900	3.18073400	2.26315200
C	-3.83604000	5.47815500	1.17508400
C	-5.53274800	3.77550300	1.15539700
C	-4.96414200	4.91191200	0.61254100
C	3.35110800	0.15086700	8.37971700
H	3.85346000	-0.71490100	8.81921400
H	3.82980500	1.05926600	8.75490100
H	2.31870400	0.14995200	8.73908400
H	0.67503600	4.22578600	8.39944900
H	-4.40526300	0.94491200	8.32009900
H	-1.09535400	-4.02399900	8.59501500
H	-0.22514600	3.23485500	2.99544300
H	-1.09818200	4.30289200	8.34116400
H	5.26821800	-3.90136200	4.16176900
H	5.24986400	3.76305700	3.82034800
H	-2.40431400	5.37127800	2.71663000
H	-3.76469800	-5.30761300	3.64690900
H	-5.43988400	2.32798700	2.68210500
H	1.64124400	2.76550700	1.72881400
H	1.79839100	-2.82139300	1.88511900
H	-2.82131700	-1.62725600	1.65718100
H	2.66301400	3.55771700	-0.40863900
H	6.26477500	4.55534800	1.67448500
H	2.86104200	-3.75468100	-0.17422200
H	6.32700700	-4.83007500	2.09239400
H	-3.57173800	-2.60960300	-0.51281600
H	-4.51346700	-6.28363900	1.46783100
H	-3.42496200	6.39189600	0.76046500
H	-6.44026400	3.36616400	0.72565700
F	-5.52937800	5.48761100	-0.46484900
F	5.05362200	4.51746300	-0.60818500
F	5.20778100	-4.83428000	-0.23687400
F	-4.47764600	-5.01432600	-0.78310500

3-TS

Zero-point correction= 0.915266 (Hartree/Particle)
Thermal correction to Energy= 0.970597
Thermal correction to Enthalpy= 0.971542
Thermal correction to Gibbs Free Energy= 0.825966
Sum of electronic and zero-point Energies= -3311.965277
Sum of electronic and thermal Energies= -3311.909946
Sum of electronic and thermal Enthalpies= -3311.909001
Sum of electronic and thermal Free Energies= -3312.054577

O	1.04863100	4.51635000	4.07205800
O	-1.29300300	4.63261100	4.16561700
O	-4.64755100	1.13721600	4.08158900
O	-4.44781300	-1.19795100	3.95813900
O	-1.12780800	-4.58417700	4.36996500
O	1.21315700	-4.56655600	4.48662300
O	4.48571500	-1.10977800	4.42512200
O	4.49226200	1.24033700	4.40472600
C	2.73917600	2.84768800	4.20008700
C	1.58552200	3.43459700	4.73874100
C	-0.15881400	4.33890600	3.37928800
C	-1.96348000	3.55384600	4.70533500
C	-3.11010700	3.02016800	4.06069100
C	-3.61209900	1.83760300	4.66536800
C	-4.28909300	0.02456300	3.28874700
C	-3.37288200	-1.71259100	4.65245600
C	-2.74148200	-2.84626800	4.12220200
C	-1.70779000	-3.43407400	4.86271100
C	0.08035500	-4.45279800	3.65810700
C	1.71345600	-3.40822400	5.04349200
C	2.80909600	-2.79994300	4.41929300
C	3.35970000	-1.65345800	5.00663700
C	4.34577900	0.05856600	3.65264200
C	3.33866700	1.80069400	4.91224500
C	1.67371700	1.95791400	6.62078100
C	1.04620200	3.01394700	5.96020000
C	-0.20049000	3.69315500	6.51069200
C	-1.44048400	3.04972900	5.90151500
C	-2.04094500	1.93648600	6.47511300
C	-3.11918800	1.30958900	5.86397200
C	-3.73769300	0.04039600	6.43760400
C	-3.00574700	-1.17820500	5.89274300
C	-1.95609400	-1.78807300	6.57961900
C	-1.29281600	-2.91312000	6.09181700
C	-0.09576500	-3.53117300	6.80048400
C	1.16128700	-2.89752500	6.22208100
C	1.74855800	-1.76047000	6.77482800
C	2.85020300	-1.12783600	6.20005900
C	3.46101800	0.13319900	6.79466700
C	2.81726700	1.33587000	6.12177600
C	3.33185100	3.32721100	2.92147100
C	2.60106700	3.26104600	1.73207900
C	3.18214200	3.71878200	0.55995600
C	4.46486000	4.23930500	0.51331100

C	5.18934900	4.29416100	1.70329000
C	4.63313600	3.84064500	2.89638700
C	-0.24331400	3.73383600	8.04050700
C	-3.82356900	0.06238800	7.96608500
C	-0.17730500	-3.45240500	8.32559800
H	-0.14067200	5.07187200	2.57003700
H	-3.25661300	0.14470600	2.93602100
H	-4.99470900	-0.00504700	2.45593100
H	0.09973300	-3.49864300	3.11444100
H	0.12071600	-5.30275600	2.97782500
H	5.17382100	0.04494900	2.94436700
H	3.37503200	0.06541000	3.14008000
H	1.25869500	1.61052800	7.56177800
H	-0.17279500	4.72731200	6.15685100
H	-1.64158700	1.53111100	7.39935500
H	-4.76006600	-0.01510000	6.05378200
H	-1.64966700	-1.37598000	7.53590700
H	-0.07436800	-4.58854400	6.51912900
H	1.33068600	-1.35021400	7.68884900
H	4.51602700	0.13732000	6.50360800
H	-0.28669200	2.74286900	8.49962800
H	-2.84806600	0.13234900	8.45421500
H	-4.30769900	-0.85002200	8.32442300
H	-0.20438600	-2.42701600	8.70356000
H	0.69145900	-3.94464400	8.77061900
C	-3.16270200	-3.42888200	2.81853500
C	-3.67754100	-4.72803800	2.75667300
C	-3.03774100	-2.68613800	1.64138500
C	-4.07506700	-5.27092500	1.53762500
C	-3.43926800	-3.25458400	0.44272200
C	-3.96069000	-4.53505200	0.35883300
C	3.38054500	-3.37774600	3.17071000
C	4.07175700	-4.59256500	3.20843800
C	3.22235900	-2.71628200	1.95035000
C	4.60970100	-5.13292600	2.04332200
C	3.76860500	-3.27980400	0.80699700
C	4.46477200	-4.47703700	0.82137500
C	-3.75042600	3.66268300	2.84983200
C	-3.26859200	4.86321500	2.28001700
C	-4.91154600	3.12997900	2.25032500
C	-3.87019600	5.45052000	1.16992900
C	-5.48306500	3.73963700	1.14730800
C	-4.98997200	4.89153700	0.56512000
C	3.39772600	0.18321800	8.32222100
H	3.90090800	-0.69026900	8.74519600
H	3.89935700	1.08437200	8.68462000
H	2.37631500	0.19624200	8.71146600
H	0.64825300	4.23692100	8.42427600
H	-4.41575300	0.92210600	8.29014900
H	-1.08156300	-3.95676900	8.67637300
H	-0.23846100	3.31537100	2.99066600
H	-1.12598600	4.28783500	8.37038100
F	3.60907900	-2.63314700	-0.36558400
F	-3.31057700	-2.52806400	-0.68624200
F	-6.59062200	3.17024300	0.62474000
F	2.46528500	3.64854800	-0.58047900
H	4.18127500	-5.11032100	4.15565900
H	5.20543000	3.87856600	3.81718800
H	-2.43506900	5.38143300	2.71757600
H	-3.76089200	-5.30879600	3.66918400
H	-5.42116700	2.26525100	2.63686400
H	-5.47378200	5.32621900	-0.30177600
H	1.59946200	2.84529700	1.70007700
H	4.87267200	4.58368100	-0.43018500
H	2.67018000	-1.78509500	1.87383500
H	4.87214200	-4.87421300	-0.10134500
H	-2.61871300	-1.68522000	1.64070700
H	-4.26098600	-4.93240400	-0.60398400
H	5.14724800	-6.07469100	2.08348900
H	-4.47794500	-6.27783800	1.50166600
H	6.19790700	4.69443600	1.69661900
H	-3.45271100	6.37216500	0.77749400

4-TS

Zero-point correction= 0.882096 (Hartree/Particle)
Thermal correction to Energy= 0.940947
Thermal correction to Enthalpy= 0.941891
Thermal correction to Gibbs Free Energy= 0.787548
Sum of electronic and zero-point Energies= -3708.840931
Sum of electronic and thermal Energies= -3708.782081
Sum of electronic and thermal Enthalpies= -3708.781137
Sum of electronic and thermal Free Energies= -3708.935480

O	1.06867600	4.47413500	4.06174400
O	-1.27250700	4.60990100	4.14683200
O	-4.66082900	1.14887900	4.08881100
O	-4.47177500	-1.18701800	3.96547900
O	-1.13756100	-4.55962200	4.33857800
O	1.20689700	-4.53235500	4.44404600
O	4.53355400	-1.13839100	4.50592100
O	4.50688700	1.20727200	4.43440100
C	2.74318000	2.79385800	4.20979900
C	1.59368400	3.39420400	4.73978200
C	-0.13661900	4.30524600	3.36448600
C	-1.94948500	3.54113300	4.69601600
C	-3.10235000	3.01327400	4.05797400
C	-3.61627900	1.83890000	4.66757400
C	-4.31795400	0.03383100	3.29230500
C	-3.39257200	-1.70003900	4.65374800
C	-2.75750200	-2.82642000	4.11481700
C	-1.72094600	-3.41860200	4.84627400
C	0.06817000	-4.40970400	3.62600500
C	1.70631900	-3.39050000	5.03318100
C	2.82573700	-2.79152200	4.44680500
C	3.39260300	-1.67284200	5.06538200
C	4.39754500	0.00898700	3.70194500
C	3.34501300	1.75670100	4.93268600
C	1.67925000	1.94026800	6.63835500
C	1.05320500	2.98972000	5.96560200
C	-0.19101800	3.68039100	6.50644200
C	-1.43234900	3.04069600	5.89611700
C	-2.04211500	1.93476200	6.47434800
C	-3.12515100	1.31196400	5.86727400
C	-3.74853000	0.04702700	6.44528100
C	-3.02177900	-1.17257900	5.89582700
C	-1.97016500	-1.78681900	6.57609500
C	-1.30594900	-2.90759200	6.07915700
C	-0.11044400	-3.53402300	6.78230700
C	1.15074000	-2.89561100	6.21796800

C	1.74520700	-1.77440100	6.79646500
C	2.86465400	-1.14773000	6.24952000
C	3.46465500	0.11770500	6.84498900
C	2.82298100	1.30977700	6.14976200
C	3.32672500	3.25233000	2.91902500
C	2.61364400	3.08952500	1.72781000
C	3.18264500	3.52846200	0.54184000
C	4.43268400	4.12266600	0.47908400
C	5.11087300	4.25959500	1.68185900
C	4.59486400	3.83858400	2.89690400
C	-0.24087100	3.73209200	8.03564000
C	-3.82782200	0.06921000	7.97393400
C	-0.19791800	-3.47641900	8.30808200
H	-0.11054800	5.03759400	2.55522600
H	-3.29037600	0.14946000	2.92422000
H	-5.03576200	0.00591500	2.47018300
H	0.07739800	-3.44524600	3.10060000
H	0.11103500	-5.24640900	2.92970300
H	5.24692700	-0.00352600	3.01996200
H	3.44266500	-0.01605200	3.15966400
H	1.26496000	1.60740000	7.58483500
H	-0.15542300	4.71183800	6.14511200
H	-1.64618400	1.53173800	7.40108000
H	-4.77253300	-0.00428500	6.06520000
H	-1.66256800	-1.38167800	7.53499700
H	-0.08846700	-4.58773300	6.48697300
H	1.31729500	-1.37149500	7.70918400
H	4.52349300	0.12445500	6.56789100
H	-0.29221300	2.74467100	8.50155900
H	-2.85001000	0.13365300	8.45813000
H	-4.31551700	-0.84053400	8.33398600
H	-0.22972100	-2.45642100	8.69999600
H	0.67032900	-3.97240700	8.74969300
C	-3.17631600	-3.39402700	2.80358300
C	-3.73743600	-4.67220100	2.74357800
C	-2.99926100	-2.65508200	1.63025500
C	-4.11978200	-5.17233700	1.50921200
C	-3.39918300	-3.20905800	0.42354700
C	-3.96761600	-4.46855000	0.32307000
C	3.40420100	-3.33318500	3.18432400
C	4.43258900	-4.27570200	3.23479600
C	2.91579400	-2.89291800	1.95121300
C	4.94820700	-4.75765200	2.04195200
C	3.47195200	-3.41198900	0.79050600
C	4.49251900	-4.34887200	0.79660400
C	-3.73974200	3.65795700	2.84845400
C	-3.23795200	4.85055700	2.28440500
C	-4.90750000	3.13720000	2.25070600
C	-3.85149800	5.42320700	1.18340900
C	-5.47438200	3.75795500	1.15078900
C	-4.97509000	4.90656200	0.56454700
C	3.37853000	0.17888700	8.37070400
H	3.88745300	-0.68452800	8.80703700
H	3.86267400	1.08903400	8.73421800
H	2.35139800	0.17990500	8.74489300
H	0.65170000	4.23280000	8.41996700
H	-4.41418700	0.93177800	8.30076500
H	-1.10193400	-3.98840300	8.64801500
H	-0.22295400	3.28182700	2.97716700
H	-1.12154900	4.29378700	8.35749100
F	5.93833100	-5.66510000	2.08633100
F	3.00108100	-2.98711200	-0.39522400
F	-3.22458400	-2.49411900	-0.70225100
F	-4.66432400	-6.39997600	1.45078700
F	-6.58607500	3.20764000	0.62598000
F	-3.31991500	6.55868200	0.69126400
F	2.49250100	3.36754900	-0.60140200
F	6.32869600	4.82846700	1.66019700
H	4.82815200	-4.62998200	4.17959200
H	5.17457300	3.96343500	3.80404200
H	-2.40090100	5.38307600	2.69849600
H	-3.87234300	-5.27164300	3.63633200
H	-5.42649300	2.27894300	2.63744200
H	-5.43496700	5.37166800	-0.29804100
H	1.63868400	2.61528000	1.70768100
H	4.85884900	4.45906700	-0.45779700
H	2.11986200	-2.15862900	1.88382800
H	4.91269400	-4.74108600	-0.12110000
H	-2.54317800	-1.67131200	1.63994100
H	-4.27351300	-4.88283200	-0.62947000

5-TS

Zero-point correction= 0.851151 (Hartree/Particle)
Thermal correction to Energy= 0.913469
Thermal correction to Enthalpy= 0.914413
Thermal correction to Gibbs Free Energy= 0.755691
Sum of electronic and zero-point Energies= -4105.646481
Sum of electronic and thermal Energies= -4105.584163
Sum of electronic and thermal Enthalpies= -4105.583219
Sum of electronic and thermal Free Energies= -4105.741941

O	1.03722600	4.35184000	3.89703000
O	-1.29272400	4.54747400	4.09043900
O	-4.73927400	1.14574700	4.16141500
O	-4.52189400	-1.18238600	3.93188700
O	-1.15850500	-4.53749700	4.25672300
O	1.19797700	-4.44874000	4.26508500
O	4.61522100	-1.14321100	4.55060300
O	4.55854300	1.20013700	4.45048100
C	2.76972100	2.75185500	4.15674200
C	1.58258600	3.32490800	4.63642700
C	-0.20958500	4.13521300	3.28049600
C	-2.02603300	3.53359600	4.67451000
C	-3.23192800	3.04410300	4.08716600
C	-3.70533100	1.85661200	4.70492200
C	-4.38956200	0.08017000	3.31142600
C	-3.44657600	-1.69867800	4.61743000
C	-2.83569900	-2.84339000	4.08375600
C	-1.76976600	-3.41943700	4.78449600
C	0.01246300	-4.30014000	3.50893200
C	1.71263400	-3.34634900	4.91185200
C	2.88831100	-2.78073500	4.39764300
C	3.44944800	-1.68067800	5.05707100
C	4.49389800	-0.00732000	3.72652000
C	3.37144300	1.73450900	4.90764100
C	1.66536100	1.91796600	6.57020100
C	1.03341000	2.94425100	5.86664200
C	-0.19970900	3.65463500	6.41015100
C	-1.47126700	3.02531300	5.85337800

C	-2.06700700	1.92778100	6.46085400
C	-3.16688300	1.31644300	5.88070800
C	-3.76719200	0.03447600	6.44277400
C	-3.04686800	-1.17115500	5.85311200
C	-1.97981600	-1.78399300	6.51120400
C	-1.32270700	-2.90109400	5.99999700
C	-0.10876100	-3.52827400	6.66489000
C	1.14438400	-2.87402600	6.10134300
C	1.73969900	-1.77540500	6.72057800
C	2.88155300	-1.15435000	6.22030700
C	3.45827800	0.11181000	6.83583800
C	2.82499000	1.29334700	6.11566200
C	3.41909000	3.24926400	2.91655500
C	2.75860600	3.22139600	1.69345200
C	3.34346500	3.70214900	0.52872700
C	4.62974700	4.21903400	0.58552200
C	5.32837000	4.25391700	1.78247000
C	4.71932500	3.76810800	2.93450600
C	-0.21481400	3.74549500	7.93925800
C	-3.81124600	0.02487500	7.97330800
C	-0.17427100	-3.50659800	8.19336500
H	-0.21181600	4.77864700	2.39825200
H	-3.36845300	0.21607800	2.94045200
H	-5.11892000	0.07706400	2.50113700
H	-0.02844400	-3.30311700	3.05874500
H	0.05562200	-5.08391200	2.75282000
H	5.37040200	-0.01326600	3.07937000
H	3.56057900	-0.05422700	3.14880100
H	1.24112600	1.60072800	7.51747400
H	-0.15743900	4.67727000	6.02639400
H	-1.63822100	1.51740900	7.36980100
H	-4.79918900	-0.01633200	6.08589500
H	-1.65321000	-1.37721500	7.46320200
H	-0.08283200	-4.57553900	6.34797500
H	1.29122900	-1.38660900	7.62929000
H	4.52494100	0.12659000	6.59186800
H	-0.28285800	2.77216200	8.43178100
H	-2.82455400	0.10280900	8.43736100
H	-4.27132800	-0.90146100	8.32761500
H	-0.22985300	-2.49708500	8.60891500
H	0.71241600	-3.98894400	8.61322200
C	-3.33214200	-3.47831500	2.83558000
C	-3.81741600	-4.79118700	2.83431000
C	-3.32686100	-2.79697800	1.62408400
C	-4.29368100	-5.39317400	1.67461200
C	-3.79805400	-3.37434100	0.45171400
C	-4.28229800	-4.67394800	0.48957600
C	3.57295600	-3.36236700	3.21279200
C	4.83515800	-3.95563100	3.32462700
C	2.98880400	-3.33067800	1.95230300
C	5.48137100	-4.51013300	2.22476600
C	3.61204300	-3.87790300	0.83750500
C	4.85865000	-4.46842300	0.98681500
C	-3.91178100	3.74495300	2.91768100
C	-3.36063800	4.94900600	2.40475700
C	-5.12075100	3.39227000	2.26728600
C	-3.86639800	5.67771400	1.33827500
C	-5.63041500	4.10417200	1.17792800
C	-5.00799200	5.23747700	0.70010800
C	3.32287200	0.17333700	8.35773100
H	3.82730900	-0.68400300	8.81100200
H	3.78474700	1.08913500	8.73590800
H	2.28447200	0.16267000	8.69900700
H	0.69753300	4.23301100	8.29332300
H	-4.40851800	0.86851800	8.32870800
H	-1.06024600	-4.04993200	8.53204700
H	-0.32898000	3.08235400	3.00711000
H	-1.07489800	4.33720500	8.26296300
F	5.44698800	-4.99186700	-0.09420300
F	5.17995600	4.67950900	-0.54301800
F	-5.53580200	5.88947300	-0.33805600
F	-4.73368300	-5.21724000	-0.64618500
F	3.01932400	-3.82829500	-0.35547700
F	-3.77675700	-2.68747300	-0.69061000
F	-6.76412300	3.67993900	0.61679900
F	2.67569300	3.65990500	-0.62444000
F	1.79706000	-2.74308700	1.76831200
H	5.31232200	-3.97622500	4.29835900
H	5.25588100	3.78581800	3.87658000
H	-2.49466100	5.36371800	2.88340600
H	-3.81601100	-5.34392000	3.76729400
F	1.52651100	2.70145800	1.59470900
F	-5.94546000	2.39822000	2.60053500
F	-2.83740100	-1.55111200	1.54444800
H	-3.38194600	6.58926500	1.00881400
H	6.33222200	4.66199200	1.79398000
H	6.45664700	-4.97526600	2.30752100
H	-4.67546100	-6.40735300	1.67089000

6-TS

Zero-point correction= 0.850285 (Hartree/Particle)
Thermal correction to Energy= 0.912918
Thermal correction to Enthalpy= 0.913862
Thermal correction to Gibbs Free Energy= 0.751778
Sum of electronic and zero-point Energies= -4105.659417
Sum of electronic and thermal Energies= -4105.596784
Sum of electronic and thermal Enthalpies= -4105.595840
Sum of electronic and thermal Free Energies= -4105.757924

O	1.06949700	4.47108300	4.06183800
O	-1.27348400	4.61046500	4.14411500
O	-4.67145100	1.16150800	4.08413400
O	-4.48654200	-1.17621400	3.95364500
O	-1.14730400	-4.55309800	4.31170400
O	1.20029000	-4.50460400	4.39318500
O	4.55025700	-1.13127900	4.51866500
O	4.52106600	1.21430300	4.45332600
C	2.75613000	2.80063500	4.21741400
C	1.59781000	3.39270000	4.74033300
C	-0.13645400	4.29942600	3.36636300
C	-1.95372500	3.54428300	4.69616500
C	-3.11147900	3.02397700	4.06164200
C	-3.62484900	1.84726300	4.66620500
C	-4.32973100	0.04749700	3.28627600
C	-3.40718800	-1.69626300	4.63683900
C	-2.77918400	-2.82650900	4.09517700
C	-1.73659200	-3.41584200	4.82213300
C	0.05090100	-4.38717000	3.59002600
C	1.69956200	-3.36857100	4.99372700

C	2.83102700	-2.77344600	4.42384900
C	3.40125000	-1.66633100	5.06141800
C	4.42314200	0.01790100	3.71587600
C	3.35320200	1.76046000	4.94206800
C	1.67586900	1.93520700	6.63694900
C	1.05185000	2.98443900	5.96247100
C	-0.19224400	3.67565900	6.50289500
C	-1.43470300	3.03861400	5.89280300
C	-2.04568500	1.93211300	6.46892900
C	-3.13112600	1.31365000	5.86150900
C	-3.75538000	0.04707400	6.43431800
C	-3.03037500	-1.17048800	5.87798400
C	-1.97646800	-1.78527300	6.55369800
C	-1.31448000	-2.90489900	6.05186000
C	-0.11461800	-3.53159400	6.74638700
C	1.14326900	-2.88539300	6.18352000
C	1.73949600	-1.77324400	6.77704200
C	2.86534900	-1.14687600	6.24387300
C	3.46172800	0.11489800	6.85008300
C	2.82346900	1.30822800	6.15363500
C	3.36245500	3.27823300	2.94499300
C	2.64427700	3.21869300	1.74762100
C	3.22543800	3.67592400	0.57582100
C	4.51383000	4.19238800	0.56406400
C	5.21987100	4.23857000	1.76053800
C	4.66469700	3.78715500	2.94538100
C	-0.24250500	3.72660400	8.03219400
C	-3.83243300	0.06183700	7.96319900
C	-0.19868400	-3.48530900	8.27283100
H	-0.10876700	5.02634700	2.55188200
H	-3.30061800	0.16321300	2.92150700
H	-5.04612300	0.02337100	2.46243800
H	0.04234400	-3.41810800	3.07341300
H	0.09621100	-5.21769200	2.88625600
H	5.28206700	0.00906000	3.04583300
H	3.47538100	-0.00764200	3.16093500
H	1.25739300	1.60050800	7.58085700
H	-0.15521500	4.70746300	6.14276900
H	-1.64915400	1.52555400	7.39379900
H	-4.78009100	-0.00142500	6.05591100
H	-1.66492500	-1.38122500	7.51175000
H	-0.08950900	-4.58322500	6.44422200
H	1.30892000	-1.37887200	7.69212900
H	4.52258600	0.12331600	6.58130700
H	1.64240500	2.80647600	1.70301700
H	-0.29712700	2.73919300	8.49768200
H	-2.85406800	0.12394400	8.44648900
H	-4.31994100	-0.84942300	8.31950500
H	-0.23807200	-2.46857000	8.67235400
H	0.67423700	-3.97773700	8.70908900
C	-3.21591500	-3.40871900	2.79700200
C	-3.70075000	-4.71916400	2.75143800
C	-3.13783000	-2.65945600	1.61983000
C	-4.11048800	-5.25192000	1.54131600
H	-3.75928900	-5.33024600	3.64483600
C	-3.55324100	-3.21858000	0.42194900
H	-2.74240600	-1.64985400	1.61101300
C	-4.04561300	-4.51507500	0.36433600
C	3.42685200	-3.31039900	3.16826600
C	4.57735100	-4.10000400	3.22412900
C	2.84004200	-3.02074400	1.93403600
C	5.11846300	-4.59455900	2.04940500
H	5.05736400	-4.33246100	4.16795100
C	3.40383900	-3.52927200	0.77359100
H	1.95663200	-2.39567400	1.85635000
C	4.54336100	-4.32054100	0.81360900
C	-3.75486300	3.67948900	2.86286100
C	-3.25750800	4.87814500	2.30795400
C	-4.92943400	3.16878700	2.27010000
C	-3.86931200	5.47730700	1.22173800
H	-2.41457900	5.40383000	2.72107500
C	-5.51810900	3.79164900	1.18446100
H	-5.44611400	2.30631100	2.65268100
C	-5.00254600	4.94923700	0.62572900
C	3.36340500	0.16996200	8.37523700
H	3.87049000	-0.69423900	8.81204800
H	3.84336000	1.07924200	8.74626900
H	2.33346300	0.16776300	8.74154600
H	0.65116900	4.22470800	8.41720700
H	-4.41838100	0.92278600	8.29483600
H	-1.09779600	-4.00702500	8.61078300
H	5.25211200	3.83278900	3.85523200
H	-0.22456600	3.27281800	2.98702800
H	-1.12164200	4.29078200	8.35373300
F	5.07645600	-4.80376900	-0.30701300
F	5.06242900	4.62924700	-0.56775200
F	-5.57675400	5.53409100	-0.42156500
F	-4.44182900	-5.04259900	-0.79211100
F	6.21749100	-5.35444400	2.07598000
F	2.85696400	-3.26179700	-0.41721300
F	-3.48236200	-2.51409900	-0.71300500
F	-4.58210300	-6.50105700	1.47571500
F	-6.63088700	3.27171000	0.65059000
F	-3.36263400	6.61269200	0.72396600
F	2.55080900	3.62358000	-0.57824800
F	6.46153700	4.73376900	1.73910300

7-TS

Zero-point correction= 0.818171 (Hartree/Particle)
Thermal correction to Energy= 0.884345
Thermal correction to Enthalpy= 0.885289
Thermal correction to Gibbs Free Energy= 0.718046
Sum of electronic and zero-point Energies= -4502.485746
Sum of electronic and thermal Energies= -4502.419573
Sum of electronic and thermal Enthalpies= -4502.418629
Sum of electronic and thermal Free Energies= -4502.585871

O	1.03667900	4.35623400	3.89994000
O	-1.29524100	4.54853700	4.08924600
O	-4.73829000	1.14341200	4.15818200
O	-4.52121500	-1.18565400	3.93146500
O	-1.15801500	-4.53929700	4.25631300
O	1.19890400	-4.45038800	4.26714000
O	4.61170700	-1.14186400	4.54491400
O	4.55569900	1.20248800	4.44753100
C	2.76686100	2.75377300	4.15813900
C	1.58023700	3.32759500	4.63750100
C	-0.20807100	4.14354100	3.27901000
C	-2.02355200	3.53135000	4.67232400

C	-3.22703300	3.03746200	4.08434500
C	-3.70344700	1.85177000	4.70222700
C	-4.39050500	0.07622200	3.30919200
C	-3.44570400	-1.70015400	4.61752500
C	-2.83351700	-2.84468100	4.08560800
C	-1.76714700	-3.42111300	4.78510300
C	0.01448800	-4.30523300	3.50930400
C	1.71144100	-3.34661000	4.91269600
C	2.88494000	-2.77839800	4.39745300
C	3.44707700	-1.67770500	5.05435900
C	4.49232900	-0.00439700	3.72258600
C	3.36928600	1.73541400	4.90676500
C	1.66462700	1.91932100	6.57036300
C	1.03212300	2.94594000	5.86779300
C	-0.20112500	3.65575200	6.41151200
C	-1.47068200	3.02465900	5.85253400
C	-2.06708700	1.92689800	6.45919300
C	-3.16619000	1.31368800	5.87917600
C	-3.76684900	0.03263300	6.44277700
C	-3.04618600	-1.17283700	5.85326500
C	-1.97923300	-1.78581800	6.51135200
C	-1.32094900	-2.90258900	6.00072200
C	-0.10763500	-3.52947900	6.66707900
C	1.14474400	-2.87451800	6.10282000
C	1.74046200	-1.77538900	6.72082300
C	2.88079400	-1.15266300	6.21887600
C	3.45818600	0.11302100	6.83462500
C	2.82369300	1.29416000	6.11494700
C	3.41518800	3.25160000	2.91733900
C	2.75595700	3.21882300	1.69526100
C	3.34457600	3.69897700	0.53069900
C	4.62855200	4.22108700	0.57549000
C	5.30338200	4.24849300	1.79195600
C	4.71512900	3.77206800	2.94785700
C	-0.21748300	3.74566700	7.94057900
C	-3.81057700	0.02396800	7.97327500
C	-0.17371500	-3.50661800	8.19544200
H	-0.20899300	4.79470800	2.40252400
H	-3.37022500	0.21171000	2.93577200
H	-5.12191600	0.07198600	2.50088100
H	-0.02594200	-3.31009800	3.05468700
H	0.05823700	-5.09293900	2.75739400
H	5.37058400	-0.00989700	3.07792300
H	3.55988200	-0.05038200	3.14314100
H	1.24181500	1.60270800	7.51847100
H	-0.15961700	4.67861100	6.02820900
H	-1.63990300	1.51844800	7.36974600
H	-4.79891700	-0.01838900	6.08606700
H	-1.65387000	-1.37977000	7.46404800
H	-0.08127700	-4.57696300	6.35089500
H	1.29414500	-1.38793300	7.63114000
H	4.52464100	0.12807500	6.58968900
H	-0.28426000	2.77205600	8.43272200
H	-2.82387700	0.10181900	8.43726500
H	-4.27108800	-0.90185500	8.32814700
H	-0.22898300	-2.49686200	8.61042000
H	0.71255500	-3.98916100	8.61573300
C	-3.33018700	-3.47956400	2.83727300
C	-3.81573600	-4.79292700	2.84956300
C	-3.32233100	-2.79974800	1.62649800
C	-4.28402000	-5.37483300	1.68713300
C	-3.79433400	-3.38174500	0.45525200
C	-4.28226300	-4.67956000	0.48206100
C	3.56513900	-3.35797100	3.20879100
C	4.82301300	-3.95994400	3.32890600
C	2.98065100	-3.31239100	1.95041000
C	5.44497100	-4.50184300	2.22001400
C	3.60301500	-3.85768100	0.83265000
C	4.84472700	-4.46077400	0.96532400
C	-3.90557800	3.73531200	2.91400400
C	-3.34227100	4.93444200	2.40485500
C	-5.11326500	3.38680600	2.26226600
C	-3.85642500	5.64938100	1.34710200
C	-5.62026400	4.10910300	1.17636000
C	-5.00521600	5.24359800	0.69076400
C	3.32419500	0.17421100	8.35660200
H	3.82916300	-0.68311700	8.80911600
H	3.78694500	1.08963400	8.73437400
H	2.28618100	0.16375500	8.69907800
H	0.69375100	4.23458400	8.29530700
H	-4.40764600	0.86784200	8.32827000
H	-1.05971400	-4.04968900	8.53425700
H	-0.32654100	3.09261100	2.99795500
H	-1.07839400	4.33618800	8.26404500
F	5.44810100	-4.98467800	-0.09762400
F	5.19980900	4.68243000	-0.53304500
F	-5.51226200	5.91377200	-0.33678600
F	-4.73577200	-5.24461900	-0.63317700
F	6.64481100	-5.08256800	2.32599300
F	3.01534500	-3.79820100	-0.36000500
F	-3.77349300	-2.70158700	-0.68862300
F	-4.75361900	-6.62730200	1.69206000
F	-6.75164200	3.69200800	0.61056400
F	-3.24392500	6.76961900	0.94146400
F	2.68375100	3.65376800	-0.62368800
F	6.54226700	4.75189800	1.81458700
F	1.79244100	-2.71566700	1.76938700
H	5.32140100	-4.00428600	4.29056300
H	5.27227900	3.80437800	3.87699900
H	-2.47350900	5.36953900	2.86366200
H	-3.82650400	-5.36600100	3.76956500
F	1.52455700	2.69650800	1.59494000
F	-5.93984000	2.39026800	2.58492300
F	-2.83187300	-1.55417600	1.54359700

8-TS

Zero-point correction= 0.987548 (Hartree/Particle)
Thermal correction to Energy= 1.069111
Thermal correction to Enthalpy= 1.070056
Thermal correction to Gibbs Free Energy= 0.855004
Sum of electronic and zero-point Energies= -5610.681062
Sum of electronic and thermal Energies= -5610.599498
Sum of electronic and thermal Enthalpies= -5610.598554
Sum of electronic and thermal Free Energies= -5610.813605

O	0.72272800	4.54782500	4.03299900
O	-1.62311400	4.47216900	4.11246700
O	-4.76580500	0.78158700	4.07542900
O	-4.46331300	-1.54169100	3.99110700

O	-0.78014900	-4.55155900	4.14796900
O	1.56023600	-4.44223000	4.37287900
O	4.59772500	-0.76606900	4.39032900
O	4.43340000	1.58239600	4.41365100
C	2.55430500	3.03843100	4.19053300
C	1.34326200	3.51945700	4.70977100
C	-0.46240600	4.26825400	3.33427300
C	-2.21130900	3.34991400	4.65835400
C	-3.31970700	2.73302900	4.02079300
C	-3.75255200	1.52939000	4.63731400
C	-4.39996600	-0.33119600	3.28271100
C	-3.31852600	-1.96749300	4.63310800
C	-2.58104400	-2.99770700	4.03538200
C	-1.44598300	-3.48003000	4.70355700
C	0.45513200	-4.33475600	3.50704400
C	1.99587400	-3.27038700	4.95603400
C	3.06068200	-2.58639800	4.35536600
C	3.51076000	-1.40016600	4.95374800
C	4.38616300	0.40701500	3.63985100
C	3.23025600	2.04269900	4.90738600
C	1.53259700	2.04833000	6.58910600
C	0.82754900	3.05175100	5.92411300
C	-0.47161700	3.63054000	6.46813400
C	-1.65725100	2.89255200	5.85843400
C	-2.18481500	1.74715500	6.44029100
C	-3.22325800	1.04675700	5.84035200
C	-3.75365400	-0.25384900	6.43296800
C	-2.95296700	-1.41515700	5.86278700
C	-1.82658600	-1.93800300	6.49708100
C	-1.06783000	-2.97401900	5.95333600
C	0.16108800	-3.53352600	6.65752400
C	1.38495100	-2.80774700	6.12222900
C	1.88433700	-1.64073700	6.69754900
C	2.94680700	-0.92650100	6.14531100
C	3.45682600	0.36622300	6.76749800
C	2.72974000	1.52460500	6.10285500
C	3.12415700	3.57636800	2.92705800
C	2.39067300	3.55462400	1.74266200
C	2.92412100	4.08073900	0.56756400
C	4.19957700	4.62708000	0.54511100
C	4.93775400	4.63427900	1.72808500
C	4.41568600	4.11657200	2.90708000
C	-0.52087000	3.67239400	7.99782200
C	-3.80113600	-0.24011800	7.96272100
C	0.05719100	-3.51072000	8.18342400
H	-0.49959700	4.99481800	2.51912700
H	-3.39660000	-0.18080000	2.86337300
H	-5.15478100	-0.40821400	2.49805000
H	0.46824000	-3.34903200	3.02299600
H	0.55433800	-5.14185200	2.78111500
H	5.22261300	0.46435300	2.94310000
H	3.42268800	0.35819600	3.11506600
H	1.13662700	1.66451300	7.52413000
H	-0.52403100	4.66299300	6.11195600
H	-1.76209700	1.37957400	7.36975700
H	-4.77911100	-0.37263000	6.07272000
H	-1.53570200	-1.53101700	7.46026100
H	0.25142800	-4.57841500	6.34456200
H	1.42501300	-1.27028000	7.60861400
H	4.51171400	0.45383600	6.48987800
H	1.39869600	3.11347700	1.72408400
H	-0.48554300	2.68294600	8.46081100
H	-2.81834300	-0.12259300	8.42645600
H	-4.22858900	-1.17734600	8.32849800
H	-0.01842100	-2.50135300	8.59620900
H	0.94214400	-3.97966900	8.62110900
C	-3.02318500	-3.58662600	2.74313200
C	-4.28236600	-4.19162600	2.63866200
C	-2.20051600	-3.55451000	1.62089400
C	-4.68275400	-4.76397800	1.43907100
H	-4.94074400	-4.21665700	3.50049200
C	-2.61314400	-4.13643800	0.42205900
H	-1.23328500	-3.06324900	1.66834200
C	-3.85286600	-4.74811800	0.31691500
C	3.70321600	-3.13328500	3.13045700
C	4.28252700	-4.40589500	3.15076800
C	3.73943700	-2.40199500	1.94415500
C	4.89718400	-4.91407300	2.01147800
H	4.25505800	-4.99497300	4.06245400
C	4.36138100	-2.92034000	0.81072000
H	3.26913900	-1.42489700	1.89175400
C	4.94820400	-4.17922200	0.82932600
C	-3.98607600	3.31405400	2.79474200
C	-3.56868900	4.52674400	2.20985900
C	-5.09747400	2.70747700	2.17385500
C	-4.15815400	5.03473500	1.05698600
H	-2.78627000	5.11375700	2.65852000
C	-5.67797200	3.22936200	1.02286500
H	-5.54849700	1.82525700	2.59358900
C	-5.21401500	4.39333900	0.42646500
C	3.37251900	0.38730600	8.29462500
H	3.93239600	-0.45411700	8.71084700
H	3.80517400	1.31577700	8.67593900
H	2.34859500	0.32203500	8.67170200
H	0.32632300	4.24708800	8.38105600
H	-4.42868100	0.58600900	8.30661700
H	-0.82679000	-4.06696800	8.50581800
H	5.00573100	4.13537100	3.81746600
H	-0.45683600	3.23754100	2.95534400
H	-1.44535100	4.15557500	8.32406400
H	5.43690100	-4.57779700	-0.05229400
H	-4.16922600	-5.20609600	-0.61419100
H	-5.65892300	4.78512000	-0.48069000
H	4.61031000	5.04160700	-0.36882900
C	4.36433500	-2.08153100	-0.43800100
C	5.47823500	-6.30194500	2.06446400
C	-1.67231800	-4.07697800	-0.74989100
C	-6.04843800	-5.38461700	1.31270500
C	-6.86652900	2.50208500	0.45351700
C	-3.61883300	6.33425400	0.52168600
C	2.06977900	4.04584400	-0.67010900
C	6.34537600	5.16784000	1.71216700
F	5.12215700	-2.61069100	-1.40665600
F	3.12285200	-1.93095900	-0.93333100
F	4.82951900	-0.84124500	-0.19098700
F	6.31906800	-6.53669600	1.04612000
F	4.51467200	-7.23970800	2.00723100
F	6.15511800	-6.51248700	3.20554400
F	-1.43772300	-2.80739300	-1.12822000
F	-2.14200100	-4.73483300	-1.81699700
F	-0.47417500	-4.61010900	-0.44045300
F	-6.89779900	-4.57124600	0.65851000
F	-6.00534100	-6.53559700	0.62073800
F	-6.59678500	-5.65088400	2.50711900

F	-7.16316800	2.91153300	-0.78794400
F	-7.96622700	2.68296200	1.20667800
F	-6.65485100	1.17264500	0.39934200
F	-4.11502400	6.62913800	-0.68794300
F	-2.27695400	6.30315600	0.41077000
F	-3.91060000	7.36450300	1.33613300
F	6.49628800	6.14978500	0.80939500
F	6.71065200	5.65607400	2.90757100
F	7.23161200	4.20541100	1.39456300
F	0.91852600	4.72075900	-0.48710700
F	1.72467400	2.78587000	-0.99331400
F	2.68556300	4.58044500	-1.73155900

9

Zero-point correction= 1.135714 (Hartree/Particle)
Thermal correction to Energy= 1.204697
Thermal correction to Enthalpy= 1.205642
Thermal correction to Gibbs Free Energy= 1.025355
Sum of electronic and zero-point Energies= -2787.589918
Sum of electronic and thermal Energies= -2787.520935
Sum of electronic and thermal Enthalpies= -2787.519991
Sum of electronic and thermal Free Energies= -2787.700277

C	-4.19631400	3.15809000	0.49910200
C	-2.81748000	3.20929700	0.31282200
C	-2.14577200	4.43737400	0.23961900
C	-2.88816800	5.61958200	0.34120200
C	-4.27225200	5.59765300	0.54566500
C	-4.90982800	4.35771000	0.63087000
H	-2.23967700	2.29065800	0.26546700
H	-2.38573300	6.57563600	0.26087500
H	-5.98105300	4.30585200	0.79440700
C	-5.02548700	6.92531200	0.66911500
C	-4.85292800	7.72659300	-0.63360100
C	-6.52310700	6.71795400	0.91854000
C	-4.43960400	7.72819100	1.84498100
H	-3.80154200	7.95438100	-0.83226100
H	-5.25017200	7.17055500	-1.48895900
H	-5.39241400	8.67669000	-0.55999700
H	-6.70798000	6.16478200	1.84521800
H	-7.01197500	7.69242000	1.01013000
H	-7.00287600	6.18288300	0.09222500
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H	-3.37860900	7.95231800	1.69890600
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C	-4.95140500	-0.63946700	-0.03302000
C	-6.25926700	-1.00572800	0.30341900
C	-4.03904900	-1.64236800	-0.39091200
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H	-6.98443700	-0.23721900	0.54159000
C	-4.40696300	-2.98474300	-0.35826200
H	-3.03978300	-1.36054700	-0.71160100
C	-5.72482300	-3.32302100	-0.01884700
H	-6.00434600	-4.37131000	-0.01807000
C	-0.69031200	4.37375400	0.06853800
C	0.27353500	5.29495500	0.28606600
N	-0.24188600	7.72248900	1.05638200
C	-0.03620900	6.63323400	0.71913000
C	2.20833600	3.70163100	0.23562200
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C	3.97308800	5.76456000	-0.46871600
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C	1.71978400	5.00239100	0.09113000
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C	5.48257500	-2.87565700	0.48773500
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C	0.30522900	-4.27590400	-0.30650000
C	0.11570900	-6.84733400	-1.41393600
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C	-0.94897300	-4.78494100	-0.65863500
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C	-1.02672300	-6.07443000	-1.21490900
H	-1.99129500	-6.48221700	-1.47951400
C	0.05413300	-8.26008400	-2.00137100
C	-1.38233000	-8.68811600	-2.32293100
C	0.87806600	-8.30380700	-3.30070700
C	0.64501300	-9.25381300	-0.98530600
H	-2.01426300	-8.70315100	-1.42891100
H	-1.85061000	-8.02920000	-3.06148000
H	-1.37193400	-9.69992400	-2.73920900
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H	0.48110000	-7.59723600	-4.03655800
H	0.60564500	-10.26967700	-1.39225800
H	1.68952900	-9.02652900	-0.75228900
H	0.07693500	-9.23616000	-0.04983500
C	-2.09949500	-3.91379000	-0.40029200
C	-3.41588300	-4.04798600	-0.67884400
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H	-1.83603400	-2.98840800	0.10836900
C	-3.96320200	-5.23314200	-1.28588800
N	-4.45177600	-6.16980000	-1.76223700
H	-3.54795500	0.87204300	-0.64640000
C	-6.09643600	1.83341800	1.37571400
N	-7.05735000	1.86611400	2.02231000

10

Zero-point correction= 0.922745 (Hartree/Particle)
Thermal correction to Energy= 0.984904
Thermal correction to Enthalpy= 0.985849
Thermal correction to Gibbs Free Energy= 0.820058
Sum of electronic and zero-point Energies= -3684.964887
Sum of electronic and thermal Energies= -3684.902727
Sum of electronic and thermal Enthalpies= -3684.901783
Sum of electronic and thermal Free Energies= -3685.067574
-1 1

Cl	19.76876100	15.57894800	14.83885700
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C	19.86987800	11.48160500	10.65943100
C	17.05857600	13.23975500	14.63361500
C	15.89074700	13.02036200	15.32555400
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C	18.96528800	9.19794400	10.29707300
C	19.14228500	7.88183700	12.42165300
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H	19.92863400	7.12393600	12.52198000

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