Electronic Supplementary Information (ESI)

π-Extended Dibenzo[*g*,*p*]chrysenes

Mohammad Mosharraf Hossain,*[1] M. Saeed Mirzaei,[2] Sergey V. Lindeman,[1] Saber Mirzaei*[3] and Rajendra Rathore[1‡]

[1]*Department of Chemistry, Marquette University, Milwaukee, WI 53201-1414, United States*
[2]*Department of Organic Chemistry, Faculty of Chemistry, Razi University, Kermanshah, Iran*
[3]*Department of Chemistry, University of Pittsburgh, Pittsburgh, PA 15260, United States*

‡Deceased February 16, 2018.
*E-mail: *hossaimm@miamioh.edu*; *saber.mirzaei@pitt.edu*.

Table of Contents

S1. General Experimental Methods and Materials. 2
S2. Synthesis of compounds. 3
S3. Crystal data and structure refinement. 13
4. NMR spectroscopy..... 18
S5. Computational details. 41
S6. Reference. 52
S7. Cartesian coordinates of optimized molecules at MN15/6-31+G(d,p)+PCM(CH_2Cl_2). 54

S1. General Experimental Methods and Materials.

All reactions were performed under an argon atmosphere unless otherwise noted. All solvents and starting materials were used without further purification unless otherwise noted. Anhydrous and nonoxygenated solvents were purchased from Sigma Aldrich (sure-seal bottle) otherwise noted. NMR spectra were recorded on Varian 400 MHz NMR spectrometers. All chemical shifts are referenced to residual protium in the NMR solvent ($CHCl_3$: δ 7.26 for protons and 77.16 for carbons).[1] For some compounds, due to the presence of several aromatic and aliphatic protons/carbons with the same environment, several ^1H NMR and ^{13}C NMR signals overlapped with each other and do not follow standard splitting patterns. Mass spectra were recorded on a Bruker Daltonics MALDI-TOF mass spectrometer with dithranol (DIT) used as the matrix. 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 (APCI) ionization sources.

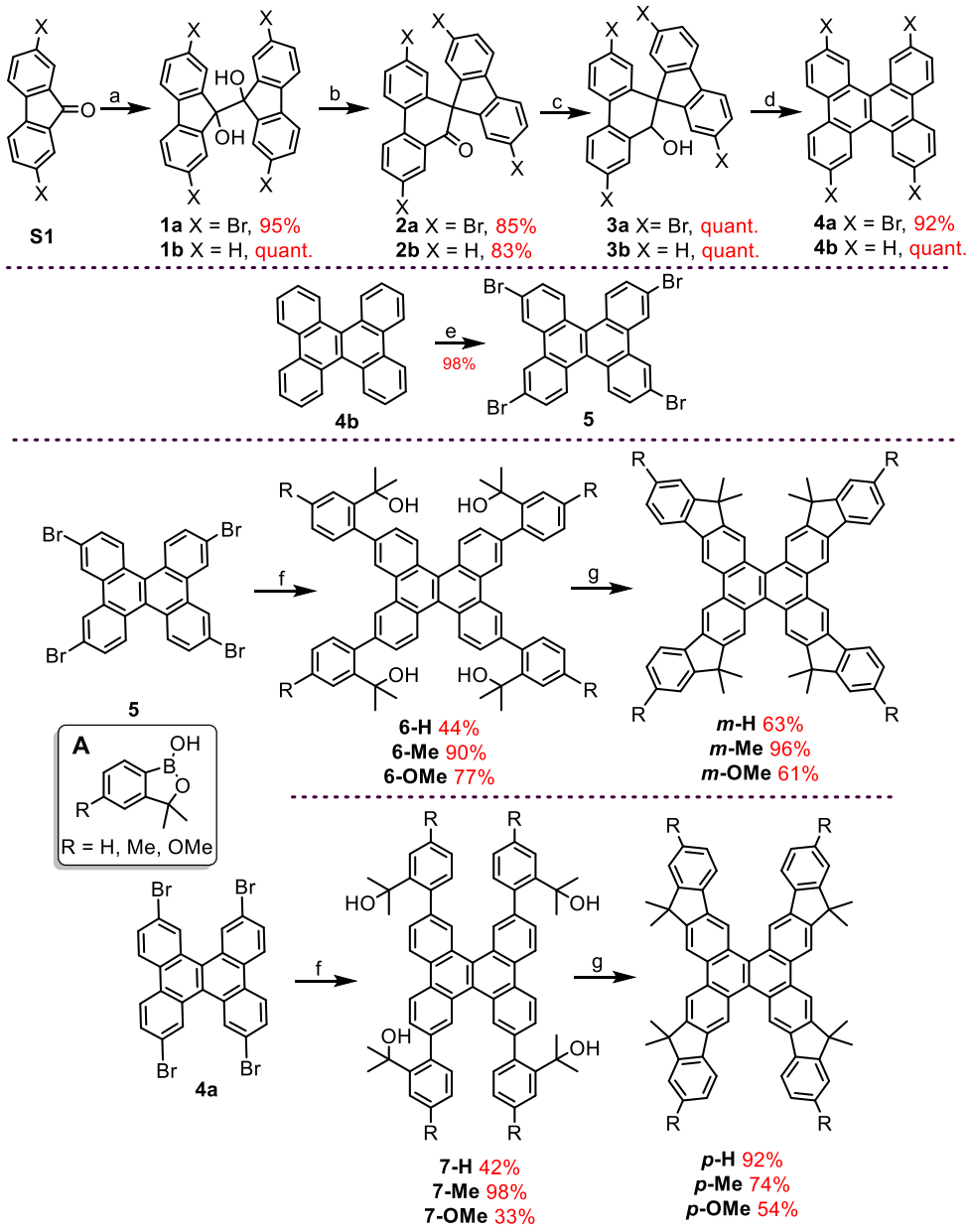
Absorption spectra (UV-vis-NIR) were obtained on a Cary 5000 spectrophotometer and emission spectra were recorded in a PTI QuantaMaster spectrofluorometer. Electronic absorption spectra of *meta*$^{+\bullet}$ and *para*$^{+\bullet}$ isomers in CH_2Cl_2 at 0 °C were obtained by quantitative redox titrations using robust aromatic oxidants (THEO$^{\bullet+}SbCl_6^-$ (E_{red} = 0.67 V vs Fc/Fc^+ and λ_{max} = 518 nm, 163 μM for ***m*-H,** 261 μM for ***m*-OMe**, 71 μM for ***p*-OMe,** 137 μM for ***m*-Me**) and NAP$^{\bullet+}SbCl_6^-$ (E_{red} = 0.94 V vs Fc/Fc^+ and λ_{max} = 672 nm, 54 μM for ***p*-H**, 123 μM for ***p*-Me**)). The redox titration experiment was carried out by incremental addition of *meta* or *para* species (Stock solution concentration: 0.116 mM of ***p*-H**, 0.675 mM of **m-H**, 0.66 mM of ***m*-OMe**, 0.08 mM of ***p*-OMe**, 0.95 mM of ***m*-Me,** 0.85 mM of ***p*-Me**) to the solution of proper oxidant.

The electrochemical cell for cyclic voltammetry (CV) was of an air-tight design with high vacuum Teflon valves and Viton O-ring seals to allow an inert atmosphere to be maintained without contamination by grease. The working electrode consisted of an adjustable platinum disk embedded in a glass seal to allow periodic polishing (with a fine emery cloth) without changing the surface area (~1 mm^2) significantly. The reference SCE electrode (saturated calomel electrode) and its salt bridge were separated from the catholyte by a sintered glass frit. The counter electrode consisted of platinum gauze that was separated from the working electrode by ~3 mm. The CV measurements were carried out in a solution of 0.1 M supporting electrolyte (tetra-*n*-butyl ammonium hexafluorophosphate, $TBAPF_6$) and 0.5×10^{-3} M for (***p*-OMe**) and 1×10^{-3} M for (***p*-H**, ***p*-Me**, ***m*-H**, ***m*-Me** and ***m*-OMe**) substrate in dry dichloromethane under an argon atmosphere. All cyclic voltammograms were recorded at a sweep rate of 200 mV s^{-1} unless otherwise specified and were IR-compensated. The oxidation potentials ($E_{1/2}$) were calibrated with added (equimolar) ferrocene ($E_{1/2}$ = 0.450 V vs. SCE).

Suitable crystals were selected, and data collected on an Oxford SuperNova diffractometer. The crystals were kept at 100 K during data collection. Using Olex2,[2] the structure was solved with the XS structure solution program using Direct Methods and refined with the XL[3] refinement package using least-squares minimization.

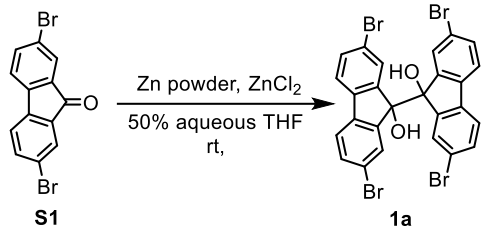
S2. Synthesis of compounds.

Scheme S1. The general synthetic approach.



(a) Zn powder, $ZnCl_2$, 50% aqueous THF, rt; (b) AcOH, H_2SO_4 (cat), 85 °C; (c) $NaBH_4$, THF, MeOH, 60 °C; (d) AcOH, H_2SO_4 (cat) 85 °C; (e) Br_2, I_2, anhydrous CH_2Cl_2, rt; (f) A, $Pd(dppf)Cl_2$, Na_2CO_3, 2:1 DME/H_2O, 100 °C; (g) CH_3SO_3H, CH_2Cl_2, rt.

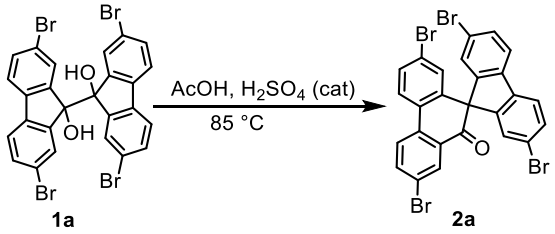
Synthesis of compound **1a**:



95%

A mixture of 2,7-dibromo-9H-fluoren-9-one (**S1**, 3.00 g, 8.87 mmol), Zn powder (15.00 g, 230 mM), $ZnCl_2$ (3.00 g, 22.01 mmol), and 50% aqueous THF (30 mL) was stirred at room temperature for 40 min. The reaction mixture was combined with 3N HCl (15 mL) and filtered to remove Zn powder. The filtrate was extracted with toluene and the Zn powder on the filter paper was washed with toluene. The combined toluene solutions were washed with water and dried over anhydrous $MgSO_4$. The solvent was evaporated to give a crude product. Then the compound was purified by recrystallization from hexane to afford pure **1a** as a white solid (2.86 g, 95%,); mp 156-158 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.21 (s, 2H from OH), 7.23 (bs, 8 H), 7.41 (bs, 4H); ^{13}C NMR (400 MHz, CD_3OD) δ 87.1, 121.9, 122.7, 129.3, 133.1, 139.4, 140.0. MALDI-TOF ([M/z]$^+$ calculated): 678.01, (exp.): 678.12.

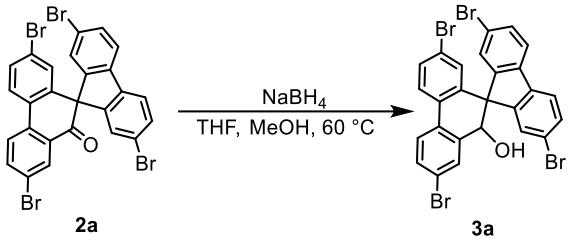
Synthesis of compound **2a**:



85%

A mixture of **1a** (1.30 g, 1.91 mmol), AcOH (30 mL), and H_2SO_4 (1.50 mL) was stirred at 85 °C for 4 h. The reaction mixture was cooled to room temperature and combined with cold water (100 mL). The mixture was extracted with dichloromethane (3×100 mL) and was washed with water. The combined dichloromethane extracts were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The crude product was recrystallized from acetonitrile to afford pure **2a** (1.07 g, 85%); mp 395-397 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.66 (d, J = 2 Hz, 1 H), 7.08 (dd, J = 1.76 Hz, 0.46 Hz, 2H), 7.55 (m, 3H), 7.64 (dd, J = 8.2 Hz, 0.46 Hz, 2H), 7.92 (m, 2H), 8.02 (d, J = 8.63 Hz, 1H), 8.10 (d, J = 2.16 Hz, 1H) ; ^{13}C NMR (400 MHz, $CDCl_3$) δ 67.8, 122.3, 122.4, 123.5, 124.2, 125.4, 126.0, 127.9, 128.7, 130.5, 131.2, 131.8, 132.2, 132.4, 135.8, 138.6, 139.7, 139.8, 148.2, 193.8. MALDI-TOF ([M/z]$^+$ calculated): 660.00 (exp.): 660.11.

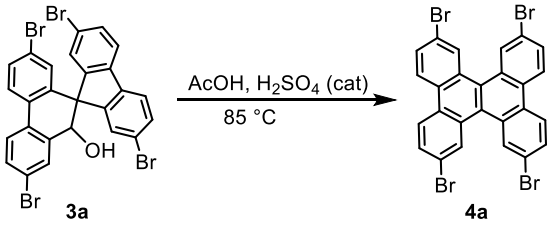
Synthesis of compound **3a**:



quant.

Compound **2a** (1.01 g, 1.53 mmol) was dissolved in THF (15 mL) and methanol (15 mL) in a Schlenk flask under an argon atmosphere and outfitted with an air condenser. The reaction mixture was heated to 60 °C and $NaBH_4$ (58.00 mg, 1.53 mmol) was added in four portions (14.50 mg each time) over 4 hours with heating. Heating at 60 °C was continued for 20 hours. The reaction mixture was cooled to 0 °C and quenched with the slow addition of 1 M HCl (30 mL). The product was then extracted with dichloromethane (3×40 mL). The combined organic extracts were washed with H_2O (2×40 mL) and saturated brine (2×30 mL). The organic phase was then dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The product **3a** was isolated as a white solid which was purified by recrystallization from hexane to afford pure compound (1.00 g, quant.); mp > 450 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.66 (d, J = 6.4 Hz, 1H), 5.23 (d, J = 6.4 Hz, 1H) 6.75 (d, J = 2.05 Hz, 1 H), 6.84 (d, J = 1.26 Hz, 1H), 7.34 (d, J = 1.26 Hz, 1H), 7.47 (dd, J = 8.16 Hz, 1.78 Hz, 1H), 7.50 (dd, J = 8.43 Hz, 2.09 Hz , 1H), 7.58 (m, 2H), 7.65 (m, 3H), 7.76 (m, 2H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 61.2, 74.1, 121.8, 121.9, 121.9, 122.5, 123.0, 123.4, 125.5, 126.2, 127.9, 129.0, 123.0, 130.3, 131.4, 131.8, 132.1, 132.2, 132.3, 132.4, 138.1, 139.0, 139.3, 140.3, 146.5, 149.0. MALDI-TOF ([M/z]$^+$ calculated): 662.01, (exp.): 662.09.

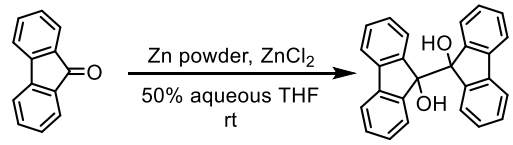
Synthesis of compound **4a**:



92%

A mixture of **3a** (1.22 g, 1.84 mmol), AcOH (30 mL), and H_2SO_4 (1.50 mL) was stirred at 85 °C for 4 h. The reaction mixture was cooled to room temperature and combined with cold water (100 mL). A white precipitate was isolated by filtration and washed with water (3×100 mL) and EtOH (100 mL), then dried under vacuum to obtain compound **4a** (1.10 g, 92%). The white solid was insoluble in all common organic solvents therefore no NMR analysis was possible; mp > 450 ºC. MALDI-TOF ([M/z]$^+$ calculated): 644.00, (exp.): 644.10.

Synthesis of compound **1b**:

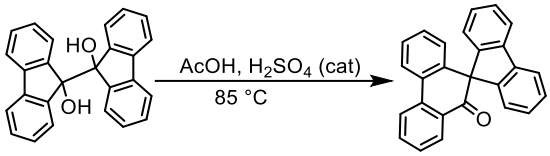


fluorenone **1b**

quant.

A mixture of fluorenone (6.00 g, 33.3 mmol), Zn powder (30.00 g, 461.53 mmol), $ZnCl_2$ (6.00 g, 44.02 mmol), and 50% aqueous THF (120 mL) was stirred at room temperature for 40 min. The reaction mixture was combined with 3N HCl (30 mL) and filtered to remove Zn powder. The filtrate was extracted with toluene and the Zn powder on the filter paper was washed with toluene. The combined toluene solutions were washed with water and dried over anhydrous $MgSO_4$. The solvent was evaporated to give crude **1b** (6.02 g, quant.). The crude product was used in the next reaction without purification. MALDI-TOF ($[M/z]^+$ calculated): 362.43, (exp.): 362.49.

Synthesis of compound **2b**:

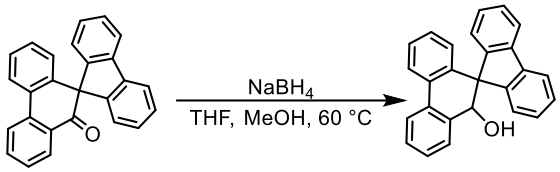


1b **2b**

83%

A mixture of **1b** (6.00 g, 16.55 mmol), AcOH (70 mL), and H_2SO_4 (6 mL) was stirred at 85 °C for 4 h. The reaction mixture was cooled to room temperature and combined with cold water (100 mL). The mixture was extracted with dichloromethane (3×100mL) and washed with water. The combined dichloromethane extracts were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The crude product was purified by washing with a mixture of acetonitrile and CH_2Cl_2 (95:5) to afford pure **2b** (4.70 g, 83%); mp 248-250 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ= 6.62 (dd, J = 7.9 Hz, 1.36 Hz, 1H), 7.07 (m, 3H), 7.18 (dt, J = 7.46 Hz, 1.18 Hz, 2H), 7.38 (m, 3H), 7.46 (dt, J = 7.61 Hz, 1.08 Hz, 1H), 7.79 (m, 3H), 8.00 (dd, J = 7.72 Hz, 1.5Hz, 1H), 8.10 (dd, J = 8.27 Hz, 1.0Hz, 1H), 8.20 (dd, J = 8.1 Hz, 0.3 Hz, 1H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 68.9, 120.7, 123.4, 124.3, 124.9, 128.1, 128.2, 128.3, 128.5, 128.5, 128.7, 129.4, 130.3, 130.7, 135.1, 138.3, 139.5, 141.8, 147.2, 197.4. MALDI-TOF ($[M/z]^+$ calculated): 344.41, (exp.): 344.48.

Synthesis of compound **3b**:

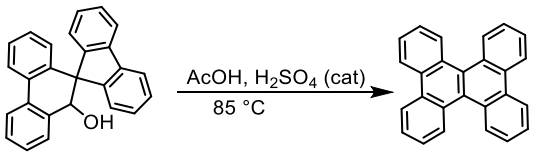


2b **3b**

quant.

Compound **2b** (4.70 g, 13.80 mmol) was dissolved in THF (60 mL) and methanol (60 mL) in a Schlenk flask under an argon atmosphere and outfitted with an air condenser. The reaction mixture was heated to 60 °C and $NaBH_4$ (520 mg, 13.80 mmol) was added in four portions (130 mg each time) over 4 hours with heating. Heating at 60 °C was continued for 20 hours. The reaction was cooled to 0 °C and quenched with the slow addition of 1 M HCl (100 mL). The product was then extracted with dichloromethane (3×100 mL). The combined organic phases were washed with H_2O (2×100 mL) and saturated brine solution (2×50 mL). The organic extracts were then dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The product **3b** was isolated as white solid (4.66 g, quant.); mp 150-152 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.6 (d, *J* = 6.8 Hz, 1H), 5.31 (d, *J* = 6.8 Hz, 1H) 6.68 (dd, *J* = 7.90 Hz, 1.38 Hz, 1 H), 6.80 (d, *J* = 7.70 Hz, 1H), 7.01 (dt, *J* = 7.72 Hz, 1.1 Hz, 1H), 7.07 (dt, *J* = 7.5 Hz, 1.28 Hz, 1H), 7.21 (d, *J* = 7.68 Hz, 1H), 7.34 (m, 5H), 7.51 (m, 2H), 7.75 (d, *J* = 7.76 Hz, 1H), 7.80 (d, *J* = 7.61 Hz, 1H), 7.95 (dt, *J* = 8.08 Hz, 1.20 Hz, 2H) ; ^{13}C NMR (400 MHz, $CDCl_3$) δ 61.6, 75.0, 120.2, 120.3, 123.8, 124.3, 124.8, 125.9, 126.7, 127.5, 127.6, 128.0, 128.3, 128.3, 128.4, 128.5, 128.6, 128.8, 133.8, 133.8, 137.2, 138.8, 141.2, 142.3, 145.7, 148.1. MALDI-TOF ($[M/z]^+$ calculated): 346.43, (exp.): 346.51.

Synthesis of compound **4b**:

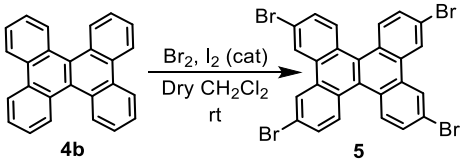


3b **4b**

quant.

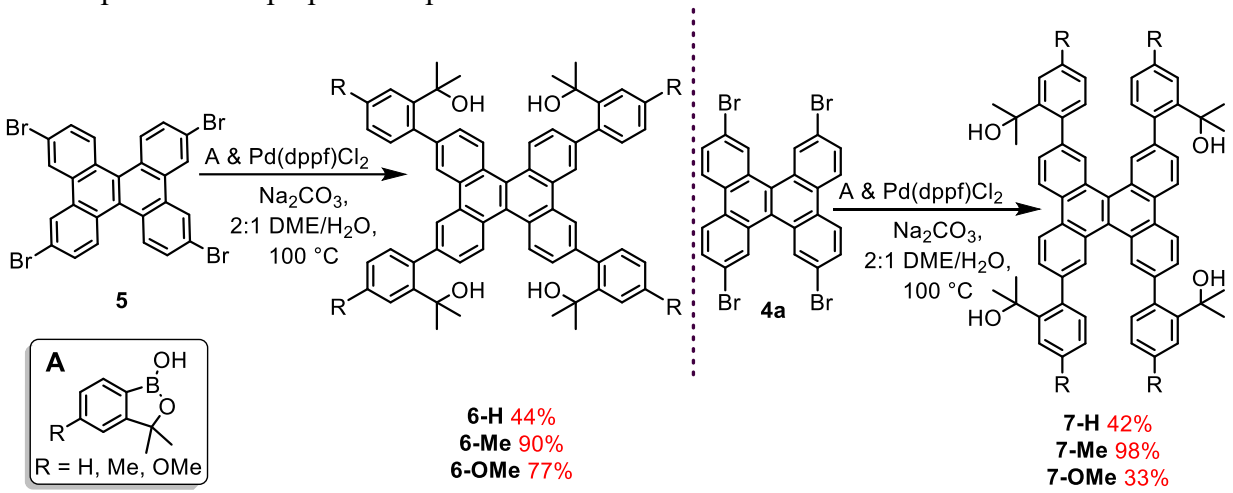
A mixture of compound **3b** (4.70 g, 13.56 mmol), AcOH (60 mL), and H_2SO_4 (6 mL) was stirred at 85 °C for 4 h. The reaction mixture was carefully neutralized with aqueous $NaHCO_3$ solution and extracted with CH_2Cl_2 (3×50 mL). The combined organic extracts were washed with water, dried over anhydrous $MgSO_4$, and filtered, and the solvent was removed under reduced pressure. The crude solid was recrystallized from ethanol to afford dibenzo[*g*,*p*]chrysene **4b** (4.40 g, quant.); mp 202-204 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (m, 8H), 8.71 (dt, *J* = 8.57 Hz, 1.65 Hz, 8H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 123.8, 126.7, 127.6, 129.1, 129.4, 131.0. MALDI-TOF ($[M/z]^+$ calculated): 328.41, (exp.): 328.48.

Synthesis of compound **5**:



In a 1000 mL round bottom flask was dissolved **4b** (1.00 g, 3.00 mmol) in anhydrous dichloromethane (140 mL). Iodine (75 mg, 0.29 mmol) was added and the mixture stirred for 30 min at room temperature. Bromine (2.43 g, 0.78 mL, 15.20 mmol) was added slowly through the rubber septum and stirring continued for an additional 75 hours at room temperature. After every 24 hours, additional dichloromethane (100 mL) and bromine (0.30 mL, 5.83 mmol) were added until 75 hours had elapsed. After the completion of the reaction, the solvent was evaporated under reduced pressure and the reddish-colored crude solid was obtained washed with ethanol. The resulting white-colored solid was dissolved in tetrahydrofuran and crystallized to afford colorless crystals of **5** (1.90 g, 98%); mp 423-425 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (dd, J = 8.8 Hz, 2.0 Hz, 4H), 8.42 (d, J = 8.8 Hz, 4H), 8.73 (d, J = 2.0 Hz, 4H). MALDI-TOF ([M/z]$^+$ calculated): 644.00, (exp.): 644.11.

General procedure to prepare compound **6s** and **7s**:



To a mixture of corresponding benzoxaborole (**A**, 6 equivalents), tetrabromo dibenzochrysene (**4a** or **5**) (1 equivalent), sodium carbonate (10 equivalents), and $Pd(dppf)Cl_2$ (0.4 equivalents) in a 250 mL Schlenk flask equipped with air condenser was added 1,2-dimethoxyethane (DME) and water (2:1). The mixture was evacuated and filled with argon three times. The mixture was heated to 100 °C for 48 h. The mixture was then cooled to room temperature and 50 mL of water was added. The blackish solution was transferred to a 1 L separatory funnel and extracted with diethyl ether (3×50 mL), CH_2Cl_2 (3×50 mL), $CHCl_3$ (3×50 mL) and ethyl acetate (3×50 mL). The combined ether extracts and ethyl acetate extracts were washed with brine and the combined dichloromethane extracts and chloroform extracts were washed with brine and both organic extracts were dried over anhydrous $MgSO_4$, filtered and the solvent was removed under reduced pressure. The blackish-brown crude solid was purified by washing with a mixture of hexane and CH_2Cl_2 (9:1) to afford the desired product that was used without further purification.

Compound **6-H**:
This compound was synthesized by using the general coupling procedure with **A-H** (0.81 g, 5.04 mmol, 6 equivalents), **5** (0.50 g, 0.77 mmol, 1 equivalent), sodium carbonate (0.82 g, 7.76 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.22 g, 0.31 mmol, 0.40 equivalents) in 1,2-dimethoxyethane (DME) (40 mL) and water (20 mL). The crude solid was washed with a mixture of hexane and chloroform (95:5) to afford **6-H** (0.30 g, 44%); mp 270-272 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.53 (s, 24H), 1.88 (s, 4H), 7.21 (dd, 4H, *J* = 7.68 Hz, 1.65 Hz), 7.30 (td, 4H, *J* = 7.48 Hz, 1.60 Hz), 7.40 (td, 4H, *J* = 8.21 Hz, 1.56 Hz), 7.68 (t, 8H, *J* = 8.63 Hz, 1.61 Hz), 8.61 (d, 4H, *J* = 1.68 Hz), 8.79 (d, 4H, *J* = 8.52 Hz). $C_{62}H_{56}O_4$, HRMS(ESI) calc.: 864.4173; exp.: 864.4185.

Compound **6-Me**:
This compound was synthesized by using the general coupling procedure with **A-Me** (0.85 g, 4.84 mmol, 6 equivalents), **5** (0.52 g, 0.80 mmol, 1 equivalent), sodium carbonate (0.85 g, 8.07 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.23 g, 0.32 mmol, 0.40 equivalents) in 1,2-dimethoxyethane (DME) (40 mL) and water (20 mL). The crude solid was washed with a mixture of hexane and CH_2Cl_2 (85:15) to afford **6 Me** (0.67 g, 90%); mp 238-240 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.52 (s, 24H), 1.81 (s, 4H), 2.44 (s, 12H), 7.10 (s, 8H), 7.52 (s, 4H), 7.64 (d, 4H, *J* = 8.54 Hz), 8.57 (d, 4H, *J* = 1.37 Hz), 8.77 (d, 4H, *J* = 8.53 Hz). $C_{66}H_{64}O_4Na$, HRMS(ESI) calc.: 943.4697; exp.: 943.4719.

Compound **6-OMe**:
This compound was synthesized by using the general coupling procedure with **A-OMe** (1.78 g, 9.30 mmol, 6 equivalents), **5** (1.0 g, 1.55 mmol, 1 equivalent), sodium carbonate (1.64 g, 15.52 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.45 g, 0.62 mmol, 0.40 equivalents) in 1,2-dimethoxyethane (DME) (60 mL) and water (30 mL).The crude solid was washed with a mixture of acetonitrile and CH_2Cl_2 (95:5) to afford **6-OMe** (0.42 g, 77%); mp 246-248 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.51 (s, 24H), 1.86 (bs, 4H), 3.88 (s, 12H), 6.83 (dd, 4H, J = 8.40 Hz, 2.70 Hz), 7.13 (d, 4H, *J* = 8.31 Hz), 7.28 (d, 4H, *J* = 2.68 Hz), 8.57 (d, 4H, *J* = 1.75 Hz), 8.76 (d, 4H, *J* = 8.44 Hz). $C_{66}H_{64}O_8$, HRMS(ESI) calc.: 984.4596; exp.: 984.4588.

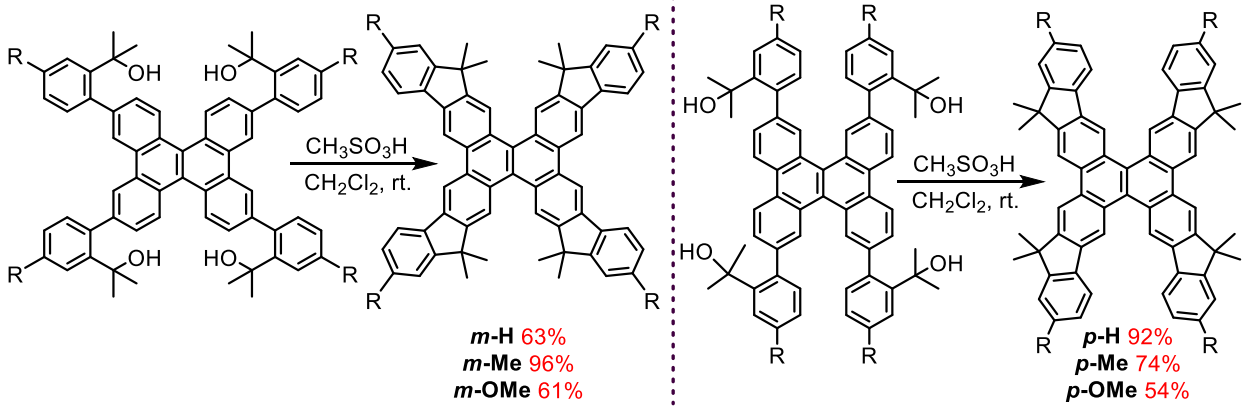
Compound **7-H**:
This compound was synthesized by using the general coupling procedure with **A-H** (0.88 g, 5.43 mmol, 6 equivalents), **4a** (0.50 g, 0.77 mmol, 1 equivalent), sodium carbonate (0.82 g, 7.76 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.45 g, 0.62 mmol, 0.40 equivalents) in in 1,2-dimethoxyethane (DME) (40 mL) and water (20 mL). The crude solid was washed with a mixture of acetonitrile and chloroform (95:5) to afford compound **7-H** (0.28 g, , 42 %); mp 336-338 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 24H), 1.70(bs, 4H), 7.04(bs, 4H), 7.19 (td, 4H, *J* = 7.47 Hz, 1.1 Hz), 7.34 (td, 4H, *J* = 7.5 Hz, 1.6 Hz), 7.60 (m, 8H), 8.67 (d, 8H, *J* = 8.73 Hz). $C_{62}H_{56}O_4Na$, HRMS(ESI) calc.: 887.4071; exp.: 887.4071.

Compound **7-Me**:
This compound was synthesized by using the general coupling procedure with **A-H** (1.05 g, 6.00 mmol, 6 equivalents), **4a** (0.64 g, 1.00 mmol, 1 equivalent), sodium carbonate (1.05 g, 10.0 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.29 g, 0.40 mmol, 0.4 equivalents) in in 1,2-dimethoxyethane (DME) (40 mL) and water (20 mL). The crude solid was washed with a mixture of hexane and

CH_2Cl_2 (90:10) to afford compound **7-Me** (0.90 g, 98%); mp above 410 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 24H), 1.66 (bs, 4H), 2.42 (s, 12H), 6.93 (d, 4H, J = 7.04 Hz), 7.01 (d, 4H, J = 7.80 Hz), 7.41 (s, 4H), 7.58 (dd, 4H, J = 8.30 Hz, 1.36 Hz), 8.65 (m, 8H). $C_{66}H_{64}O_4Na$, HRMS(ESI) calc.: 943.4697; exp.: 943.4688.

Compound **7-OMe**:
This compound was synthesized by using the general coupling procedure with **A-H** (1.78 g, 9.30 mmol, 6 equivalents), **4a** (1.00 g, 1.55 mmol, 1 equivalent), sodium carbonate (1.64 g, 15.52 mmol, 10 equivalents), and Pd(dppf)Cl_2 (0.45 g, 0.62 mmol, 0.40 equivalents) in 1,2-dimethoxyethane (DME) (60 mL) and water (300 mL). The solid crude was washed with acetonitrile to afford **7-OMe** (0.50 g, 33 %); mp above 410 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.33 (s, 24H), 1.72 (bs, 4H), 3.87 (s, 12 H), 6.74 (dd, 4H, J = 8.29 Hz, 2.76 Hz), 6.96 (bs, 4H), 7.18 (d, 4H, J = 2.54 Hz), 7.58 (d, 4H, J = 8.40 Hz), 8.65 (d, 8H, J = 8.86 Hz). $C_{66}H_{64}O_8Na$, HRMS(ESI) calc.: 1007.4493; exp.: 1007.4493.

General procedure to prepare the final compounds (***m*s** and ***p*s**):



To a solution of the corresponding tetrahydroxy compounds (**6s** and **7s**) in 100 to 200 mL of anhydrous CH_2Cl_2 (depending on solubility) was added 10-15 mL of CH_3SO_3H at room temperature and the reaction mixture stirred for 2 h. The reaction was neutralized carefully with 5% $NaHCO_3$ solution and extracted with $CHCl_3$ (4×50 mL). The combined organic extracts were dried over anhydrous $MgSO_4$, filtered, and the solvent was removed under reduced pressure. The crude solid was purified by silica gel column chromatography using hexane and ethyl acetate (98:2) as eluent or recrystallization from different solvent systems to afford compounds ***m*-H, *m*-Me, *m*-OMe, *p*-H, *p*-Me and *p*-OMe**.

Compound ***p*-H**:
This compound was synthesized by using the general procedure with **7-H** (0.75 g, 0.86 mmol, 1 equivalent) in the mixture of CH_3SO_3H (15.0 mL, 231 mmol) and anhydrous CH_2Cl_2 (200 mL). The crude product was purified through recrystallization from acetonitrile to afford ***p*-H** (0.63 g, 92%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.79 (s, 24H), 7.39 (m, 8H), 7.56 (m, 4H), 7.87 (m, 4H), 8.81 (s, 4H), 9.14 (s, 4H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 28.1, 47.3, 117.6, 120.1, 120.6, 123.1, 127.5, 128.0, 129.4, 131.1, 138.5, 139.4, 152.3, 154.4. $C_{62}H_{48}$, HRMS(ESI) calc.:

792.3751; exp.: 792.3743. Slow evaporation of a 1,2-dichloroethane solution of ***p*-H** at room temperature affords high quality colorless crystals.

Compound ***p*-Me**:
This compound was synthesized by using the general procedure with **7-Me** (0.50 g, 0.54 mmol, 1 equivalent) in the mixture of CH_3SO_3H (10.0 mL, 154 mmol) and anhydrous CH_2Cl_2 (80 mL). The crude was passed through short silica pad with hexane as an eluent to afford a yellow colored ***p*-Me** (0.34 g, 74%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.76 (s, 24H), 2.48 (s, 12 H), 7.18 (d, 4H, *J* = 8.07 Hz), 7.36 (s, 4H), 7.74 (d, 4H, *J* = 7.65 Hz), 8.76 (s, 4H), 9.08 (s, 4H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 22.0, 28.1, 47.2, 117.4, 119.6, 120.3, 123.7, 128.3, 129.3, 130.8, 136.8, 137.9, 138.4, 152.2, 154.7. $C_{66}H_{56}$, HRMS(ESI) calc.: 848.4382; exp.: 848.4362.

Compound ***p*-OMe**:
This compound was synthesized by using the general procedure with **7-OMe** (0.50 g, 0.50 mmol, 1 equivalent) in the mixture of CH_3SO_3H (15.0 mL, 231 mmol) and anhydrous CH_2Cl_2 (100 mL). The crude was heated in the mixture of CH_2Cl_2 and acetonitrile (30:70) and cooled to room temperature. The solid suspension was filtered to afford an off-white-colored ***p*-OMe** (0.25 g, 54%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.75 (s, 24H), 3.91 (s, 12H), 6.90 (dd, 4H, *J* = 8.48 Hz, 2.30 Hz), 7.07 (d, 4H, *J* = 2.30 Hz), 7.75 (d, 4H, *J* = 8.37 Hz), 8.72 (s, 4H), 9.01 (s, 4H). Due to the poor solubility, no ^{13}C NMR is provided. $C_{66}H_{56}O_4$, HRMS(ESI) calc.: 912.4173; exp.: 912.4196.

Compound ***m*-H**:
This compound was synthesized by using the general procedure with **6-H** (0.27 g, 0.31 mmol, 1 equivalent) in the mixture of CH_3SO_3H (6.0 mL, 92.40 mmol) and anhydrous CH_2Cl_2 (70 mL). The crude solid was purified through silica gel column chromatography using hexane and ethyl acetate (98:2) as eluent to afford ***m*-H** (0.15 g, 63%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64 (s, 24H), 7.43 (td, 4H, *J* = 7.33 Hz, 1.12 Hz), 7.50 (td, 4H, *J* = 7.40 Hz, 1.15 Hz), 7.55 (d, 4H, *J* = 7.27 Hz), 8.15 (d, 4H, *J* = 7.4 Hz), 8.78 (s, 4H), 9.15 (s, 4H); ^{13}C NMR (300 MHz, $CDCl_3$) δ 27.8, 47.1, 114.9, 120.8, 123.0, 123.1, 127.5, 128.1, 128.5, 129.3, 131.1, 138.5, 139.3, 152.2, 154.4. $C_{62}H_{48}$, HRMS(ESI) calc.: 792.3751; exp.: 792.3745. Slow evaporation of a dichloromethane/acetonitrile solution of ***m*-H** at room temperature affords high-quality pale-yellow crystals.

Compound ***m*-Me**:
This compound was synthesized by using the general procedure with **6-Me** (0.50 g, 0.54 mmol, 1 equivalent) in the mixture of CH_3SO_3H (8.0 mL, 123.20 mmol) and anhydrous CH_2Cl_2 (70 mL). The crude solid was purified through silica gel column chromatography using hexane and ethyl acetate (98:2) as eluent to afford ***m*-Me** (0.442 g, 96%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.61 (s, 24H), 2.51 (s, 12H), 7.31 (d, 4H, *J* = 7.70 Hz), 7.34 (s, 4H), 8.01 (d, 4H, *J* = 7.70 Hz), 8.75 (s, 4H), 9.08 (s, 4H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 22.1, 28.0, 47.0, 114.4, 120.6, 122.9, 123.8, 128.4, 128.9, 131.1, 136.7, 138.0, 138.5, 152.2, 154.6. $C_{66}H_{57}$, HRMS(ESI) calc.: 849.4455; exp.: 849.4452. Slow evaporation of a dichloromethane/acetonitrile solution of ***m*-Me** at room temperature affords high-quality pale-yellow crystals.

Compound ***m*-OMe**:
This compound was synthesized by using the general procedure with **6-OMe** (0.40 g, 0.40 mmol, 1 equivalent) in the mixture of CH_3SO_3H (10.0 mL, 154 mmol) and anhydrous CH_2Cl_2 (75 mL). The crude solid was purified through silica gel column chromatography using hexane and ethyl acetate (94:6) as eluent to afford ***m*-OMe** (0.23 g, 61%); mp above 420 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.60 (s, 24H), 3.94 (s, 12H), 7.04 (dd, 4H, J = 8.30 Hz, 2.30 Hz), 7.06 (d, 4H, J = 2.30 Hz), 8.03 (d, 4H, J = 8.30 Hz), 8.72 (s, 4H), 9.01 (s, 4H); ^{13}C NMR (400 MHz, $CDCl_3$) δ 27.9, 47.1, 55.8, 109.1, 113.1, 113.8, 121.6, 122.9, 128.5, 131.1, 132.2, 138.3, 151.8, 156.4, 160.4. $C_{66}H_{56}O_4$, HRMS(ESI) calc.: 912.4173; exp.: 912.4156. Slow evaporation of a dichloromethane/acetonitrile solution of ***m*-OMe** at room temperature affords high-quality pale-yellow crystals.

S3. Crystal data and structure refinement.

Figure S1. Crystal structures (obtained at 100 K) of *m*-Me (top left) and *m*-OMe (top right) and crystal packing arrangement of *m*-Me (bottom left) and *m*-OMe (bottom right).; hydrogen atoms and solvent molecules are deleted for clarity; thermal ellipsoids are set at the 50% probability level; the C and O atoms are colored grey and red, respectively.

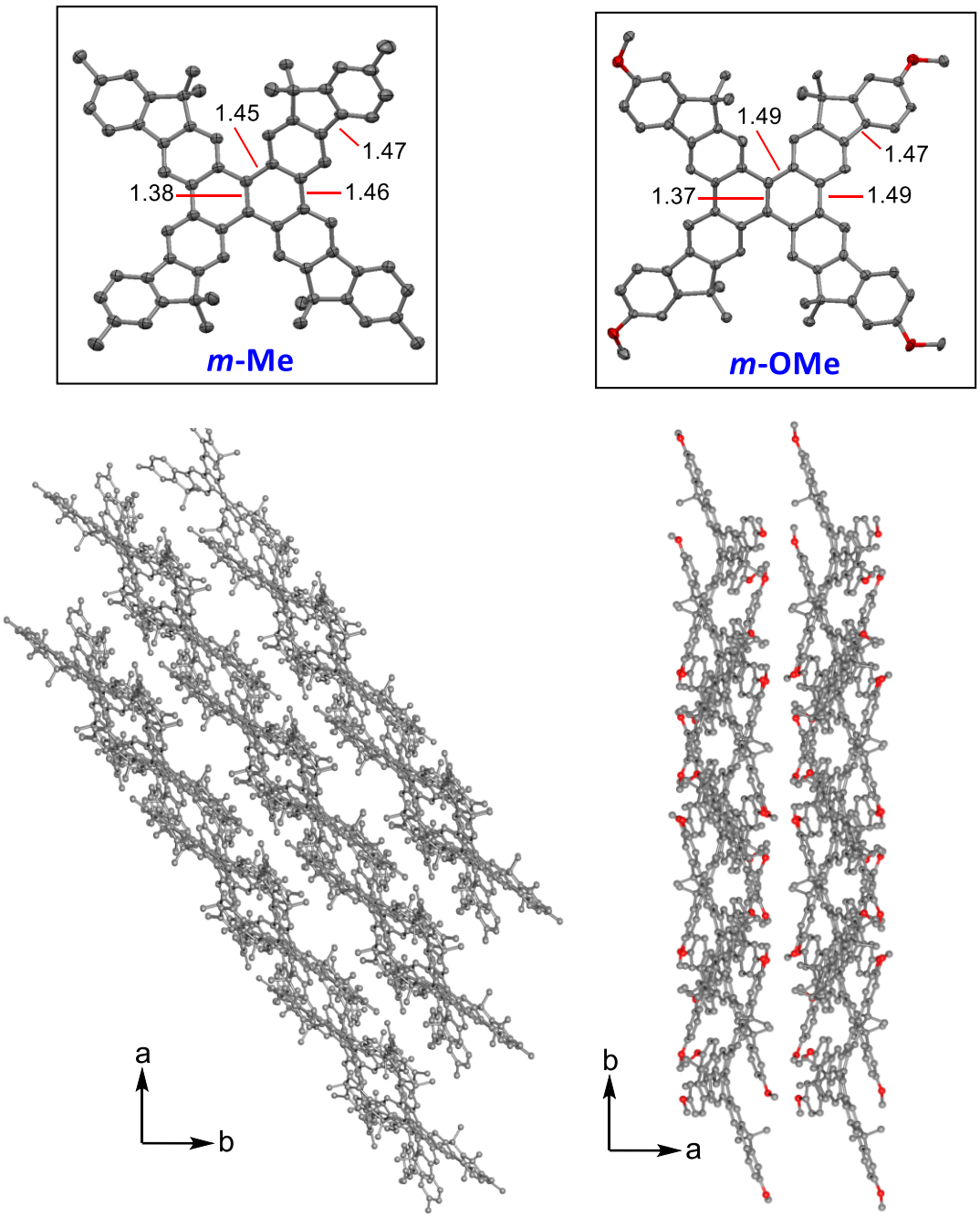


Table S1. Summary of X-ray crystallographic data collection and structure refine.

Identification code	raj25u (*p*-H)	raj25w (*m*-H)	raj26r (*m*-Me)	raj26b (*m*-OMe)
CCDC number	2039941	2039942	2039943	2039944
Empirical formula	$C_{62}H_{48}$	$C_{62.7}H_{49.39}Cl_{1.39}$	$C_{66}H_{56}$	$C_{66}H_{56}O_4$
Formula weight	793.00	851.94	849.11	913.11
Temperature/K	99.8(4)	100.00(10)	99.9(3)	99.95(10)
Crystal system	tetragonal	monoclinic	triclinic	orthorhombic
Space group	$P\text{-}42_1c$	$P2_1/c$	P-1	$P2_12_12_1$
a/Å	15.21984(10)	13.76405(18)	14.4517(6)	18.64163(18)
b/Å	15.21984(10)	26.5563(2)	15.0266(6)	22.60353(19)
c/Å	23.2343(3)	13.26570(13)	26.3973(10)	27.5670(2)
α/°	90.00	90.00	81.001(3)	90.00
β/°	90.00	104.2936(11)	81.996(3)	90.00
γ/°	90.00	90.00	80.366(3)	90.00
Volume/Å^3	5382.07(8)	4698.81(9)	5544.2(4)	11615.82(17)
Z	4	4	4	8
ρ_{calc}g/cm^3	0.979	1.204	1.017	1.044
μ/mm^{-1}	0.417	1.220	0.431	0.495
F(000)	1680.0	1797.0	1808.0	3872.0
Crystal size/mm^3	0.4635 × 0.2418 × 0.1755	0.3 × 0.28 × 0.04	0.28 × 0.05 × 0.03	0.6965 × 0.0779 × 0.0478
2Θ range for data collection/°	6.94 to 148.48	6.62 to 148.32	6.02 to 148.62	6.42 to 148.54
Index ranges	$-18 \le h \le 18$, $-16 \le k \le 18$, $-19 \le l \le 28$	$-17 \le h \le 17$, $-32 \le k \le 32$, $-14 \le l \le 16$	$-16 \le h \le 18$, $-18 \le k \le 17$, $-32 \le l \le 32$	$-22 \le h \le 23$, $-27 \le k \le 20$, $-33 \le l \le 33$
Reflections collected	26252	45255	78503	65960
Independent reflections	5219 [R_{int} = 0.0314, R_{sigma} = 0.0199]	9442 [R_{int} =0.0246, R_{sigma} = 0.0155]	22037 [R_{int} = 0.0706, R_{sigma} = 0.0587]	22347 [R_{int} = 0.0392, R_{sigma} = 0.0415]
Data/restraints/parameters	5219/0/285	9442/0/595	22037/0/1213	22347/0/1285
Goodness-of-fit on F^2	1.106	1.059	1.005	1.105
Final R indexes [I>=2σ (I)]	R_1 = 0.0526, wR_2 = 0.1539	R_1 = 0.0622, wR_2 = 0.1938	R_1 = 0.0742, wR_2 = 0.2106	R_1 = 0.0600, wR_2 = 0.1727
Final R indexes [all data]	R_1 = 0.0553, wR_2 = 0.1565	R_1 = 0.0661, wR_2 = 0.1988	R_1 = 0.1061, wR_2 = 0.2312	R_1 = 0.0692, wR_2 = 0.1799
Largest diff. peak/hole / e Å^{-3}	0.21/-0.27	1.45/-0.27	0.40/-0.28	0.29/-0.30

Figure S2. Center-to-center distances (in Å) in *m*-Me (top) and *m*-OMe (bottom). Thermal ellipsoids are set at the 50% probability level.

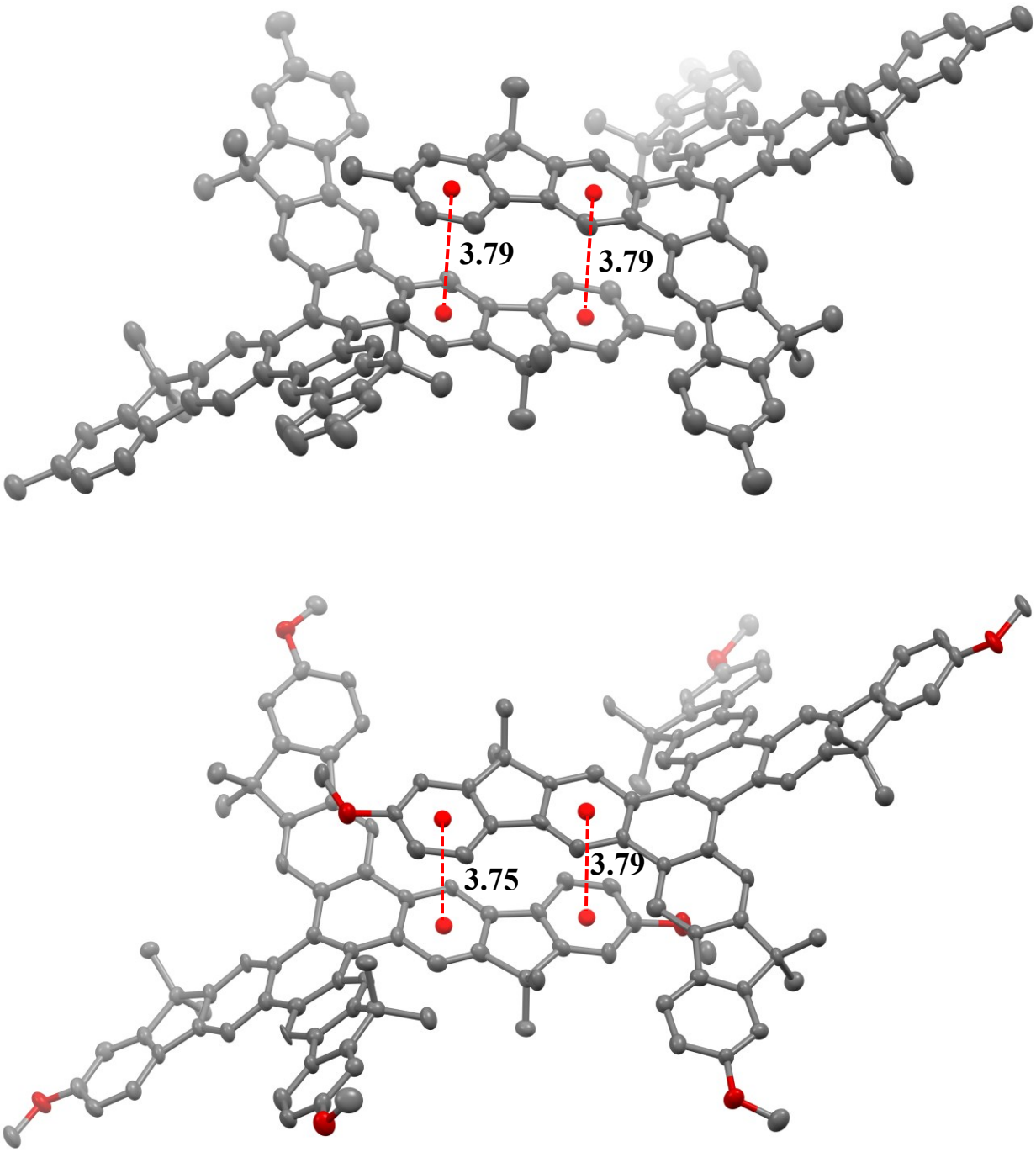


Figure S3. Top and side views of the π-π stacking in the *m*-Me. The least-squares-fit planes defined by the orange fluorene moieties in each molecule are shown. Thermal ellipsoids are set at 50% probability.

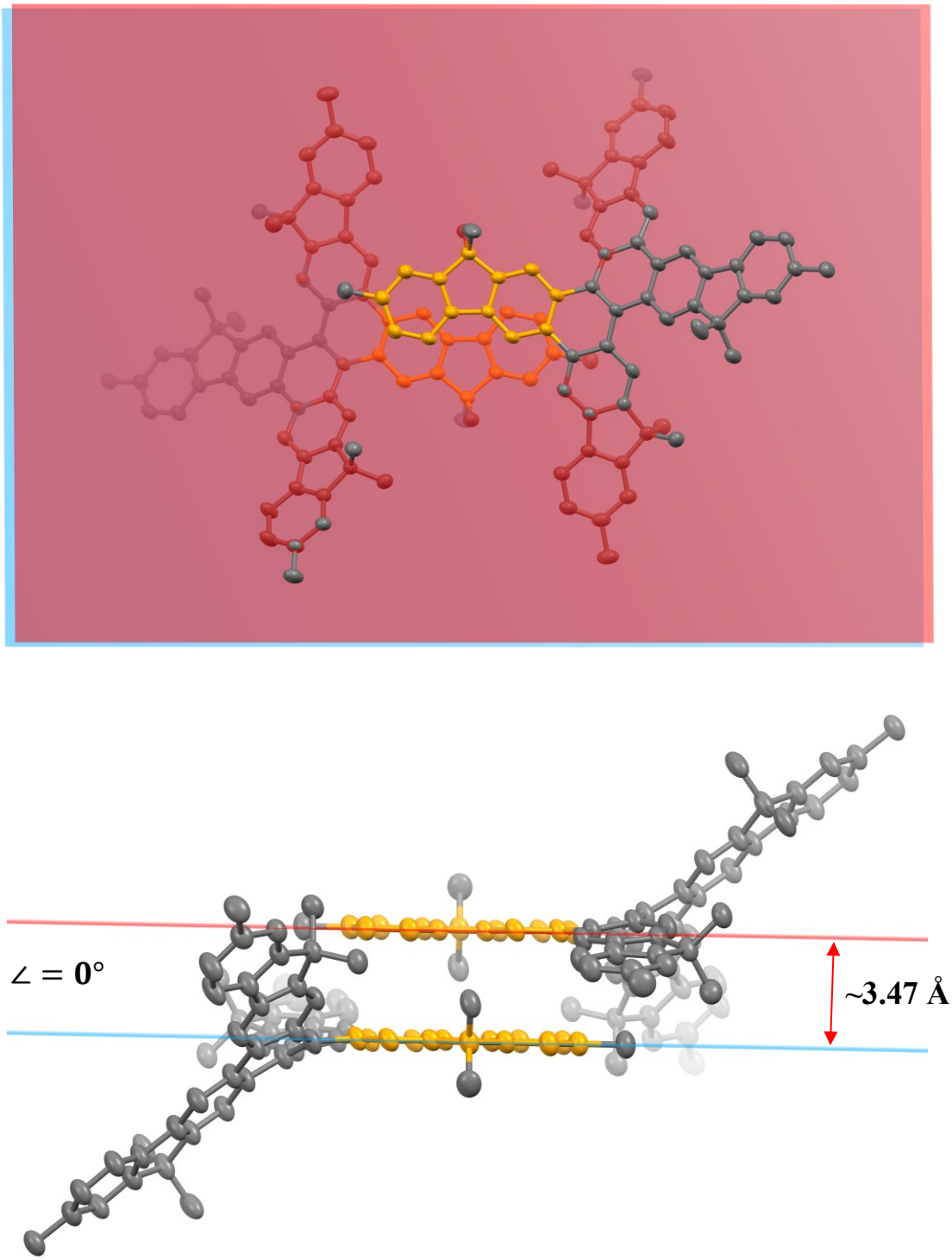
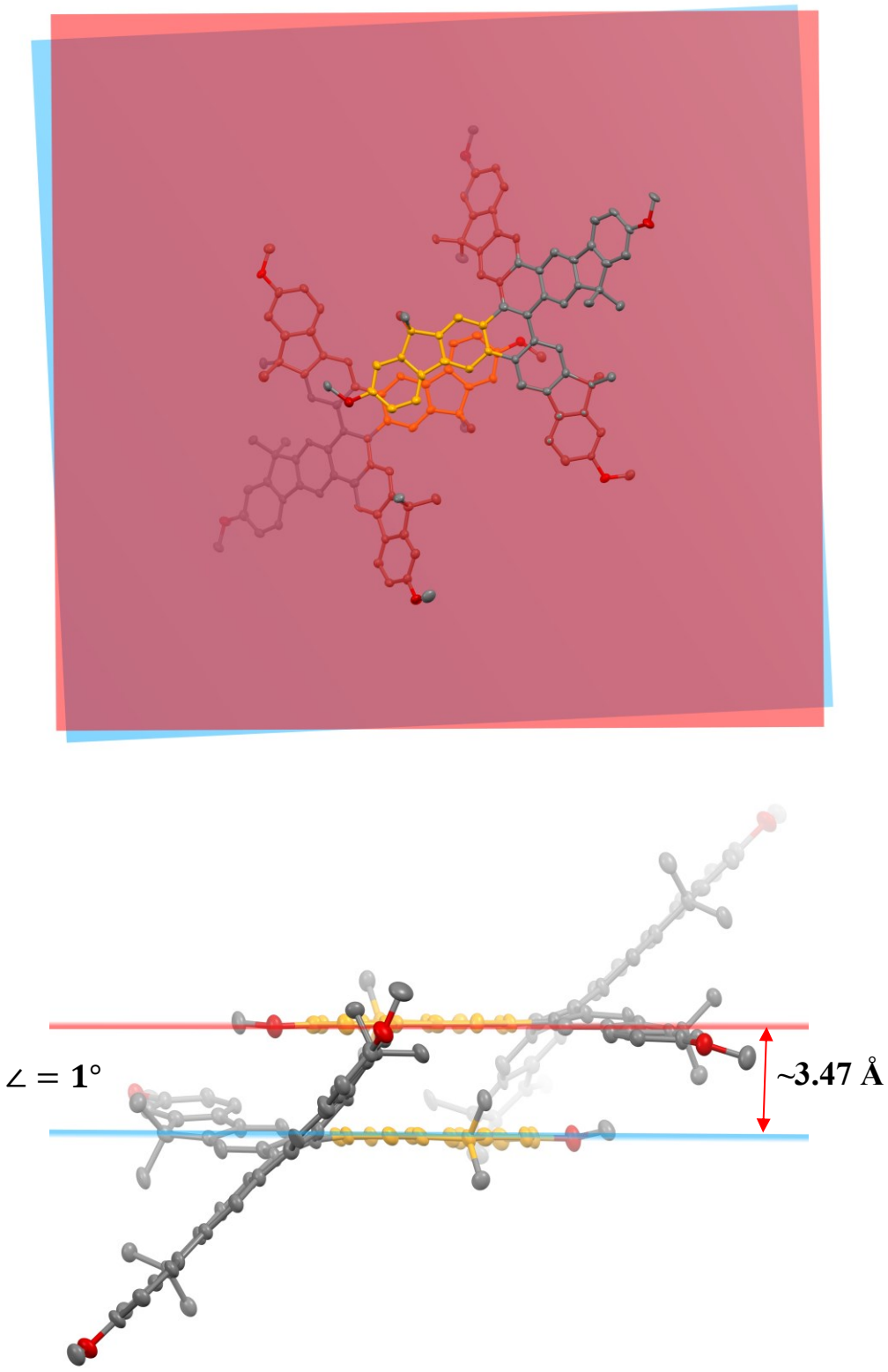
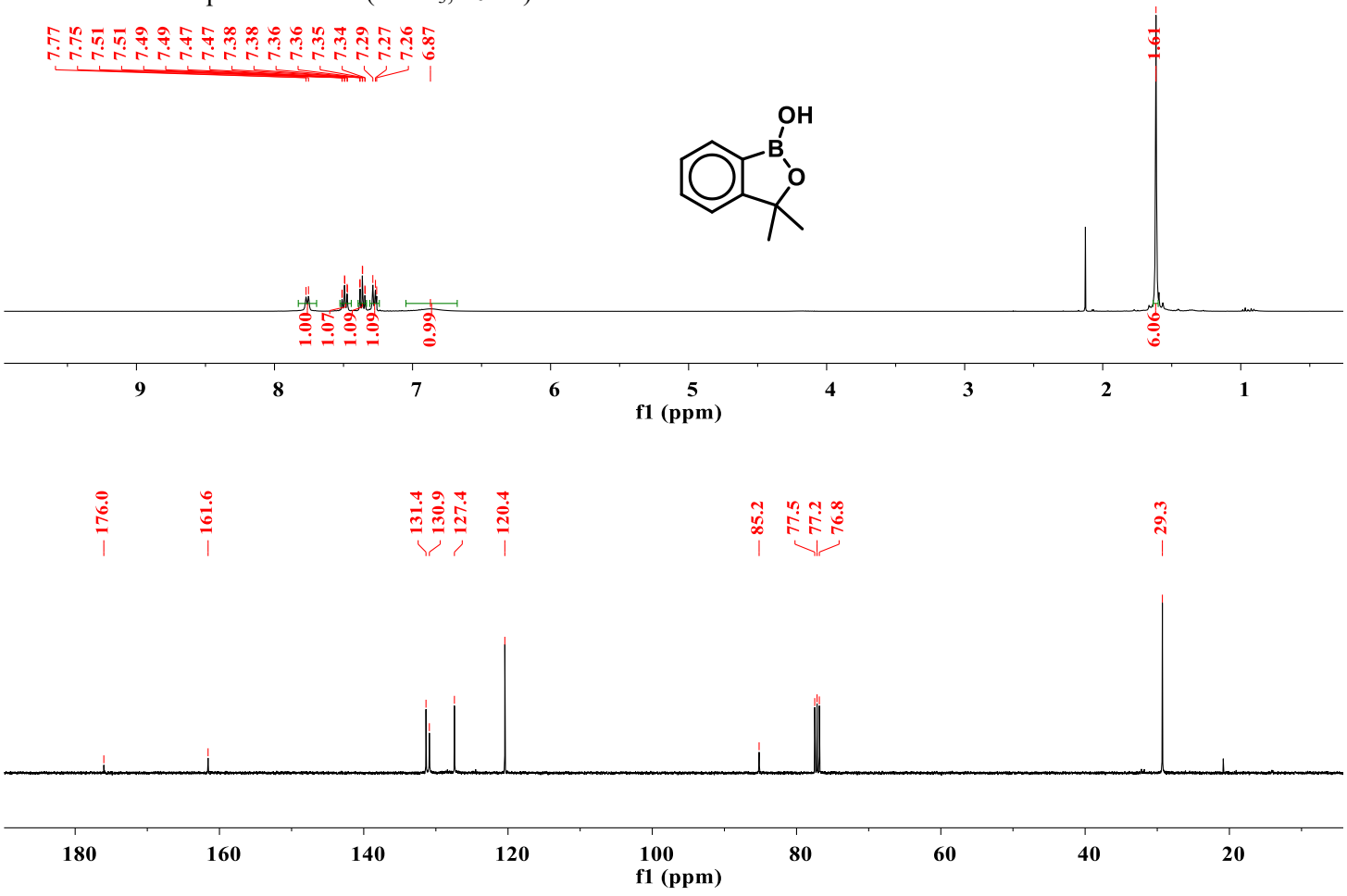


Figure S4. Top and side views of the π-π stacking in the *m*-OMe. The least-squares-fit planes defined by the orange fluorene moieties in each molecule are shown. Thermal ellipsoids are set at 50% probability.

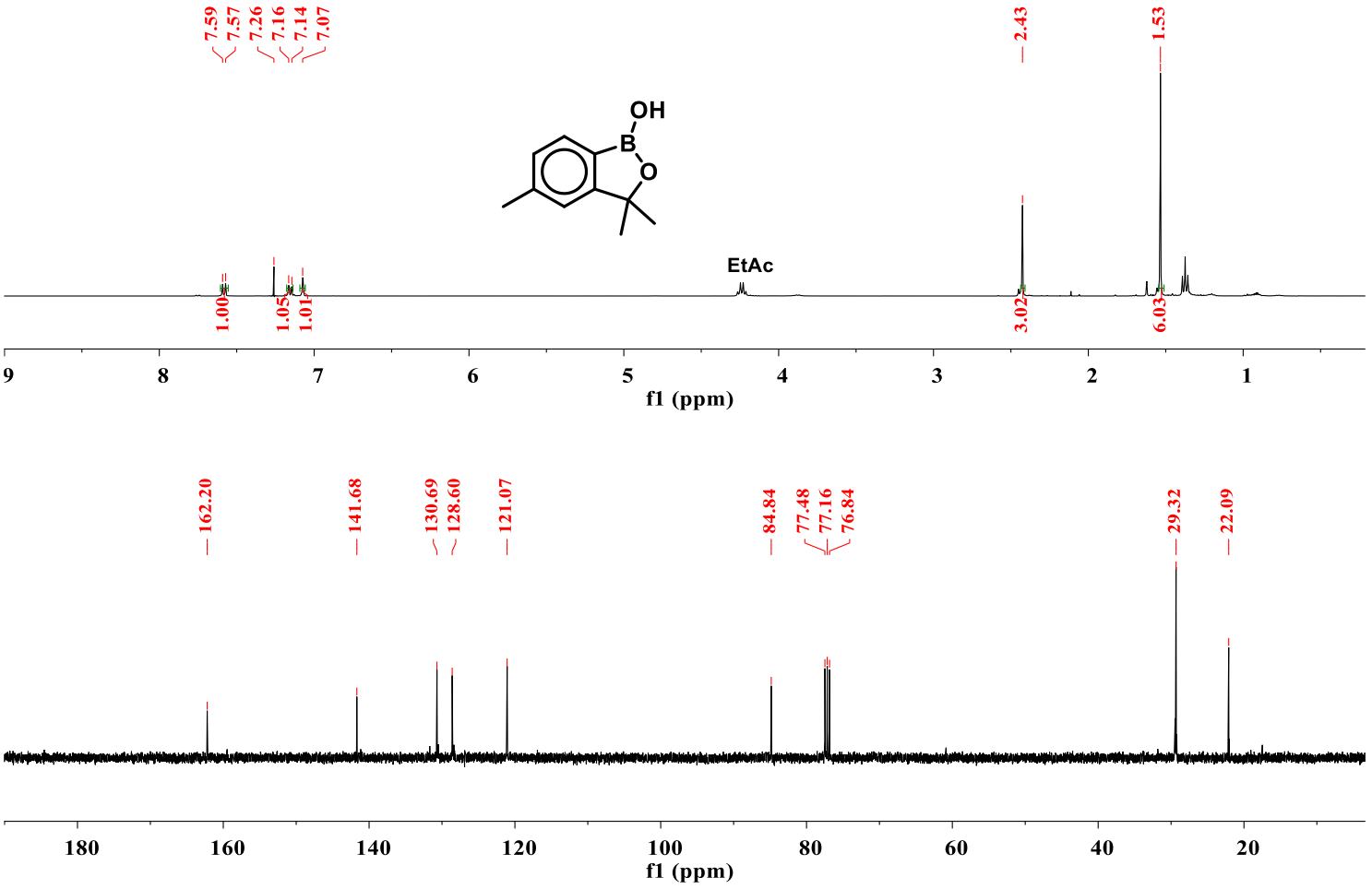


4. NMR spectroscopy.

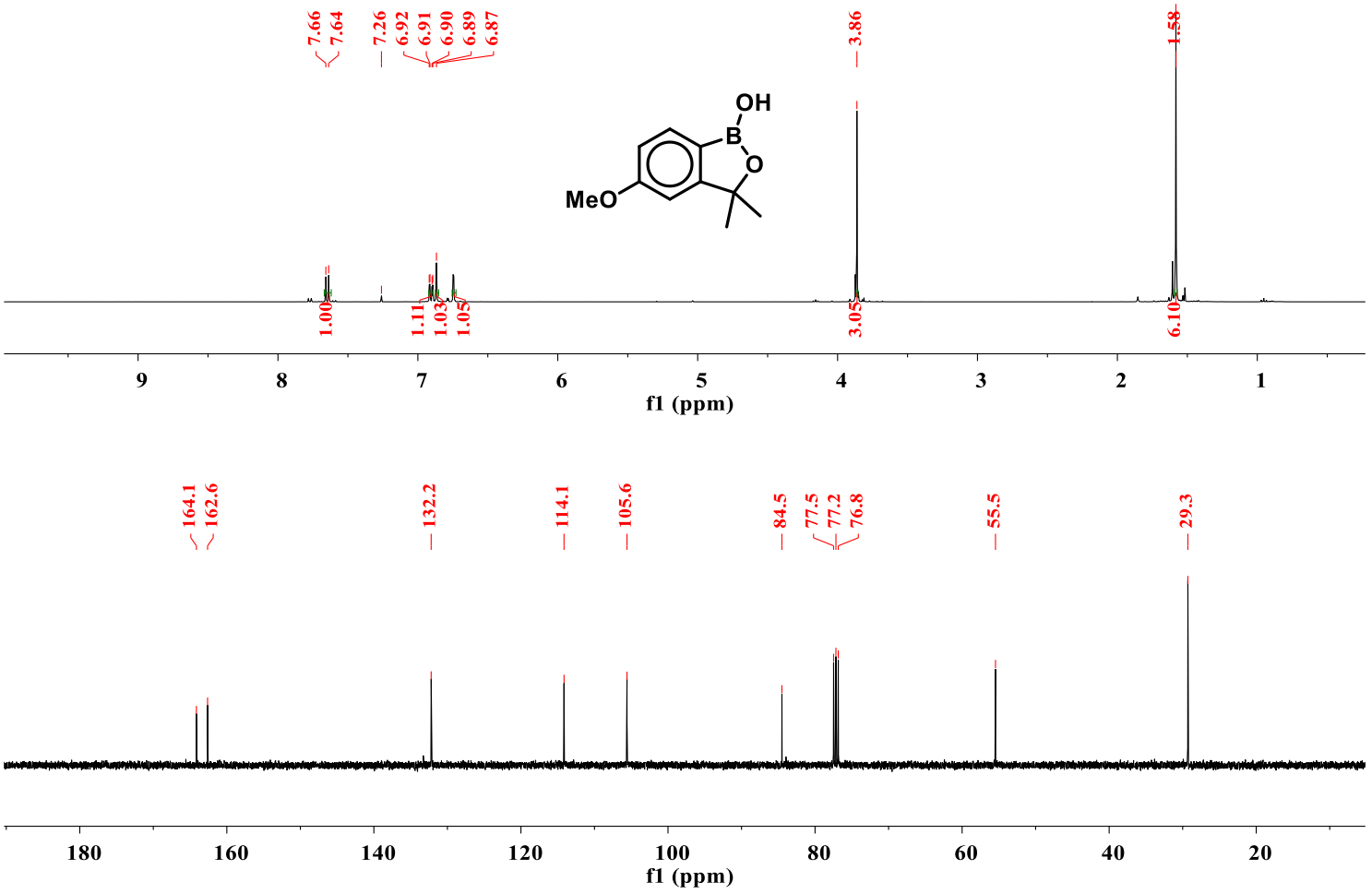
^{1}H and ^{13}C NMR spectra of **A-H** ($CDCl_3$, 20 °C)[4]



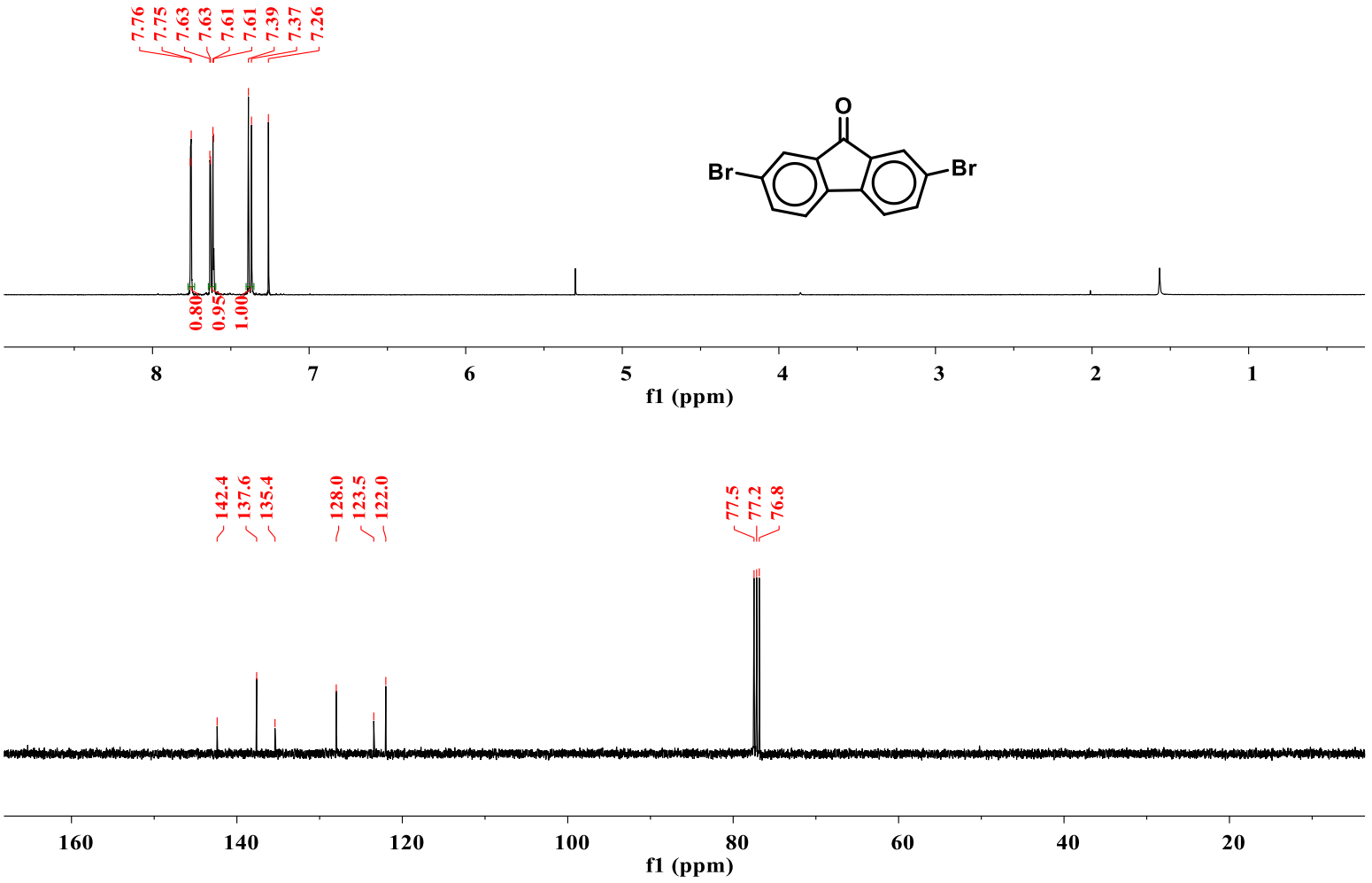
^{1}H and ^{13}C NMR spectra of **A-Me** ($CDCl_3$, 20 °C)[5]



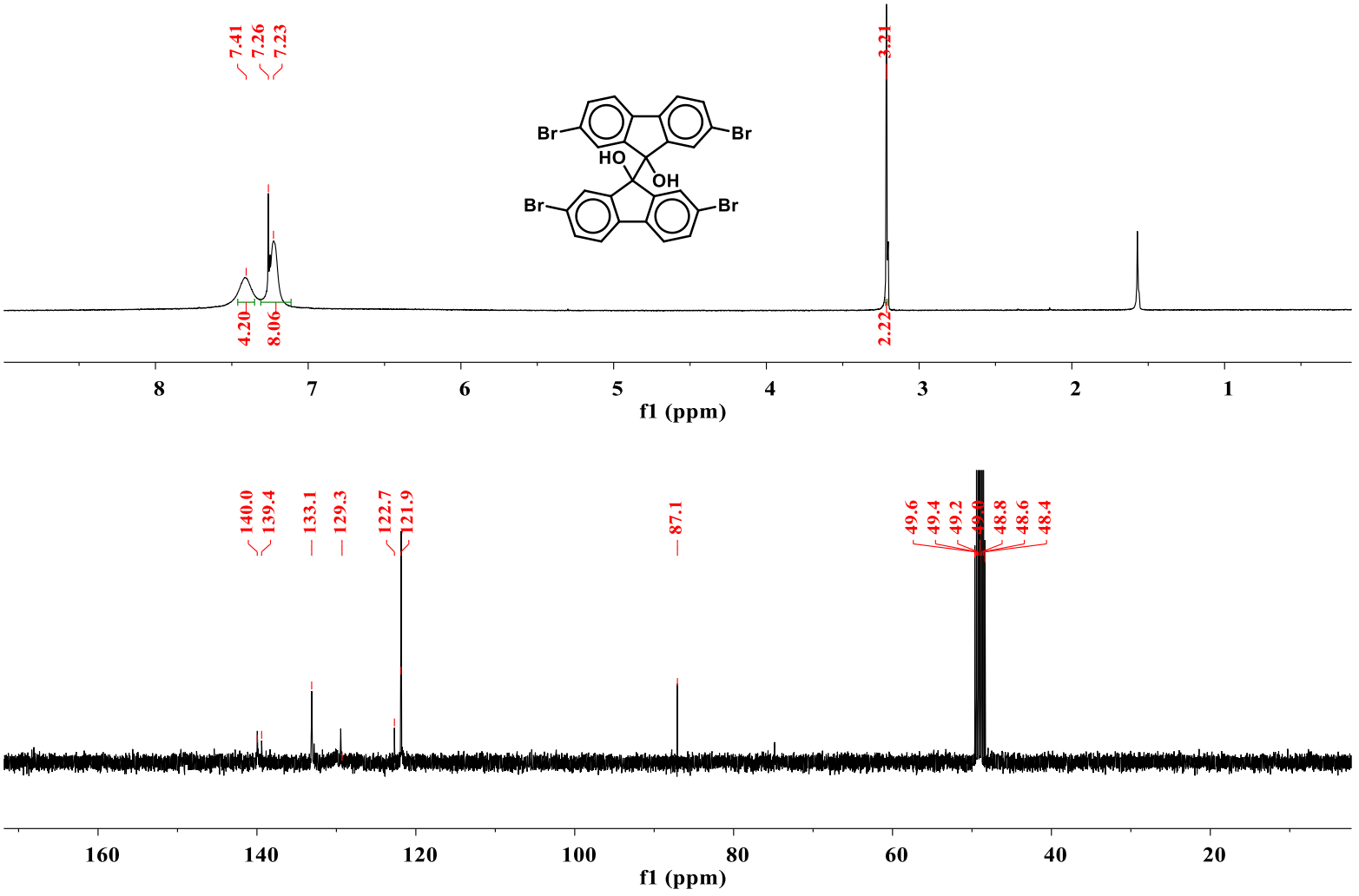
^{1}H and ^{13}C NMR spectra of **A-OMe** ($CDCl_3$, 20 °C)[6]



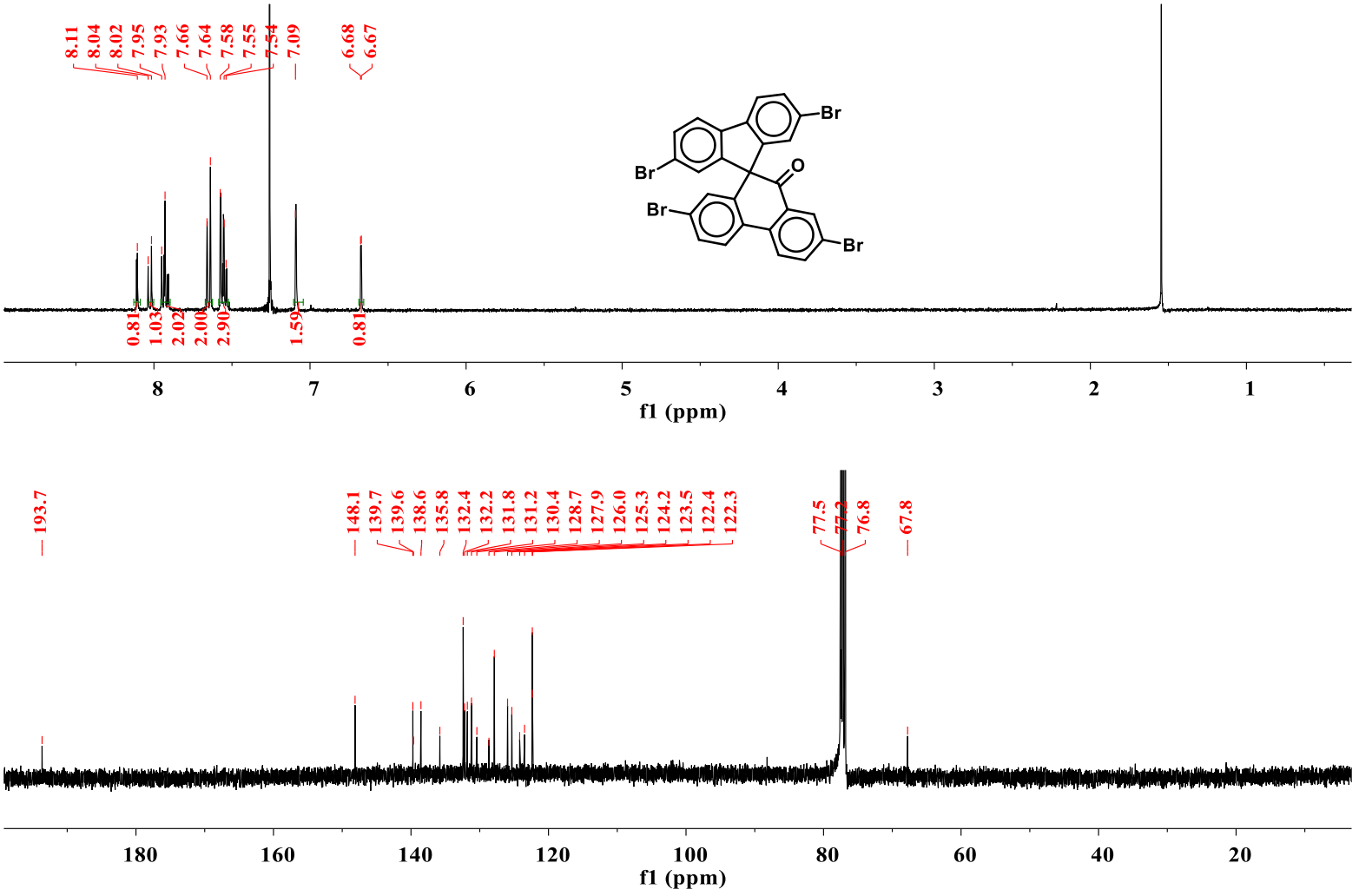
^{1}H and ^{13}C NMR spectra of **S1** (X = Br, $CDCl_3$, 20 °C)



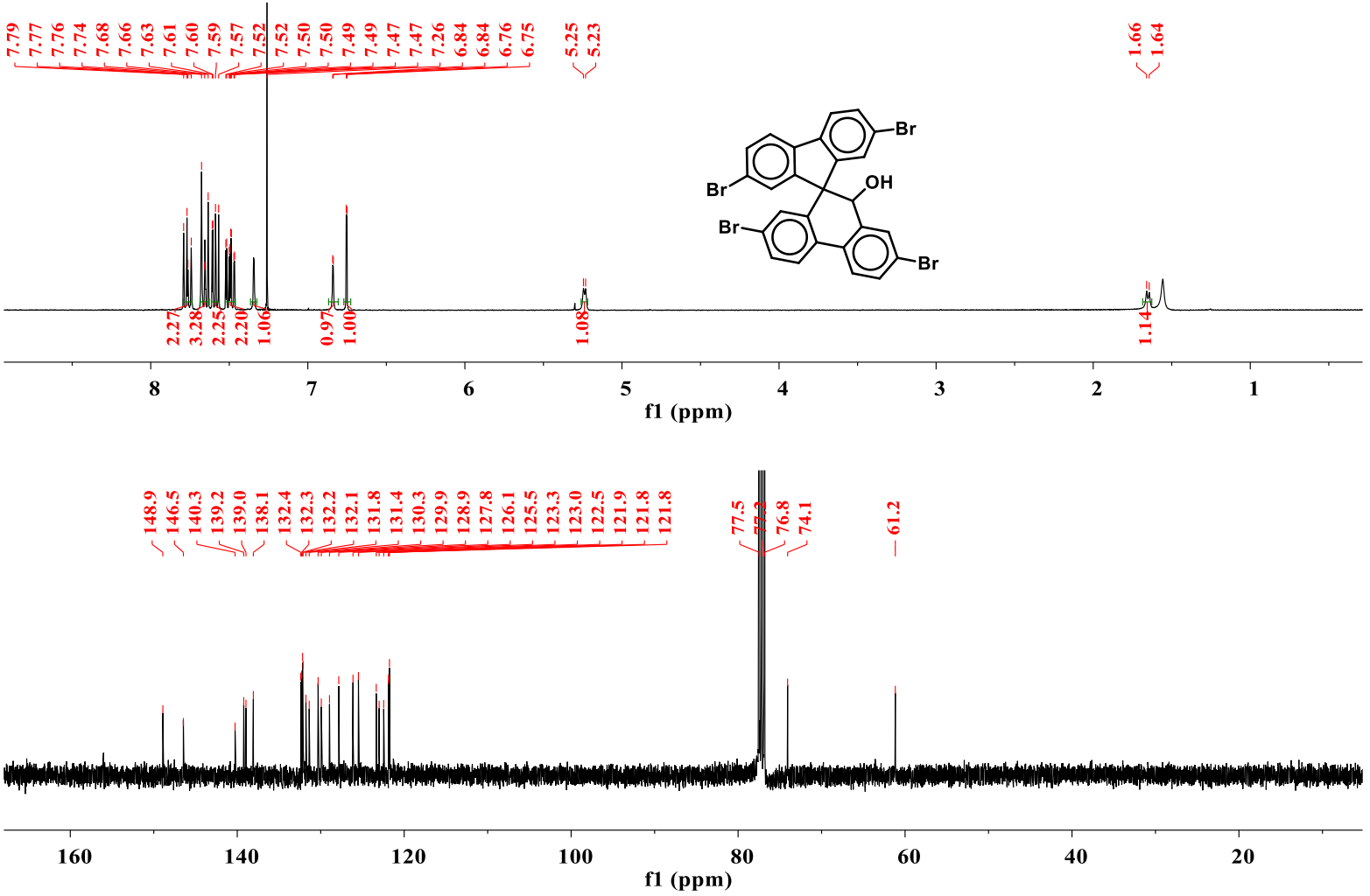
^{1}H ($CDCl_3$) and ^{13}C (CD_3OD) NMR spectra of **1a** at 20 °C



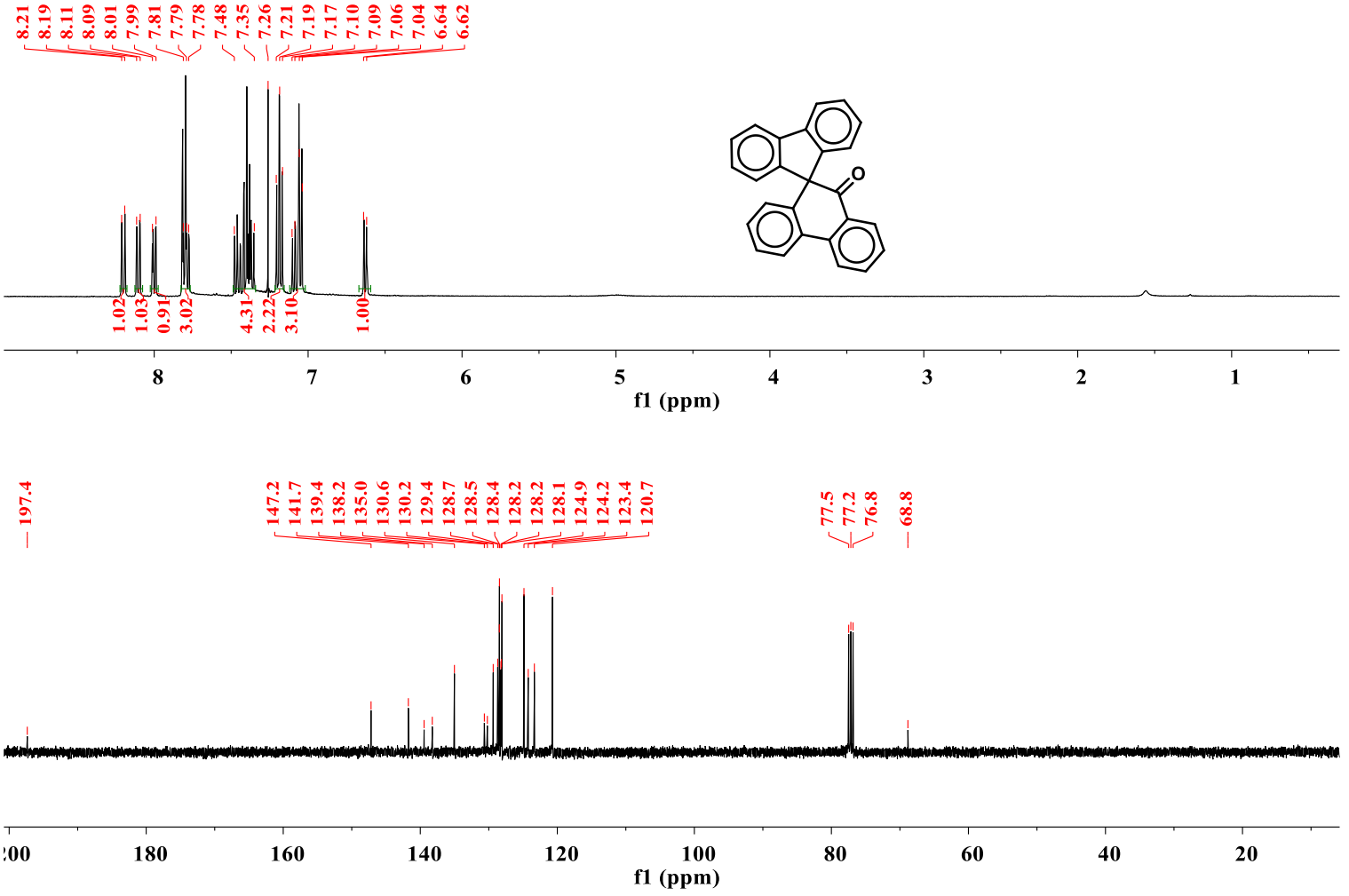
^{1}H and ^{13}C NMR spectra of **2a** ($CDCl_3$, 20 °C)



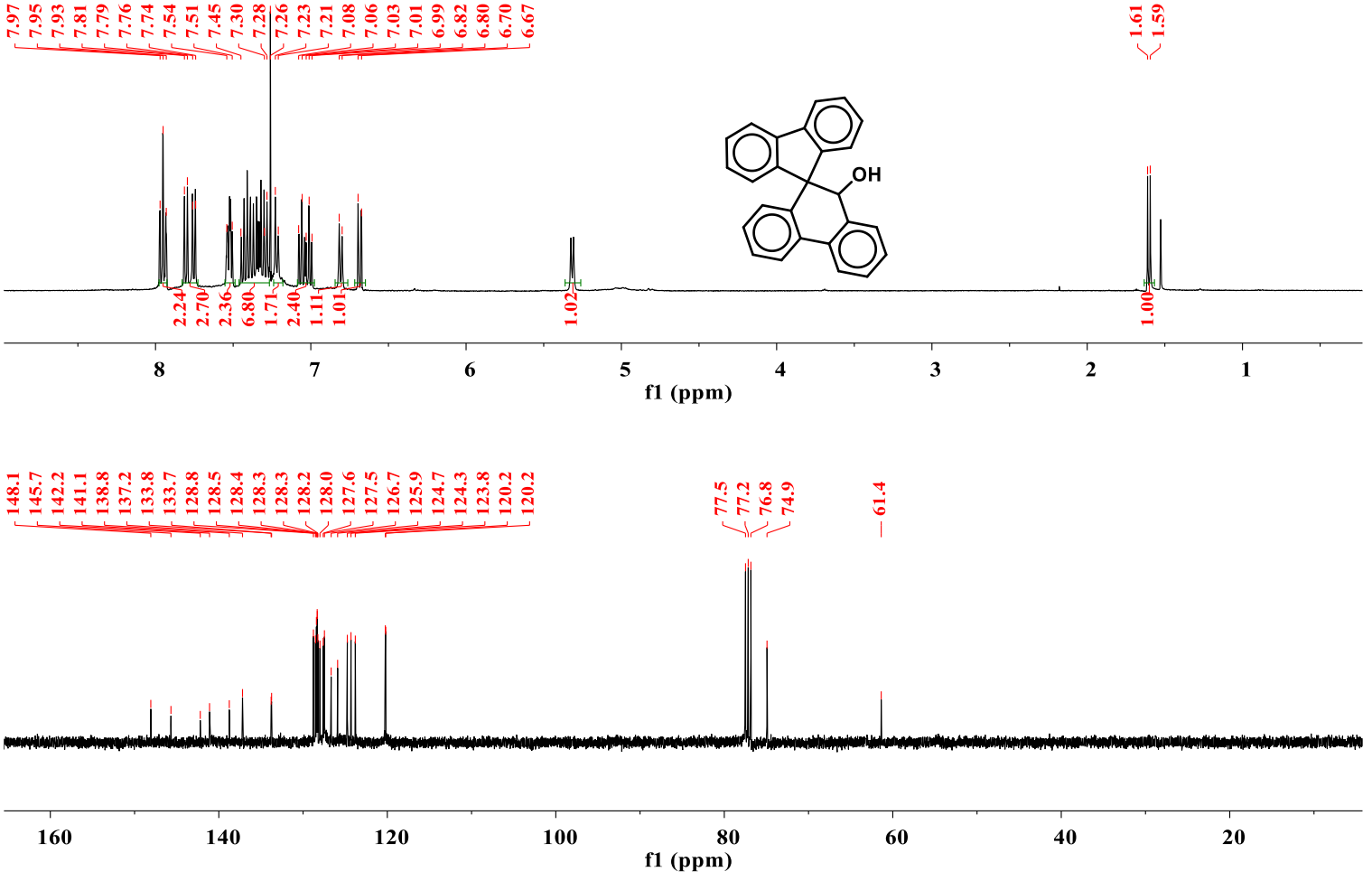
^{1}H and ^{13}C NMR spectra of **3a** ($CDCl_3$, 20 °C)



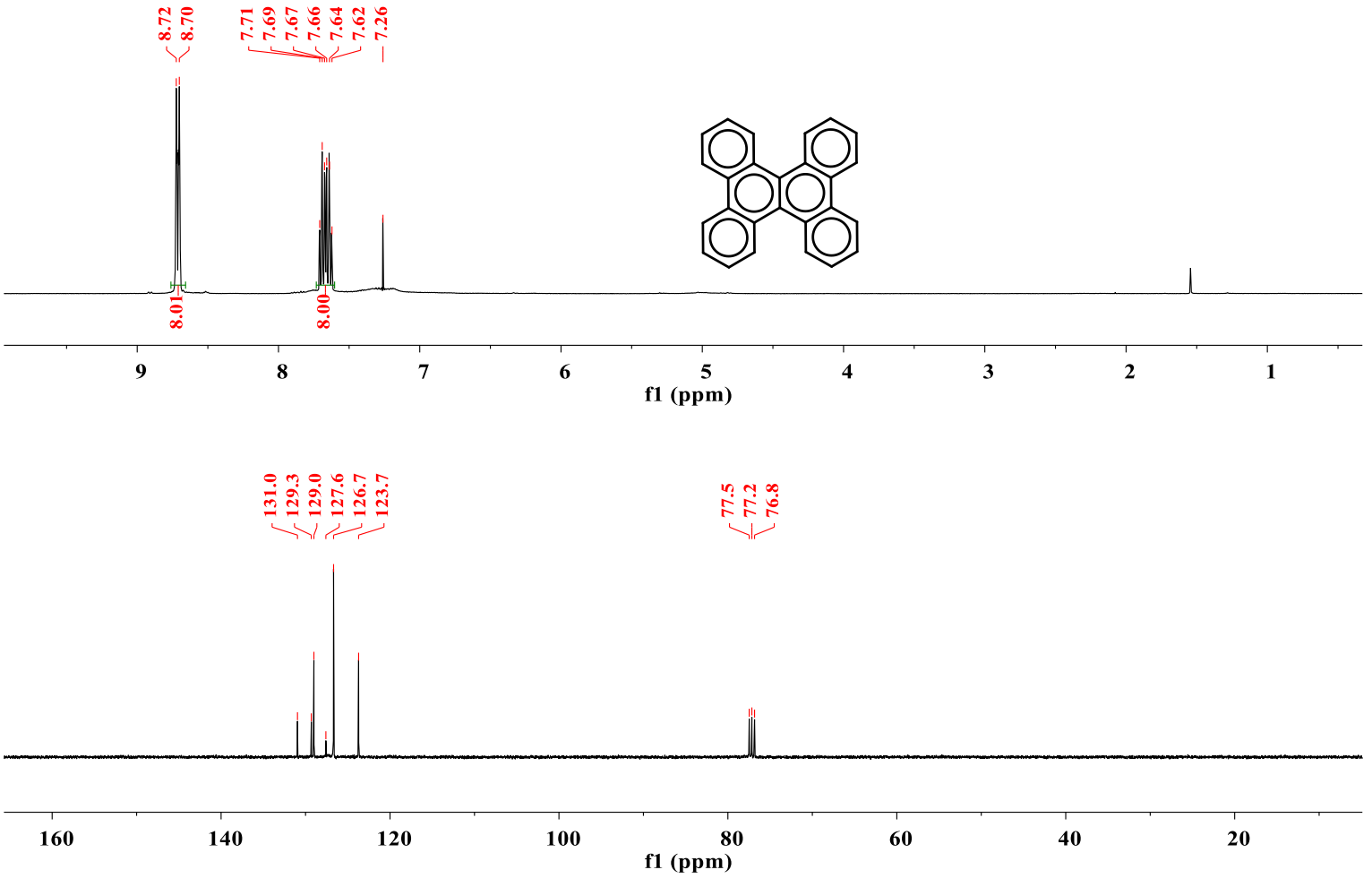
^{1}H and ^{13}C NMR spectra of **2b** ($CDCl_3$, 20 °C)



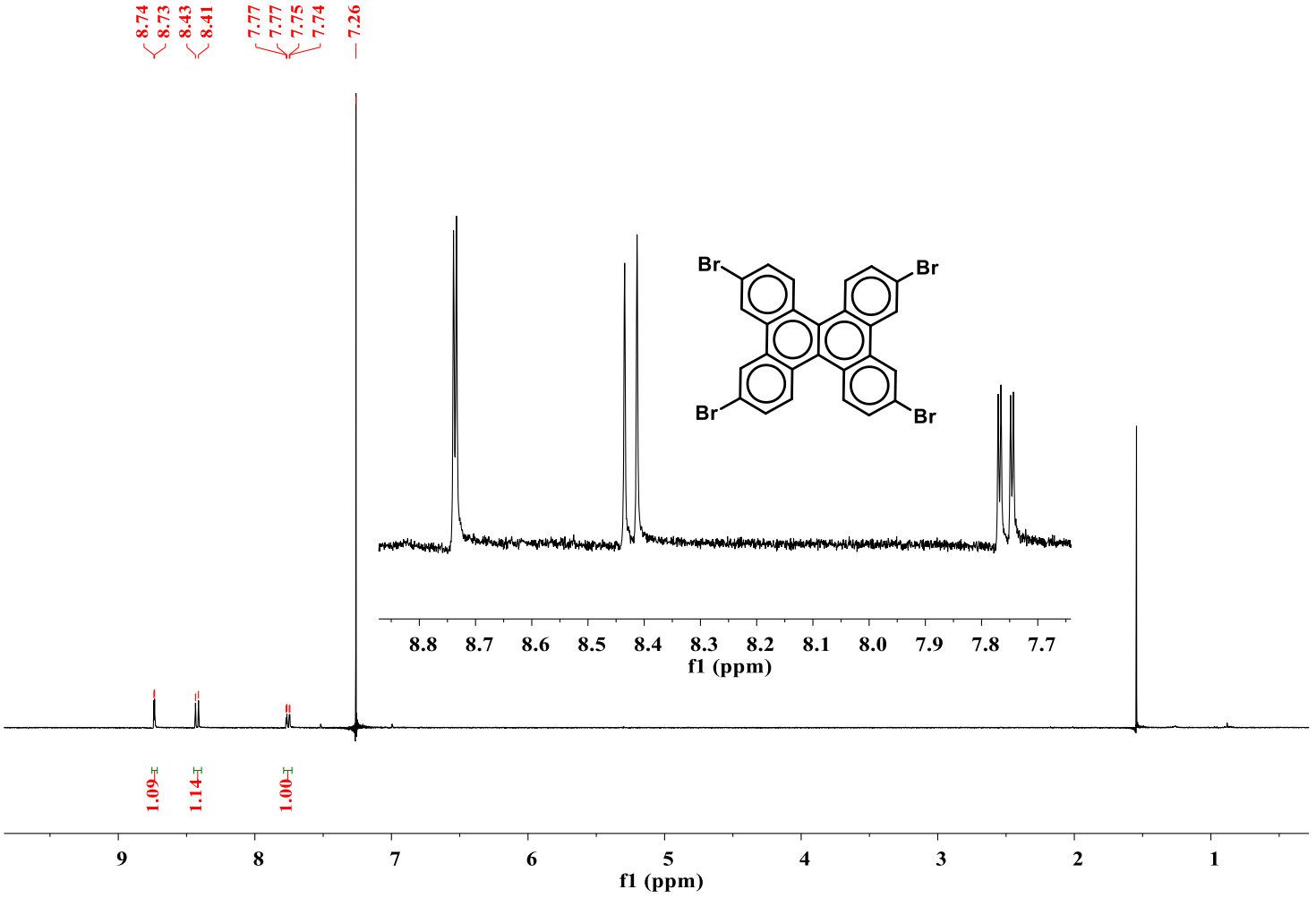
^{1}H and ^{13}C NMR spectra of **3b** ($CDCl_3$, 20 °C)



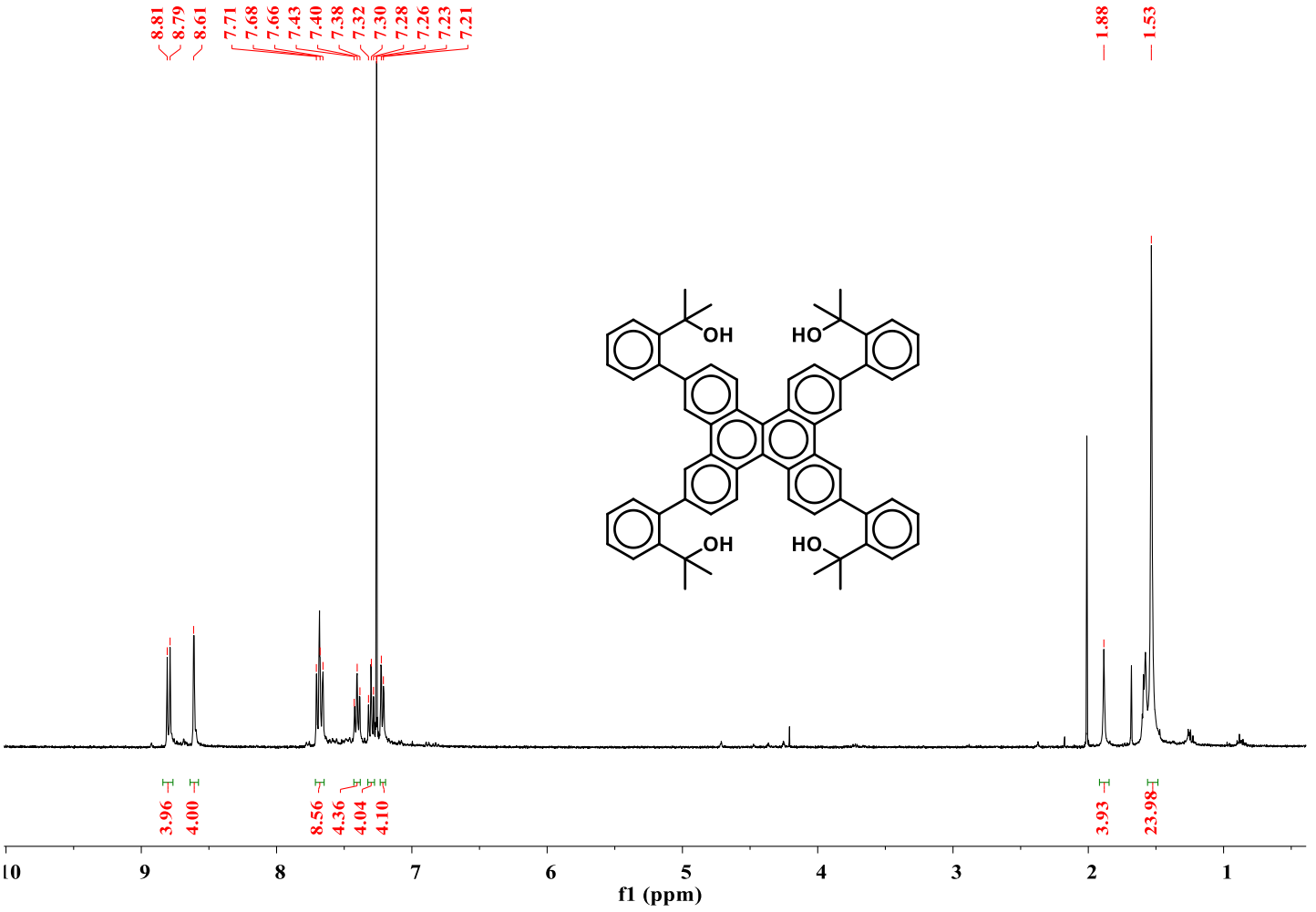
^{1}H and ^{13}C NMR spectra of **4b** ($CDCl_3$, 20 °C)



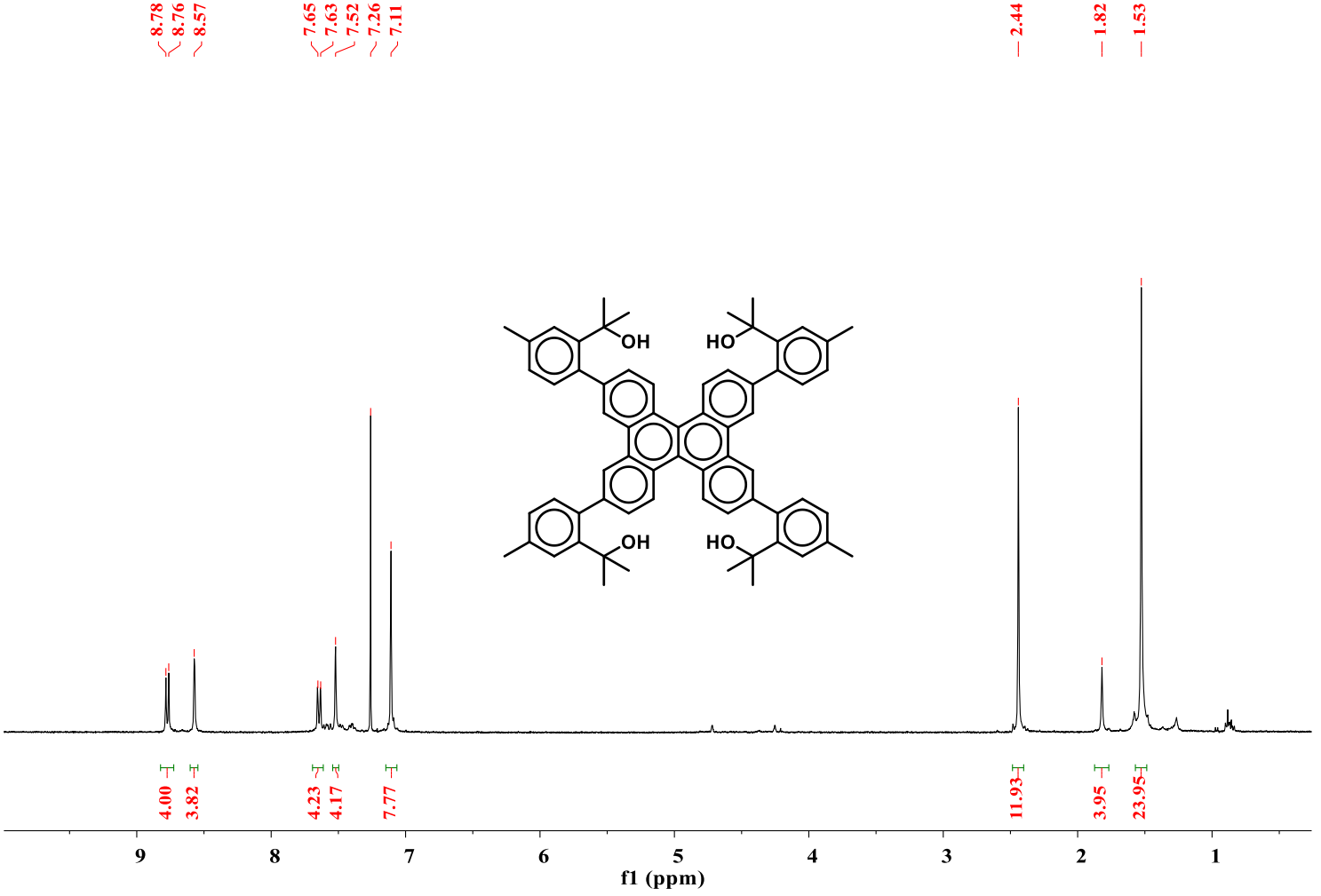
^{1}H NMR spectrum of **5** ($CDCl_3$, 20 °C)



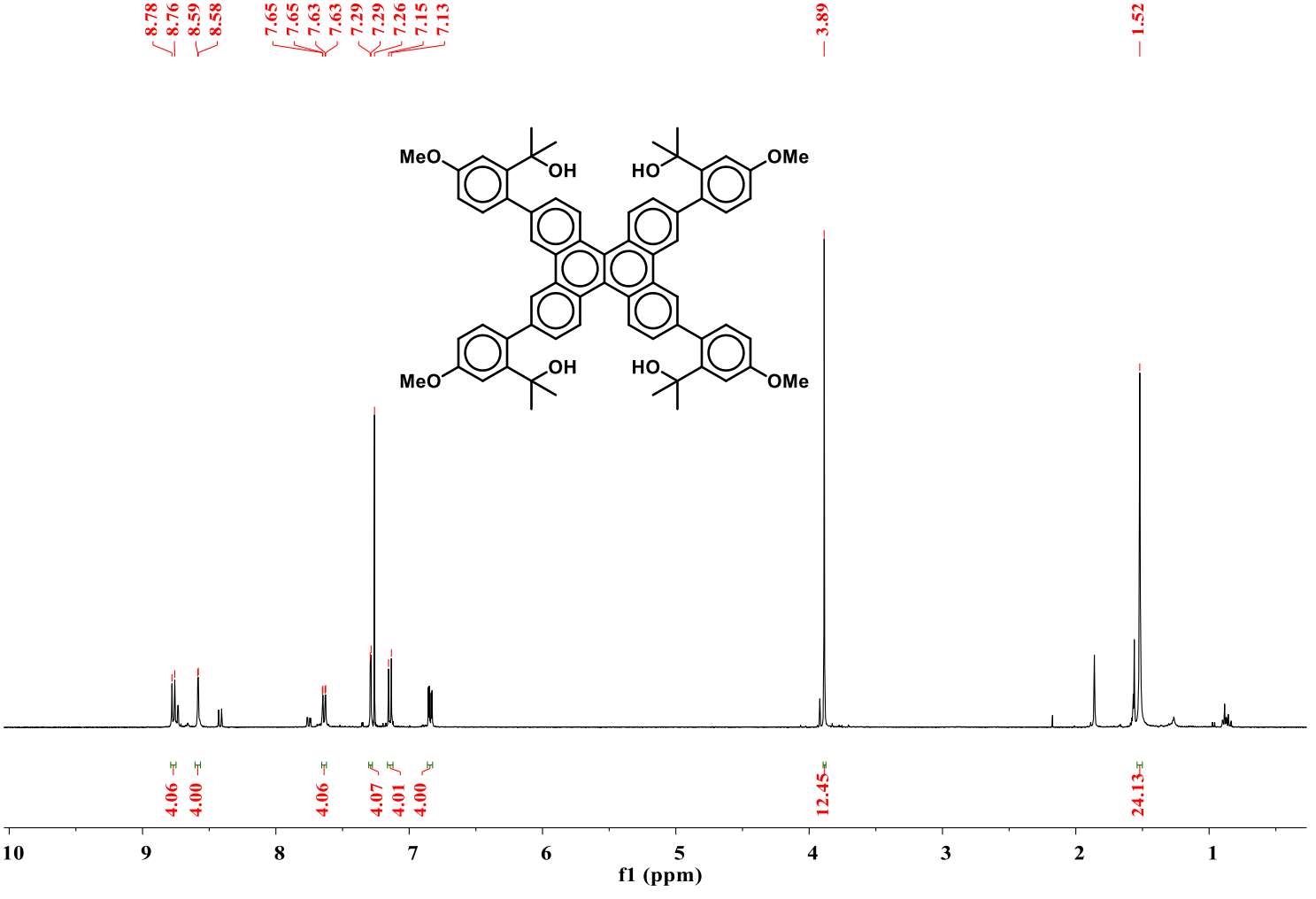
^{1}H NMR spectrum of **6-H** ($CDCl_3$, 20 °C)



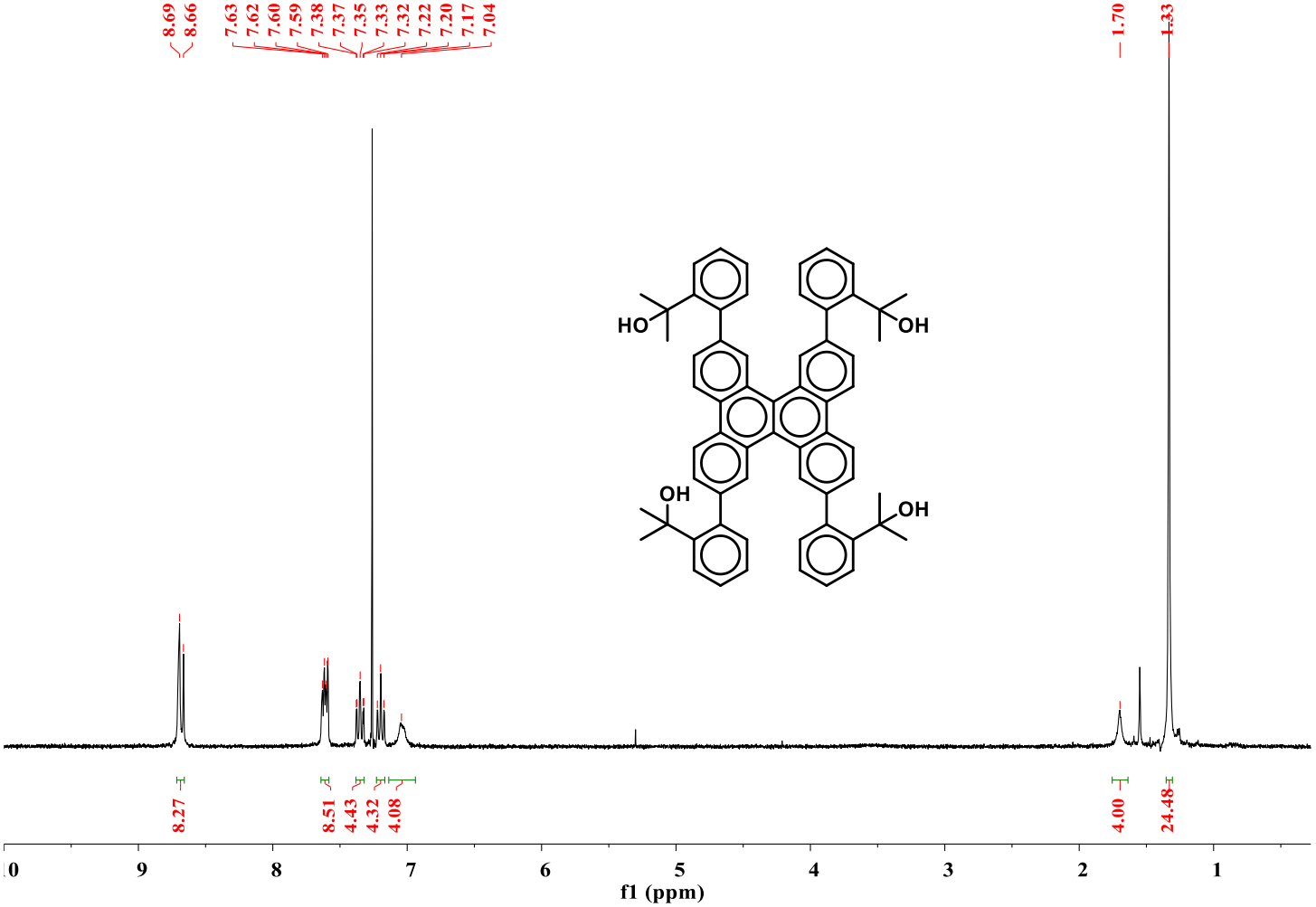
^{1}H NMR spectrum of **6-Me** ($CDCl_3$, 20 °C)



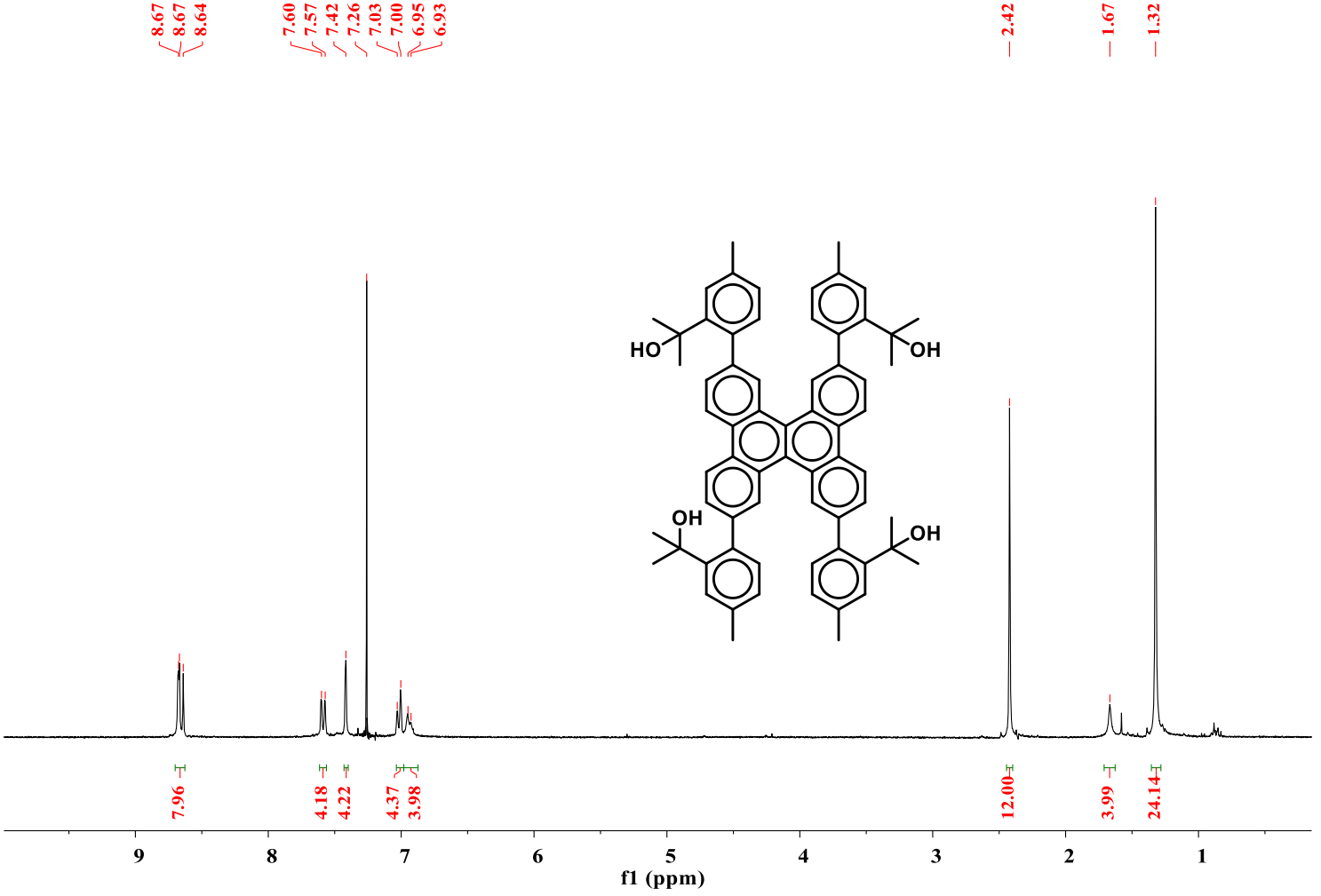
^{1}H NMR spectrum of **6-OMe** ($CDCl_3$, 20 °C)



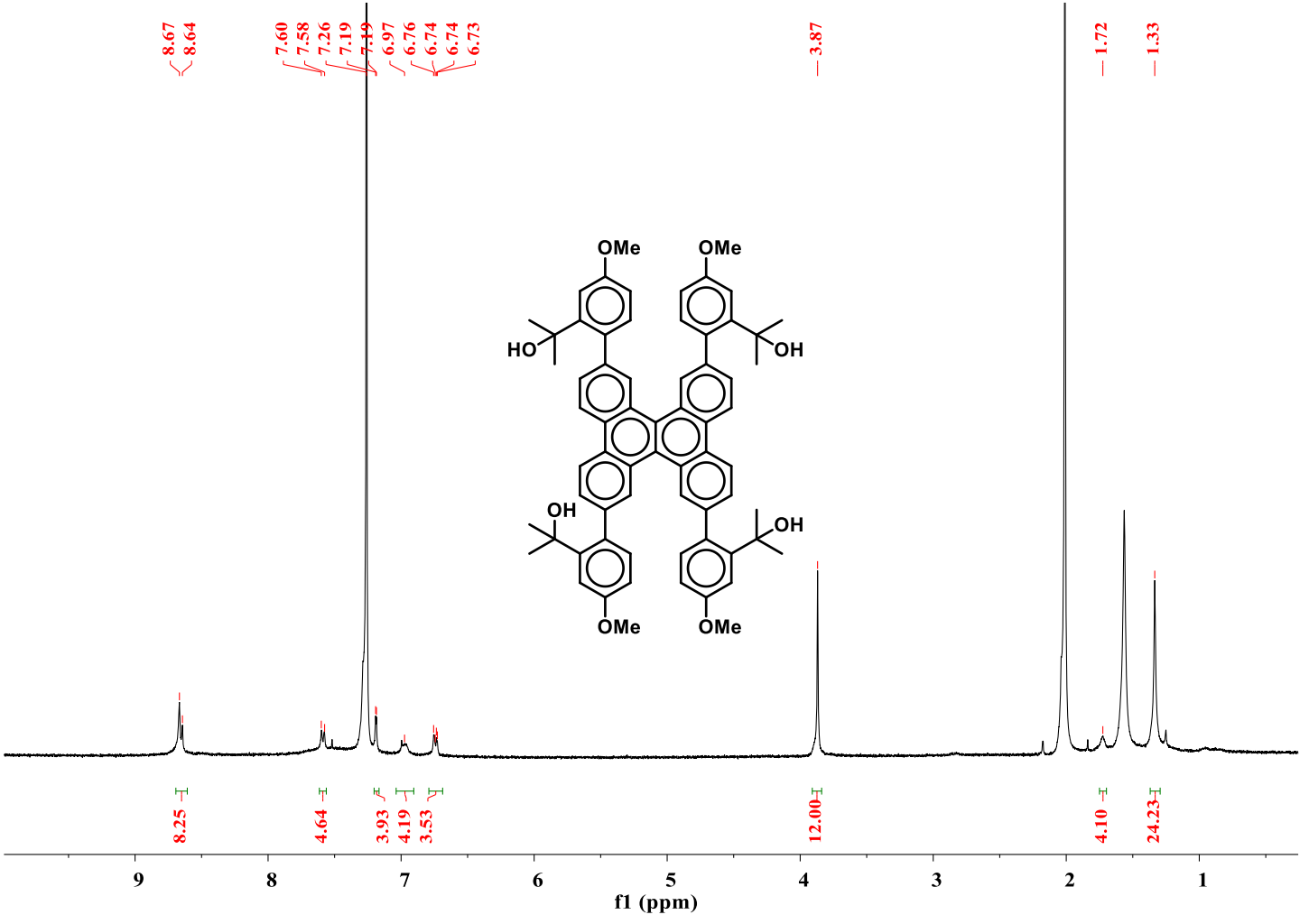
^{1}H NMR spectrum of **7-H** ($CDCl_3$, 20 °C)



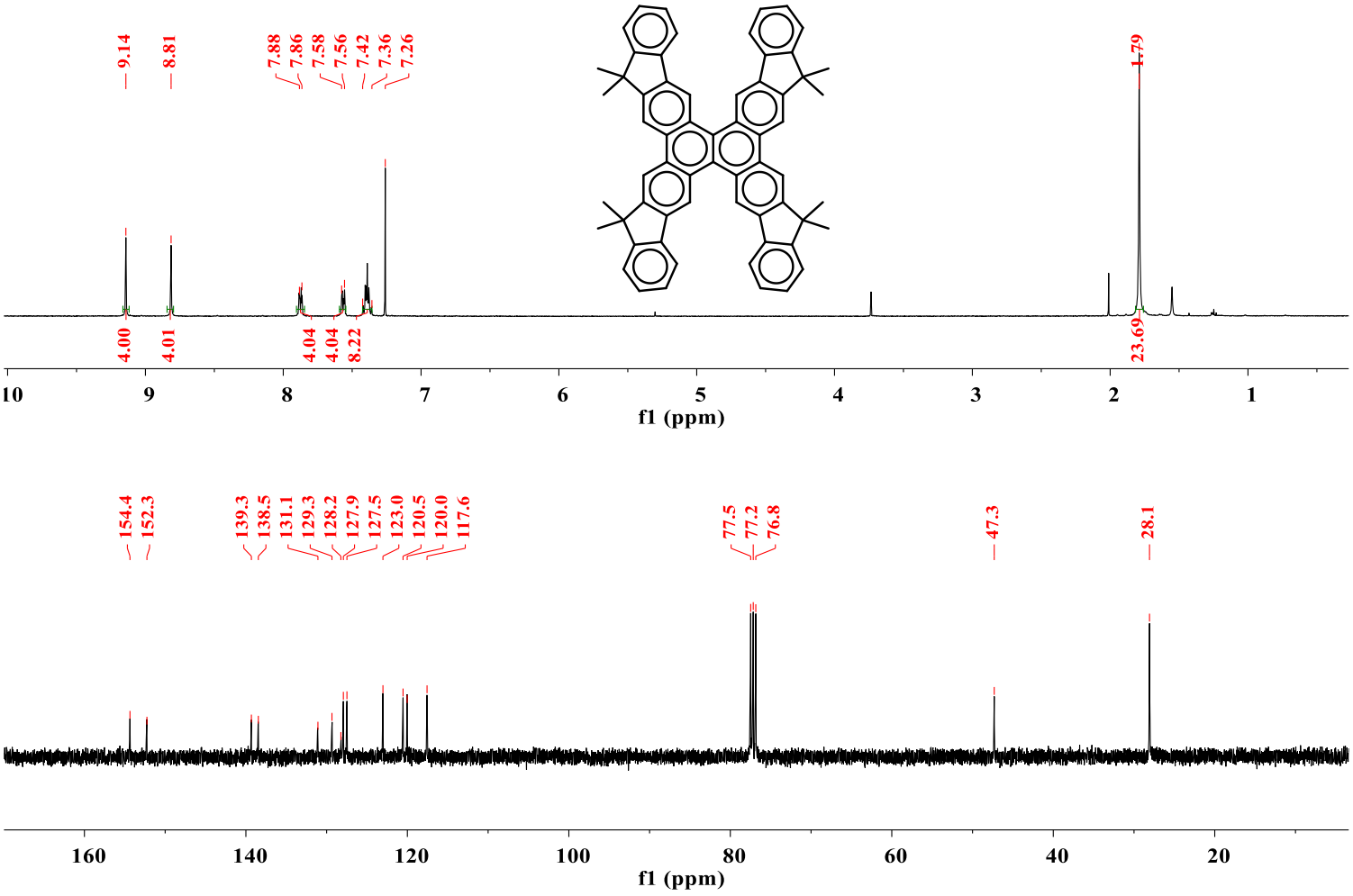
^{1}H NMR spectrum of **7-Me** ($CDCl_3$, 20 °C)



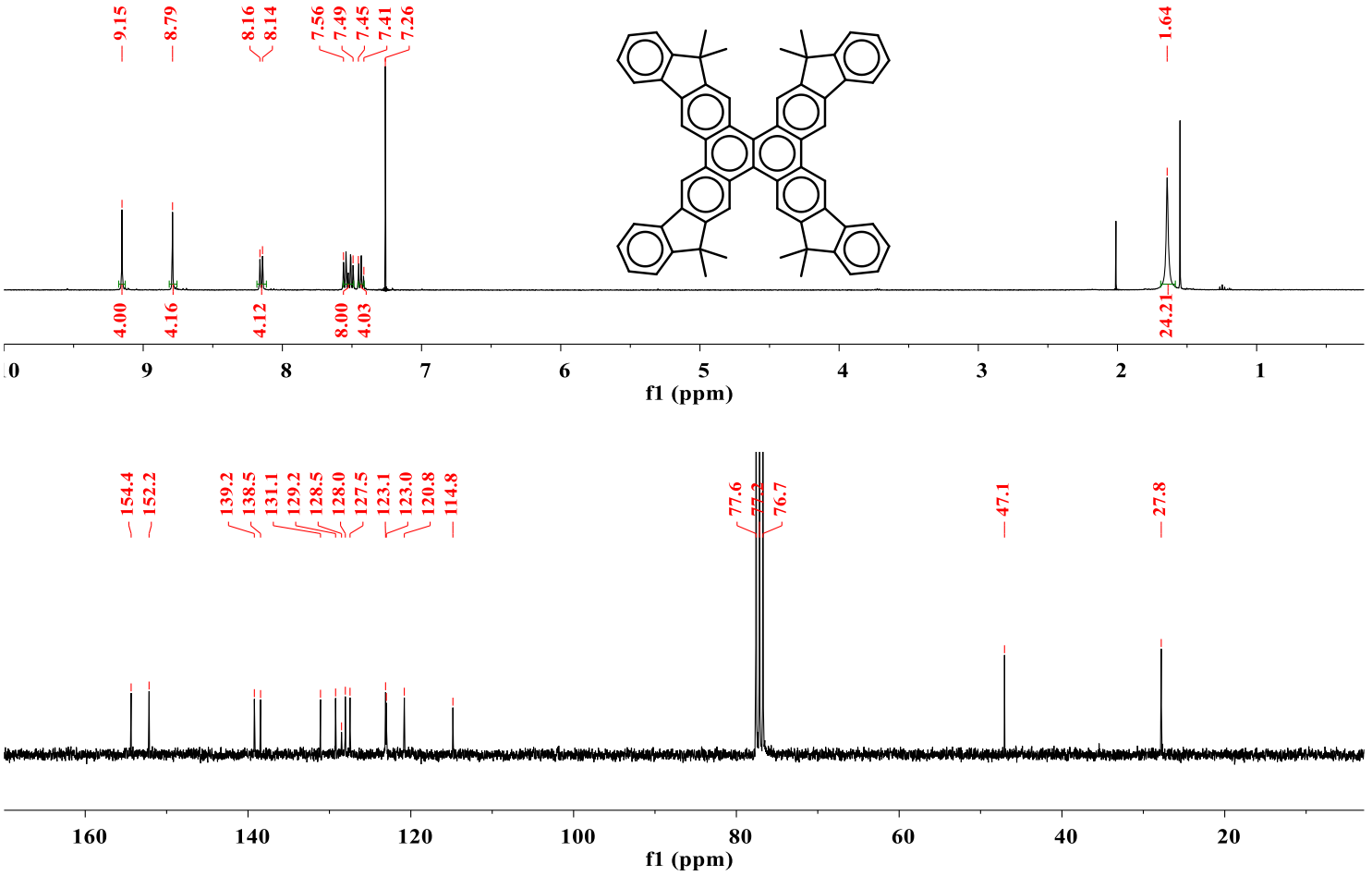
^{1}H NMR spectrum of **7-OMe** ($CDCl_3$, 20 °C)



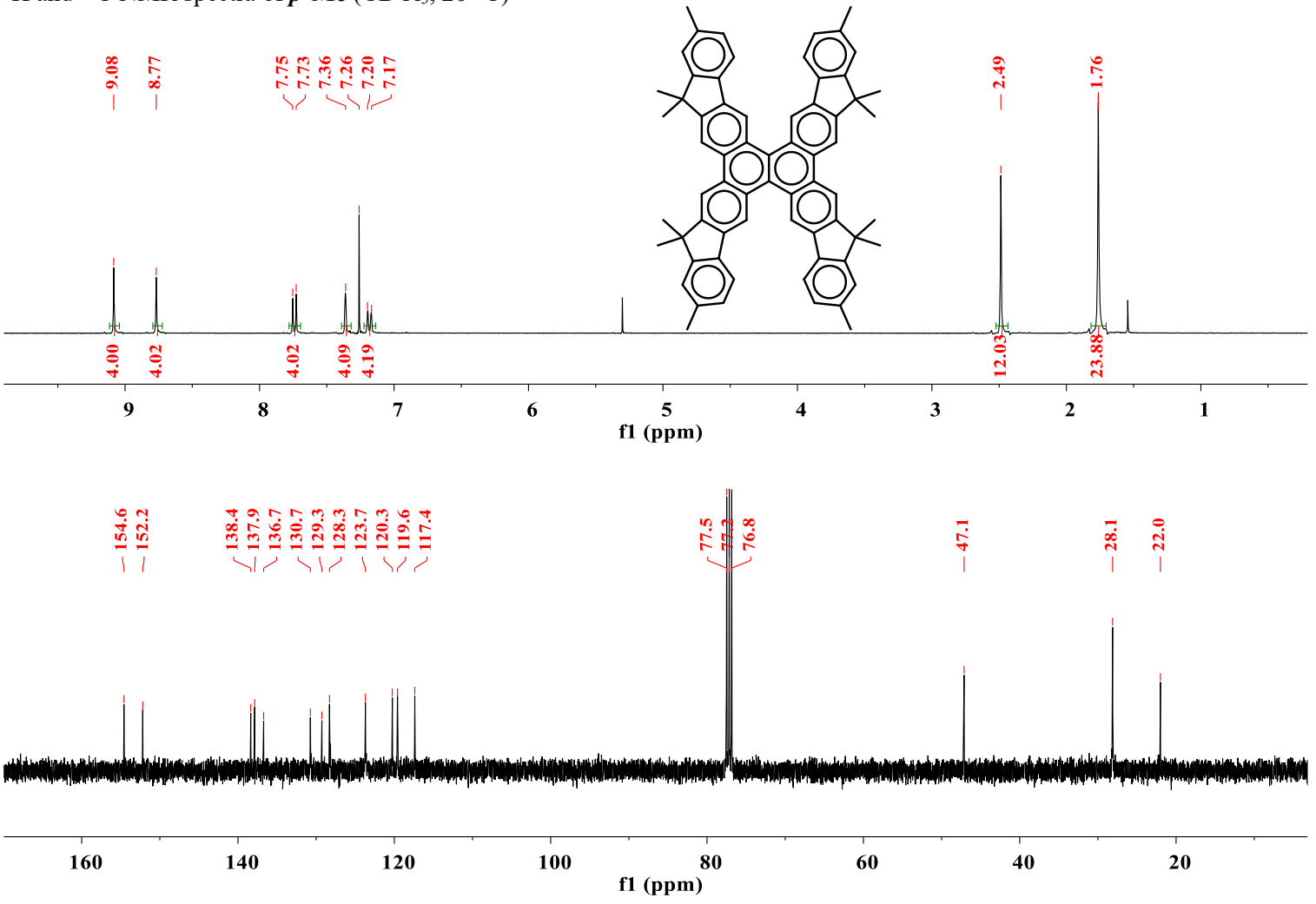
^{1}H and ^{13}C NMR spectra of ***p*-H** ($CDCl_3$, 20 °C)



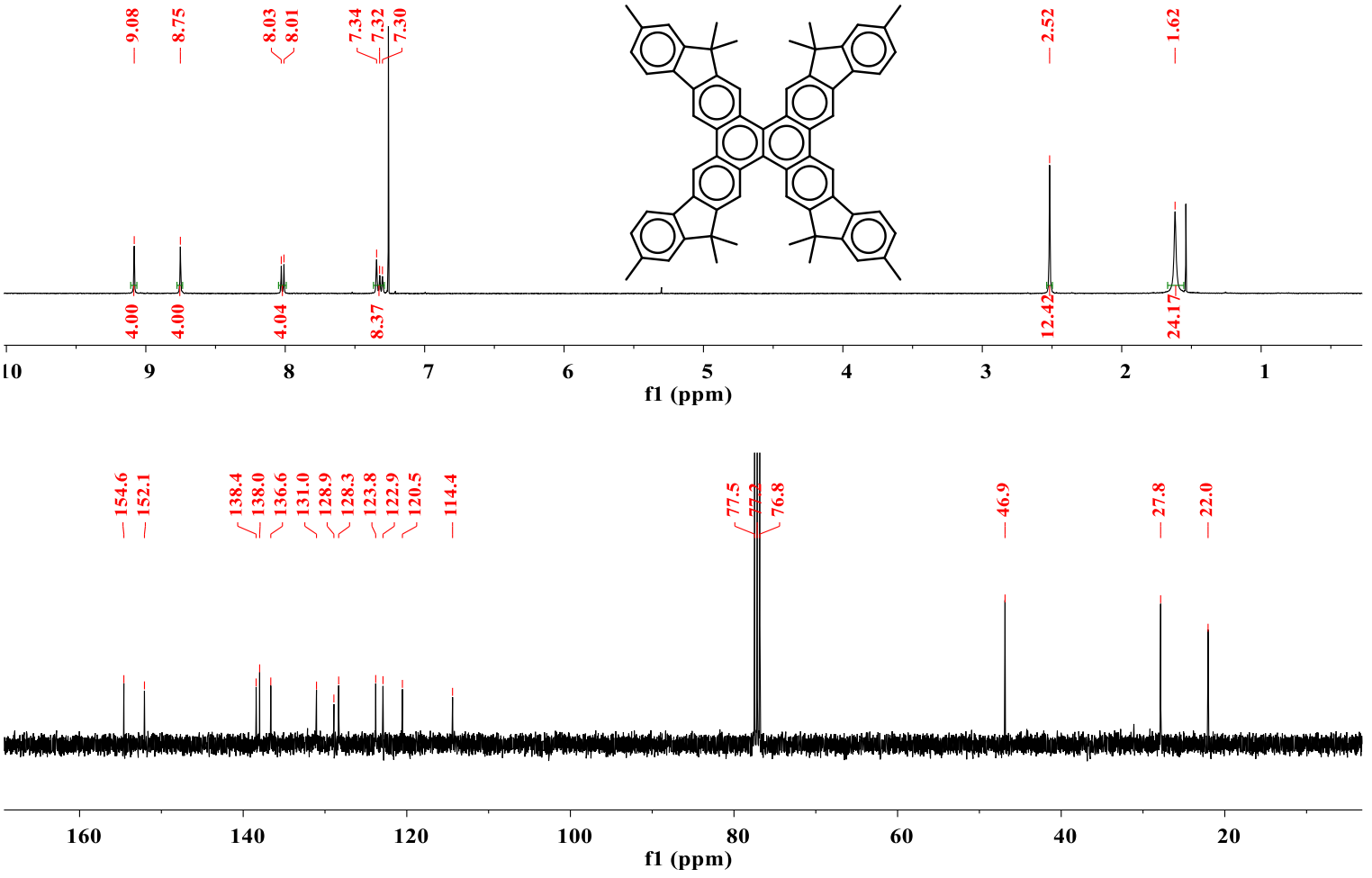
^{1}H and ^{13}C NMR spectra of ***m*-H** ($CDCl_3$, 20 °C)



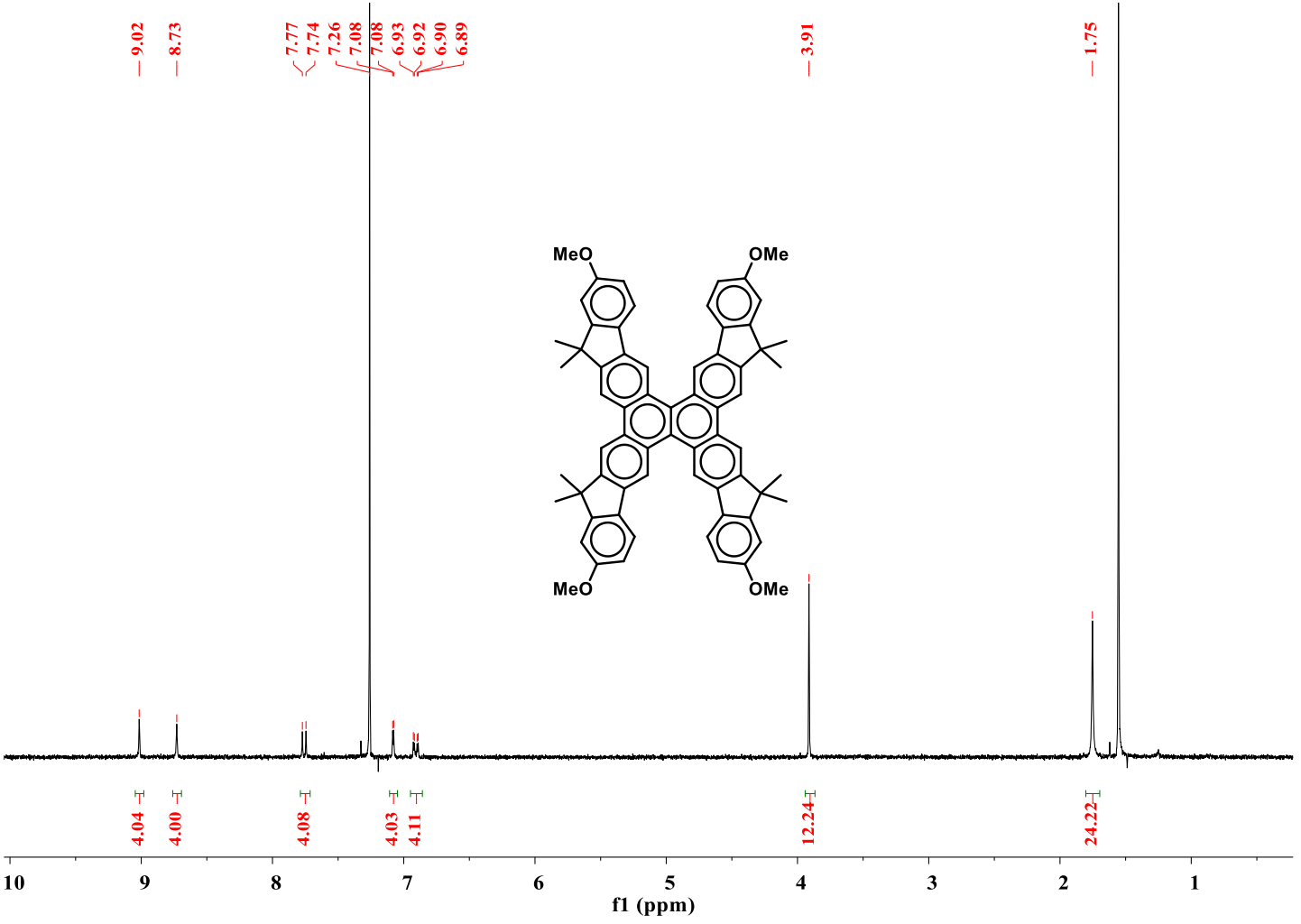
^{1}H and ^{13}C NMR spectra of ***p*-Me** ($CDCl_3$, 20 °C)



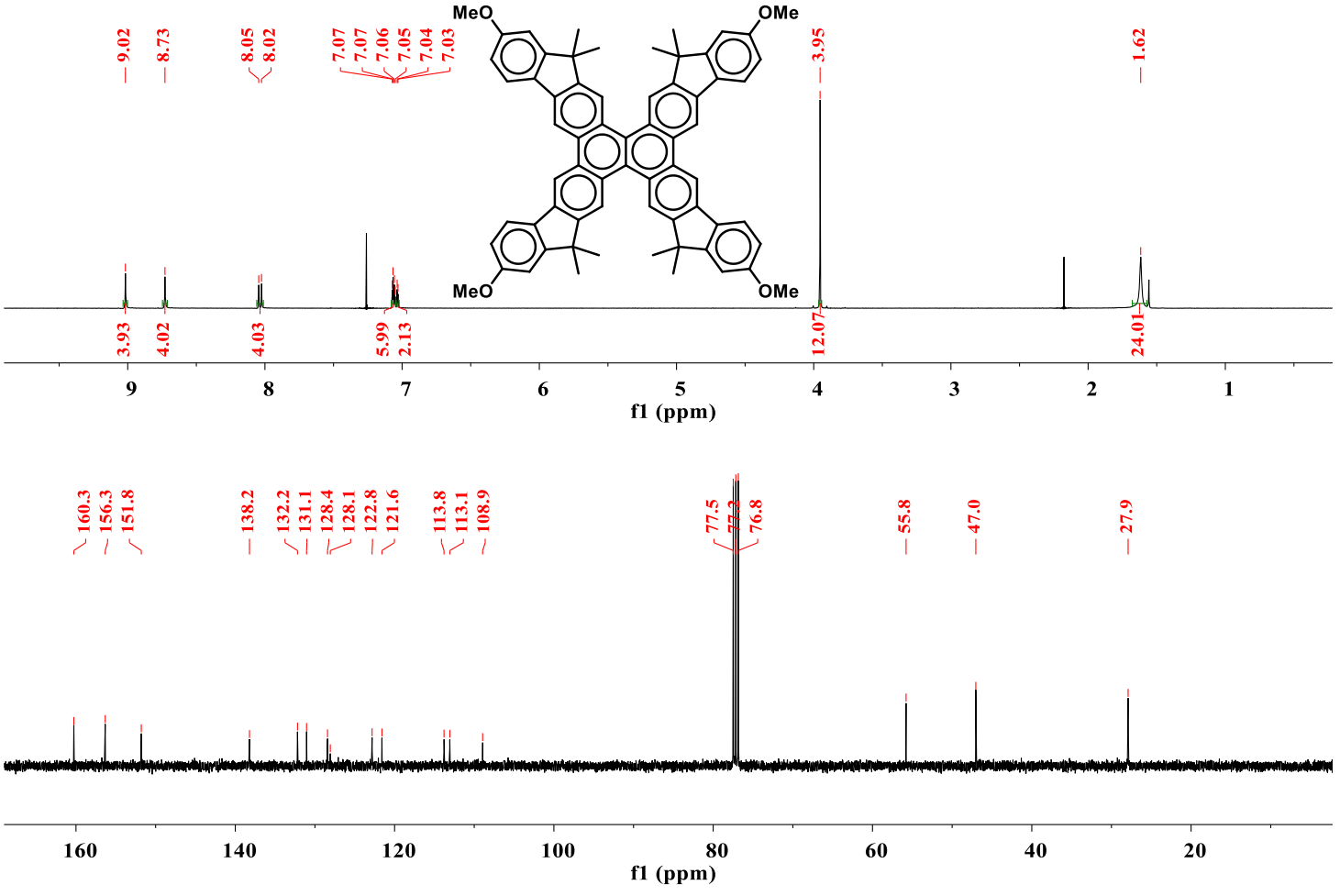
^{1}H and ^{13}C NMR spectra of ***m*-H** ($CDCl_3$, 20 °C)



^{1}H NMR spectrum of ***p*-OMe** ($CDCl_3$, 20 °C)



^{1}H and ^{13}C NMR spectra of ***m*-OMe** ($CDCl_3$, 20 °C)



S5. Computational details.

All density functional theory (DFT) calculations were performed using the Gaussian 16 software package.[7] The analysis of TD-DFT studies have been carried out using the GaussSum 3.0 software package.[8] The orbital contribution analysis carried out using Hirshfeld[9] method as implemented in MultiWFN.[10] This method showed the lowest basis set dependency for orbital contribution analysis.[11]
Since modification of the exact Hartree-Fock (HF) exchange term improves the accuracy of hybrid DFT methods for delocalized mixed-valence systems via healing the self-interaction error (SIE) problem,[12] we selected the MN15[13] functional which has 45% HF. In addition to the MN15 functional, we also assessed the performance of the PBE0-D3BJ,[14, 15] B3LYP-D3BJ[16], CAM-B3LYP-D3BJ[17] and ωB97XD[18] functionals. All of the calculations were carried out using the 6-31+G(d,p) basis set. In order to include bulk solvation effects, the integral equation formalism variant of the polarizable continuum model (IEF-PCM) with standard parameters for dichloromethane (CH_2Cl_2) was used.[19]

The optical gaps (E_g) were obtained by using the absorption edge wavelength ($\lambda_{a.e}$) of each spectrum according to Eq. 1.[20, 21]

$$E_g(\text{eV}) = h \times f = h \times \frac{c}{\lambda_{a.e}} \approx \frac{1240}{\lambda_{a.e}(\text{nm})} \qquad \text{(Eq. 1)}$$

For the calculation of coupling energy through the series, we employed Hückel molecular orbital (MO) theory[22] using the tight-binding Hamiltonian as described in detail in the previous work.[23] Accordingly, the coupling energy is provided by DFT calculations of the HOMO and HOMO-1 according to Eq. 2.

$$V_{12} = \frac{1}{2}[\varepsilon_{\text{HOMO}} - \varepsilon_{\text{HOMO}-1}] \qquad \text{(Eq. 2)}$$

The internal reorganization energy (λ_{reorg}) of radical cations for DBC compounds were calculated using the neutral in cation geometry (NICG) method[24, 25] with the MN15 functional by Eq. 3.

$$\lambda_{\text{reorg}} = (n^+ + c^0) - (n^0 + c^+) \qquad \text{(Eq. 3)}$$

where $n^+$is the energy of the radical cation in the optimized neutral geometry, c^0 is the neutral energy in the optimized oxidized geometry etc.

Table S2. The relative Gibbs free energies (ΔG, kcal mol^{-1}) for neutral and cation radical *meta* and *para* DBC isomers calculated at the DFT/6-31+G**+PCM(CH_2Cl_2) level.

Neutral	MN15	CAM-BLYP-D3BJ	B3LYP-D3BJ	PBE0-D3BJ	ω**B97XD**
***m*-H**	0.0	0.0	0.0	0.0	0.0
(*p*-H)	(0.8)	(0.9)	(1.2)	(0.8)	(0.8)
***m*-Me**	0.0	0.0	0.0	0.0	0.0
(*p*-Me)	(0.3)	(1.4)	(0.2)	(1.4)	(1.4)
***m*-OMe**	0.0	0.0	0.0	0.0	0.0
(*p*-OMe)	(1.1)	(1.1)	(1.3)	(1.1)	(1.4)

Cation Radical	MN15	CAM-BLYP-D3BJ	B3LYP-D3BJ	PBE0-D3BJ	ω**B97XD**
***m*-H+•**	0.0	0.0	0.0	0.0	0.0
(*p*-H)+•	(5.5)	(4.2)	(5.0)	(4.9)	(4.0)
***m*-Me+•**	0.0	0.0	0.0	0.0	0.0
(*p*-Me)+•	(7.3)	(6.7)	(5.0)	(5.0)	(5.6)
***m*-OMe+•**	0.0	0.0	0.0	0.0	0.0
(*p*-OMe)+•	(7.5)	(8.1)	(7.5)	(7.4)	(8.7)

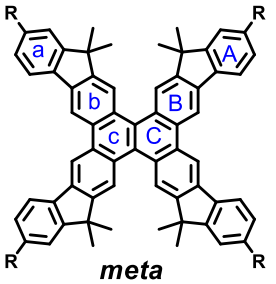
Table S3. Calculated E_g ($E_g = E_{LUMO} - E_{HOMO}$, eV) of *meta* and *para* DBC compounds at the DFT/6-31+G(d,p)+PCM(CH_2Cl_2) level of theory and corresponding R-squared (R^2) values from the correlation diagram between the calculated and experimental data.

	MN15	CAM-BLYP-D3BJ	B3LYP-D3BJ	PBE0-D3BJ	ω**B97XD**	Exp.
***m*-H**	4.43	5.43	3.21	3.50	6.51	2.84
***m*-Me**	4.41	5.40	3.18	3.47	6.49	2.83
***m*-OMe**	4.37	5.36	3.15	3.43	6.44	2.79
***p*-H**	5.00	6.01	3.71	4.03	7.11	3.30
***p*-Me**	5.00	6.01	3.71	4.03	7.12	3.25
***p*-OMe**	4.88	5.91	3.58	3.89	7.01	3.16
R^2	0.996	0.990	0.995	0.995	0.990	----

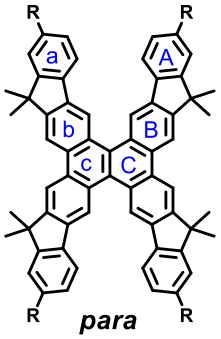
Table S4. Calculated HOMO (eV) of *meta* and *para* DBC compounds at the DFT/6-31+G(d,p)+PCM(CH_2Cl_2) level of theory and corresponding R-squared (R^2) values from the correlation diagram between the calculated and experimental data.

	MN15	CAM-BLYP-D3BJ	B3LYP-D3BJ	PBE0-D3BJ	ωB97XD	Exp.
***m*-H**	-5.98	-6.42	-5.27	-5.50	-6.99	-5.33
***m*-Me**	-5.88	-6.32	-5.17	-5.40	-6.89	-5.26
***m*-OMe**	-5.77	-6.21	-5.05	-5.27	-6.78	-5.17
***p*-H**	-6.25	-6.71	-5.52	-5.76	-7.28	-5.50
***p*-Me**	-6.18	-6.64	-5.43	-5.67	-7.21	-5.47
***p*-OMe**	-6.04	-6.49	-5.28	-5.51	-7.06	-5.39
R^2	0.970	0.988	0.967	0.967	0.990	----

Table S5. NICS values for substituted *meta* and *para* DBC isomers calculated at the MN15/6-31+G**+PCM(CH_2Cl_2) level; values in parentheses are for cation radical species.



meta



para

	***m*-H**	***m*-Met**	***m*-OMet**	***p*-H**	***p*-Met**	***p*-OMet**
A	-6.8	-6.8	-7.8	-7.0	-6.8	-7.9
	(-6.7)	(-6.5)	(-7.2)	(-7.4)	(-5.2)	(-5.6)
B	-6.8	-6.8	-6.8	-6.8	-6.8	-6.8
	(-1.7)	(-2.0)	(-2.3)	(-1.9)	(11.8)	(-5.4)
C	-1.3	-1.4	-1.4	-1.3	-1.4	-1.4
	(6.2)	(5.9)	(5.3)	(10.8)	(18.8)	(11.0)
a	-6.8	-6.8	-7.8	-7.0	-6.8	-7.9
	(-6.7)	(-6.5)	(-7.2)	(-7.4)	(-6.9)	(-7.8)
b	-6.8	-6.8	-6.8	-6.8	-6.8	-6.8
	(-1.7)	(-2.0)	(-2.3)	(-1.9)	(-3.5)	(-5.3)
c	-1.3	-1.4	-1.4	-1.3	-1.4	-1.4
	(6.2)	(5.9)	(5.3)	(10.8)	(1.7)	(0.1)

Figure S5. Comparison of reorganization energy ($1/2\lambda_{reog}$) versus coupling energy (V_{12}) of *meta* and *para* DBC compounds at the MN15/6-31+G(d,p)+PCM(CH_2Cl_2) level of theory; all values are in eV.

Compound	1/2 $\boldsymbol{\lambda_{reorg}}$	$\boldsymbol{V_{12}}$
m-H	0.102	0.288
m-Me	0.103	0.281
m-OMe	0.105	0.262
p-H	0.125	0.027
p-Me	0.128	0.045
p-OMe	0.135	0.081

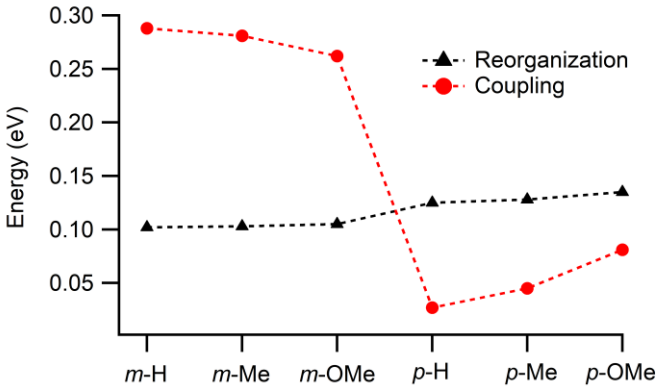


Figure S6. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-H. The calculated highest transition is 327 nm with an oscillator strength of 3.16 for which the major contribution (56%) is from H-1→LUMO.

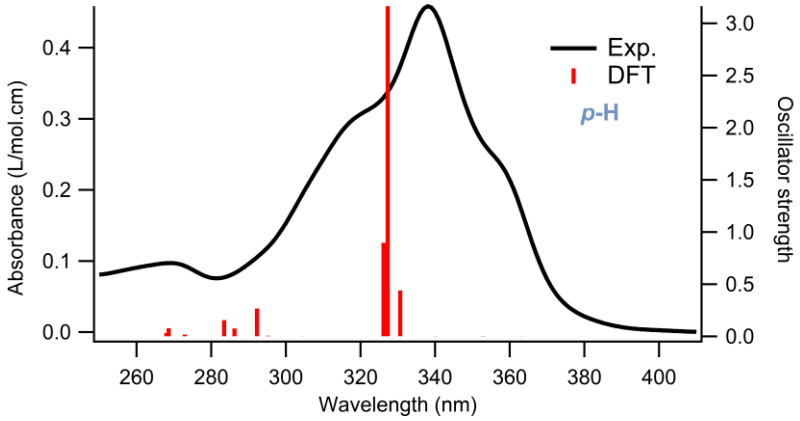


Figure S7. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-Me. The calculated highest transition is 331 nm with an oscillator strength of 3.43 for which the major contribution (51%) is from HOMO→LUMO (51%).

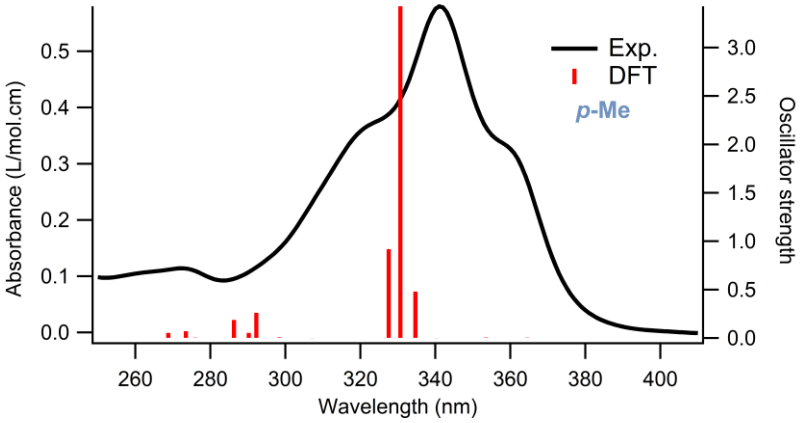


Figure S8. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-OMe. The calculated highest transition is 335 nm with an oscillator strength of 3.50 for which the major contributions are from H-1→LUMO (37%) and HOMO→L+1 (42%).

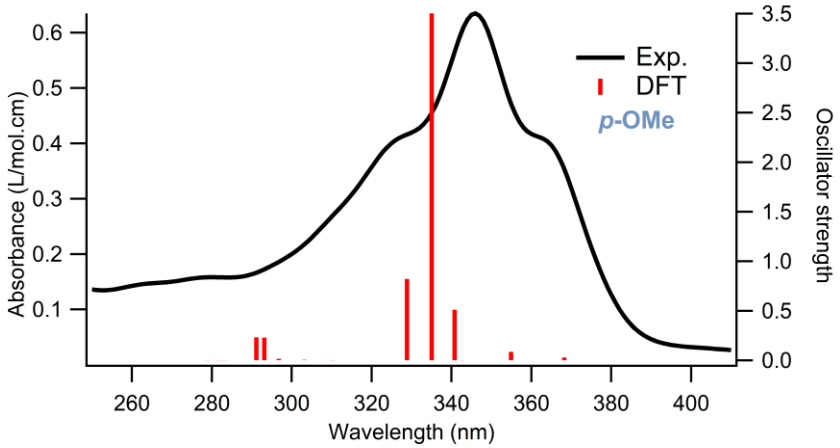


Figure S9. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-H. The calculated highest transition is 396 nm with an oscillator strength of 0.92 for which the major contribution (94%) is from HOMO→LUMO.

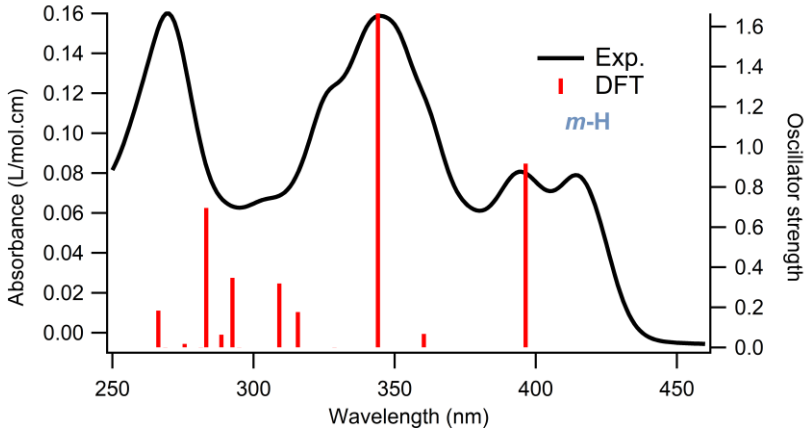


Figure S10. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-Me. The calculated highest transition is 399 nm with an oscillator strength of 1.00 for which the major contribution (94%) is from HOMO→LUMO.

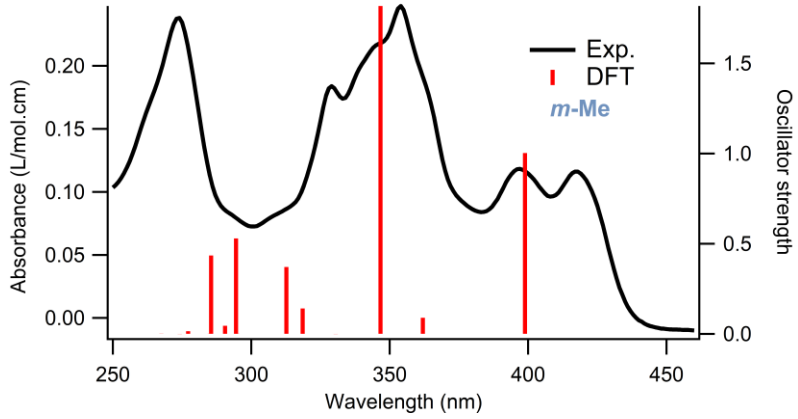


Figure S11. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-OMe. The calculated highest transition is 402 nm with an oscillator strength of 1.04 for which the major contribution (93%) is from HOMO→LUMO.

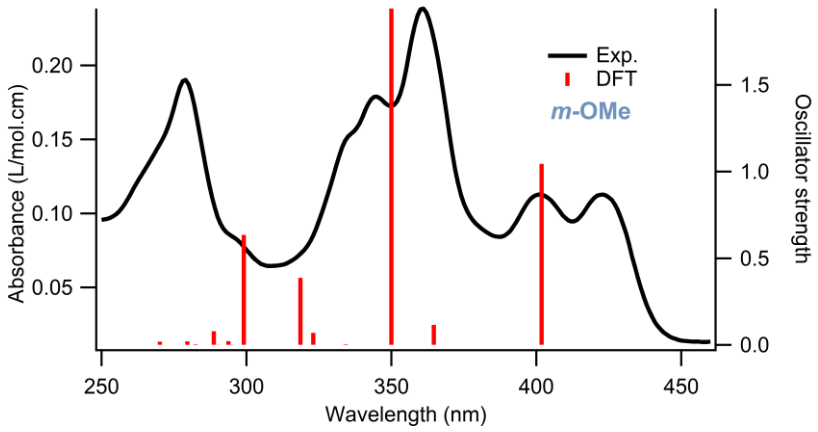


Figure S12. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-H cation radical. The calculated highest transition is 618 nm with an oscillator strength of 0.23 for which the major contribution (77%) is from. H-9(β)→LUMO(β).

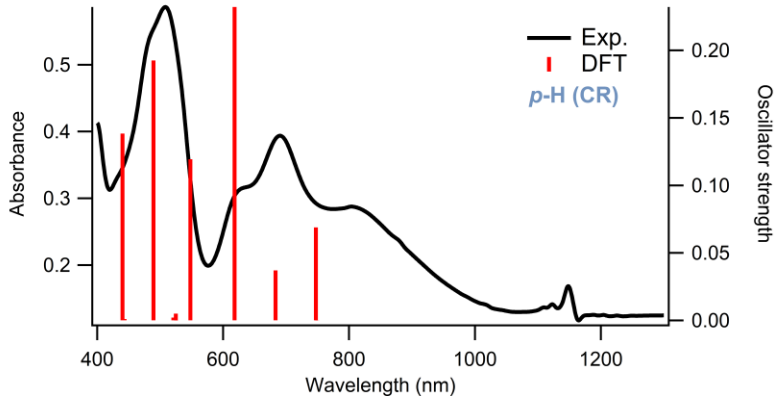


Figure S13. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-Me cation radical. The calculated highest transition is 1192 nm with an oscillator strength of 0.68 for which the major contribution (94%) is from H-2(β)→LUMO(β).

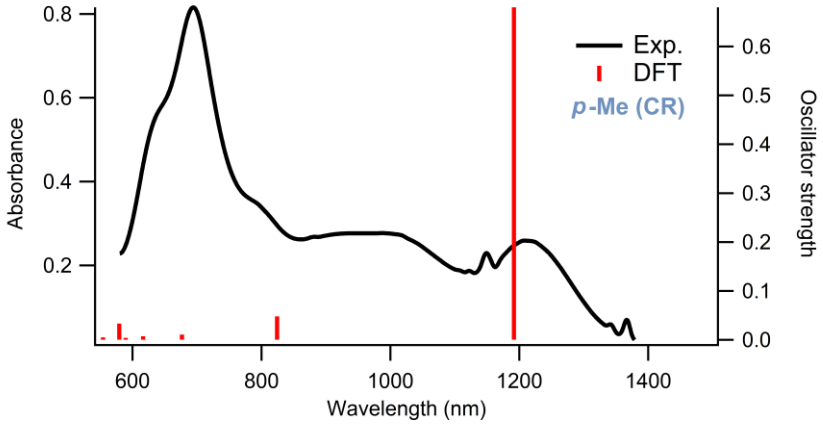


Figure S14. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *p*-OMe cation radical. The calculated highest transition is 1388 nm with an oscillator strength of 0.77 for which the major contribution (87%) is from H-2(β)→LUMO(β).

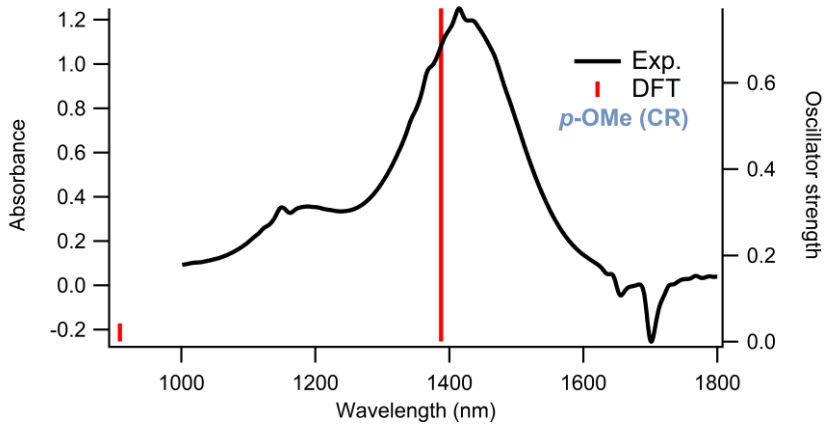


Figure S15. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-H cation radical. The calculated highest transition is 893 nm with an oscillator strength of 0.48 for which the major contribution (95%) is from H-1(β)→LUMO(β).

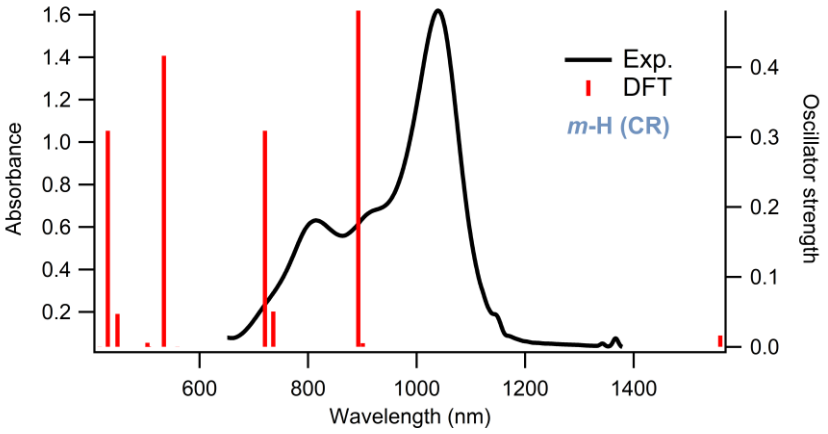


Figure S16. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-Me cation radical. The calculated highest transition is 958 nm with an oscillator strength of 0.522 for which the major contribution (95%) is from H-1(β)→LUMO(β).

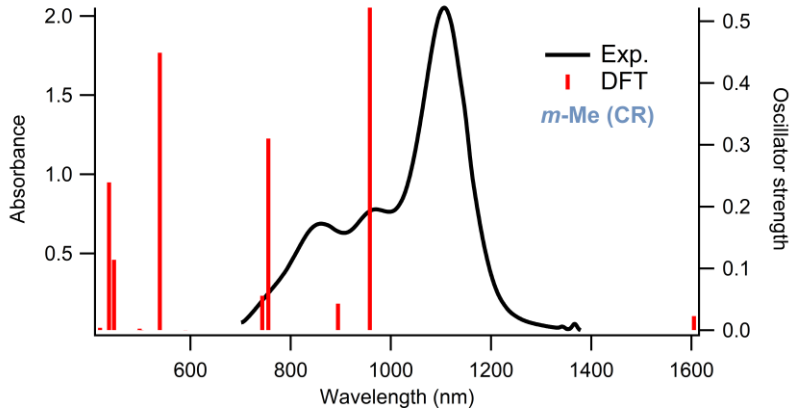


Figure S17. Experimental and simulated [MN15/6-31+G(d,p)+PCM(CH_2Cl_2)] UV-Vis spectrum of *m*-OMe cation radical. The calculated highest transition is 1075 nm with an oscillator strength of 0.56 for which the major contribution (96%) is from H-1(β)→LUMO(β).

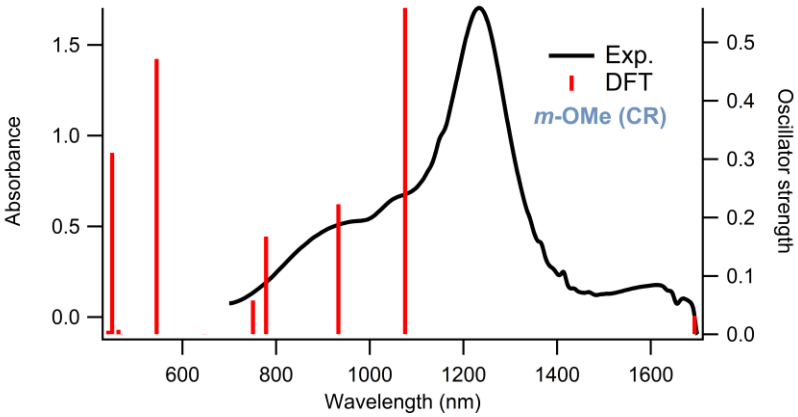
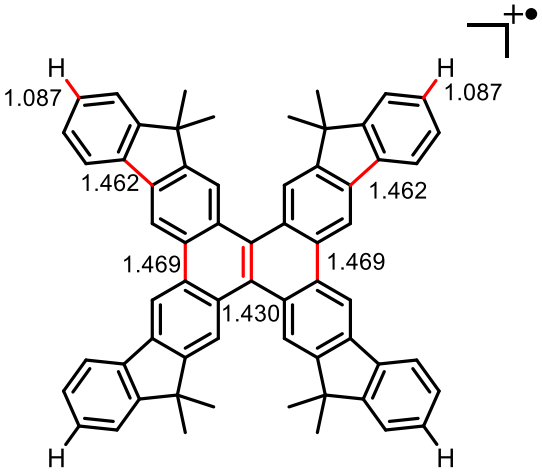
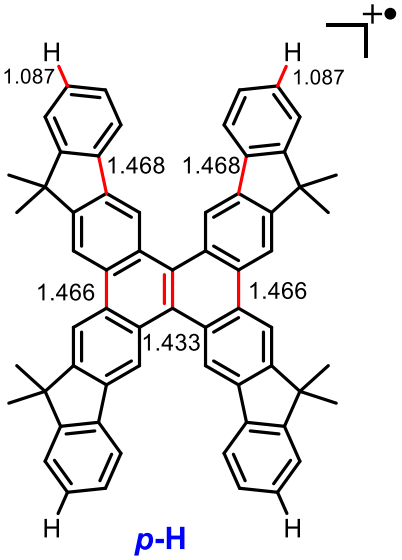


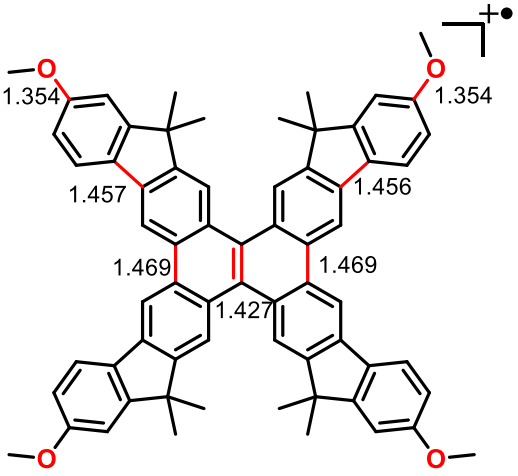
Figure S18. Key bond length values (in angstrom) of one-electron-oxidized *meta/para* H and OMe obtained at the MN15/6-31+G(d,p)+PCM(CH_2Cl_2) level. Despite symmetric bond alteration in *m*-OMe, the *para* isomer shows an asymmetric bond length alteration.



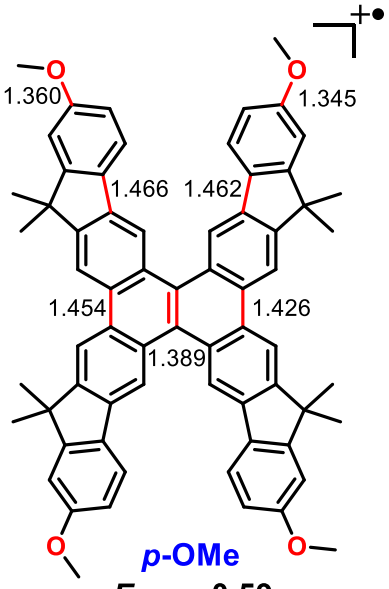
***m*-H**
E_{ox1} = 0.53



***p*-H**
E_{ox1} = 0.70



***m*-OMe**
E_{ox1} = 0.37



***p*-OMe**
E_{ox1} = 0.59

S6. Reference.

1. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, NMR Chemical Shifts of Trace Impurities: Common Laboratory Solvents, Organics, and Gases in Deuterated Solvents Relevant to the Organometallic Chemist, *Organometallics.*, 2010, **29**, 2176–2179.
2. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, 2009, **42**, 339-341.
3. G. M. Sheldrick, Crystal structure refinement with SHELXL, *Acta Cryst.*, 2015, **C71**, 3-8.
4. W. H. Parsons, R. R. Calvo, W. Cheung, Y.-K. Lee, S. Patel, J. Liu, M. A. Youngman, S. L. Dax, D. Stone, N. Qin, T. Hutchinson, M. L. Lubin, S.-P. Zhang, M. Finley, Y. Liu, M. R. Brandt, C. M. Flores and M. R. Player, Benzo[d]imidazole Transient Receptor Potential Vanilloid 1 Antagonists for the Treatment of Pain: Discovery of trans-2-(2-{2-[2-(4-Trifluoromethyl-phenyl)-vinyl]-1H-benzimidazol-5-yl}-phenyl)-propan-2-ol (Mavatrep), *J. Med. Chem.*, 2015, **58**, 3859–3874.
5. T. Akama, Y. R. Freund, P. W. Berry, D. S. Carter, E. E. Easom, K. Jarnagin, C. S. Lunde, J. J. Plattner, F. Rock, R. Stefanakis, C. Fischer, C. A. Bulman, K. C. Lim, B. M. Suzuki, N. Tricoche, A. Mansour, U. DiCosty, S. McCall, B. Carson, J. W. McCall, J. McKerrow, M. P. Hübner, S. Specht, A. Hoerauf, S. Lustigman, J. A. Sakanari and R. T. Jacobs, Macrofilaricidal Benzimidazole–Benzoxaborole Hybrids as an Approach to the Treatment of River Blindness: Part 1. Amide Linked Analogs, *ACS Infect. Dis.*, 2020, **6**, 173–179.
6. S. Kusano, S. Miyamoto, A. Matsuoka, Y. Yamada, R. Ishikawa and O. Hayashida, Benzoxaborole Catalyst for Site-Selective Modification of Polyols, *Eur. J. Org. Chem.*, 2020, 1598-1602.
7. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, F. Ogliaro, M. Bearpark, J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 16. Revision B.01. Gaussian, Inc., 2016, Wallingford CT.
8. N. M. O'Boyle, A. L. Tenderholt and K. M. Langner, cclib: A library for package-independent computational chemistry algorithms, *J. Comp. Chem.*, 2008, **29**, 839–845.
9. F. L. Hirshfeld, Bonded-atom fragments for describing molecular charge densities, *Theor. Chim. Acta.*, 1977, **44**, 129–138.
10. T. Lu and F. Chen, Multiwfn: A multifunctional wavefunction analyzer, *J. Comput. Chem.*, 2012, **33**, 580-592.
11. S. Mirzaei and H. Khosravi, Predicting the regioselectivity of nucleophilic addition to arynes using frontier molecular orbital contribution analysis, *Tetrahedron Lett.*, 2017, **58**, 3362-3365.
12. Y. Zhang and W. Yang, A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons, *J. Chem. Phys.*, 1998, **109**, 2604–2608.
13. H. S. Yu, X. He, S. L. Li and D. G. Truhlar, MN15: A Kohn–Sham global-hybrid exchange–correlation density functional with broad accuracy for multi-reference and single-reference systems and noncovalent interactions, *Chem. Sci.*, 2016, **7**, 5032–5051.
14. C. Adamo and V. Barone, Toward Reliable Density Functional Methods without Adjustable Parameters: The PBE0 Model., *J. Chem. Phys.*, 1999, **110**, 6158−6170.
15. S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, *J. Comput. Chem.*, 2006, **27**, 1787-1799.

16. A. D. Becke, Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior, *Phys. Rev. A*, 1988, **38**, 3098−3100.
17. T. Yanai, D. P. Tew and N. C. Handy, A new hybrid exchange–correlation functional using theCoulomb-attenuating method (CAM-B3LYP), *Chem. Phys. Lett.*, 2004, **393**, 51–57.
18. J.-D. Chai and M. Head-Gordon, Long-Range Corrected Hybrid Density Functionals with Damped Atom−Atom Dispersion Corrections, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615−6620.
19. E. Cancès, B. Mennucci and J. Tomasi, A New Integral Equation Formalism for the Polarizable Continuum Model: Theoretical Background and Applications to Isotropic and Anisotropic Dielectrics, *J. Chem. Phys.*, 1997, **107**, 3032−3041.
20. N. Ghobadi, Band gap determination using absorption spectrum fitting procedure, *Int. Nano. Lett.*, 2013, **3**, 2-4.
21. J. C. S. Costa, R. J. S. Taveira, C. F. R. A. C. Lima, A. Mendes and L. M. N. B. F. Santos, Optical Band Gaps of Organic Semiconductor Materials, *Opt. Matt.*, 2016, **58**, 51-60.
22. W. Kutzelnigg, What I Like About Hückel Theory, *J. Comput. Chem.*, 2007, **28**, 25-34.
23. M. M. Hossain, M. V. Ivanov, D. Wang, S. A. Reid and R. Rathore, Spreading Electron Density Thin: Increasing the Chromophore Size in Polyaromatic Wires Decreases Interchromophoric Electronic Coupling, *J. Phys. Chem. C.*, 2018, **122**, 17668-17675.
24. S. F. Nelsen, A. E. Konradsson and J. P. Telo, Pseudo-para-dinitro[2.2]paracyclophane Radical Anion, a Mixed-Valence System Poised on the Class II/Class III Borderline, *J. Am. Chem. Soc.*, 2005, **127**, 920–925.
25. A. Heckmann and C. Lambert, Organic Mixed-Valence Compounds: A Playground for Electrons and Holes, *Angew. Chem. Int. Ed.*, 2012, **51**, 326-392.

S7. Cartesian coordinates of optimized molecules at MN15/6-31+G(d,p)+PCM(CH_2Cl_2).

m-H (neutral)

Zero-point correction= 0.907239 (Hartree/Particle)
Thermal correction to Energy= 0.957150
Thermal correction to Enthalpy= 0.958095
Thermal correction to Gibbs Free Energy= 0.825118
Sum of electronic and zero-point Energies= -2387.966350
Sum of electronic and thermal Energies= -2387.916438
Sum of electronic and thermal Enthalpies= -2387.915494
Sum of electronic and thermal Free Energies= -2388.048470

C	1.32871900	1.31250400	0.30180200
C	0.56703500	2.51287400	0.23327900
C	-0.81310800	2.44565700	-0.24193000
C	-1.45115700	1.17586400	-0.31823100
C	-1.32873700	-1.31251600	0.30165800
C	-0.56701600	-2.51287000	0.23332600
C	0.81314600	-2.44567000	-0.24185000
C	1.45122800	-1.17588700	-0.31804800
C	0.69538300	0.03434700	-0.00929500
C	-0.69535900	-0.03435500	-0.00941300
C	2.63898300	1.36498800	0.84852700
H	3.19226900	0.44375000	1.01480500
C	3.18918200	2.56767000	1.23174900
C	2.44811800	3.76384100	1.11038600
C	1.14826700	3.73524500	0.63686600
H	0.56471800	4.65157100	0.61400600
C	3.27948900	4.86971000	1.60565700
C	3.02140400	6.23958000	1.69857900
H	2.06849400	6.65130500	1.37290700
C	4.01474500	7.07406500	2.21819600
H	3.83370800	8.14279200	2.29826800
C	5.24363300	6.54677100	2.63722600
H	6.00443200	7.21122800	3.03860500
C	5.49896600	5.17291400	2.54373200
H	6.45488500	4.76724400	2.87189900
C	4.51204100	4.33850700	2.02706400
C	-2.75890700	1.09997700	-0.86779700
H	-3.21600200	0.12870100	-1.04165700
C	-3.42682500	2.24403400	-1.24318200
C	-2.81061100	3.50803700	-1.11065200
C	-1.51410900	3.60654400	-0.63705300
H	-1.02540300	4.57656800	-0.60674500
C	-3.75095900	4.52855200	-1.59469300
C	-3.63569400	5.91879600	-1.67162100
H	-2.73024700	6.42326700	-1.34103800
C	-4.71067000	6.65238000	-2.18103800
H	-4.64086300	7.73495100	-2.24834700
C	-5.87949600	6.00638000	-2.60570500
H	-6.70544800	6.59366300	-2.99856600
C	-5.99178900	4.61256400	-2.52819100
H	-6.90157200	4.11404600	-2.85984500
C	-4.92319100	3.87855800	-2.02179600
C	-2.63904900	-1.36500300	0.84823800
H	-3.19242900	-0.44378900	1.01434800
C	-3.18920900	-2.56767300	1.23158400
C	-2.44807200	-3.76381600	1.11050300
C	-1.14817600	-3.73520800	0.63707200
H	-0.56452500	-4.65147800	0.61442400
C	-3.27941400	-4.86964500	1.60590300
C	-3.02123200	-6.23947900	1.69911500
H	-2.06825400	-6.65118700	1.37362200
C	-4.01456100	-7.07393600	2.21880300
H	-3.83345800	-8.14263500	2.29909000
C	-5.24352000	-6.54664500	2.63763100
H	-6.00430900	-7.21107700	3.03907100
C	-5.49893900	-5.17282200	2.54387100
H	-6.45489800	-4.76715700	2.87192200
C	-4.51203600	-4.33844500	2.02710900
C	2.75900200	-1.10003100	-0.86753300
H	3.21621600	-0.12879200	-1.04129000
C	3.42686400	-2.24411400	-1.24298300
C	2.81058400	-3.50809100	-1.11063700
C	1.51405400	-3.60656100	-0.63707400
H	1.02523500	-4.57653600	-0.60691200
C	3.75083700	-4.52858800	-1.59489700
C	3.63545700	-5.91880800	-1.67208700
H	2.72998400	-6.42326500	-1.34155800
C	4.71034800	-6.65237800	-2.18170700
H	4.64045400	-7.73493200	-2.24922300
C	5.87919900	-6.00638300	-2.60631900
H	6.70507800	-6.59365100	-2.99935700
C	5.99160900	-4.61259300	-2.52852900
H	6.90141200	-4.11408700	-2.86014700
C	4.92310800	-3.87860000	-2.02191300
C	4.55806700	2.83004700	1.83735900
C	5.68249700	2.41544900	0.87470200
H	5.65519000	1.33102800	0.70628000
H	6.66181600	2.66982800	1.29832500
H	5.57847200	2.92066200	-0.09192100
C	4.72633000	2.10233900	3.18112800
H	3.93349200	2.38543600	3.88214400
H	5.69517100	2.35263900	3.63035700
H	4.68919700	1.01612700	3.03289600
C	-4.81414900	2.37139500	-1.84975600
C	-4.90309600	1.64766000	-3.20332500
H	-4.13899700	2.01693900	-3.89613300
H	-5.88983700	1.80731100	-3.65493200
H	-4.75940700	0.56861200	-3.06822100
C	-5.89207700	1.83060600	-0.89690800
H	-5.75154800	0.75321400	-0.74039400
H	-6.89116700	1.98548700	-1.32234400
H	-5.84497100	2.33292400	0.07565400
C	-4.55813500	-2.83002700	1.83712600
C	-4.72643000	-2.10216000	3.18081800
H	-3.93360000	-2.38518000	3.88187700
H	-5.69528000	-2.35242000	3.63005600
H	-4.68929400	-1.01596300	3.03246500
C	-5.68255600	-2.41557500	0.87442000

H	-5.65531300	-1.33116500	0.70592800
H	-6.66187000	-2.66997500	1.29804000
H	-5.57849000	-2.92084700	-0.09216400
C	4.81423500	-2.37147200	-1.84945200
C	4.90355600	-1.64725200	-3.20271100
H	4.13952800	-2.01612800	-3.89581000
H	5.89035300	-1.80689400	-3.65419700
H	4.76003400	-0.56822800	-3.06723400
C	5.89208900	-1.83124000	-0.89617100
H	5.75169800	-0.75389200	-0.73922400
H	6.89123400	-1.98610800	-1.32148600
H	5.84471300	-2.33397000	0.07616500

m-Me (neutral)

Zero-point correction= 1.015596 (Hartree/Particle)
Thermal correction to Energy= 1.073403
Thermal correction to Enthalpy= 1.074347
Thermal correction to Gibbs Free Energy= 0.921231
Sum of electronic and zero-point Energies= -2544.925225
Sum of electronic and thermal Energies= -2544.867418
Sum of electronic and thermal Enthalpies= -2544.866474
Sum of electronic and thermal Free Energies= -2545.019590

C	1.59280300	-1.07262200	0.27285800
C	2.61075700	-0.07970100	0.21634800
C	2.25920600	1.26426500	-0.23682100
C	0.88504300	1.62886500	-0.30056300
C	-1.52426100	0.98496400	0.30895900
C	-2.54228800	-0.00550600	0.21981900
C	-2.19113300	-1.33327000	-0.27911200
C	-0.81701700	-1.69548700	-0.35629900
C	0.21112800	-0.71193600	-0.03022800
C	-0.14284600	0.63477300	-0.00727900
C	1.91541500	-2.35183800	0.80073800
H	1.12780700	-3.08487100	0.95884600
C	3.20611600	-2.64809800	1.17697700
C	4.22531300	-1.67582600	1.06621600
C	3.92802800	-0.40301400	0.61164600
H	4.70425600	0.35735100	0.59785700
C	5.47818700	-2.27122500	1.54914300
C	6.76908500	-1.74841800	1.65477400
H	6.98546600	-0.72646800	1.35030300
C	7.78307800	-2.56183900	2.16462700
H	8.79313100	-2.16636800	2.25630700
C	7.53435000	-3.88512900	2.56847800
C	6.22975600	-4.39317700	2.46115700
H	6.02168000	-5.41512900	2.78067400
C	5.21298400	-3.59104900	1.95379000
C	0.54058100	2.90345000	-0.82581200
H	-0.50461300	3.15536700	-0.98916100
C	1.52129200	3.79734100	-1.19227300
C	2.88607300	3.45074500	-1.07536600
C	3.24990100	2.19433200	-0.62346600
H	4.29948700	1.91340700	-0.60486200
C	3.68743600	4.58680900	-1.54946800
C	5.06929500	4.76622800	-1.64714600
H	5.75820800	3.98133800	-1.34177700
C	5.55532500	5.97475800	-2.14988300
H	6.62985300	6.12697200	-2.23528400
C	4.69045000	7.00681400	-2.55410600
C	3.30423800	6.80805700	-2.45445700
H	2.62242700	7.59730900	-2.77382600
C	2.81024100	5.60769300	-1.95435300
C	-1.84645000	2.24559500	0.88004100
H	-1.05881700	2.97303700	1.06215500
C	-3.13682300	2.52885200	1.26718500
C	-4.15614000	1.56081400	1.12475400
C	-3.85918200	0.30407200	0.62725300
H	-4.63532800	-0.45553100	0.58854300
C	-5.40849500	2.13959300	1.62888700
C	-6.69940400	1.61356300	1.71862700
H	-6.91622700	0.60245100	1.38019600
C	-7.71260300	2.40934700	2.25679000
H	-8.72257700	2.01104400	2.33645700
C	-7.46330200	3.71853600	2.70440400
C	-6.15898800	4.22983900	2.61236000
H	-5.95033600	5.24052100	2.96552800
C	-5.14282800	3.44501700	2.07720900
C	-0.47300400	-2.95141600	-0.92501600
H	0.57200300	-3.19764300	-1.09796600
C	-1.45400000	-3.83231500	-1.32091800
C	-2.81867800	-3.48992800	-1.19120300
C	-3.18213000	-2.24958700	-0.69664100
H	-4.23165500	-1.96924900	-0.66825200
C	-3.62037200	-4.60896600	-1.70364000
C	-5.00242500	-4.78516000	-1.80589200
H	-5.69108400	-4.01170000	-1.47207600
C	-5.48881900	-5.97533900	-2.35004900
C	-4.62416700	-6.99239600	-2.79146400
C	-3.23798700	-6.79719100	-2.68608100
H	-2.55640000	-7.57465500	-3.03353300
C	-2.74355100	-5.61494300	-2.14466100
C	3.74480800	-3.94189200	1.76525900
C	3.56366200	-5.11566200	0.78962700
H	2.49560600	-5.30798900	0.62414200
H	4.01455100	-6.02763000	1.19979000
H	4.03218600	-4.89897100	-0.17682700
C	3.07218100	-4.27040300	3.10800500
H	3.19011700	-3.44418100	3.81772700
H	3.51758800	-5.17236900	3.54546400
H	2.00067400	-4.45441600	2.96204500
C	1.35820800	5.19211600	-1.77363100
C	0.61461900	5.15748900	-3.11854300
H	1.12448000	4.50038800	-3.83162900
H	0.56125400	6.16510400	-3.54880600
H	-0.40979100	4.79137300	-2.97775100
C	0.62215200	6.12098800	-0.79485000
H	-0.40397400	5.76499200	-0.63520700
H	0.57084100	7.13918200	-1.19964800
H	1.13338000	6.15573600	0.17362300
C	-3.67488200	3.80202100	1.89926500
C	-3.00123800	4.08486000	3.25186200

H	-3.11872100	3.23508300	3.93327600
H	-3.44645400	4.97145200	3.71985200
H	-1.92984700	4.27375900	3.11149900
C	-3.49452100	5.00822200	0.96389900
H	-2.42660500	5.20531200	0.80317300
H	-3.94403900	5.90595500	1.40581300
H	-3.96484500	4.82495700	-0.00857700
C	-1.29135900	-5.20618300	-1.95018500
C	-0.54802000	-5.12507700	-3.29324400
H	-1.05728200	-4.44258300	-3.98251100
H	-0.49602200	-6.11687700	-3.75897400
H	0.47689000	-4.76539400	-3.13991200
C	-0.55538800	-6.16852700	-1.00416900
H	0.47070800	-5.81827300	-0.83214600
H	-0.50402100	-7.17215300	-1.44386500
H	-1.06675200	-6.23678300	-0.03754600
C	8.65678800	-4.75121200	3.08454900
H	8.28237500	-5.51955000	3.76821400
H	9.16643400	-5.26459900	2.25987300
H	9.40776800	-4.15521800	3.61271000
C	5.24575400	8.31427100	-3.06252800
H	4.53314700	8.81687100	-3.72388700
H	5.46277800	8.99721300	-2.23195400
H	6.17966000	8.16218200	-3.61294000
C	-8.58539000	4.56617300	3.25094600
H	-8.20718000	5.32791400	3.93980700
H	-9.11329600	5.08627000	2.44213000
H	-9.32220400	3.95535800	3.78223000
H	-6.56341400	-6.12478600	-2.43937100
C	-5.18055100	-8.28059600	-3.34580700
H	-4.45916000	-8.77190300	-4.00604300
H	-5.42088000	-8.98328800	-2.53848500
H	-6.10169500	-8.10509200	-3.91067800

m-OMe (neutral)

Zero-point correction= 1.037528 (Hartree/Particle)
Thermal correction to Energy= 1.098157
Thermal correction to Enthalpy= 1.099101
Thermal correction to Gibbs Free Energy= 0.942084
Sum of electronic and zero-point Energies= -2845.477199
Sum of electronic and thermal Energies= -2845.416570
Sum of electronic and thermal Enthalpies= -2845.415626
Sum of electronic and thermal Free Energies= -2845.572644

O	6.90970100	-6.59535100	3.21694400
O	6.90010800	6.60510300	-3.21734000
O	-7.20142400	6.58218900	2.98421600
O	-7.19201900	-6.59231700	-2.98446500
C	1.18014100	-1.38652300	0.32545700
C	2.41657100	-0.68667300	0.24510600
C	2.41559200	0.69004400	-0.24516000
C	1.17817500	1.38816700	-0.32537500
C	-1.31395900	1.39397700	0.29067200
C	-2.55048500	0.69271300	0.22697600
C	-2.54949800	-0.69627300	-0.22714400
C	-1.31199400	-1.39585500	-0.29061400
C	-0.06645700	-0.69642100	0.00833100
C	-0.06743100	0.69630100	-0.00824100
C	1.17090800	-2.69094300	0.88959100
H	0.22394800	-3.19533900	1.06694200
C	2.34574900	-3.29529500	1.27576300
C	3.57866800	-2.61783700	1.14038800
C	3.61079900	-1.32355900	0.65119500
H	4.55433100	-0.78550400	0.61770900
C	2.53872300	-4.66737900	1.90156000
C	2.05892000	-5.78409800	0.96118700
H	0.97659100	-5.70091000	0.79830300
H	2.26306800	-6.76828100	1.40049900
H	2.56285800	-5.72377900	-0.00982000
C	1.81374400	-4.77447200	3.25286800
H	2.14367300	-3.98592100	3.93809600
H	2.01617500	-5.74743700	3.71707200
H	0.73004600	-4.68193500	3.11089300
C	1.16708600	2.69261600	-0.88940000
H	0.21942300	3.19571000	-1.06668500
C	2.34105500	3.29863500	-1.27560400
C	3.57492600	2.62288500	-1.14041600
C	3.60889400	1.32860900	-0.65131900
H	4.55316900	0.79185100	-0.61795200
C	2.53204100	4.67106000	-1.90125400
C	2.05100000	5.78694400	-0.96050800
H	0.96881800	5.70229600	-0.79739400
H	2.25377000	6.77149900	-1.39962400
H	2.55524300	5.72704000	0.01036600
C	1.80658800	4.77748000	-3.25235100
H	2.13728500	3.98943000	-3.93778400
H	2.00772200	5.75075500	-3.71647200
H	0.72303600	4.68362700	-3.11011300
C	-1.30469100	2.71286600	0.82088900
H	-0.35765500	3.22118000	0.98640800
C	-2.47975500	3.32731600	1.18861100
C	-3.71318000	2.64759100	1.06830600
C	-3.74548400	1.34093400	0.61376600
H	-4.68941100	0.80308000	0.59198100
C	-2.67630200	4.71478600	1.77697700
C	-2.18785700	5.80673600	0.81239500
H	-1.10472700	5.71718100	0.65879900
H	-2.39167900	6.80240900	1.22539700
H	-2.68559700	5.72336800	-0.16007800
C	-1.96165200	4.85494200	3.13101400
H	-2.29529100	4.08163000	3.83165800
H	-2.16939500	5.83785800	3.57160300
H	-0.87672700	4.76168000	2.99941000
C	-1.30087800	-2.71479400	-0.82067000
H	-0.35315200	-3.22188300	-0.98597700
C	-2.47506900	-3.33087100	-1.18847500
C	-3.70942600	-2.65278600	-1.06847700
C	-3.74355100	-1.34612100	-0.61409200
H	-4.68819300	-0.80951500	-0.59252800
C	-2.66965800	-4.71874600	-1.77655700
C	-1.95442400	-4.85848900	-3.13031800
H	-2.28892000	-4.08593900	-3.83139400

H	-2.16067100	-5.84188200	-3.57054800
H	-0.86966400	-4.76368400	-2.99844600
C	-2.18014200	-5.80976100	-0.81145900
H	-1.09718600	-5.71872600	-0.65750500
H	-2.38251800	-6.80583100	-1.22421500
H	-2.67834100	-5.72672900	0.16080900
C	4.04889900	-4.69942500	2.08227800
C	4.82073000	-5.72371400	2.60556300
H	4.38499100	-6.65913600	2.95235000
C	6.21273700	-5.54909300	2.69275900
C	6.81118000	-4.35668500	2.25671000
H	7.88540300	-4.22006000	2.32278900
C	6.02077000	-3.32919500	1.72899500
H	6.49335200	-2.40908800	1.39201700
C	4.64091900	-3.49902000	1.64059100
C	8.31739300	-6.47716100	3.33461300
H	8.59036100	-5.64088100	3.98995600
H	8.78600100	-6.33784800	2.35258300
H	8.66983300	-7.41053900	3.77395000
C	4.04213900	4.70517600	-2.08225400
C	4.81245900	5.73055000	-2.60562800
H	4.37536500	6.66536900	-2.95234600
C	6.20469400	5.55786600	-2.69304500
C	6.80487000	4.36630400	-2.25706800
H	7.87927300	4.23118600	-2.32329700
C	6.01597300	3.33770500	-1.72924700
H	6.48990200	2.41826400	-1.39234000
C	4.63589300	3.50558200	-1.64067600
C	8.30794000	6.48887800	-3.33528700
H	8.65898400	7.42275500	-3.77468100
H	8.58195000	5.65299100	-3.99069600
H	8.77692800	6.35021100	-2.35334700
C	-4.18761700	4.75142000	1.94671500
C	-4.95610900	5.80511300	2.43947000
H	-4.48116100	6.73315100	2.74794200
C	-6.34471800	5.62984000	2.52232900
C	-6.93943100	4.42003700	2.11783300
H	-8.01900800	4.32837900	2.19974000
C	-6.16237200	3.37700500	1.62715900
H	-6.63458500	2.44779800	1.31594900
C	-4.77484000	3.54477700	1.53987200
C	-6.66096100	7.82284900	3.40560900
H	-7.50369800	8.43269500	3.73146500
H	-6.14314500	8.32844200	2.58111400
H	-5.96518800	7.68671200	4.24283100
C	-4.18088200	-4.75737500	-1.94665600
C	-4.94787300	-5.81216700	-2.43937200
H	-4.47162700	-6.73962500	-2.74758800
C	-6.33669200	-5.63874100	-2.52257800
C	-6.93309800	-4.42966200	-2.11842100
H	-8.01277700	-4.33945000	-2.20057300
C	-6.15752800	-3.38553100	-1.62772500
H	-6.63104700	-2.45690800	-1.31675500
C	-4.76979300	-3.55144800	-1.54012700
C	-6.64972800	-7.83216900	-3.40588000
H	-5.95395100	-7.69496500	-4.24292300
H	-7.49154400	-8.44314700	-3.73199600
H	-6.13140500	-8.33713800	-2.58132100

p-H (neutral)

Zero-point correction= 0.907320 (Hartree/Particle)
Thermal correction to Energy= 0.957297
Thermal correction to Enthalpy= 0.958241
Thermal correction to Gibbs Free Energy= 0.824543
Sum of electronic and zero-point Energies= -2387.964383
Sum of electronic and thermal Energies= -2387.914406
Sum of electronic and thermal Enthalpies= -2387.913462
Sum of electronic and thermal Free Energies= -2388.047160

C	0.69517700	0.00000000	0.00000100
C	-0.69519000	0.00000000	0.00000100
C	-1.39197500	-1.24736500	0.31058200
C	-0.68887900	-2.48270100	0.23797000
C	0.68886600	-2.48269800	-0.23800000
C	1.39196200	-1.24736000	-0.31059500
C	1.33097500	-3.67790600	-0.64448600
H	0.79096000	-4.62180200	-0.61810200
C	2.62260000	-3.64809100	-1.12293900
C	3.30377700	-2.41664300	-1.24556900
C	2.69895300	-1.23480900	-0.85833400
H	3.20558300	-0.28927000	-1.02728100
C	-1.33099000	-3.67791300	0.64444000
H	-0.79097800	-4.62181000	0.61803900
C	-2.62261000	-3.64810000	1.12290300
C	-3.30379400	-2.41665500	1.24554500
C	-2.69897000	-1.23481800	0.85832000
H	-3.20559700	-0.28927800	1.02726500
C	4.73484000	-4.06273100	-2.06573500
C	5.89524700	-4.59323700	-2.62212700
H	5.98962900	-5.66397100	-2.79762400
C	6.94367200	-3.72683500	-2.95616000
H	7.85578400	-4.12599800	-3.39226000
C	6.82811300	-2.34812800	-2.73358500
H	7.65167200	-1.69032700	-2.99892500
C	5.66527700	-1.81178400	-2.17368200
H	5.57809000	-0.74106400	-2.00122200
C	4.62115300	-2.67881500	-1.84225900
C	-4.73484400	-4.06275300	2.06570800
C	-5.89525300	-4.59326400	2.62209400
H	-5.98963500	-5.66399900	2.79758800
C	-6.94368900	-3.72686600	2.95610700
H	-7.85580200	-4.12604100	3.39219300
C	-6.82813700	-2.34815800	2.73354300
H	-7.65170300	-1.69036200	2.99887300
C	-5.66529500	-1.81181100	2.17364800
H	-5.57810700	-0.74109000	2.00119100
C	-4.62116800	-2.67883700	1.84223300
C	3.47689600	-4.79856400	-1.62957800
C	-3.47688600	-4.79857500	1.62957300
C	3.77684800	-5.80812900	-0.50941800
H	2.84863700	-6.28223000	-0.16739400
H	4.25201700	-5.31555200	0.34607800
H	4.44799300	-6.59460200	-0.87572000

C	2.80869700	-5.51577100	-2.81364700
H	2.58539800	-4.81201700	-3.62301200
H	1.87171600	-5.98781700	-2.49363600
H	3.46883800	-6.29949900	-3.20488300
C	-2.80866400	-5.51569400	2.81368900
H	-2.58536000	-4.81187700	3.62299800
H	-1.87168000	-5.98775500	2.49370300
H	-3.46879500	-6.29939700	3.20498900
C	-3.77680600	-5.80821400	0.50947700
H	-2.84859600	-6.28236600	0.16752300
H	-4.25193400	-5.31569700	-0.34607500
H	-4.44798100	-6.59464500	0.87581800
C	-1.39197400	1.24736700	-0.31058000
C	-0.68887600	2.48270100	-0.23797000
C	0.68886800	2.48269700	0.23800000
C	1.39196300	1.24735800	0.31059600
C	1.33097800	3.67790500	0.64448600
H	0.79096400	4.62180100	0.61810100
C	2.62260400	3.64808900	1.12293900
C	3.30378000	2.41664000	1.24557000
C	2.69895500	1.23480700	0.85833500
H	3.20558400	0.28926700	1.02728300
C	-1.33098600	3.67791400	-0.64444100
H	-0.79097200	4.62181000	-0.61804000
C	-2.62260500	3.64810200	-1.12290400
C	-3.30379100	2.41665800	-1.24554300
C	-2.69896900	1.23482100	-0.85831700
H	-3.20559800	0.28928100	-1.02726100
C	4.73484400	4.06272600	2.06573600
C	5.89525200	4.59323100	2.62212800
H	5.98963400	5.66396600	2.79762500
C	6.94367500	3.72682800	2.95616200
H	7.85578700	4.12599100	3.39226300
C	6.82811400	2.34812100	2.73358800
H	7.65167300	1.69031900	2.99892800
C	5.66527800	1.81177900	2.17368400
H	5.57809000	0.74105900	2.00122400
C	4.62115600	2.67881100	1.84226000
C	-4.73483900	4.06275700	-2.06570900
C	-5.89524700	4.59326900	-2.62209500
H	-5.98962800	5.66400400	-2.79759100
C	-6.94368500	3.72687200	-2.95610600
H	-7.85579700	4.12604800	-3.39219400
C	-6.82813500	2.34816500	-2.73354000
H	-7.65170200	1.69036900	-2.99886900
C	-5.66529400	1.81181600	-2.17364500
H	-5.57810800	0.74109600	-2.00118600
C	-4.62116500	2.67884100	-1.84223100
C	3.47690100	4.79856100	1.62957700
C	-3.47688000	4.79857800	-1.62957500
C	3.77685700	5.80812200	0.50941300
H	2.84864700	6.28222200	0.16738400
H	4.25202900	5.31554300	-0.34607900
H	4.44800100	6.59459700	0.87571500
C	2.80870300	5.51577400	2.81364200
H	2.58540500	4.81202300	3.62301100
H	1.87172100	5.98781700	2.49363000
H	3.46884400	6.29950300	3.20487400
C	-2.80865600	5.51569400	-2.81369300
H	-2.58535400	4.81187400	-3.62300100
H	-1.87167100	5.98775300	-2.49370800
H	-3.46878700	6.29939700	-3.20499400
C	-3.77679800	5.80822000	-0.50948200
H	-2.84858700	6.28237100	-0.16752900
H	-4.25192600	5.31570500	0.34607200
H	-4.44797100	6.59465200	-0.87582400

p-Me (neutral)

Zero-point correction= 1.015576 (Hartree/Particle)
Thermal correction to Energy= 1.073536
Thermal correction to Enthalpy= 1.074480
Thermal correction to Gibbs Free Energy= 0.919489
Sum of electronic and zero-point Energies= -2544.923167
Sum of electronic and thermal Energies= -2544.865207
Sum of electronic and thermal Enthalpies= -2544.864263
Sum of electronic and thermal Free Energies= -2545.019253

C	-0.69535500	-0.00002000	0.00003800
C	0.69533800	-0.00004800	0.00002300
C	1.39217700	1.24733000	0.31068900
C	0.68880400	2.48237000	0.23796800
C	-0.68870000	2.48239400	-0.23796600
C	-1.39214200	1.24738700	-0.31063300
C	-1.33127100	3.67771000	-0.64465200
H	-0.79117500	4.62165300	-0.61836400
C	-2.62272800	3.64809500	-1.12291500
C	-3.30505900	2.41667600	-1.24518500
C	-2.69964300	1.23509700	-0.85794300
H	-3.20651500	0.28956400	-1.02622200
C	1.33144600	3.67766900	0.64459700
H	0.79140700	4.62164200	0.61825600
C	2.62289700	3.64799600	1.12287500
C	3.30513600	2.41653400	1.24525600
C	2.69965900	1.23497800	0.85804400
H	3.20645700	0.28941500	1.02637900
C	-4.73634000	4.06369700	-2.06378400
C	-5.89396200	4.59619800	-2.62144300
H	-5.98086000	5.66886500	-2.79960800
C	-6.96015700	3.74859900	-2.96323100
C	-6.82859500	2.36738800	-2.73867400
H	-7.65232500	1.71040400	-3.01215700
C	-5.67096900	1.82308100	-2.17817700
H	-5.59139800	0.75013600	-2.01518300
C	-4.62209800	2.68081600	-1.83989600
C	4.73646000	4.06349900	2.06390800
C	5.89403500	4.59593200	2.62170700
H	5.98099200	5.66860000	2.79983900
C	6.96011900	3.74825900	2.96369600
C	6.82849000	2.36705800	2.73916700
H	7.65213200	1.71002400	3.01279000
C	5.67089500	1.82281200	2.17852500
H	5.59126500	0.74986700	2.01556600

C	4.62213800	2.68060800	1.84007700
C	-3.47657000	4.79888000	-1.63073300
C	3.47685300	4.79877100	1.63052700
C	-3.77313600	5.81165100	-0.51277100
H	-2.84369100	6.28498600	-0.17292200
H	-4.24803200	5.32185800	0.34451800
H	-4.44356400	6.59833800	-0.88006500
C	-2.80903200	5.51209300	-2.81749700
H	-2.58795500	4.80572400	-3.62524100
H	-1.87081400	5.98362700	-2.50025700
H	-3.46880600	6.29556200	-3.21000900
C	2.80929600	5.51261300	2.81687100
H	2.58789800	4.80663900	3.62487200
H	1.87125300	5.98425900	2.49928100
H	3.46918600	6.29608700	3.20917800
C	3.77385100	5.81103400	0.51218800
H	2.84457800	6.28445000	0.17198400
H	4.24877800	5.32076500	-0.34481200
H	4.44441500	6.59769900	0.87928400
C	1.39213800	-1.24743700	-0.31067000
C	0.68868600	-2.48243100	-0.23801000
C	-0.68878900	-2.48241300	0.23799600
C	-1.39219700	-1.24739100	0.31070800
C	-1.33136600	-3.67772000	0.64471700
H	-0.79128600	-4.62167100	0.61842700
C	-2.62280400	-3.64807200	1.12301300
C	-3.30512900	-2.41664300	1.24527700
C	-2.69970000	-1.23507300	0.85803200
H	-3.20655600	-0.28953100	1.02631000
C	1.33122400	-3.67774800	-0.64477500
H	0.79110700	-4.62167900	-0.61853000
C	2.62266400	-3.64812500	-1.12305600
C	3.30503800	-2.41671100	-1.24527300
C	2.69965000	-1.23513900	-0.85798600
H	3.20653000	-0.28960300	-1.02622100
C	-4.73640800	-4.06357300	2.06385200
C	-5.89419700	-4.59611300	2.62145700
H	-5.98114400	-5.66876400	2.79959300
C	-6.96032700	-3.74860500	2.96309000
C	-6.82876000	-2.36725800	2.73849500
H	-7.65255400	-1.71027000	3.01184900
C	-5.67118600	-1.82302200	2.17816400
H	-5.59157900	-0.75008800	2.01510700
C	-4.62217300	-2.68082500	1.83996700
C	4.73622400	-4.06361800	-2.06397600
C	5.89402000	-4.59618100	-2.62168000
H	5.98092000	-5.66882700	-2.79984900
C	6.96012000	-3.74872000	-2.96328700
C	6.82863100	-2.36733200	-2.73853100
H	7.65247100	-1.71037000	-3.01183100
C	5.67113900	-1.82311700	-2.17815000
H	5.59156300	-0.75020000	-2.01496300
C	4.62205300	-2.68093400	-1.84000500
C	-3.47667000	-4.79881400	1.63086700
C	3.47652700	-4.79887200	-1.63091100
C	-3.77325800	-5.81162600	0.51294300
H	-2.84382900	-6.28502200	0.17314000
H	-4.24811100	-5.32184700	-0.34437700
H	-4.44373400	-6.59826400	0.88025700
C	-2.80916700	-5.51199300	2.81767200
H	-2.58805200	-4.80558800	3.62537500
H	-1.87097300	-5.98359200	2.50045700
H	-3.46898000	-6.29540500	3.21023200
C	2.80899000	-5.51222600	-2.81757600
H	2.58775300	-4.80593500	-3.62534500
H	1.87085900	-5.98386700	-2.50023600
H	3.46882500	-6.29563700	-3.21010100
C	3.77326400	-5.81153900	-0.51288000
H	2.84389100	-6.28494500	-0.17294000
H	4.24816300	-5.32162200	0.34433600
H	4.44375900	-6.59818000	-0.88015600
C	-8.23632300	-4.31212200	3.53817900
H	-8.95772400	-4.53891900	2.74347100
H	-8.04809500	-5.24113200	4.08542900
H	-8.71316300	-3.60049300	4.21957800
C	-8.23585600	4.31277800	-3.53833200
H	-8.94599600	4.56706500	-2.74179500
H	-8.04325600	5.22636300	-4.10961900
H	-8.72772600	3.59057400	-4.19745600
C	8.23575200	4.31240700	3.53897500
H	8.94536200	4.56823200	2.74245700
H	8.04288200	5.22509700	4.11160500
H	8.72835000	3.58959100	4.19687900
C	8.23612200	-4.31196600	-3.53863200
H	8.96128800	-4.52982900	-2.74486100
H	8.04933100	-5.24582100	-4.07803800
H	8.70787200	-3.60387500	-4.22725700

p-OMe (neutral)

Zero-point correction= 1.037759 (Hartree/Particle)
Thermal correction to Energy= 1.098422
Thermal correction to Enthalpy= 1.099366
Thermal correction to Gibbs Free Energy= 0.941520
Sum of electronic and zero-point Energies= -2845.474696
Sum of electronic and thermal Energies= -2845.414033
Sum of electronic and thermal Enthalpies= -2845.413089
Sum of electronic and thermal Free Energies= -2845.570935

C	-0.69543600	-0.00000600	-0.00003500
C	0.69542100	0.00000600	-0.00003800
C	1.39219200	-1.24732600	-0.31095300
C	0.68872100	-2.48212900	-0.23776700
C	-0.68869100	-2.48214200	0.23773100
C	-1.39218800	-1.24734900	0.31089700
C	-1.33241200	-3.67727100	0.64388200
H	-0.79312300	-4.62169300	0.61665400
C	-2.62350600	-3.64726200	1.12262900
C	-3.30583400	-2.41564400	1.24680000
C	-2.69956700	-1.23463300	0.85881300
H	-3.20537600	-0.28855000	1.02732200
C	1.33247100	-3.67724700	-0.64390600
H	0.79320400	-4.62168200	-0.61665500

C	2.62355600	-3.64721400	-1.12266900
C	3.30586600	-2.41558400	-1.24684800
C	2.69957500	-1.23458600	-0.85886300
H	3.20536900	-0.28848700	-1.02734600
C	-4.73480800	-4.06582300	2.06894600
C	-5.88397800	-4.60430900	2.62462400
H	-5.99507500	-5.67175100	2.80750400
C	-6.94139300	-3.74343100	2.96612400
C	-6.83580100	-2.36110000	2.74715700
H	-7.65065000	-1.69499000	3.01022800
C	-5.67041700	-1.82896800	2.18336700
H	-5.59696800	-0.75631500	2.01670900
C	-4.62048900	-2.67942000	1.84468400
C	4.73485600	-4.06576000	-2.06898800
C	5.88403500	-4.60425600	-2.62460900
H	5.99516200	-5.67170700	-2.80742100
C	6.94145200	-3.74337600	-2.96612200
C	6.83585300	-2.36105500	-2.74718600
H	7.65068500	-1.69494200	-3.01030300
C	5.67046300	-1.82890800	-2.18340600
H	5.59703100	-0.75624400	-2.01680200
C	4.62052200	-2.67934100	-1.84474100
C	-3.47644600	-4.79980100	1.62932700
C	3.47646600	-4.79974000	-1.62945100
C	-3.77889900	-5.80737500	0.50833900
H	-2.85094000	-6.27926300	0.16271500
H	-4.25688200	-5.31341900	-0.34481400
H	-4.44823400	-6.59525600	0.87494100
C	-2.80696500	-5.51842500	2.81141700
H	-2.58368300	-4.81584600	3.62182000
H	-1.86965400	-5.98839200	2.48948000
H	-3.46590200	-6.30360400	3.20178600
C	2.80696500	-5.51809900	-2.81170900
H	2.58381800	-4.81535200	-3.62200400
H	1.86957500	-5.98800100	-2.48990800
H	3.46583900	-6.30328500	-3.20216800
C	3.77878300	-5.80753300	-0.50864400
H	2.85077800	-6.27946100	-0.16319900
H	4.25670500	-5.31377200	0.34465800
H	4.44811800	-6.59537400	-0.87533200
C	1.39217700	1.24734700	0.31088100
C	0.68867400	2.48213800	0.23774600
C	-0.68873900	2.48213300	-0.23775200
C	-1.39220500	1.24732800	-0.31096200
C	-1.33248600	3.67725800	-0.64387900
H	-0.79321900	4.62169200	-0.61661900
C	-2.62356700	3.64722800	-1.12265700
C	-3.30586000	2.41559300	-1.24688700
C	-2.69956700	1.23459000	-0.85891800
H	-3.20533600	0.28849300	-1.02747500
C	1.33239200	3.67725900	0.64391800
H	0.79309800	4.62167900	0.61670700
C	2.62349200	3.64725000	1.12264600
C	3.30584200	2.41563700	1.24675000
C	2.69958000	1.23463100	0.85874400
H	3.20541800	0.28854700	1.02717300
C	-4.73485800	4.06576500	-2.06901300
C	-5.88402800	4.60424800	-2.62466600
H	-5.99517500	5.67170000	-2.80746200
C	-6.94141200	3.74335000	-2.96624000
C	-6.83579600	2.36102500	-2.74731900
H	-7.65061900	1.69490600	-3.01045100
C	-5.67041400	1.82889300	-2.18351300
H	-5.59696300	0.75623000	-2.01690800
C	-4.62050200	2.67934400	-1.84480100
C	4.73480900	4.06581700	2.06891600
C	5.88399400	4.60431500	2.62455100
H	5.99507000	5.67175300	2.80745700
C	6.94144400	3.74345300	2.96598100
C	6.83587400	2.36112900	2.74697500
H	7.65074400	1.69502700	3.01000000
C	5.67047500	1.82898300	2.18322800
H	5.59704600	0.75633200	2.01655400
C	4.62051200	2.67941800	1.84461400
C	-3.47652400	4.79976100	-1.62933700
C	3.47638100	4.79977700	1.62946200
C	-3.77901700	5.80730200	-0.50833400
H	-2.85107400	6.27919700	-0.16267800
H	-4.25701200	5.31331900	0.34479800
H	-4.44835600	6.59518200	-0.87492900
C	-2.80703300	5.51842600	-2.81140000
H	-2.58372600	4.81586900	-3.62181500
H	-1.86973500	5.98840100	-2.48943500
H	-3.46597800	6.30360200	-3.20176200
C	2.80689100	5.51805400	2.81177500
H	2.58377600	4.81525800	3.62203600
H	1.86948400	5.98795400	2.49002000
H	3.46575500	6.30323400	3.20226100
C	3.77863600	5.80763900	0.50869800
H	2.85060200	6.27954400	0.16329500
H	4.25656200	5.31393700	-0.34463600
H	4.44794500	6.59548800	0.87541400
O	-8.03950100	4.33938600	-3.50910300
O	-8.03954500	-4.33949300	3.50888500
O	8.03955500	-4.33941400	-3.50893800
O	8.03964900	4.33953300	3.50860500
C	9.13705000	3.52228500	3.87880700
H	9.54810100	2.99429100	3.00948200
H	9.89542000	4.19034300	4.28748800
H	8.84569800	2.79167900	4.64351200
C	9.13741800	-3.52226000	-3.87791500
H	9.54761700	-2.99447600	-3.00806400
H	9.89608500	-4.19035500	-4.28598000
H	8.84697600	-2.79146600	-4.64279900
C	-9.13722300	3.52221100	-3.87846500
H	-9.54753700	2.99420300	-3.00880500
H	-9.89587500	4.19032700	-4.28652200
H	-8.84657800	2.79161100	-4.64345500
C	-9.13687800	-3.52223100	3.87926000
H	-9.54805900	-2.99423600	3.00999800
H	-9.89519200	-4.19028000	4.28806000
H	-8.84539900	-2.79162600	4.64391800

m-H (cation radical)

Zero-point correction= 0.907444
(Hartree/Particle)

Thermal correction to Energy= 0.957482
Thermal correction to Enthalpy= 0.958426
Thermal correction to Gibbs Free Energy= 0.824741
Sum of electronic and zero-point Energies= -2387.768082
Sum of electronic and thermal Energies= -2387.718044
Sum of electronic and thermal Enthalpies= -2387.717099
Sum of electronic and thermal Free Energies= -2387.850785

C	1.46864700	1.12987100	0.36029700
C	0.84821800	2.41277100	0.27312500
C	-0.52261300	2.50266000	-0.24887500
C	-1.30648800	1.31228400	-0.33432200
C	-1.46856700	-1.12985800	0.36026400
C	-0.84815700	-2.41276700	0.27320800
C	0.52266800	-2.50267600	-0.24881400
C	1.30659700	-1.31233400	-0.33415600
C	0.71332500	-0.04704800	0.01499400
C	-0.71320700	0.04704800	0.01490600
C	2.77300000	1.01794700	0.91743600
H	3.20088000	0.03372100	1.09324600
C	3.45784700	2.14823700	1.29972800
C	2.85957400	3.42060500	1.16272200
C	1.56061200	3.54994900	0.67232300
H	1.10073900	4.53266800	0.62879200
C	3.80315800	4.42630200	1.64876300
C	3.69807600	5.81980300	1.71938000
H	2.79996700	6.33216000	1.38242900
C	4.77724100	6.54072200	2.23055500
H	4.72143800	7.62377200	2.29497200
C	5.93753500	5.88020800	2.66252300
H	6.76705800	6.46078500	3.05712200
C	6.03970000	4.48616400	2.59201900
H	6.94321200	3.98170700	2.92982800
C	4.96583100	3.76180800	2.08363000
C	-2.61152400	1.37061500	-0.89830200
H	-3.16451200	0.45058800	-1.07274900
C	-3.13893300	2.57918900	-1.29049300
C	-2.37924300	3.76211600	-1.15336100
C	-1.07763500	3.72208400	-0.65491000
H	-0.49338100	4.63650300	-0.61361100
C	-3.17794800	4.88106100	-1.65035700
C	-2.88698400	6.24748900	-1.72648600
H	-1.93041800	6.63630200	-1.38507900
C	-3.85660300	7.10318100	-2.24906900
H	-3.65665100	8.16879300	-2.31789900
C	-5.09128700	6.60059100	-2.68734400
H	-5.83311200	7.28429000	-3.09125100
C	-5.37888300	5.23290100	-2.61211600
H	-6.33861100	4.85239200	-2.95683800
C	-4.41532700	4.37436200	-2.09160300
C	-2.77290000	-1.01788200	0.91741400
H	-3.20081100	-0.03365400	1.09315100
C	-3.45772500	-2.14815600	1.29981900
C	-2.85947000	-3.42053800	1.16295000
C	-1.56049700	-3.54991300	0.67256400
H	-1.10053100	-4.53260100	0.62921600
C	-3.80308800	-4.42617500	1.64903800
C	-3.69805900	-5.81967700	1.71971000
H	-2.79994800	-6.33207800	1.38283000
C	-4.77727100	-6.54053900	2.23087300
H	-4.72150700	-7.62358900	2.29532000
C	-5.93755200	-5.87997000	2.66278600
H	-6.76710100	-6.46050300	3.05739100
C	-6.03966600	-4.48592200	2.59222200
H	-6.94316900	-3.98141400	2.92999000
C	-4.96576300	-3.76162700	2.08382000
C	2.61164500	-1.37074000	-0.89807100
H	3.16475100	-0.45078400	-1.07250100
C	3.13897300	-2.57934900	-1.29030900
C	2.37920000	-3.76223300	-1.15334500
C	1.07755600	-3.72211000	-0.65497700
H	0.49313300	-4.63643100	-0.61386400
C	3.17786200	-4.88119000	-1.65038300
C	2.88683800	-6.24760000	-1.72658300
H	1.93020500	-6.63636000	-1.38530300
C	3.85647100	-7.10332900	-2.24907800
H	3.65647300	-8.16892900	-2.31796900
C	5.09124300	-6.60078900	-2.68717400
H	5.83308800	-7.28451800	-3.09099500
C	5.37889700	-5.23311600	-2.61187900
H	6.33870000	-4.85265300	-2.95643800
C	4.41531400	-4.37453500	-2.09148100
C	4.83940800	2.25675700	1.91861600
C	5.91894800	1.69353500	0.98012600
H	5.76728600	0.61663500	0.83266900
H	6.91383000	1.83949800	1.41695900
H	5.89045000	2.18869100	0.00342300
C	4.89983900	1.54021500	3.27840500
H	4.13170200	1.92270600	3.95910200
H	5.88234600	1.69298600	3.74005100
H	4.74793600	0.46204900	3.14792800
C	-4.48901100	2.86596100	-1.92238600
C	-4.62842600	2.16065300	-3.28248100
H	-3.81540000	2.44594400	-3.95870600
H	-5.58235900	2.43074700	-3.75030600
H	-4.60918900	1.07220000	-3.15119300
C	-5.64147600	2.44922500	-0.99424100
H	-5.63474000	1.36141600	-0.84801700
H	-6.60493500	2.72545400	-1.43850900
H	-5.55605600	2.93479000	-0.01608000
C	-4.83934900	-2.25659800	1.91858300
C	-4.90017100	-1.53968500	3.27811600
H	-4.13230100	-1.92201600	3.95920200
H	-5.88283300	-1.69224700	3.73950200
H	-4.74814900	-0.46156500	3.14740400
C	-5.91872100	-1.69370700	0.97963700
H	-5.76702400	-0.61685500	0.83186300
H	-6.91369600	-1.83955100	1.41629900
H	-5.88995300	-2.18921000	0.00312100
C	4.48900000	-2.86613100	-1.92231200
C	4.62789400	-2.16103200	-3.28261300
H	3.81461900	-2.44650400	-3.95846300
H	5.58166500	-2.43117900	-3.75073700

H	4.60863900	-1.07255800	-3.15149200
C	5.64169900	-2.44914700	-0.99464200
H	5.63501300	-1.36130500	-0.84867800
H	6.60503300	-2.72546200	-1.43912600
H	5.55660700	-2.93446500	-0.01632800

m-Me (cation radical)

Zero-point correction= 1.015625 (Hartree/Particle)
Thermal correction to Energy= 1.073602
Thermal correction to Enthalpy= 1.074546
Thermal correction to Gibbs Free Energy= 0.919449
Sum of electronic and zero-point Energies= -2544.730327
Sum of electronic and thermal Energies= -2544.672349
Sum of electronic and thermal Enthalpies= -2544.671405
Sum of electronic and thermal Free Energies= -2544.826502

C	-1.71041300	-0.71395400	-0.35011200
C	-2.51550400	0.46199800	-0.26511900
C	-1.91348000	1.69594800	0.25845300
C	-0.49107600	1.78581200	0.34226400
C	1.70961200	0.71287900	-0.35061700
C	2.51459800	-0.46326300	-0.26713900
C	1.91297800	-1.69735500	0.25656500
C	0.49065600	-1.78703500	0.34173000
C	-0.31351000	-0.64292700	-0.00472000
C	0.31290700	0.64185800	-0.00469200
C	-2.26227600	-1.90088400	-0.90951700
H	-1.62170100	-2.76268900	-1.08210600
C	-3.58066800	-1.93087000	-1.29957900
C	-4.38719200	-0.77734200	-1.16838900
C	-3.85443400	0.41176500	-0.67161400
H	-4.47715900	1.30056100	-0.63108500
C	-5.72253300	-1.09285000	-1.66707200
C	-6.88088500	-0.31138000	-1.75937900
H	-6.88578900	0.72517500	-1.43001600
C	-8.03253400	-0.89053800	-2.28411700
H	-8.94260300	-0.29951800	-2.36552700
C	-8.05379000	-2.23173700	-2.71804700
C	-6.88349700	-2.99907600	-2.62347500
H	-6.88898100	-4.03495700	-2.96236900
C	-5.72623000	-2.43048700	-2.10109100
C	0.10465600	2.95113000	0.90216800
H	1.17828700	2.97682300	1.07401500
C	-0.68310500	4.00793200	1.29435100
C	-2.08878700	3.93253000	1.16518100
C	-2.69800900	2.78118300	0.66730600
H	-3.78179300	2.72417000	0.62855500
C	-2.66245700	5.17751500	1.66741500
C	-3.99154900	5.60943700	1.75826000
H	-4.81085900	4.97676700	1.42455700
C	-4.24449400	6.87324700	2.28306300
H	-5.27028500	7.22826100	2.35975700
C	-3.20106500	7.71437800	2.72069500
C	-1.87558200	7.26633200	2.62324400
H	-1.06267600	7.91057100	2.95821700
C	-1.61072800	6.00406900	2.10126000
C	2.26179000	1.90033600	-0.90848300
H	1.62160500	2.76262700	-1.08022800
C	3.58025500	1.93065100	-1.29813400
C	4.38635900	0.77656500	-1.16965900
C	3.85326600	-0.41307900	-0.67445300
H	4.47542500	-1.30234500	-0.63549500
C	5.72144700	1.09257100	-1.66864700
C	6.88008900	0.31124400	-1.76152600
H	6.88519000	-0.72534700	-1.43229000
C	8.03187900	0.89125800	-2.28439400
H	8.94268400	0.30104500	-2.36426200
C	8.05294700	2.23305800	-2.71727400
C	6.88347000	3.00085600	-2.61974300
H	6.88994300	4.03825300	-2.95400200
C	5.72562900	2.43112500	-2.09928700
C	-0.10475900	-2.95178000	0.90324800
H	-1.17825000	-2.97703700	1.07595800
C	0.68330900	-4.00827400	1.29571000
C	2.08880200	-3.93335300	1.16440100
C	2.69776100	-2.78253300	0.66503800
H	3.78153300	-2.72581400	0.62505900
C	2.66291500	-5.17817400	1.66649700
C	3.99189200	-5.61067400	1.75479900
H	4.81085100	-4.97852800	1.41926500
C	4.24525900	-6.87470400	2.27907100
C	3.20235500	-7.71531400	2.71870000
C	1.87678300	-7.26669900	2.62359200
H	1.06413600	-7.91073900	2.95966000
C	1.61158700	-6.00424900	2.10241000
C	-4.36125100	-3.07418900	-1.92288300
C	-4.42234100	-4.28776100	-0.98142400
H	-3.41578700	-4.69587800	-0.82499300
H	-5.04409700	-5.07689100	-1.42030200
H	-4.84350200	-4.01183000	-0.00855200
C	-3.76066100	-3.48954800	-3.27665500
H	-3.70471100	-2.63572300	-3.96044900
H	-4.37949600	-4.26725400	-3.73957200
H	-2.75103000	-3.89433100	-3.13772600
C	-0.26265500	5.32666400	1.91826400
C	0.44040500	5.10843700	3.26873400
H	-0.19475100	4.53850400	3.95537900
H	0.67509500	6.07457500	3.73095400
H	1.38017500	4.56175700	3.12502700
C	0.65146100	6.12483900	0.97448400
H	1.59419200	5.58602100	0.81584800
H	0.88857000	7.10108700	1.41329900
H	0.17201900	6.28579100	0.00278500
C	4.36167300	3.07579500	-1.91686700
C	3.76015000	3.50092300	-3.26688100
H	3.70171900	2.65179300	-3.95627800
H	4.37959200	4.28072600	-3.72543700
H	2.75143500	3.90657900	-3.12385800
C	4.42592100	4.28318000	-0.96734400
H	3.41981200	4.69018700	-0.80493100
H	5.04654900	5.07513500	-1.40271900
H	4.84991500	4.00040300	0.00232500

C	0.26357600	-5.32591800	1.92241300
C	-0.43410700	-5.10470700	3.27527100
H	0.20438800	-4.53442900	3.95854100
H	-0.66792500	-6.06991600	3.73987200
H	-1.37378400	-4.55715000	3.13436300
C	-0.65517600	-6.12440200	0.98355500
H	-1.59758300	-5.58430300	0.82751500
H	-0.89237500	-7.09935000	1.42520200
H	-0.17963300	-6.28806700	0.01039900
C	-9.32642200	-2.82661200	-3.26385500
H	-9.14570700	-3.80829300	-3.71073300
H	-10.07081400	-2.94990300	-2.46835700
H	-9.77103300	-2.17680200	-4.02511900
C	-3.51897100	9.07149700	3.29376500
H	-2.60784100	9.64770700	3.47739800
H	-4.15902000	9.64573600	2.61516000
H	-4.05726700	8.97708500	4.24406400
C	9.32224400	2.82322600	-3.27572500
H	9.17514200	3.86294200	-3.58101900
H	10.12699300	2.79623900	-2.53233000
H	9.66813900	2.25638400	-4.14735200
C	3.52050600	-9.07138400	3.29412000
H	2.61232000	-9.66232900	3.44208000
H	4.19333700	-9.63125400	2.63574300
H	4.02244300	-8.97499400	4.26404100
H	5.27099000	-7.23035500	2.35339100

m-OMe (cation radical)

Zero-point correction= 1.037783 (Hartree/Particle)
Thermal correction to Energy= 1.098494
Thermal correction to Enthalpy= 1.099438
Thermal correction to Gibbs Free Energy= 0.942176
Sum of electronic and zero-point Energies= -2845.285250
Sum of electronic and thermal Energies= -2845.224539
Sum of electronic and thermal Enthalpies= -2845.223595
Sum of electronic and thermal Free Energies= -2845.380857

O	6.88418800	-6.53583600	3.28385400
O	6.88446200	6.53573400	-3.28368200
O	-7.17023200	6.52477000	3.05278400
O	-7.17016400	-6.52457900	-3.05317900
C	1.15786400	-1.38486900	0.36371800
C	2.39768400	-0.68357600	0.26954300
C	2.39767500	0.68358000	-0.26968500
C	1.15786700	1.38493800	-0.36375600
C	-1.29199900	1.39507400	0.32209700
C	-2.53229800	0.69133600	0.24909300
C	-2.53229300	-0.69132100	-0.24902200
C	-1.29198400	-1.39503800	-0.32206500
C	-0.06760400	-0.71367000	0.01046000
C	-0.06760500	0.71373500	-0.01049600
C	1.13364800	-2.68453600	0.94364500
H	0.17991300	-3.17468100	1.12500000
C	2.30431400	-3.28552300	1.34079200
C	3.53752400	-2.60824400	1.19575500
C	3.57937300	-1.31196000	0.68258300
H	4.52881700	-0.78674700	0.63415000
C	2.49935700	-4.64472200	1.98996400
C	2.00536000	-5.77964200	1.07917000
H	0.92092000	-5.69988600	0.93046200
H	2.21438400	-6.75281900	1.53893600
H	2.49671300	-5.74276200	0.10082600
C	1.79056100	-4.71774000	3.35305300
H	2.12908000	-3.91371400	4.01542400
H	2.00082500	-5.67931500	3.83589400
H	0.70525900	-4.63059600	3.22271900
C	1.13370400	2.68464600	-0.94361700
H	0.18000100	3.17491200	-1.12482400
C	2.30438700	3.28558200	-1.34079400
C	3.53757000	2.60823000	-1.19584100
C	3.57937400	1.31191900	-0.68275700
H	4.52879700	0.78666200	-0.63441900
C	2.49950000	4.64477400	-1.98997300
C	2.00543300	5.77977800	-1.07934500
H	0.92099500	5.70004500	-0.93063400
H	2.21442000	6.75289900	-1.53925300
H	2.49677200	5.74307500	-0.10098900
C	1.79084700	4.71767900	-3.35315500
H	2.12934700	3.91353300	-4.01538800
H	2.00127800	5.67917500	-3.83608300
H	0.70552500	4.63066100	-3.22293500
C	-1.26782200	2.71273900	0.86164200
H	-0.31419700	3.20845900	1.02783800
C	-2.43825300	3.32477400	1.23971100
C	-3.67192400	2.64327900	1.11635900
C	-3.71407200	1.33182700	0.64245100
H	-4.66351000	0.80549800	0.60934200
C	-2.63679900	4.70287800	1.84474900
C	-2.14467600	5.80906900	0.89813400
H	-1.06048100	5.72496000	0.75041400
H	-2.35290500	6.79634700	1.32735600
H	-2.63734800	5.74128000	-0.07785600
C	-1.92938700	4.82138900	3.20551000
H	-2.26344800	4.03581700	3.89181400
H	-2.14543600	5.79585500	3.65920400
H	-0.84353000	4.73726800	3.07823400
C	-1.26782100	-2.71272300	-0.86157600
H	-0.31419900	-3.20843100	-1.02784100
C	-2.43825500	-3.32479100	-1.23956000
C	-3.67193000	-2.64329500	-1.11620900
C	-3.71407800	-1.33183800	-0.64232100
H	-4.66353400	-0.80553800	-0.60920200
C	-2.63682400	-4.70291700	-1.84453800
C	-1.92928600	-4.82158900	-3.20520400
H	-2.26329200	-4.03615100	-3.89168400
H	-2.14526000	-5.79614500	-3.65873800
H	-0.84344600	-4.73742500	-3.07781500
C	-2.14488100	-5.80912600	-0.89783400
H	-1.06068900	-5.72515400	-0.74998500
H	-2.35318000	-6.79637600	-1.32709400
H	-2.63764400	-5.74129000	0.07810400
C	4.00991300	-4.67309600	2.15691600

C	4.78845500	-5.68810900	2.68318600
H	4.36187800	-6.62292900	3.04117600
C	6.18113100	-5.50349100	2.75864800
C	6.77419300	-4.30910100	2.30828600
H	7.84812900	-4.16980700	2.36749700
C	5.97950400	-3.29234500	1.77817700
H	6.44437600	-2.37311000	1.42970100
C	4.59698800	-3.47336600	1.69989800
C	8.29500500	-6.41727100	3.39557800
H	8.56837700	-5.57657900	4.04393600
H	8.75772900	-6.28731200	2.41023800
H	8.64593700	-7.34782200	3.84099100
C	4.01006800	4.67309100	-2.15689600
C	4.78865700	5.68809600	-2.68311900
H	4.36211000	6.62294700	-3.04106200
C	6.18132000	5.50340700	-2.75857800
C	6.77431200	4.30893400	-2.30832700
H	7.84823700	4.16958400	-2.36759500
C	5.97957900	3.29219000	-1.77827500
H	6.44440300	2.37290100	-1.42987700
C	4.59707200	3.47330300	-1.69995900
C	8.29527900	6.41707300	-3.39529700
H	8.64633800	7.34771400	-3.84042500
H	8.56862300	5.57652600	-4.04385400
H	8.75789700	6.28679400	-2.40995200
C	-4.14727900	4.73266400	2.00989300
C	-4.92121500	5.77685300	2.50782600
H	-4.45503200	6.70665800	2.82292500
C	-6.30953600	5.58830000	2.58820300
C	-6.89936000	4.37383400	2.17606400
H	-7.97804500	4.27786800	2.25902700
C	-6.11921400	3.34133300	1.68026800
H	-6.58378400	2.41076500	1.36333600
C	-4.73006400	3.52332700	1.59398900
C	-6.64805000	7.77251600	3.48511900
H	-7.50165900	8.36636200	3.81068800
H	-6.13555100	8.28831300	2.66452200
H	-5.95515100	7.63806300	4.32415900
C	-4.14728500	-4.73264000	-2.00981000
C	-4.92119000	-5.77678700	-2.50789000
H	-4.45496800	-6.70656700	-2.82300000
C	-6.30949400	-5.58818400	-2.58840500
C	-6.89932800	-4.37372900	-2.17623400
H	-7.97800400	-4.27773600	-2.25929500
C	-6.11921100	-3.34127500	-1.68030100
H	-6.58377900	-2.41070900	-1.36335900
C	-4.73007200	-3.52331300	-1.59389000
C	-6.64793900	-7.77231100	-3.48549800
H	-5.95511800	-7.63783700	-4.32460000
H	-7.50152900	-8.36623700	-3.81096600
H	-6.13531900	-8.28802700	-2.66492600

p-H (cation radical)

Zero-point correction= 0.907481
(Hartree/Particle)
Thermal correction to Energy= 0.957514
Thermal correction to Enthalpy= 0.958458
Thermal correction to Gibbs Free Energy= 0.824906
Sum of electronic and zero-point Energies= -2387.759430
Sum of electronic and thermal Energies= -2387.709397
Sum of electronic and thermal Enthalpies= -2387.708452
Sum of electronic and thermal Free Energies= -2387.842004

C	0.71670500	0.00009100	-0.00014700
C	-0.71664600	-0.00009200	-0.00013900
C	-1.39055800	-1.22318800	0.35665000
C	-0.68182000	-2.45896000	0.26815400
C	0.68248200	-2.45882600	-0.26811500
C	1.39086900	-1.22285300	-0.35687900
C	1.31406400	-3.63984600	-0.68801000
H	0.78753100	-4.59012300	-0.64800900
C	2.60542200	-3.59736100	-1.19414400
C	3.29496000	-2.37227700	-1.31905300
C	2.69383100	-1.19199900	-0.91807000
H	3.18515600	-0.23883100	-1.09040200
C	-1.31304800	-3.64001300	0.68847700
H	-0.78628900	-4.59016600	0.64877100
C	-2.60438800	-3.59775300	1.19465300
C	-3.29438500	-2.37289000	1.31896900
C	-2.69354300	-1.19253500	0.91770500
H	-3.18508900	-0.23941200	1.08976500
C	4.69995800	-4.02078000	-2.16586700
C	5.84970000	-4.55727400	-2.73854500
H	5.93505200	-5.62677900	-2.92328100
C	6.89925100	-3.69499700	-3.07653000
H	7.80356200	-4.09757000	-3.52494700
C	6.79828000	-2.31636500	-2.84360600
H	7.62467400	-1.66446700	-3.11324300
C	5.64703900	-1.77412000	-2.26803700
H	5.57001000	-0.70435200	-2.08676000
C	4.60198700	-2.63823100	-1.93292200
C	-4.69916400	-4.02166000	2.16563200
C	-5.84908800	-4.55836300	2.73775100
H	-5.93424800	-5.62783100	2.92276700
C	-6.89916000	-3.69635700	3.07484700
H	-7.80361900	-4.09914400	3.52277200
C	-6.79852400	-2.31776100	2.84161500
H	-7.62529400	-1.66605600	3.11056400
C	-5.64710800	-1.77529000	2.26660500
H	-5.57031200	-0.70555300	2.08507900
C	-4.60157400	-2.63913600	1.93232600
C	3.43983000	-4.74738100	-1.72371400
C	-3.43828500	-4.74784900	1.72489100
C	3.73239400	-5.77492800	-0.61673800
H	2.80188500	-6.24542200	-0.27714800
H	4.22078900	-5.30200600	0.24190600
H	4.39120700	-6.56147700	-1.00260200
C	2.74228000	-5.43656400	-2.90921400
H	2.51846300	-4.71899900	-3.70577900
H	1.80552200	-5.90403400	-2.58346400
H	3.39008500	-6.22045100	-3.31832700
C	-2.74087200	-5.43465800	2.91194900
H	-2.51879000	-4.71576100	3.70779600

H	-1.80316500	-5.90124600	2.58766200
H	-3.38798700	-6.21891500	3.32144700
C	-3.72902000	-5.77727800	0.61927200
H	-2.79783200	-6.24762400	0.28129100
H	-4.21695700	-5.30610800	-0.24059700
H	-4.38756000	-6.56378100	1.00569600
C	-1.39083100	1.22283100	-0.35690700
C	-0.68246900	2.45882200	-0.26815800
C	0.68183100	2.45897800	0.26811000
C	1.39060000	1.22322100	0.35660500
C	1.31301500	3.64006200	0.68841400
H	0.78617400	4.59017300	0.64873000
C	2.60436700	3.59786400	1.19455700
C	3.29441900	2.37301500	1.31884300
C	2.69360800	1.19263400	0.91762600
H	3.18521200	0.23954500	1.08969000
C	-1.31408100	3.63980700	-0.68809700
H	-0.78761800	4.59012700	-0.64809400
C	-2.60543300	3.59726200	-1.19425700
C	-3.29492300	2.37217000	-1.31915700
C	-2.69375400	1.19190600	-0.91812900
H	-3.18503400	0.23871400	-1.09048300
C	4.69913800	4.02183500	2.16551500
C	5.84906800	4.55859800	2.73755700
H	5.93415800	5.62806500	2.92260400
C	6.89923700	3.69665300	3.07450000
H	7.80370500	4.09948400	3.52236700
C	6.79867400	2.31805500	2.84123300
H	7.62551300	1.66639100	3.11007100
C	5.64725000	1.77553100	2.26629700
H	5.57052900	0.70579700	2.08471500
C	4.60162100	2.63931400	1.93215400
C	-4.69997800	4.02061600	-2.16596600
C	-5.84974400	4.55705600	-2.73864600
H	-5.93516200	5.62655900	-2.92336500
C	-6.89924000	3.69472800	-3.07668400
H	-7.80357300	4.09726300	-3.52509100
C	-6.79820300	2.31610000	-2.84377300
H	-7.62456000	1.66417100	-3.11344800
C	-5.64694400	1.77390200	-2.26819700
H	-5.56984700	0.70413500	-2.08694800
C	-4.60194800	2.63806500	-1.93303400
C	3.43816300	4.74796000	1.72493600
C	-3.43987000	4.74726500	-1.72384000
C	3.72872100	5.77771300	0.61959000
H	2.79743600	6.24789700	0.28166100
H	4.21684300	5.30688000	-0.24035800
H	4.38702700	6.56430200	1.00624200
C	2.74068900	5.43436000	2.91220500
H	2.51859200	4.71518800	3.70780200
H	1.80298500	5.90103600	2.58802600
H	3.38778900	6.21848100	3.32198700
C	-2.74233100	5.43631000	-2.90945200
H	-2.51879700	4.71868700	-3.70604200
H	-1.80541400	5.90356600	-2.58385600
H	-3.39001500	6.22034400	-3.31847700
C	-3.73236000	5.77491700	-0.61696500
H	-2.80183300	6.24541500	-0.27742700
H	-4.22075100	5.30210000	0.24173900
H	-4.39114800	6.56145700	-1.00288900

p-Me (cation radical)

Zero-point correction= 1.015151 (Hartree/Particle)
Thermal correction to Energy= 1.073296
Thermal correction to Enthalpy= 1.074240
Thermal correction to Gibbs Free Energy= 0.919125
Sum of electronic and zero-point Energies= -2544.716038
Sum of electronic and thermal Energies= -2544.657893
Sum of electronic and thermal Enthalpies= -2544.656949
Sum of electronic and thermal Free Energies= -2544.812063

C	-0.69462000	-0.00008600	0.00925200
C	0.69464000	-0.00010800	-0.00918400
C	1.39713500	-1.23993600	-0.30924200
C	0.68927200	-2.47485000	-0.23138400
C	-0.68935000	-2.47483300	0.23137900
C	-1.39715300	-1.23989200	0.30930900
C	-1.34098500	-3.67366000	0.61631300
H	-0.80500800	-4.61909100	0.58552700
C	-2.63688400	-3.64511400	1.07791300
C	-3.32157600	-2.41278000	1.20820500
C	-2.71156000	-1.22865900	0.84111800
H	-3.21975300	-0.28508100	1.01663500
C	1.34085000	-3.67368500	-0.61638800
H	0.80482600	-4.61909100	-0.58567300
C	2.63675800	-3.64517900	-1.07796300
C	3.32153300	-2.41287900	-1.20812700
C	2.71156500	-1.22874700	-0.84099500
H	3.21982300	-0.28519000	-1.01643700
C	-4.76066600	-4.06820100	1.98956600
C	-5.92523900	-4.60642500	2.52884900
H	-6.01656500	-5.68089100	2.69114400
C	-6.99168000	-3.76149200	2.87197800
C	-6.85640100	-2.37600300	2.66705000
H	-7.68212000	-1.72198200	2.94141700
C	-5.69396100	-1.82677300	2.12584400
H	-5.61069800	-0.75191400	1.97831100
C	-4.64305300	-2.68337600	1.78608000
C	4.76056600	-4.06834200	-1.98952300
C	5.92513900	-4.60659800	-2.52875200
H	6.01640200	-5.68105400	-2.69115000
C	6.99168100	-3.76170500	-2.87170500
C	6.85647300	-2.37623100	-2.66669900
H	7.68225300	-1.72224300	-2.94095800
C	5.69401600	-1.82696100	-2.12554600
H	5.61080800	-0.75210700	-1.97795200
C	4.64303300	-2.68351600	-1.78593100
C	-3.49905000	-4.80062800	1.55850500
C	3.49882800	-4.80070300	-1.55870500
C	-3.78575500	-5.79212700	0.41864600
H	-2.85463900	-6.26488700	0.08309400
H	-4.24763900	-5.28561500	-0.43594400

H	-4.46469100	-6.58073700	0.76466600
C	-2.84531300	-5.53597300	2.73946900
H	-2.62979600	-4.84491300	3.56171000
H	-1.90662000	-6.00686300	2.42330600
H	-3.51256700	-6.32283500	3.11121100
C	2.84508400	-5.53561700	-2.73994700
H	2.62975200	-4.84428100	-3.56200400
H	1.90628600	-6.00645000	-2.42400700
H	3.51225600	-6.32246900	-3.11185700
C	3.78526000	-5.79255700	-0.41909900
H	2.85403700	-6.26527300	-0.08377800
H	4.24712900	-5.28636100	0.43568600
H	4.46410700	-6.58118100	-0.76526200
C	1.38303600	1.25043900	0.30761700
C	0.67910400	2.50737200	0.21524500
C	-0.67901200	2.50738300	-0.21530100
C	-1.38298700	1.25046800	-0.30758100
C	-1.34888200	3.72130500	-0.57710100
H	-0.82523400	4.67058300	-0.51401900
C	-2.62599700	3.68747500	-1.05818500
C	-3.28789000	2.43561300	-1.22801200
C	-2.66767100	1.23824300	-0.86396900
H	-3.16989100	0.29532300	-1.05331700
C	1.34901500	3.72129500	0.57697300
H	0.82540600	4.67058800	0.51380300
C	2.62611500	3.68744800	1.05809300
C	3.28795600	2.43557100	1.22803500
C	2.66769800	1.23820000	0.86404900
H	3.16987800	0.29527200	1.05346900
C	-4.74053500	4.07420500	-1.98774100
C	-5.91298800	4.58746200	-2.52695400
H	-6.03979400	5.66037000	-2.66708600
C	-6.94667700	3.71287600	-2.89683500
C	-6.77949600	2.32005000	-2.71255500
H	-7.58982100	1.65489700	-3.00253000
C	-5.61537800	1.79379900	-2.17401900
H	-5.50273800	0.72110200	-2.03791100
C	-4.58746400	2.68165800	-1.80940600
C	4.74063600	4.07415700	1.98768000
C	5.91309600	4.58742300	2.52689400
H	6.03992000	5.66033700	2.66694900
C	6.94673700	3.71283800	2.89686300
C	6.77950200	2.31998500	2.71270900
H	7.58979500	1.65483700	3.00279000
C	5.61539400	1.79373800	2.17418100
H	5.50270100	0.72103600	2.03816000
C	4.58751800	2.68161200	1.80944900
C	-3.50943200	4.83215400	-1.52165400
C	3.50958000	4.83212500	1.52151000
C	-3.84515300	5.78227000	-0.35950800
H	-2.93423500	6.27454900	0.00043800
H	-4.30316000	5.24012700	0.47462900
H	-4.54237600	6.55774500	-0.69697000
C	-2.86158100	5.61739200	-2.67351600
H	-2.61171500	4.95707700	-3.51071200
H	-1.94432700	6.10846400	-2.32796600
H	-3.54767700	6.39323100	-3.03252500
C	2.86172500	5.61744900	2.67331600
H	2.61179700	4.95718100	3.51053200
H	1.94450700	6.10855000	2.32771000
H	3.54784900	6.39326800	3.03231300
C	3.84537200	5.78216800	0.35932900
H	2.93448700	6.27446800	-0.00066800
H	4.30338100	5.23996800	-0.47477000
H	4.54261700	6.55762900	0.69677500
C	-8.22568600	4.23672900	-3.48983000
H	-9.09129300	3.89664200	-2.91060300
H	-8.23472900	5.32935200	-3.51718700
H	-8.35776000	3.86607500	-4.51293300
C	-8.27324500	-4.32581300	3.43251000
H	-9.04517700	-4.38931100	2.65597100
H	-8.12087200	-5.33304900	3.83160600
H	-8.66882400	-3.69308300	4.23364700
C	8.27329100	-4.32613600	-3.43202400
H	9.04431700	-4.39198100	-2.65477600
H	8.12037800	-5.33243300	-3.83328500
H	8.67034200	-3.69217900	-4.23145100
C	8.22579400	4.23667800	3.48976700
H	9.09128200	3.89728200	2.90994800
H	8.23450500	5.32928500	3.51786900
H	8.35839600	3.86532900	4.51254400

p-OMe (cation radical)

Zero-point correction= 1.037605 (Hartree/Particle)
Thermal correction to Energy= 1.098480
Thermal correction to Enthalpy= 1.099424
Thermal correction to Gibbs Free Energy= 0.940684
Sum of electronic and zero-point Energies= -2845.271976
Sum of electronic and thermal Energies= -2845.211102
Sum of electronic and thermal Enthalpies= -2845.210158
Sum of electronic and thermal Free Energies= -2845.368898

C	0.69456900	0.00418300	-0.00885500
C	-0.69457400	0.00419600	0.00874200
C	-1.39661800	-1.23633200	0.31024800
C	-0.68929100	-2.47086500	0.23181600
C	0.68929200	-2.47085500	-0.23208100
C	1.39663500	-1.23631600	-0.31036900
C	1.34134500	-3.66917100	-0.61819500
H	0.80599000	-4.61504300	-0.58625600
C	2.63653800	-3.64028000	-1.08194500
C	3.32083000	-2.40796800	-1.21401400
C	2.71013200	-1.22457400	-0.84445500
H	3.21699600	-0.28026400	-1.02004400
C	-1.34133900	-3.66920800	0.61786500
H	-0.80600200	-4.61508800	0.58581500
C	-2.63649800	-3.64034100	1.08170200
C	-3.32076400	-2.40803100	1.21394900
C	-2.71006500	-1.22461400	0.84445400
H	-3.21688000	-0.28030300	1.02018200
C	4.75780500	-4.06669300	-2.00063500
C	5.91286100	-4.61009400	-2.53829600

H	6.02853800	-5.67933000	-2.70615100
C	6.97140100	-3.75107800	-2.88179000
C	6.86089500	-2.36514800	-2.68317400
H	7.67658700	-1.70140400	-2.94914400
C	5.69028500	-1.82830400	-2.13745500
H	5.61254600	-0.75353500	-1.98731400
C	4.63952400	-2.67752000	-1.79619900
C	-4.75769700	-4.06681900	2.00051600
C	-5.91270200	-4.61026700	2.53821200
H	-6.02837600	-5.67952300	2.70594800
C	-6.97122300	-3.75128200	2.88187100
C	-6.86073900	-2.36533800	2.68334300
H	-7.67642700	-1.70161300	2.94937400
C	-5.69016400	-1.82844800	2.13758300
H	-5.61245000	-0.75366500	1.98752000
C	-4.63941700	-2.67762200	1.79619700
C	3.49700200	-4.79747700	-1.56338000
C	-3.49693200	-4.79757600	1.56310300
C	3.78881500	-5.78623900	-0.42266700
H	2.85857100	-6.25675100	-0.08175500
H	4.25486500	-5.27787100	0.42855100
H	4.46535900	-6.57643800	-0.76969700
C	2.84026900	-5.53535200	-2.74083900
H	2.62329900	-4.84630500	-3.56437000
H	1.90179400	-6.00383400	-2.42067100
H	3.50553800	-6.32411700	-3.11203200
C	-2.84011700	-5.53553200	2.74047000
H	-2.62316600	-4.84655600	3.56406400
H	-1.90162300	-6.00392500	2.42022500
H	-3.50532800	-6.32437600	3.11160000
C	-3.78882500	-5.78626300	0.42235000
H	-2.85860400	-6.25674600	0.08133600
H	-4.25494500	-5.27784800	-0.42880100
H	-4.46533400	-6.57649200	0.76938300
C	-1.38367500	1.25477300	-0.30854900
C	-0.67912900	2.50953900	-0.21868500
C	0.67925500	2.50955000	0.21823400
C	1.38369900	1.25476000	0.30838500
C	1.34648100	3.72141400	0.58615600
H	0.82092400	4.67014900	0.52735800
C	2.62390100	3.68806600	1.06825300
C	3.28934600	2.43764000	1.23267100
C	2.66945700	1.24156100	0.86330800
H	3.17191200	0.29789300	1.04864100
C	-1.34627600	3.72138600	-0.58679400
H	-0.82060500	4.67007100	-0.52828600
C	-2.62377000	3.68807600	-1.06869400
C	-3.28938700	2.43769000	-1.23268100
C	-2.66955100	1.24162600	-0.86323600
H	-3.17214900	0.29798800	-1.04831500
C	4.73735300	4.08084600	2.00266800
C	5.89690300	4.59653500	2.54270400
H	6.04688800	5.66226300	2.70019900
C	6.92835300	3.70563700	2.90644300
C	6.78446700	2.31113100	2.72395900
H	7.58317700	1.63487600	3.00707700
C	5.61448500	1.80103900	2.17811500
H	5.50554000	0.72861400	2.03789700
C	4.58478800	2.68352900	1.81515200
C	-4.73745000	4.08091300	-2.00257500
C	-5.89714900	4.59661800	-2.54229200
H	-6.04711500	5.66232800	-2.69992800
C	-6.92880200	3.70575200	-2.90552000
C	-6.78501000	2.31128100	-2.72282700
H	-7.58389900	1.63506000	-3.00552200
C	-5.61488300	1.80116900	-2.17728900
H	-5.50600900	0.72875800	-2.03690400
C	-4.58497900	2.68361800	-1.81484900
C	3.50197300	4.83480300	1.53892400
C	-3.50173400	4.83480200	-1.53959900
C	3.83410200	5.79329500	0.38302800
H	2.92002400	6.27983000	0.02327700
H	4.29790600	5.25866800	-0.45277900
H	4.52442300	6.57263600	0.72579000
C	2.84990400	5.60925900	2.69545800
H	2.60400100	4.94225200	3.52854100
H	1.92936600	6.09585800	2.35244300
H	3.53078600	6.38742100	3.05933000
C	-2.84982900	5.60828400	-2.69690800
H	-2.60456600	4.94064100	-3.52967300
H	-1.92893600	6.09469100	-2.35457700
H	-3.53052500	6.38651200	-3.06098500
C	-3.83306700	5.79414100	-0.38420800
H	-2.91869500	6.28070700	-0.02522500
H	-4.29659700	5.26019500	0.45218600
H	-4.52334900	6.57344100	-0.72714100
O	8.03125700	4.27215500	3.42763000
O	8.07424300	-4.35086300	-3.40535900
O	-8.07397200	-4.35111700	3.40553000
O	-8.03187300	4.27228500	-3.42636000
C	-9.12327000	3.44677300	-3.82012900
H	-9.51936700	2.89108100	-2.96324000
H	-9.88859900	4.11998000	-4.20399200
H	-8.81928300	2.74917200	-4.60812200
C	-9.17526000	-3.53846700	3.77702000
H	-9.57699700	-2.99796900	2.91121900
H	-9.93744100	-4.21257600	4.16787400
H	-8.89100900	-2.82004300	4.55558400
C	9.12245100	3.44666000	3.82202700
H	9.51880800	2.89072700	2.96541700
H	9.88769000	4.11991300	4.20598500
H	8.81812500	2.74929200	4.61009100
C	9.17536300	-3.53809100	-3.77712200
H	9.57728800	-2.99756200	-2.91142900
H	9.93752300	-4.21211600	-4.16816700
H	8.89082400	-2.81970000	-4.55560500