Supporting Information

Relevant Synthesis to Manipulating Non-Planarity in Dibenzo[*g*,*p*]chrysene: Substitution Reactions at the Bay.

Shinsuke Kamiguchi, [a] Ryuhei Akasaka, [a] Naruhiro Yoshida, [a] Tomoya Imai, [b]
Yousuke Yamaoka, [c] Toru Amaya, [b] Tetsuo Iwasawa* [a]

[a] *Department of Materials Chemistry, Faculty of Science and Technology, Ryukoku University, Seta, Otsu, 520-2194, Japan*

[b] *Department of Information and Basic Science, Graduate School of Science, Nagoya City University, Mizuho-ku, Nagoya, Aichi, 467-8501, Japan*

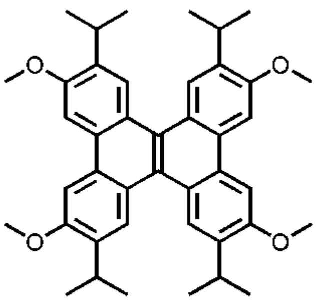
[c] *Department of Synthetic Medicinal Chemistry, Graduate School of Pharmaceutical Sciences, Kyoto University, Sakyo-ku, Kyoto, 606-8501, Japan*

Corresponding author's email address: iwasawa@rins.ryukoku.ac.jp

Contents

1. General Information. All reactions sensitive to air or moisture were carried out under an argon or a nitrogen atmosphere and anhydrous conditions unless otherwise noted. Dry solvents were purchased and used without further purification and dehydration. All reagents were purchased and used without further purification. Analytical thin layer chromatography was carried out on Merck silica $60F_{254}$. Column chromatography was carried out with silica gel 60 $_N$ (Kanto Chemical Co.). HRMS were reported on the basis of TOF (time of flight)-MS (MALDI-TOF or LCMS-IT-TOF), and DART (Direct Analysis in Real Time)-MS. ^{1}H and ^{13}C NMR spectra were recorded with a 5 mm QNP probe at 400 MHz and 100 MHz, respectively. Chemical shifts are reported in δ (ppm) with reference to residual solvent signals [^{1}H NMR: $CHCl_3$ (7.26), DMSO (2.50); ^{13}C NMR: $CDCl_3$ (77.0), DMSO (39.5)]. Signal patterns are indicated as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad. All melting points were recorded on the melting point apparatus of Stanford Research Systems OptiMelt and are not corrected.

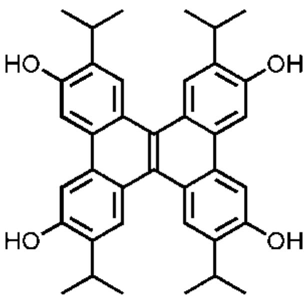
2. Synthesis of **3** (Scheme 1). Under an Ar atmosphere, to a suspension of 2,7,10,15-tetramethoxy-DBC (4.19 g, 9.3 mmol) in 2-Chloropropane (50 mL, 514 mmol) at room temperature was added $AlCl_3$ (5.97 g, 44.8 mmol). After stirred at room temperature for 89 h, the mixture was quenched with 1 M aq. HCl (150 mL) at 0 °C. The aqueous phase was extracted with $CHCl_3$ (20 mL x 3), and combined organic phases were washed with brine (40 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-gel column chromatography (eluent, hexane/toluene, 2:1) gave 3.46 g of **3** (60%) as brownish yellow solid materials. Data of **3**: Rf value 0.58 (hexane/EtOAc, 2:1); M.p. 256-257 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) 8.49 (s, 4H), 7.89 (s, 4H), 4.12 (s, 12H), 3.54



3

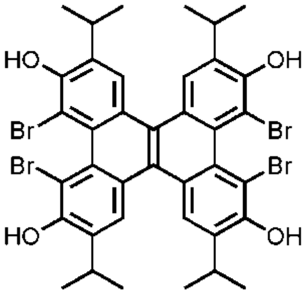
(sept, J = 6.8 Hz, 4H), 1.32 (d, J = 6.8 Hz, 24H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 155.9, 137.1, 129.5, 126.7, 125.1, 124.1, 103.2, 55.9, 27.3, 23.4 ppm; MS (DART-TOFMS) *m*/*z*: 617 $[MH]^+$; IR (neat): 2946, 2862, 1611, 1458, 1411, 1236, 1164, 1065, 829, 753 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{42}H_{49}O_4$: 617.3631 $[MH]^+$, Found: 617.3614; Anal. Calcd. for $C_{42}H_{48}O_4$; C, 81.78; H, 7.84. Found: C, 82.08; H, 7.88.

3. Synthesis of **4** (Scheme 1). Under an Ar atmosphere, to a suspension of **3** (6.2 g, 10.0 mmol) in dry CH_2Cl_2 (40 mL) at 0 °C was added BBr_3 (60 mL, 60 mmol, 1 M in CH_2Cl_2) dropwise over 10 min. After stirred at 0 °C for 15 min, the reaction mixture was allowed to warm to room temperature, and conducted over 1 h. The mixture was quenched with water (100 mL) at 0 °C. The aqueous phase was extracted with EtOAc (40 mL x 3), and combined organic phases were washed with brine (30 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-gel column chromatography (eluent, toluene/EtOAc, 2:1) gave 5.1 g of **4** (90%) as whitish green solid materials. Data of **4**: Rf value 0.35 (hexane/EtOAc, 1:1); ^{1}H NMR (400 MHz, DMSO-d_6) 9.96 (s, 4H), 8.30 (s, 4H), 7.84 (s, 4H), 3.44 (sept, J = 6.9 Hz, 4H), 1.28 (d, J = 6.9 Hz, 24H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) 153.3, 134.9, 128.6, 125.4, 123.5, 122.1, 107.0, 26.5, 22.9 ppm; MS (DART-TOFMS) *m*/*z*: 561 $[MH]^+$; IR (neat): 3518 (OH), 3367 (OH), 2955, 1610, 1420, 1155, 1053, 843 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{38}H_{41}O_4$: 561.3005 $[MH]^+$, Found: 561.2993.



4

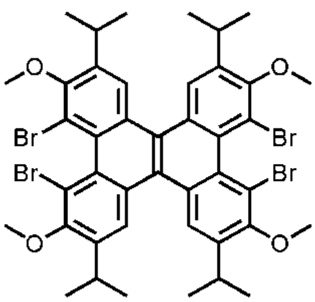
4. Synthesis of **5** (Scheme 1). Under an Ar atmosphere, to a suspension of **4** (1.12 g, 2.0



5

mmol) in CH_2Cl_2 (40 mL) at 0 °C was added Br_2 (15.2 mL, 64 mmol, 4.2 M in CH_2Cl_2) dropwise over 9 min. After stirred at 0 °C for 15 min, the reaction mixture was allowed to warm to room temperature, and conducted over 24 h. The mixture was quenched with 3 M aq. $Na_2S_2O_3$ (100 mL) and 3 M aq. HCl (50 mL) at 0 °C. The aqueous phase was extracted with $CHCl_3$ (20 mL x 3), and combined organic phases were washed with brine (35 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-gel column chromatography (eluent, $CHCl_3$/Hexane, 2:1) gave 1.33 g of **5** (76%) as greenish yellow solid materials. Data of **5**: Rf value 0.51 (hexane/EtOAc, 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) 8.29 (s, 4H), 6.20 (s, 4H), 3.52 (qq, *J* = 6.9, 6.9 Hz, 4H), 1.47 (d, *J* = 6.9 Hz, 12H), 1.24 (d, *J* = 6.9 Hz, 12H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6) 150.5, 137.8, 128.8, 125.3, 124.5, 123.0, 112.2, 27.5, 22.8, 22.6 ppm; MS (DART-TOFMS) *m/z*: 873 $[MH]^+$; IR (neat): 3482 (OH), 2956, 2865, 1372, 1204, 1169, 615 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{38}H_{37}Br_4O_4$: 872.9425 $[MH]^+$, Found: 872.9378.

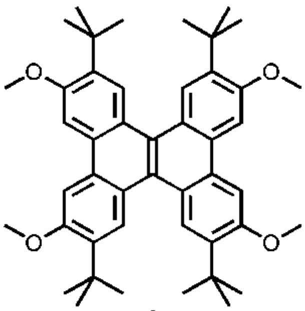
5. Synthesis of **1** (Scheme 1). To a suspension of **5** (1.92 g, 2.19 mmol) in acetone (45



1

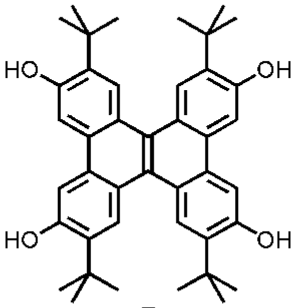
mL) at room temperature was added Iodomethane (5.46 mL, 87.6 mmol) and DBU (6.60 mL, 43.8 mmol). After stirred at room temperature for 17 h, the mixture was quenched with 1 M aq. HCl (48 mL). The aqueous phase was extracted with toluene (25 mL x 3), and combined organic phases were washed with brine (40 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by column chromatography (eluent, hexane/EtOAc, 19:1) gave 1.59 g of **1** (78%) as yellow solid materials**.** Data of **1**: Rf value 0.53 (hexane/EtOAc, 4:1); M.p. 250 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.27 (s, 4H), 4.11 (s, 12H), 3.53 (qq, *J* = 6.8, 6.9 Hz, 4H), 1.49 (d, *J* = 6.9 Hz, 12H), 1.22 (d, *J* = 6.8 Hz, 12H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 155.3, 143.5, 131.2, 129.0, 128.3, 125.0, 119.4, 62.9, 28.6, 24.4 ppm; MS (DART-TOFMS) *m/z*: 929 $[MH]^+$; IR (neat): 2955, 2924, 1389, 1314, 1061, 1006, 803, 634 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{42}H_{45}Br_4O_4$: 929.0051 $[MH]^+$, Found: 929.0047; Anal. Calcd. for $C_{42}H_{44}Br_4O_4$, C, 54.10; H, 4.76. Found: C, 54.20; H, 4.87.

6. Synthesis of **6** (Scheme 1). Under an Ar atmosphere, to a suspension of 2,7,10,15-tetramethoxy-DBC (1.79 g, 4.00 mmol) in *tert*-butyl chloride (20 mL, 180 mmol) at room temperature was added $AlCl_3$ (133 mg, 1.0 mmol). After stirred at room temperature for 23 h, the mixture was quenched with H_2O (20 mL) at 0 °C. The aqueous phase was extracted with toluene (10 mL x 3), and combined organic phases were washed with brine (20 mL x 3), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by silica-gel column chromatography (eluent, hexane/toluene, 4:1) gave 1.81 g of **6** (67%) as yellowish white solid materials. Data of **6**: Rf value 0.51 (hexane/EtOAc, 4:1); ^{1}H NMR (400 MHz, $CDCl_3$) 8.52 (s, 4H), 7.90 (s, 4H), 4.13 (s, 12H), 1.49 (s, 36H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 157.6, 138.1, 129.4, 127.4, 125.6, 123.8, 104.3, 55.5, 35.8, 30.5 ppm; MS (DART-TOFMS) m/z: 673 $[MH]^+$; IR (neat): 2949, 1447, 1412, 1212, 1073, 1013, 890, 830, 786, 750 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{46}H_{57}O_4$ $[MH]^+$: 673.4257, Found: 673.4243; Anal. Calcd. for $C_{46}H_{56}O_4$; C, 82.10; H, 8.39. Found: C, 82.00; H, 8.64.



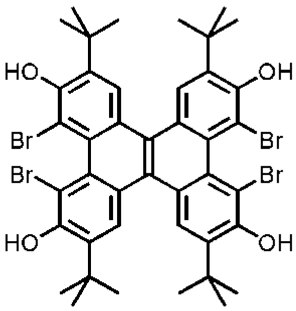
6

7. Synthesis of **7** (Scheme 2). Under an Ar atmosphere, to a solution of 1-decanethiol (14 mL, 67.2 mmol) in anhydrous *N,N*-dimethyl formamide (84 mL) was added Potassium *tert*-butoxide (5.66 g, 50.4 mmol). After stirred for 15 min at 0 °C, the reaction was allowed to warm to room temperature, and **6** (2.83 g, 4.2 mmol) was added. The mixture was stirred for 36 h at 145 °C, the mixture was quenched with 1 M aq. HCl (105 mL) at 0 °C. The aqueous phase was extracted with EtOAc (60 mL x 3), and combined organic phases were washed with brine (60 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-gel column chromatography (eluent, hexane/EtOAc, 2:1) gave 2.13 g of **7** (82%) as dark purple solid materials. Data of **7**: Rf value 0.28 (hexane/EtOAc, 2:1); ^{1}H NMR (400 MHz, CD_3CN) 8.44 (s, 4H), 7.88 (s, 4H), 7.45 (s, 4H), 1.51 (s, 36H) ppm; ^{13}C NMR (100 MHz, CD_3CN) 155.1, 137.1, 129.7, 127.8, 125.7, 123.9, 109.6, 35.8, 30.1 ppm; MS (DART-TOFMS) m/z: 617 $[MH]^+$; IR (neat): 3526 (OH), 2952, 1615, 1419, 1356, 1161, 1057, 583 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{42}H_{49}O_4$: 617.3631 $[MH]^+$, Found: 617.3616.



7

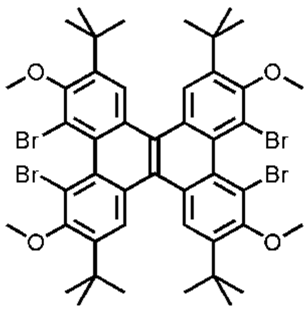
8. Synthesis of **8** (Scheme 2). Under an Ar atmosphere, to a suspension of **7** (2.13 g, 3.50 mmol) in anhydrous CH_2Cl_2 (70 mL) at 0 °C was added Br_2 (26.7 mL, 112 mmol, 4.2 M in CH_2Cl_2) dropwise over 7 min. After stirred at 0 °C for 15 min, the reaction mixture was allowed to warm to room temperature, and conducted over 58 h. The mixture was quenched with 3 M aq. $Na_2S_2O_3$ (100 mL) and 1 M aq. HCl (50 mL) at 0 °C. The aqueous phase was extracted with EtOAc (60 mL x 3), and combined organic phases were washed with brine (60 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-



8

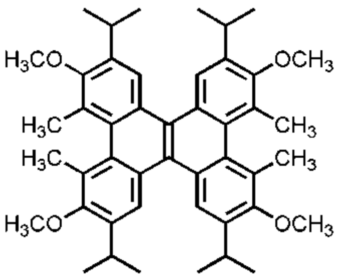
gel column chromatography (eluent, hexane/$CHCl_3$, 4:1) gave 2.40 g of **8** (74%) as yellow solid materials. Data of **8**: Rf value 0.51 (hexane/EtOAc, 2:1); ^{1}H NMR (400 MHz, $CDCl_3$) 8.35 (s, 4H), 6.41 (s, 4H), 1.52 (s, 36H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 150.0, 138.4, 128.9, 127.2, 125.6, 125.3, 113.0, 36.4, 30.0 ppm; MS (DART-TOFMS) m/z: 933 $[MH]^+$; IR (neat): 3459 (OH), 2952, 1408, 1328, 1189, 922, 882, 754 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{42}H_{45}Br_4O_4$ $[MH]^+$: 933.0010, Found: 932.9922.

9. Synthesis of **2** (Scheme 2). To a suspension of **8** (2.91 g, 3.10 mmol) in Acetone (66 mL) was added Iodomethane (7.7 mL, 124 mmol), and DBU (9.2 mL, 62 mmol). After stirred at room temperature for 1 h, the mixture was quenched with 1 M aq. HCl (66 mL). The aqueous phase was extracted with CH_2Cl_2 (60 mL x 3), and combined organic phases were washed with brine (60 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by short-plugged silica-gel column chromatography (eluent, hexane/EtOAc, 19:1) gave 2.08 g of **2** (68%) as orangish yellow solid materials. Data of **2**: Rf value 0.53 (hexane/EtOAc, 4:1); M.p. 284 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.32 (s, 4H), 4.25 (s, 4H), 1.51 (s, 36H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 157.6, 144.3, 131.6, 128.5, 127.8, 125.4, 119.8, 62.8, 36.3, 31.2 ppm; MS (DART-TOFMS) *m/z*: 989 $[MH]^+$; IR (neat): 2949, 1380, 1225, 1065, 993, 754 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{46}H_{53}Br_4O_4$ $[MH]^+$: 989.0636, found: 989.0625; Anal. Calcd. for $C_{46}H_{52}Br_4O_4$; C, 55.89; H, 5.30. Found: C, 55.73; H, 5.22.



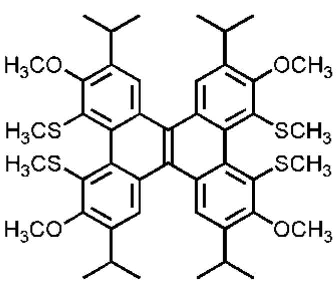
2

10. Synthesis of **9** (Scheme 3(a)). Under an Ar atmosphere, to a solution of **1** (932 mg, 1 mmol) in dry THF (20 mL) at -78 °C was added MeLi (4.2 mL, 5 mmol, 1.2 M in Et_2O) dropwise over 4 min. After stirred at -78 °C for 30 min, the reaction mixture was allowed to warm to room temperature, and conducted over 2 h. The reaction was quenched with H_2O (20 mL) at 0 °C. The aqueous phase was extracted with toluene (10 mL x 3), combined organic phases were washed with brine (30 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by silica-gel column chromatography (eluent, hexane/toluene, 1:2) gave 341 mg of **9** (51%) as white solid materials. Data of **9**: Rf value 0.35 (hexane/toluene, 1:4); M.p. 293 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.27 (s, 4H), 3.99 (s, 12H), 3.51 (qq, *J* = 6.9, 6.8 Hz, 4H), 2.52 (s, 12H), 1.49 (d, *J* = 6.9, 12H), 1.19 (d, *J* = 6.8, 12H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 155.9, 140.7, 130.9, 129.5, 128.3, 128.2, 123.7, 61.8, 27.7, 24.7, 17.9 ppm; MS (DART-TOFMS) m/z: 673 $[MH]^+$; IR (neat): 2955, 1397, 1318, 1247, 1124, 1072, 1006, 871 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{46}H_{57}O_4$ $[MH]^+$: 673.4257, Found: 673.4238; Anal. Calcd. for $C_{46}H_{56}O_4$; C, 82.10; H, 8.39. Found: C, 82.12; H, 8.32.



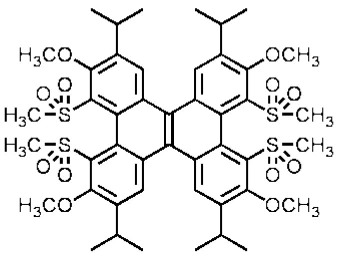
9

11. Synthesis of **10** and **11** (Scheme 3(b)). Under an Ar atmosphere, to a suspension of **1** (466 mg, 0.5 mmol) in dry Et_2O (10 mL) at 0 °C was added MeLi (2.1 mL, 2.5 mmol, 1.2 M in Et_2O) dropwise over 4 min. The mixture was stirred at 0 °C for 30 min, and dimethyl disulfide (0.9 mL, 10 mmol) was slowly added over 2 min. After stirred at 0 °C for 30 min, the reaction mixture was allowed to warm to room temperature, and conducted over 2 h. The reaction was quenched with H_2O (10 mL) at 0 °C. The aqueous phase was extracted with toluene (10 mL x 3), combined



10

organic phases were washed with brine (10 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by silica-gel column chromatography (eluent, hexane/toluene, 1:1) gave 267 mg of **10** (67%) as yellowish white solid materials. Data of **10**: Rf value 0.53 (hexane/toluene, 1:4); M.p. 192 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.32 (s, 4H), 4.28 (s, 12H), 3.58 (qq, *J* = 7.0, 6.9 Hz, 4H), 1.99 (s, 12H), 1.52 (d, *J* = 7.0, 12H), 1.18 (d, *J* = 6.9, 12H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 157.0, 142.0, 132.7, 132.1, 127.9, 127.2, 125.1, 62.1, 28.2, 24.5, 23.7, 20.7 ppm; MS (DART-TOFMS) m/z: 801 $[MH]^+$; IR (neat): 2952, 2917, 1388, 1308, 1057, 1006, 754 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{46}H_{57}O_4S_4$ $[MH]^+$: 801.3140, Found: 801.3141; Anal. Calcd. for $C_{46}H_{56}O_4S_4$; C, 68.96; H, 7.05. Found: C, 68.78; H, 7.22. For **11**: **10**

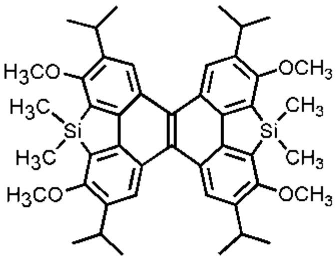


11

(300 mg, 0.37 mmol) and hydrogen peroxide (7.4 mL, 95 mmol, 30% aq.) were dissolved in the mixed solvent of CH_2Cl_2 (3.7 mL) and acetic acid (7.4 mL). After stirred at 60 °C for 19 h, the reaction was quenched with satd. aq. $NaHCO_3$ (20 mL) at 0 °C, and the mixture was diluted with toluene. The aqueous phase was extracted with toluene (20 mL x 3), combined organic phases were washed with satd. aq. $NaHCO_3$ (20 mL x 3), washed with brine (20 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by silica-gel column chromatography (eluent, hexane/EtOAc, 1:1) gave 263 mg of **11** (77%) as whitish yellow solid materials. Data of **11**: Rf value 0.35 (hexane/EtOAc, 1:1); M.p. 292 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.44 (s, 4H), 4.18 (s, 12H), 3.54 (qq, *J* = 6.8, 6.8 Hz, 4H), 3.21 (s, 12H), 1.53 (d, *J* = 6.8, 12H), 1.23 (d, *J* = 6.8, 12H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 155.1, 144.6, 137.8, 129.7, 127.7, 127.5, 124.3, 65.2, 46.1, 27.4, 24.5, 23.8 ppm; MS (DART-TOFMS) m/z: 946 $[MNH_4]^+$; IR (neat): 2965, 1460, 1304 ($-SO_2-$), 1137, 1122, 957, 742, 473 cm^{-1}; HRMS (DART-TOF) calcd. for

$C_{46}H_{60}NO_{12}S_4$ $[MNH_4]^+$: 946.2998, Found: 946.2991; Anal. Calcd. for $C_{46}H_{56}O_{12}S_4$; C, 59.46; H, 6.07. Found: C, 59.46; H, 6.19.

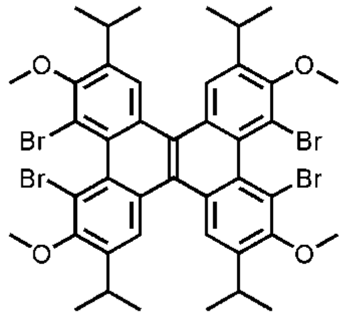
12. Synthesis of **12** (Scheme 3(c)). Under an Ar atmosphere, to a solution of **1** (1.86 g, 2 mmol) in dry THF (40 mL) at 0 °C was added *n*-BuLi (6.4 mL, 10 mmol, 1.56 M in hexane) dropwise over 4 min. After the mixture was stirred for 15 min at 0 °C, dichlorodimethylsilane (0.57 mL, 4.8 mmol) was added over 2.5 min. After stirred for 30 min at 0 °C, the reaction mixture was heated at 60 °C for 24 h. The reaction was quenched with H_2O (40 mL) at 0 °C. The aqueous phase was extracted with toluene (30 mL x 3), combined organic phases were washed with brine (50 mL), dried over Na_2SO_4, and concentrated *in vacuo* to give crude products. Purification by silica-gel column chromatography (eluent, hexane/toluene, 1:1) gave 310 mg of **12** (21%) as orangish yellow solid materials. Data of **12**: Rf value 0.35 (hexane/toluene, 1:1); M.p. 148 ºC (dec.); ^{1}H NMR (400 MHz, $CDCl_3$) 8.68 (s, 4H), 4.09 (s, 12H), 3.59 (sept, J = 7.0 Hz, 4H), 1.40(d, J = 7.0 Hz, 24H), 0.81 (s, 12H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) 160.9, 141.6, 140.1, 128.4, 125.9, 124.7, 123.7, 61.8, 27.6, 24.6, 0.14 ppm; MS (DART-TOFMS) *m/z*: 729 $[MH]^+$; IR (neat): 2956, 1451, 1395, 1240, 1165, 1061, 886, 834, 786, 750 cm^{-1}; HRMS (DART-TOF) calcd. for $C_{46}H_{57}O_4Si_2$ $[MH]^+$:729.3795, found: 729.3791; Anal. Calcd. for $C_{46}H_{56}O_4Si_2$; C, 75.78; H, 7.74. Found: C, 75.77; H, 7.83.

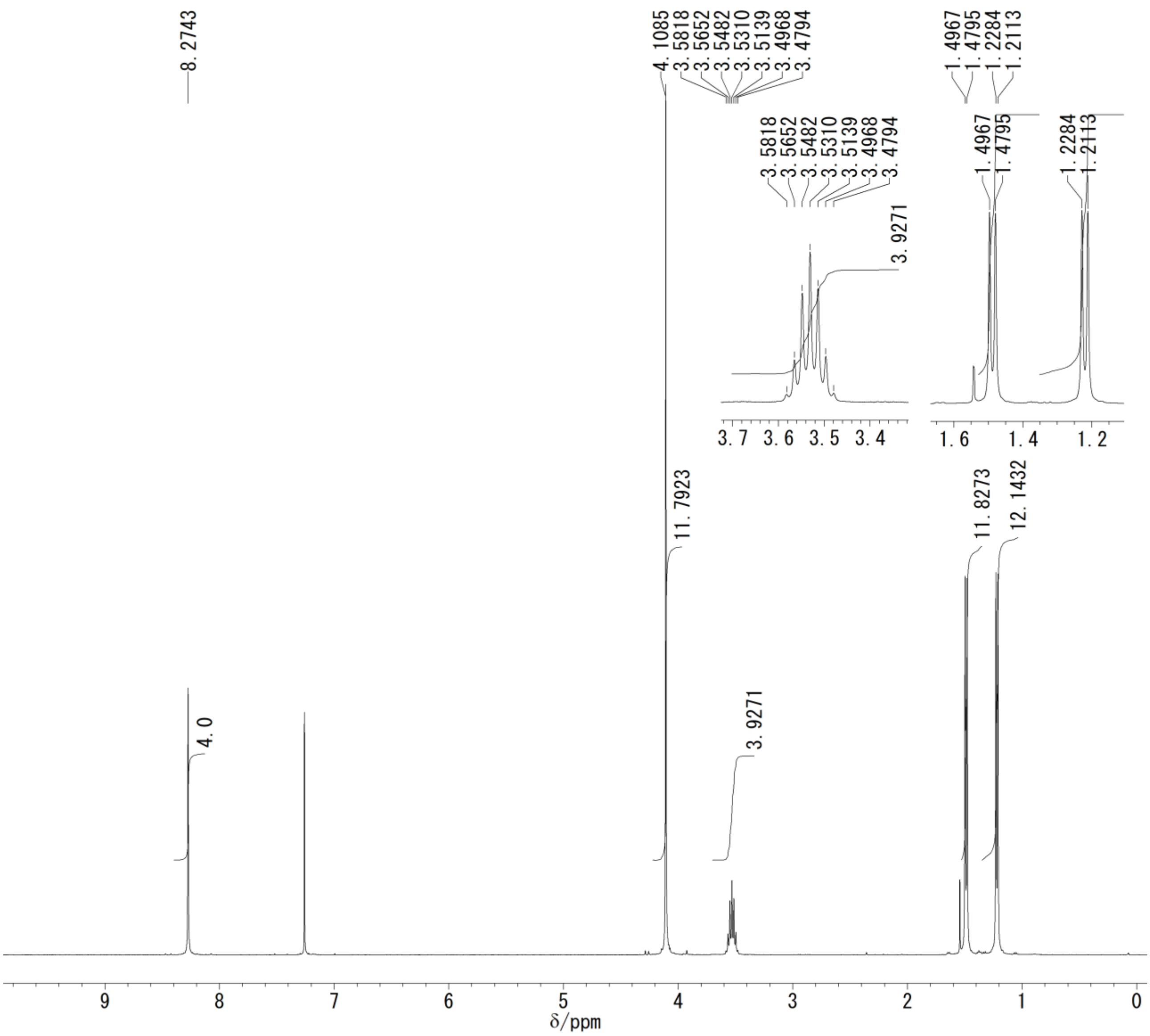


12

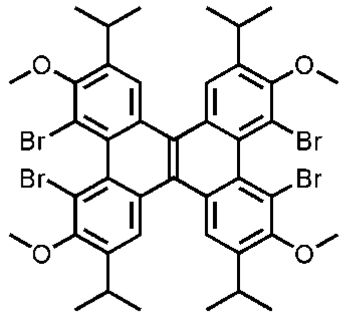
13. ^{1}H NMR and ^{13}C NMR spectra for all new compounds of **1**-**12**.

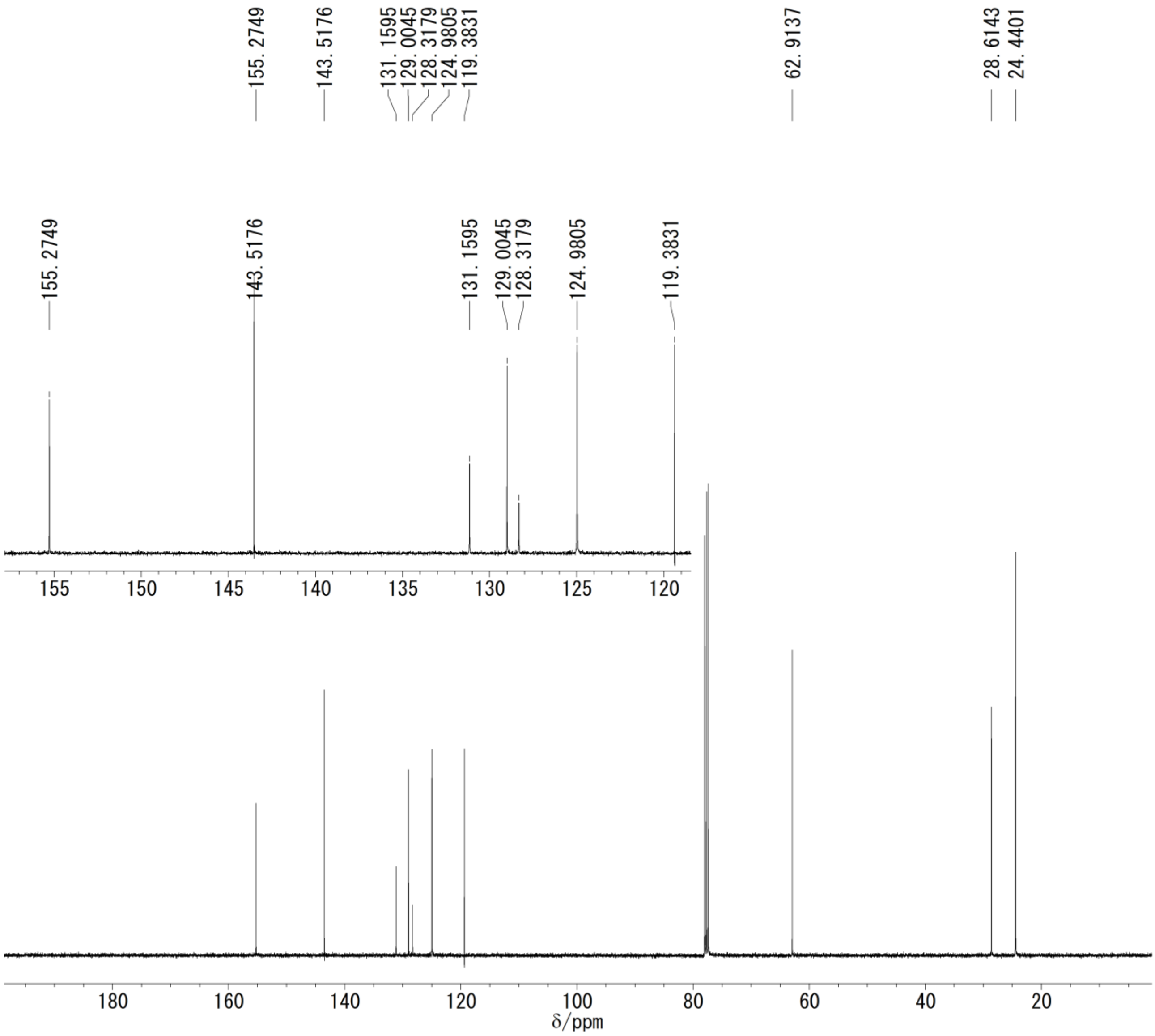
Compound **1** (^{1}H NMR spectrum in $CDCl_3$)



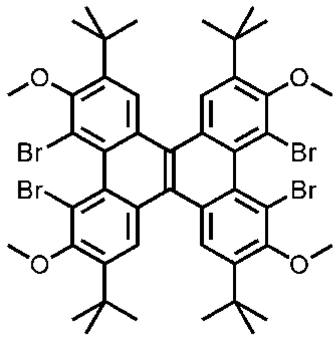


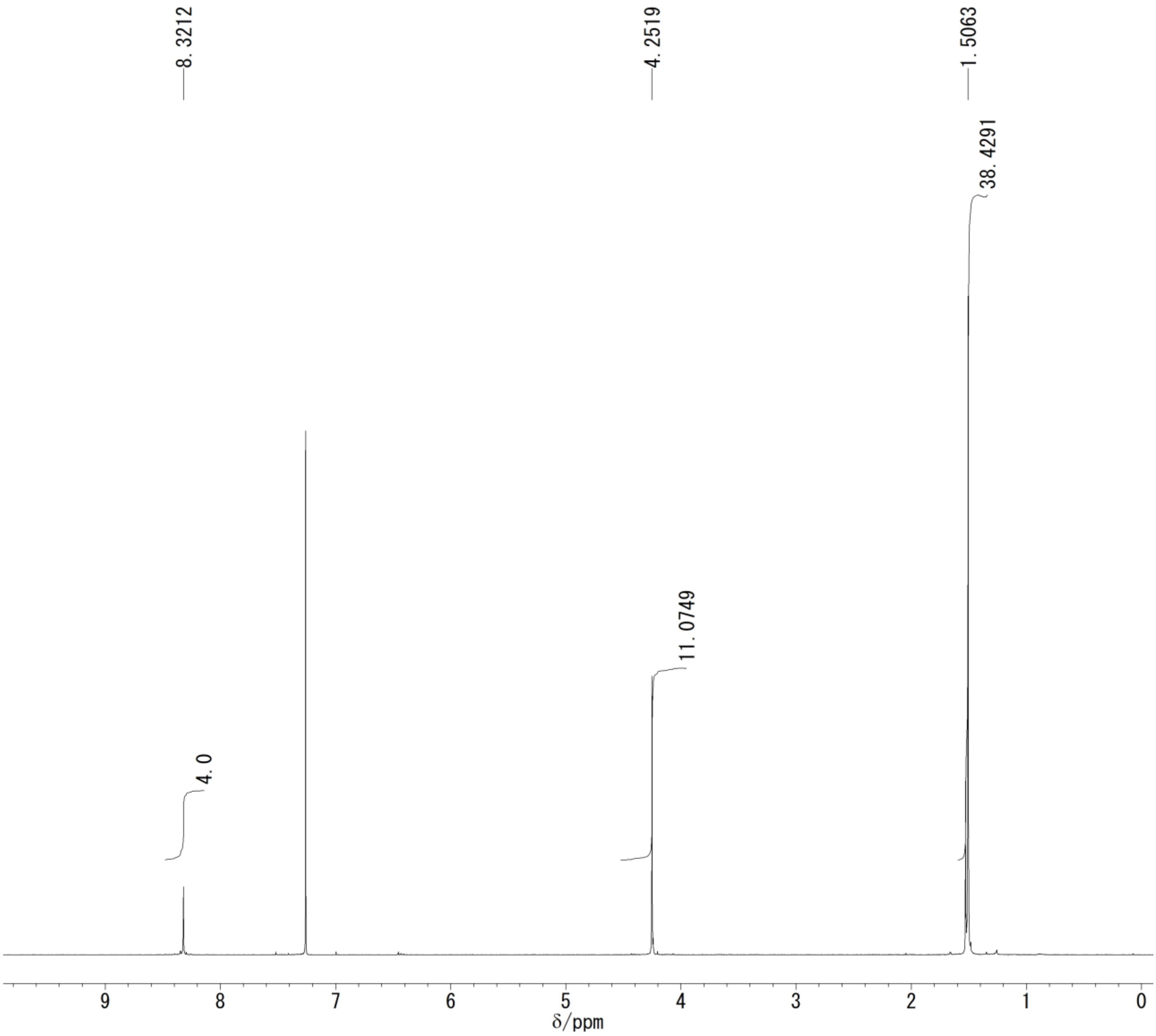
Compound **1** (^{13}C NMR spectrum in $CDCl_3$)



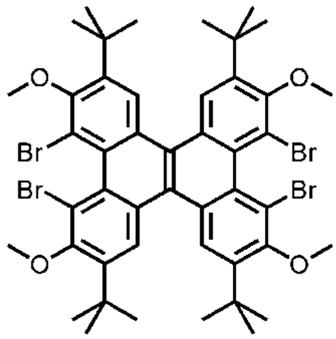


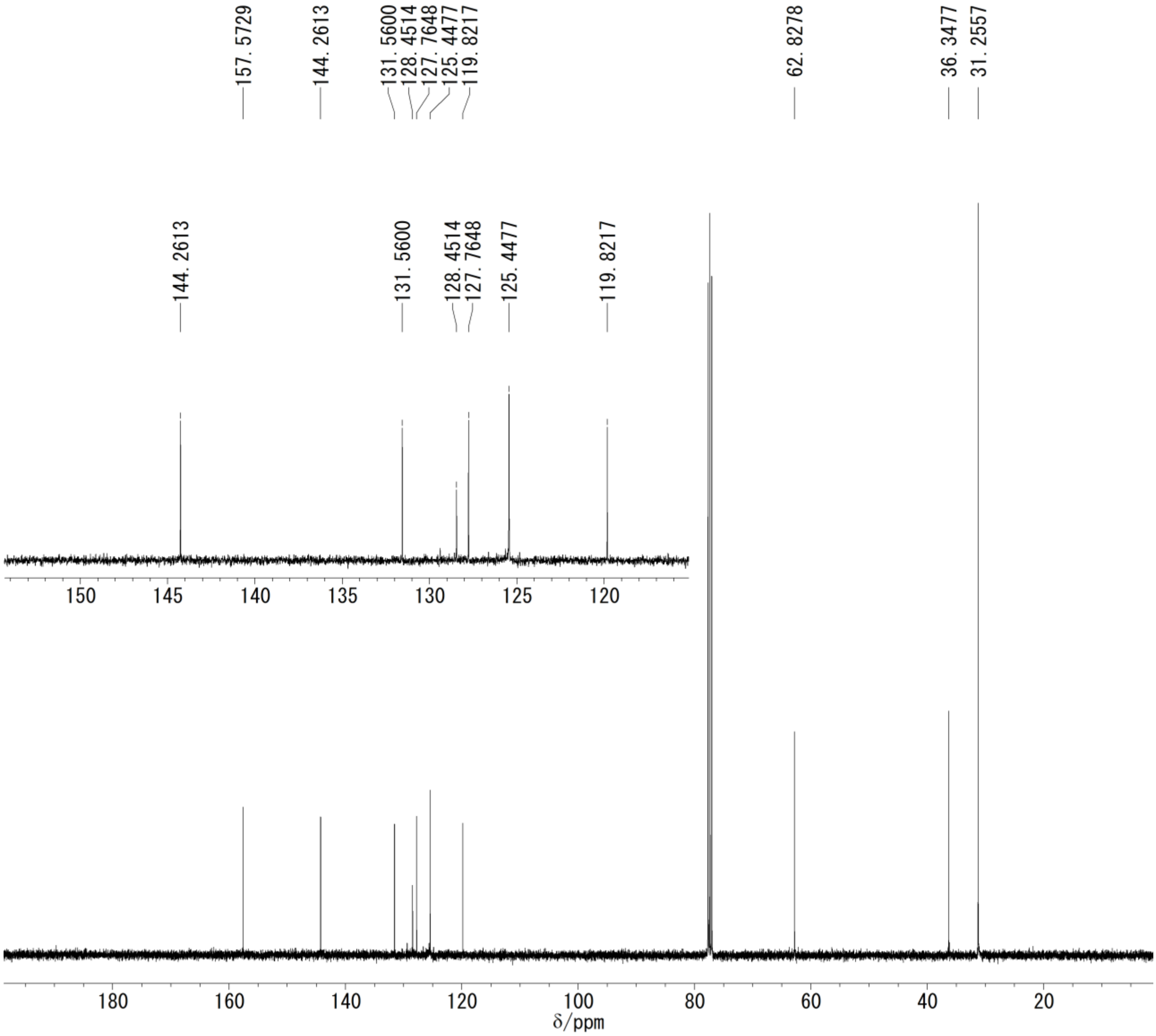
Compound **2** ([1]H NMR spectrum in $CDCl_3$)



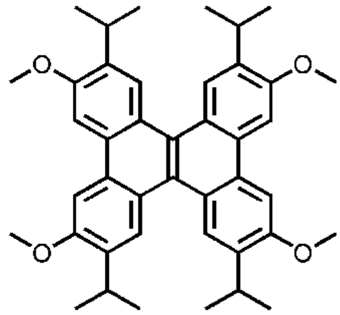


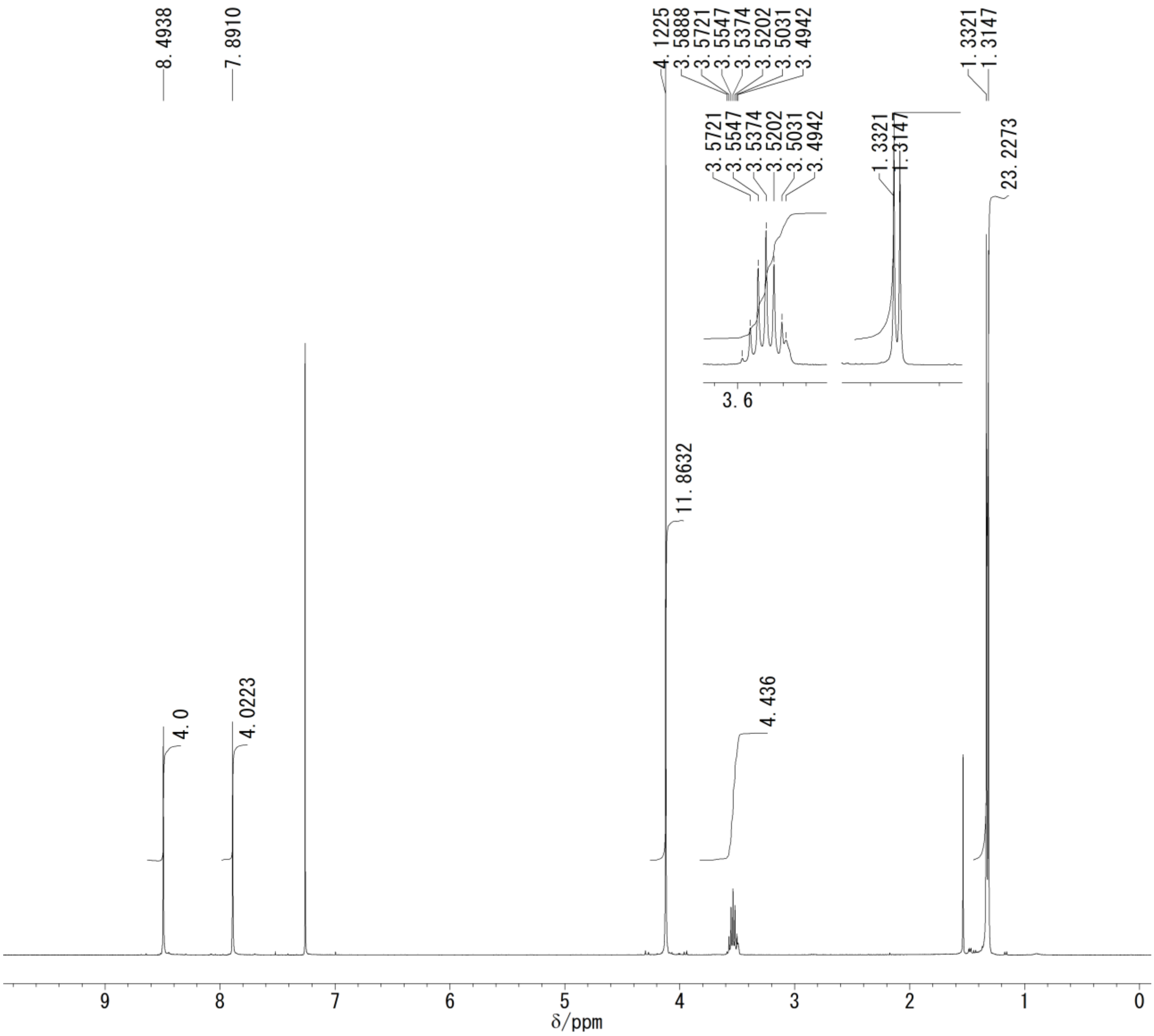
Compound **2** (^{13}C NMR spectrum in $CDCl_3$)



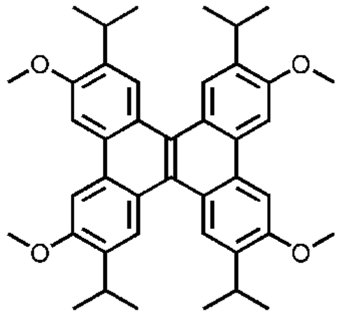


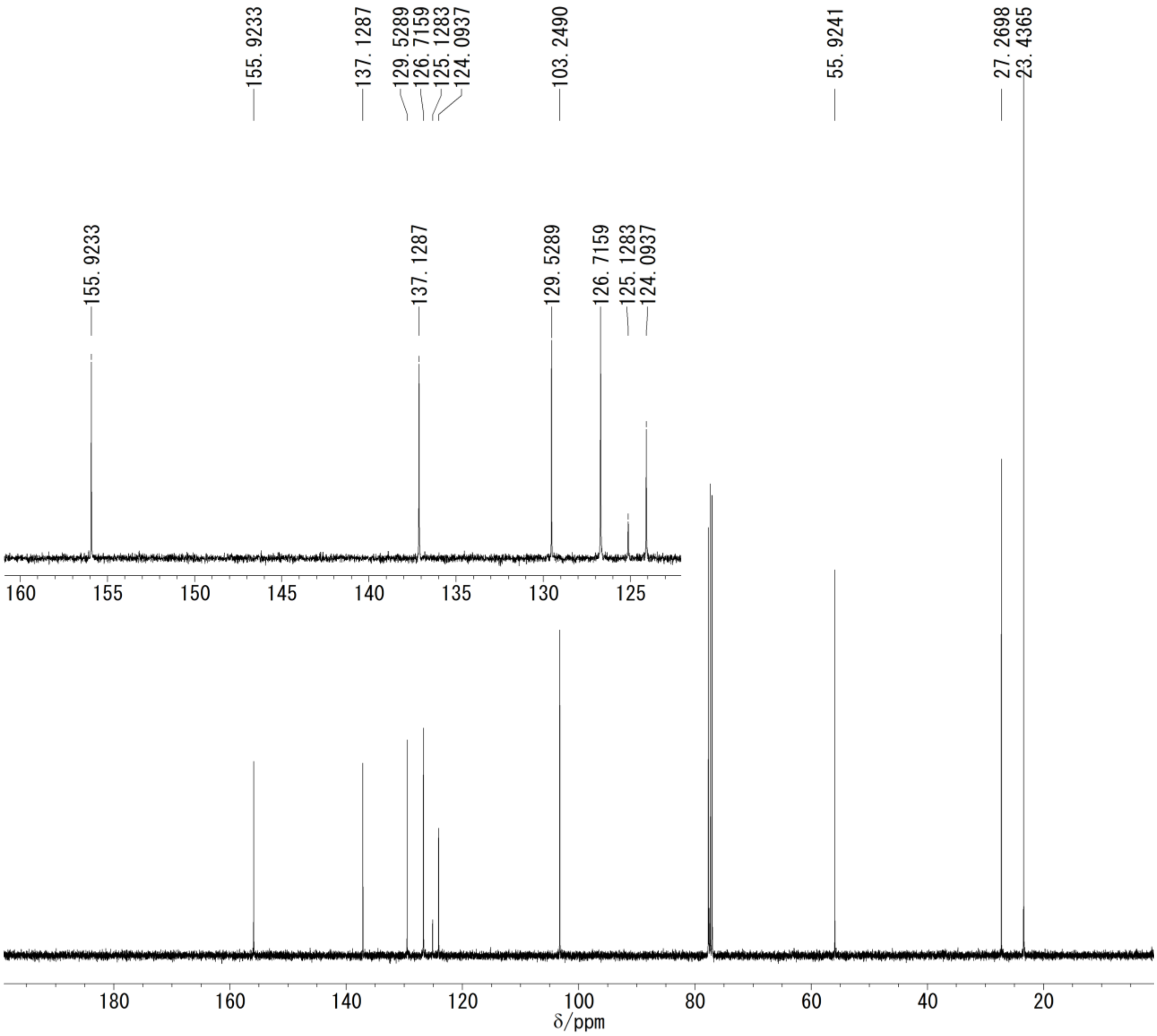
Compound **3** (^1H NMR spectrum in $CDCl_3$)



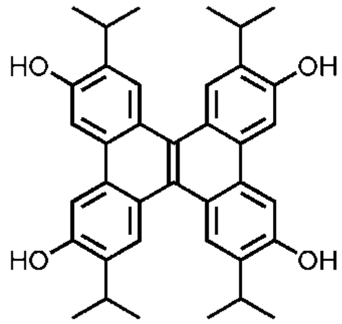


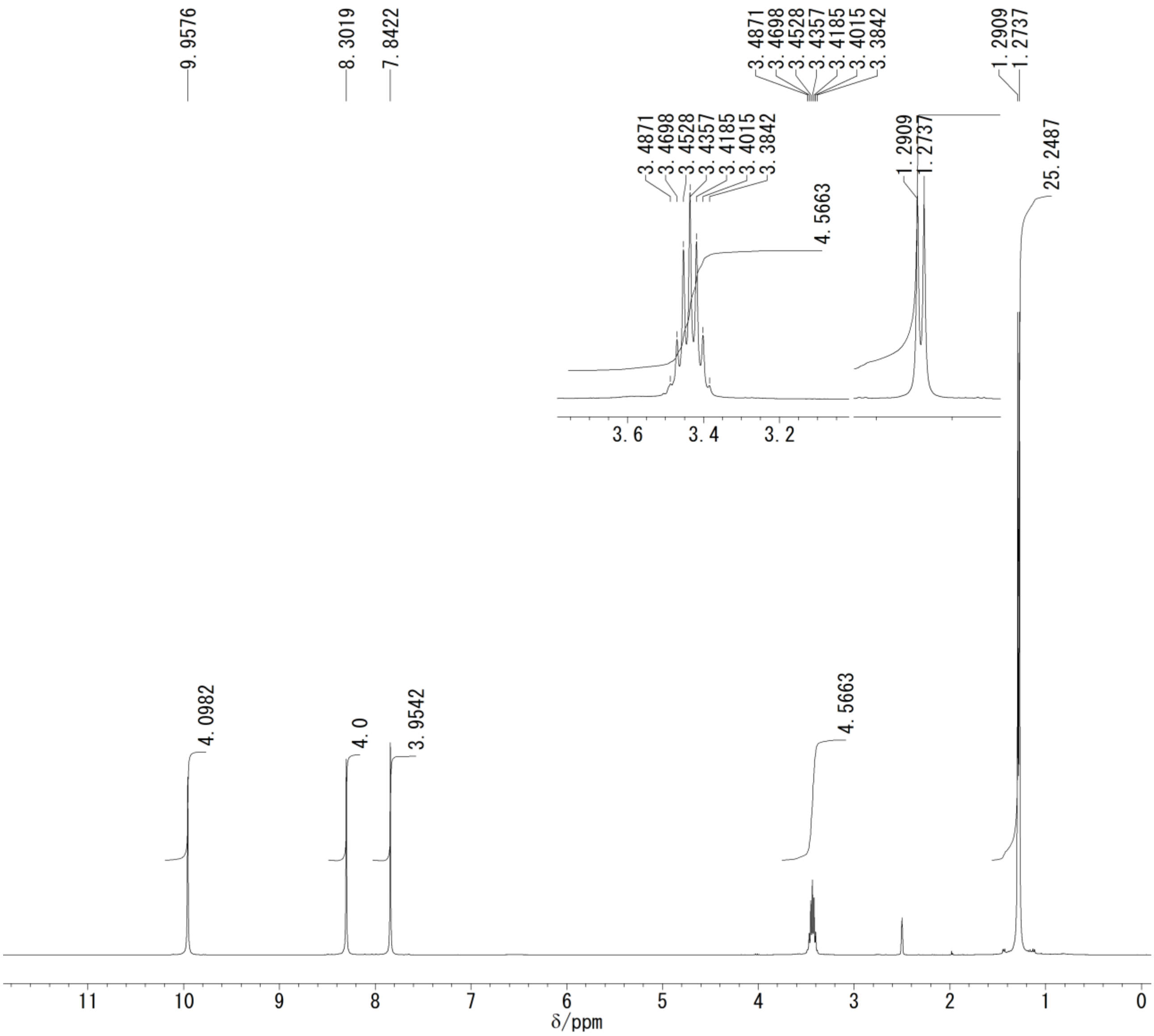
Compound **3** (^{13}C NMR spectrum in $CDCl_3$)



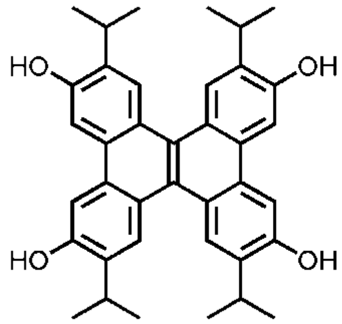


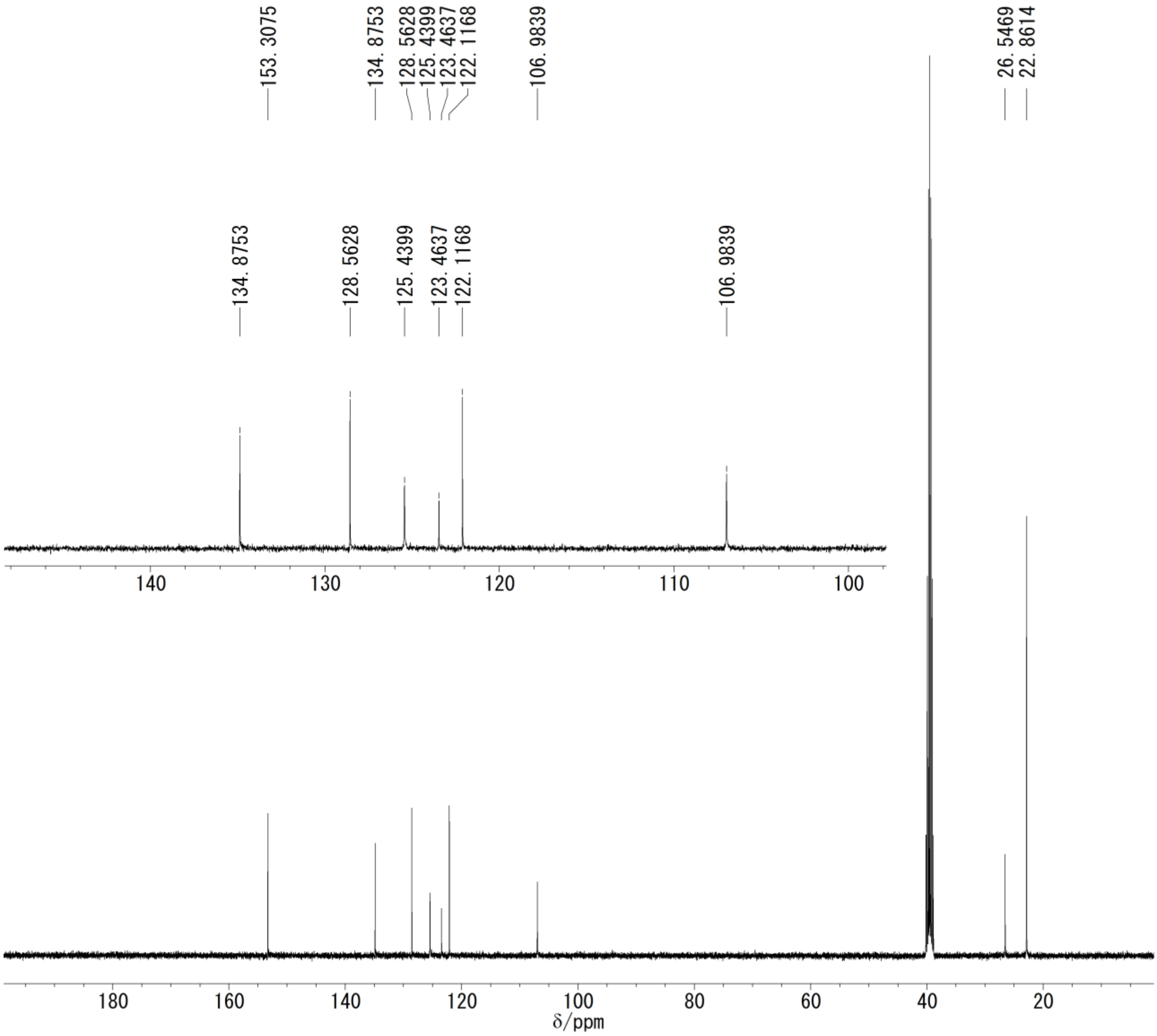
Compound **4** (^{1}H NMR spectrum in DMSO-d_6)



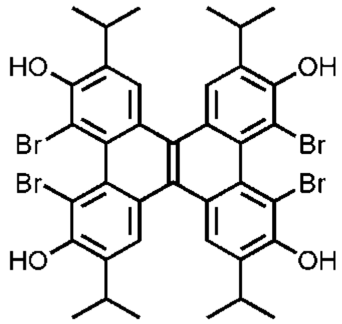


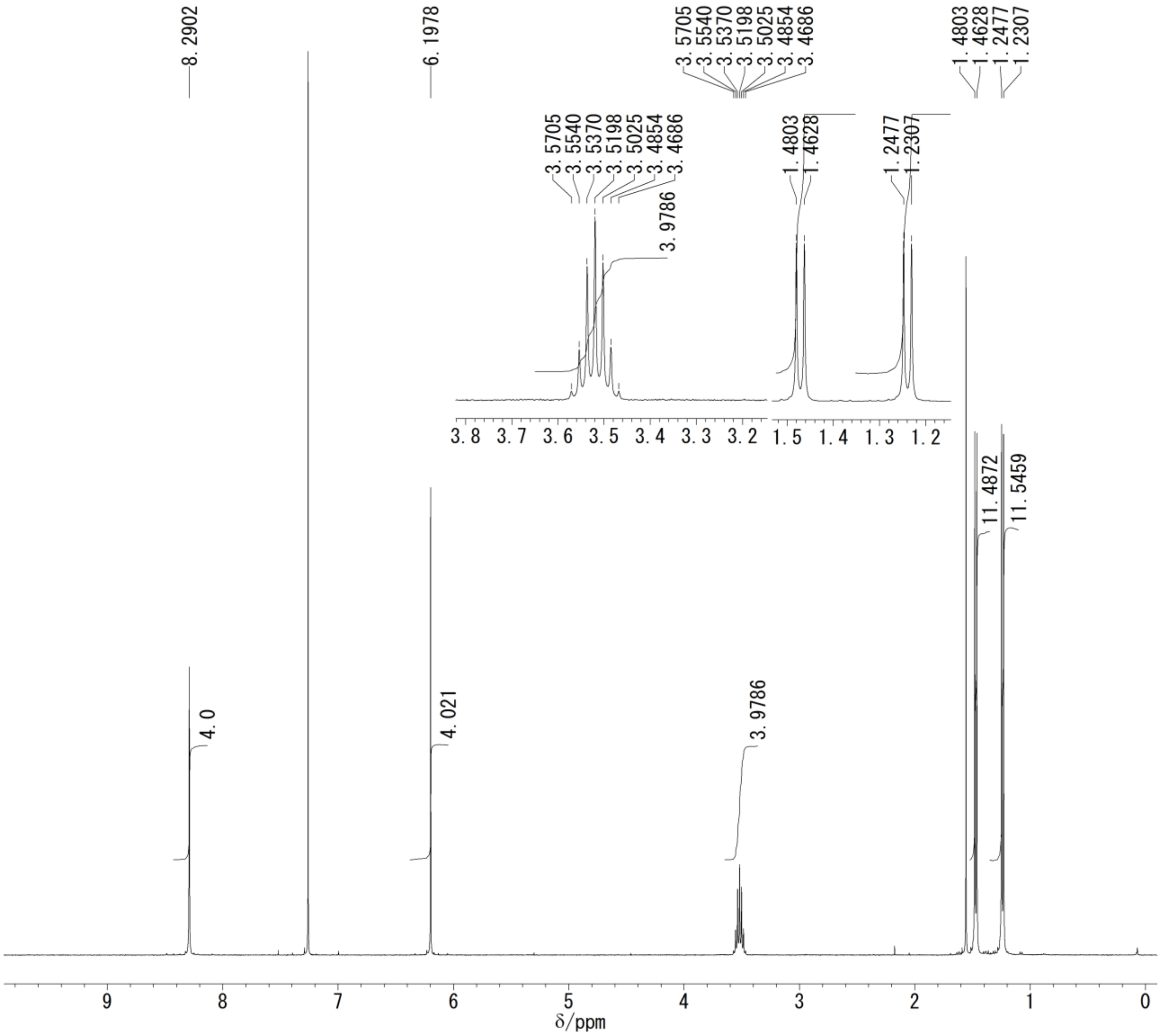
Compound **4** (^{13}C NMR spectrum in DMSO-d_6)



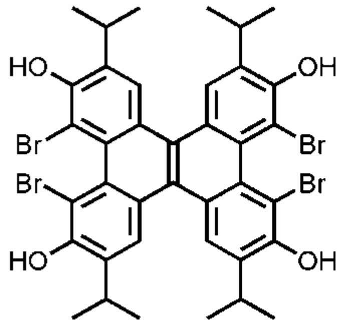


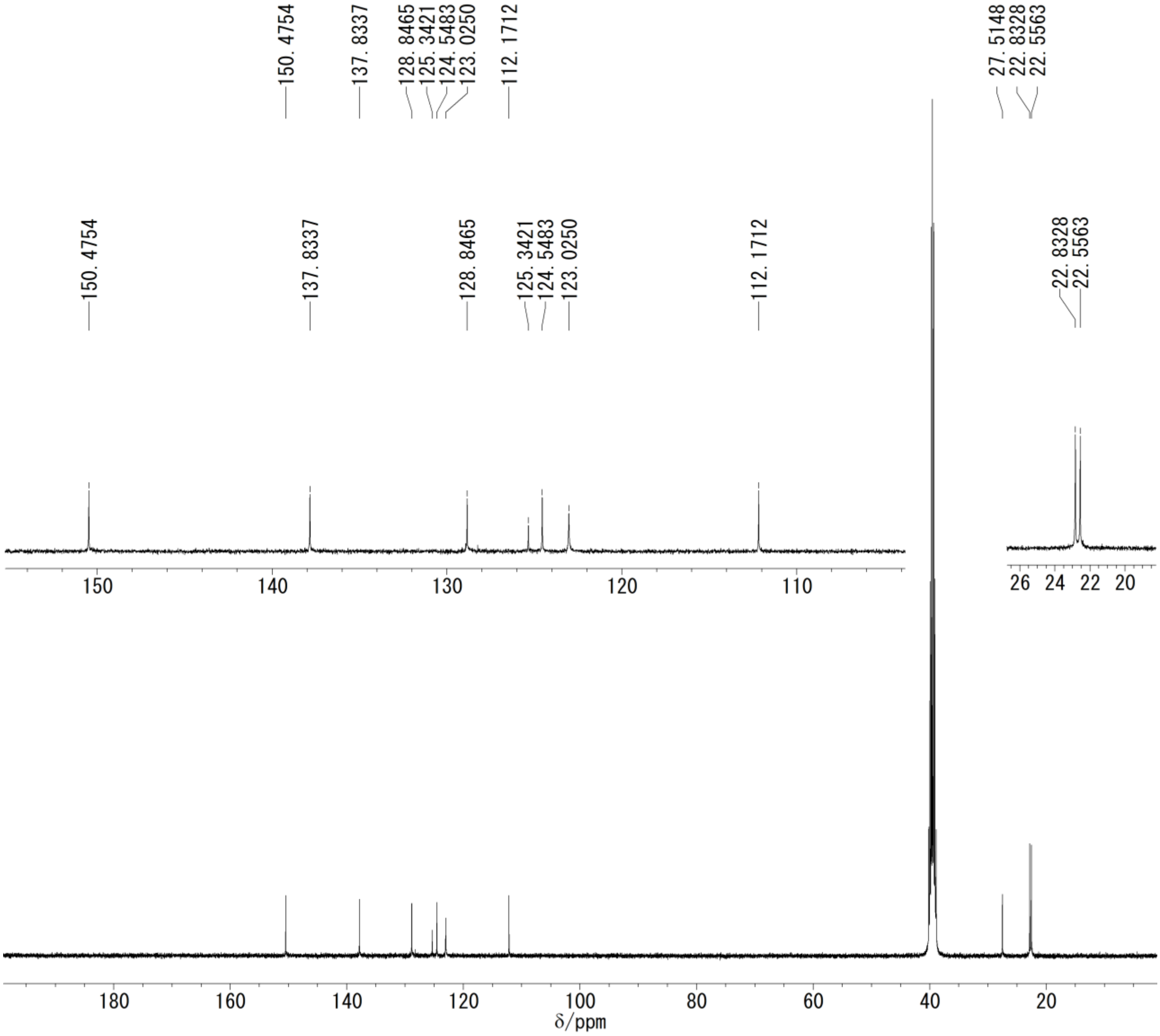
Compound **5** ([1]H NMR spectrum in $CDCl_3$)



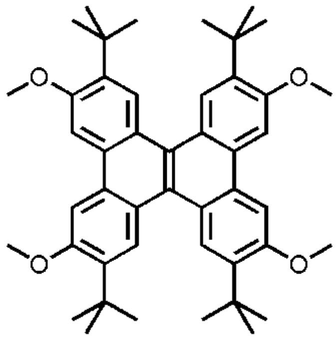


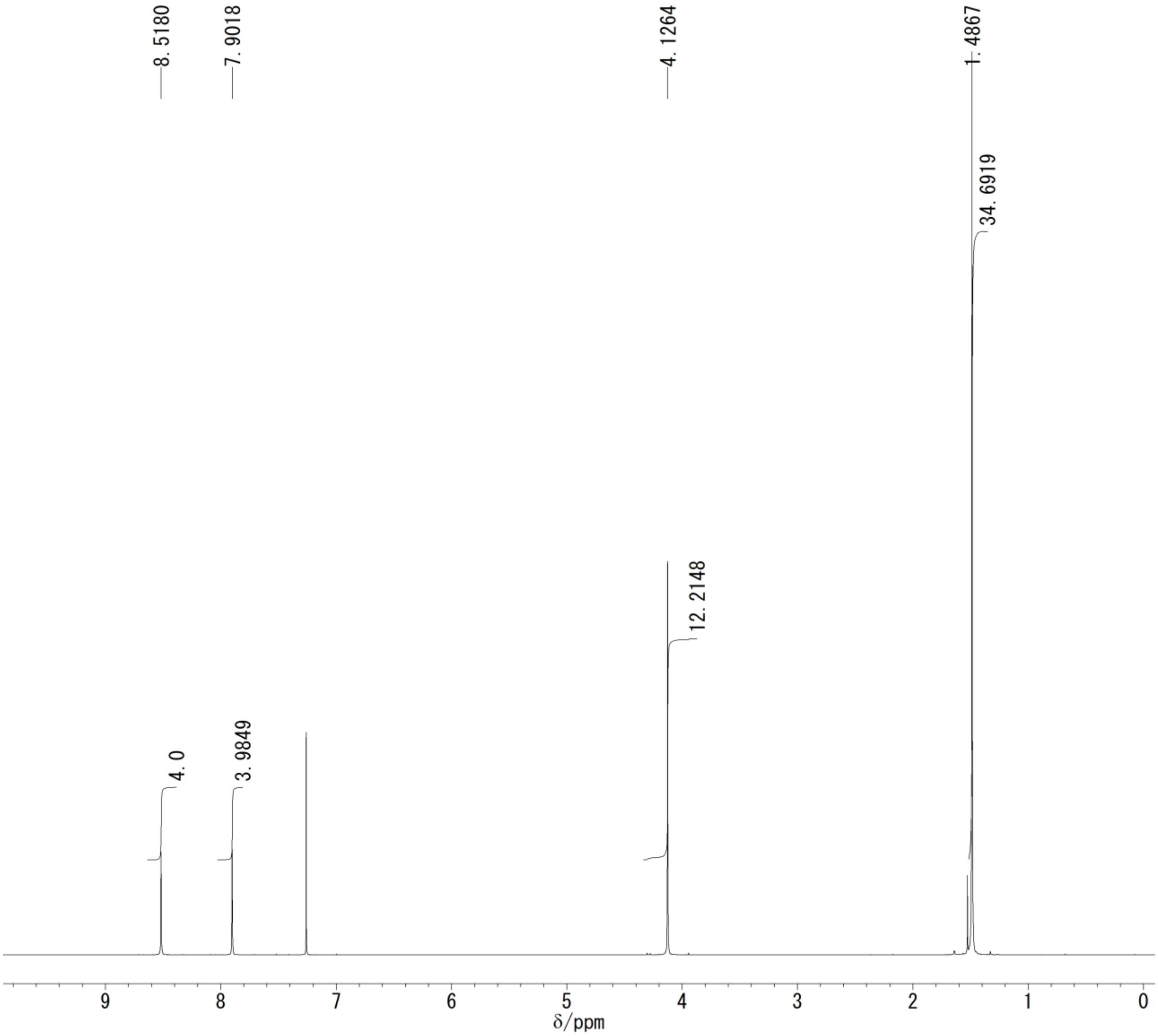
Compound **5** (^{13}C NMR spectrum in DMSO-d_6)



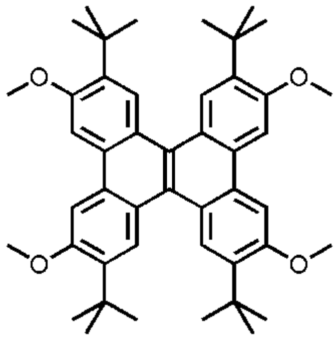


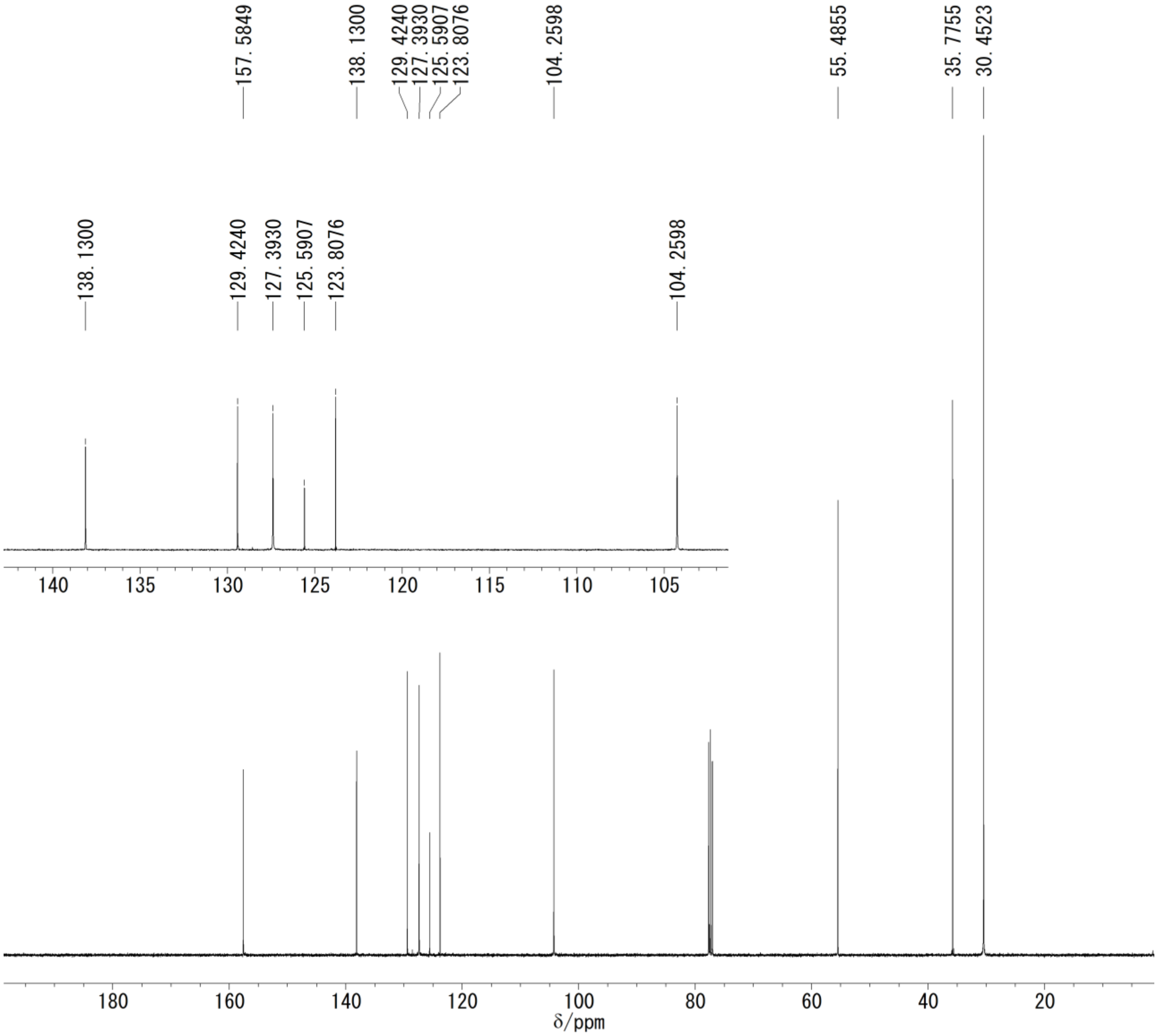
Compound **6** (^{1}H NMR spectrum in $CDCl_3$)



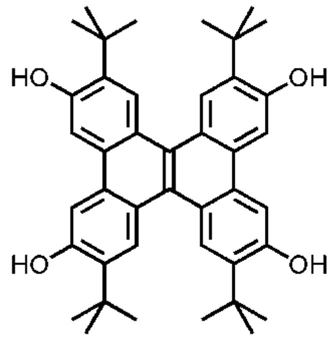


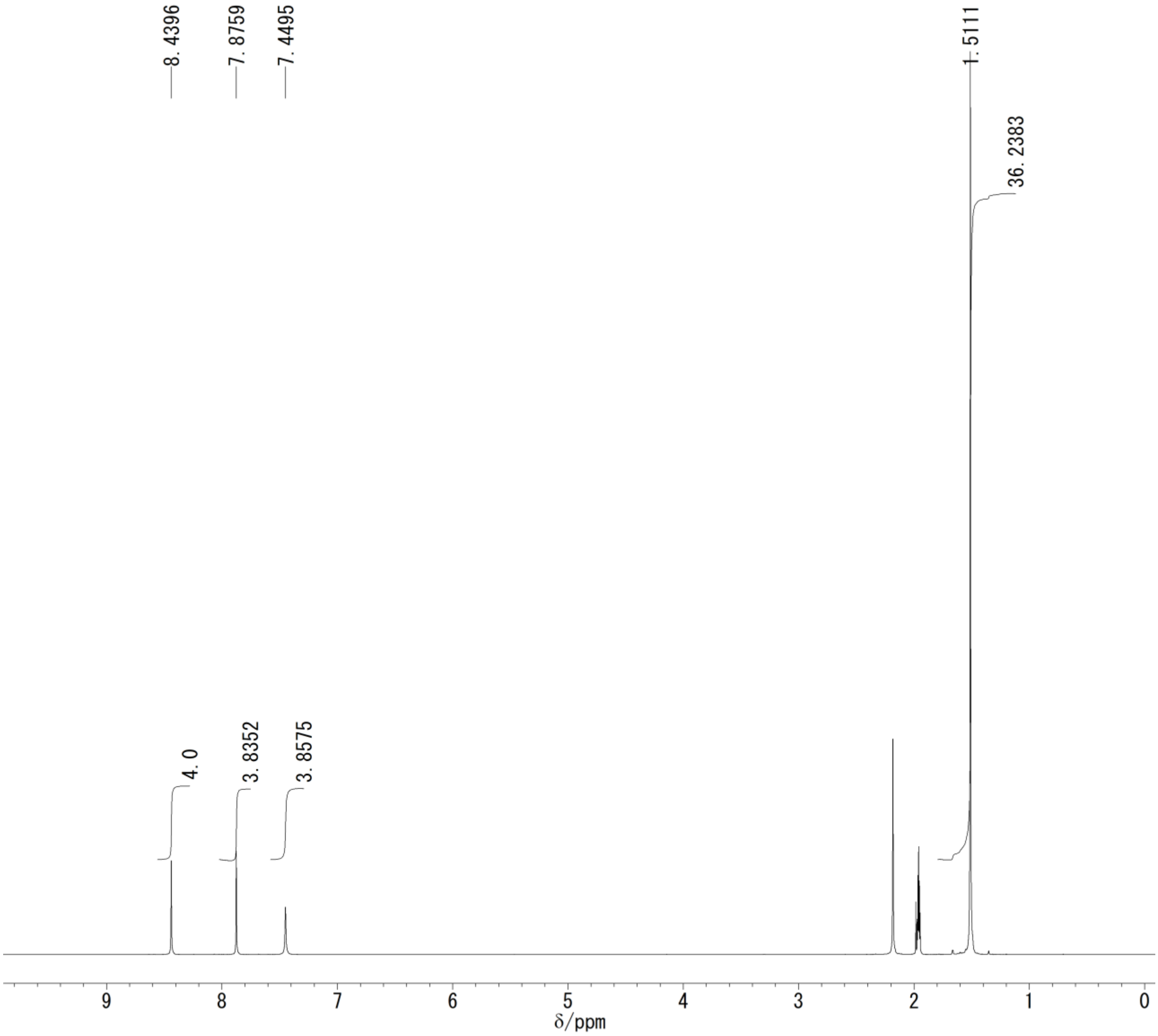
Compound **6** (^{13}C NMR spectrum in $CDCl_3$)



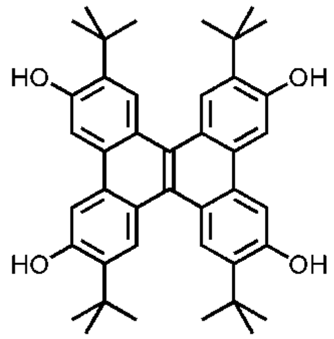


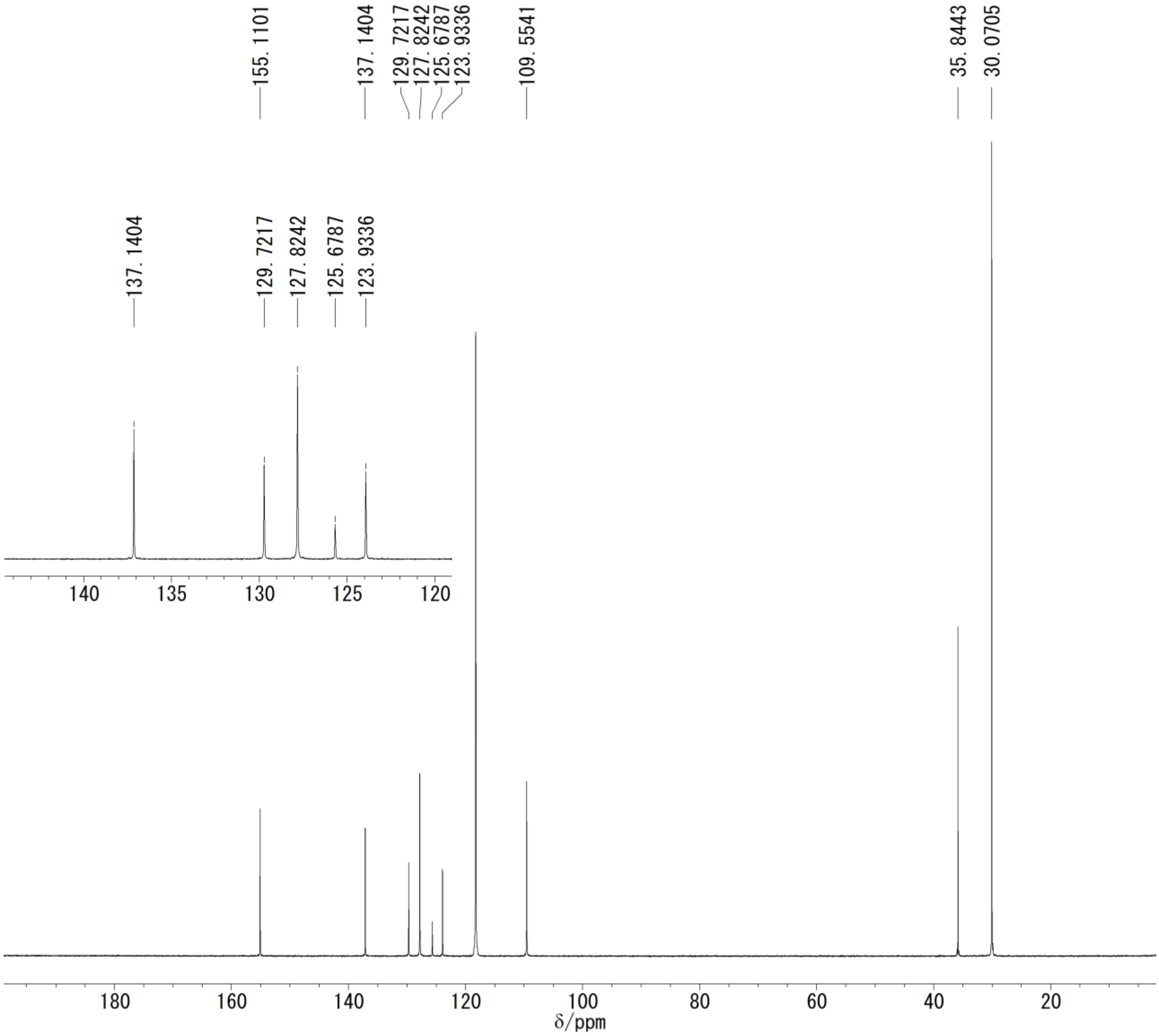
Compound **7** ([1]H NMR spectrum in CD_3CN)



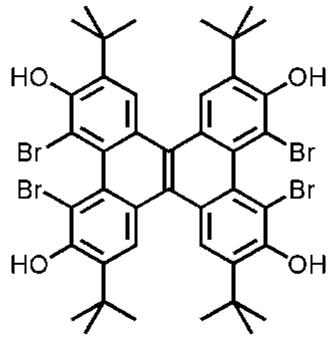


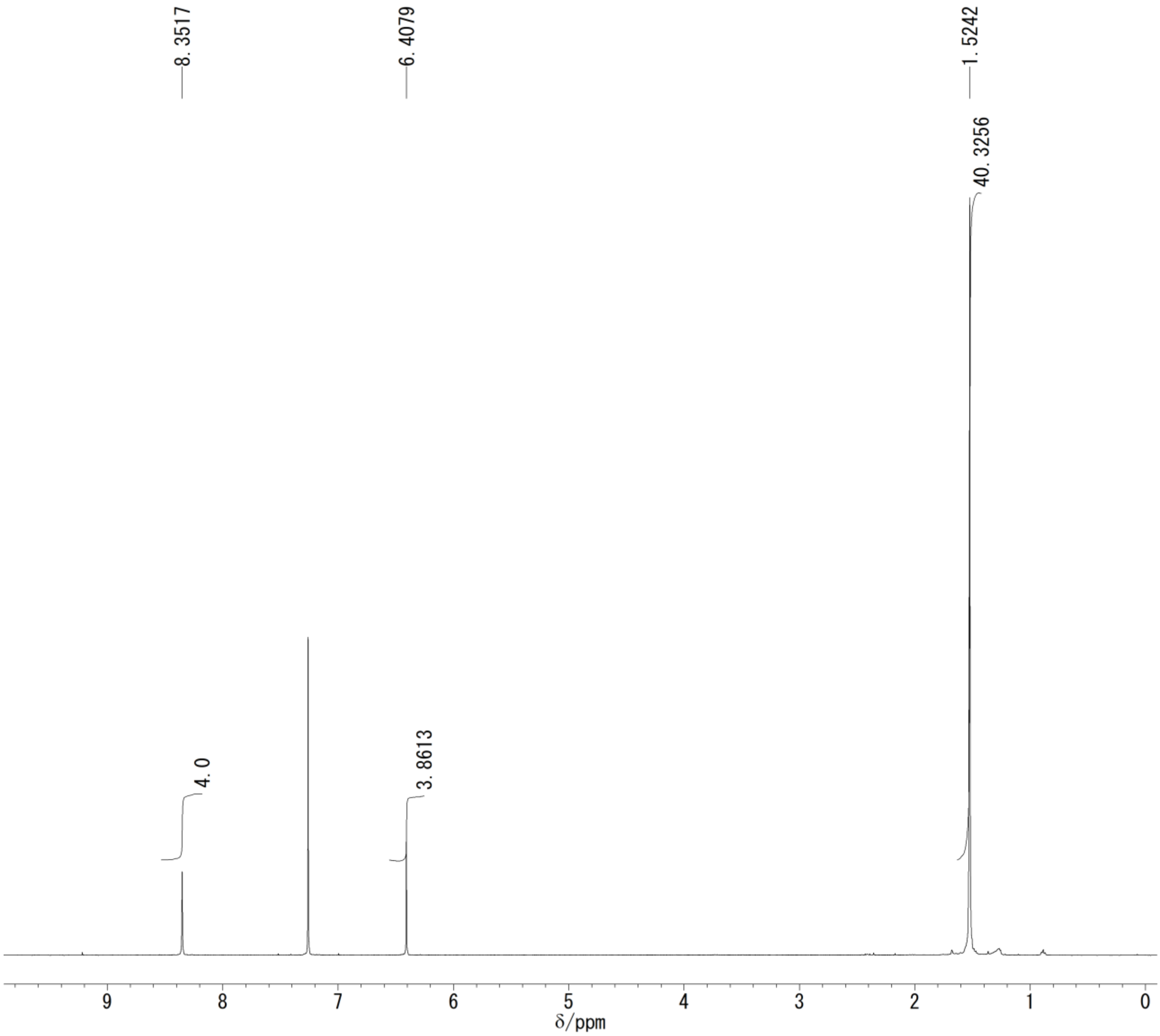
Compound **7** (^{13}C NMR spectrum in CD_3CN)



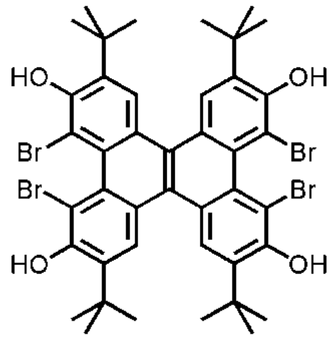


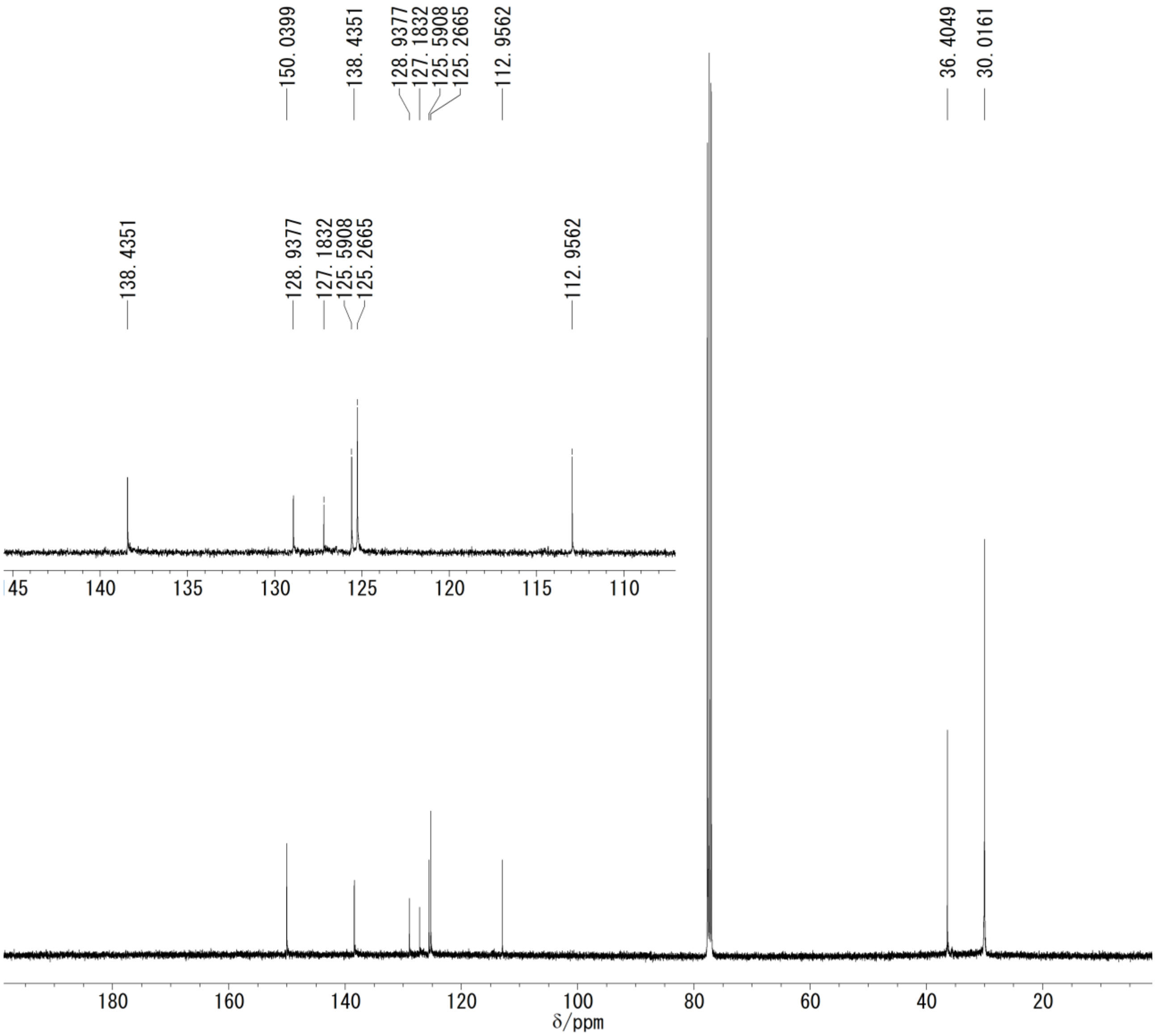
Compound **8** (^{1}H NMR spectrum in $CDCl_3$)



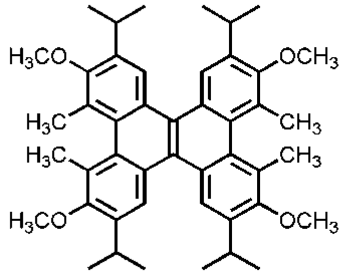


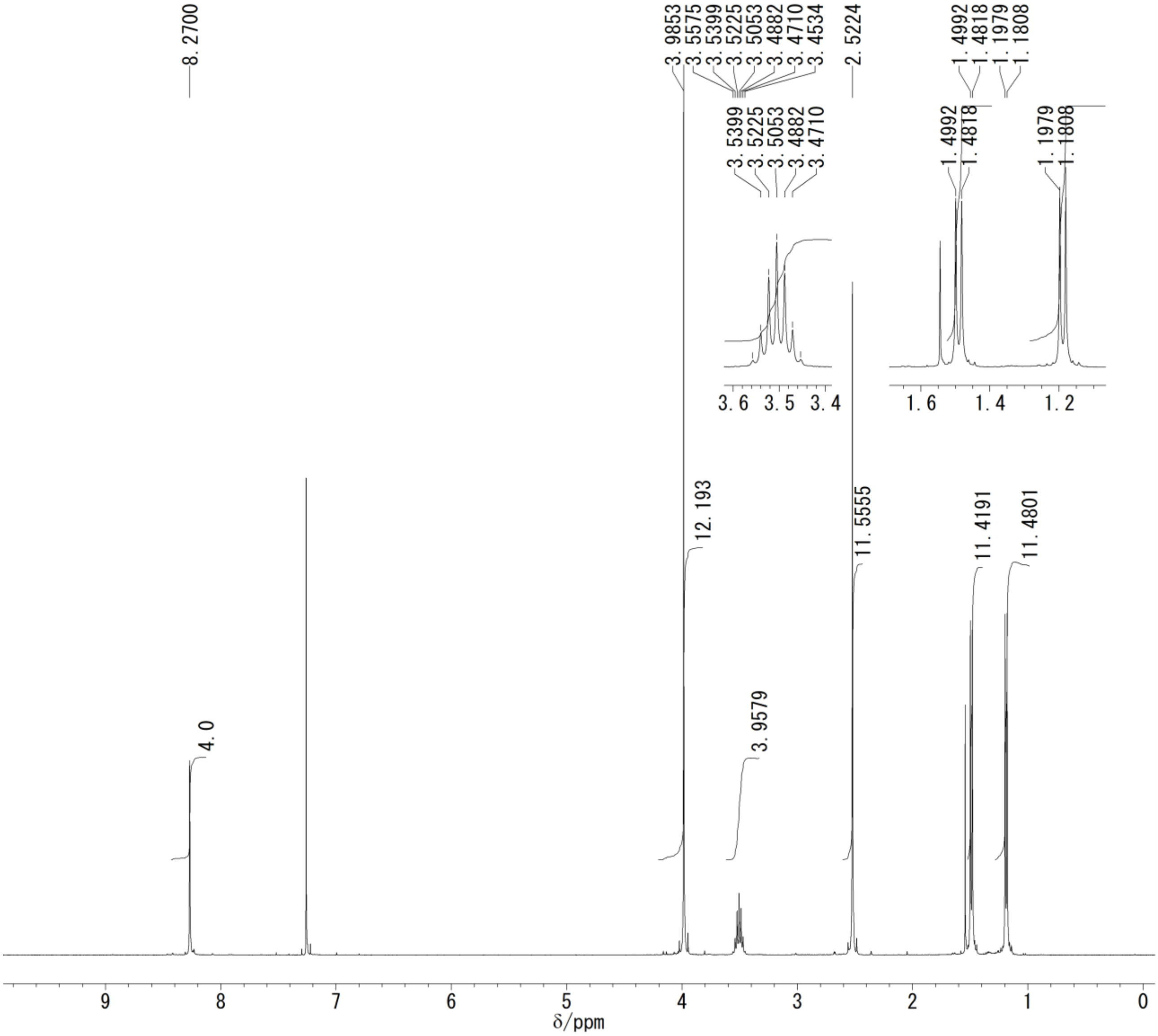
Compound **8** (^{13}C NMR spectrum in $CDCl_3$)



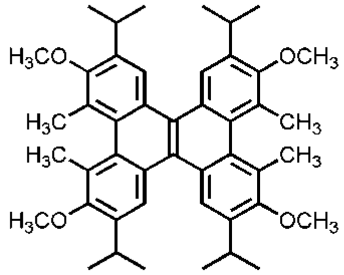


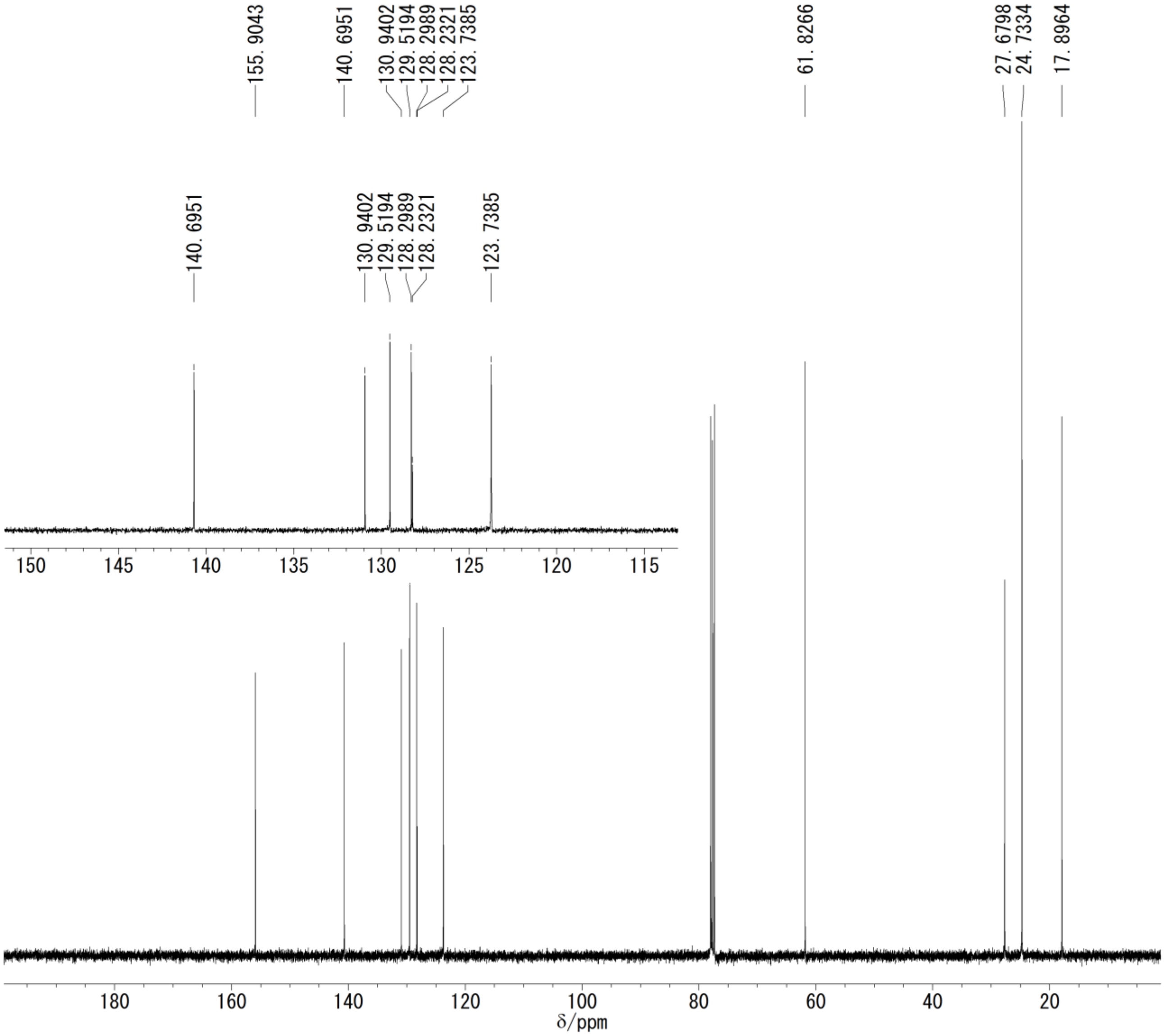
Compound **9** (^{1}H NMR spectrum in $CDCl_3$)



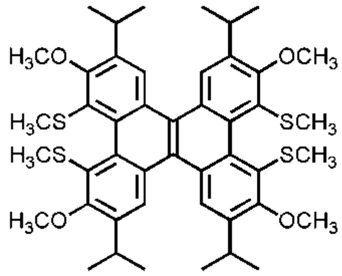


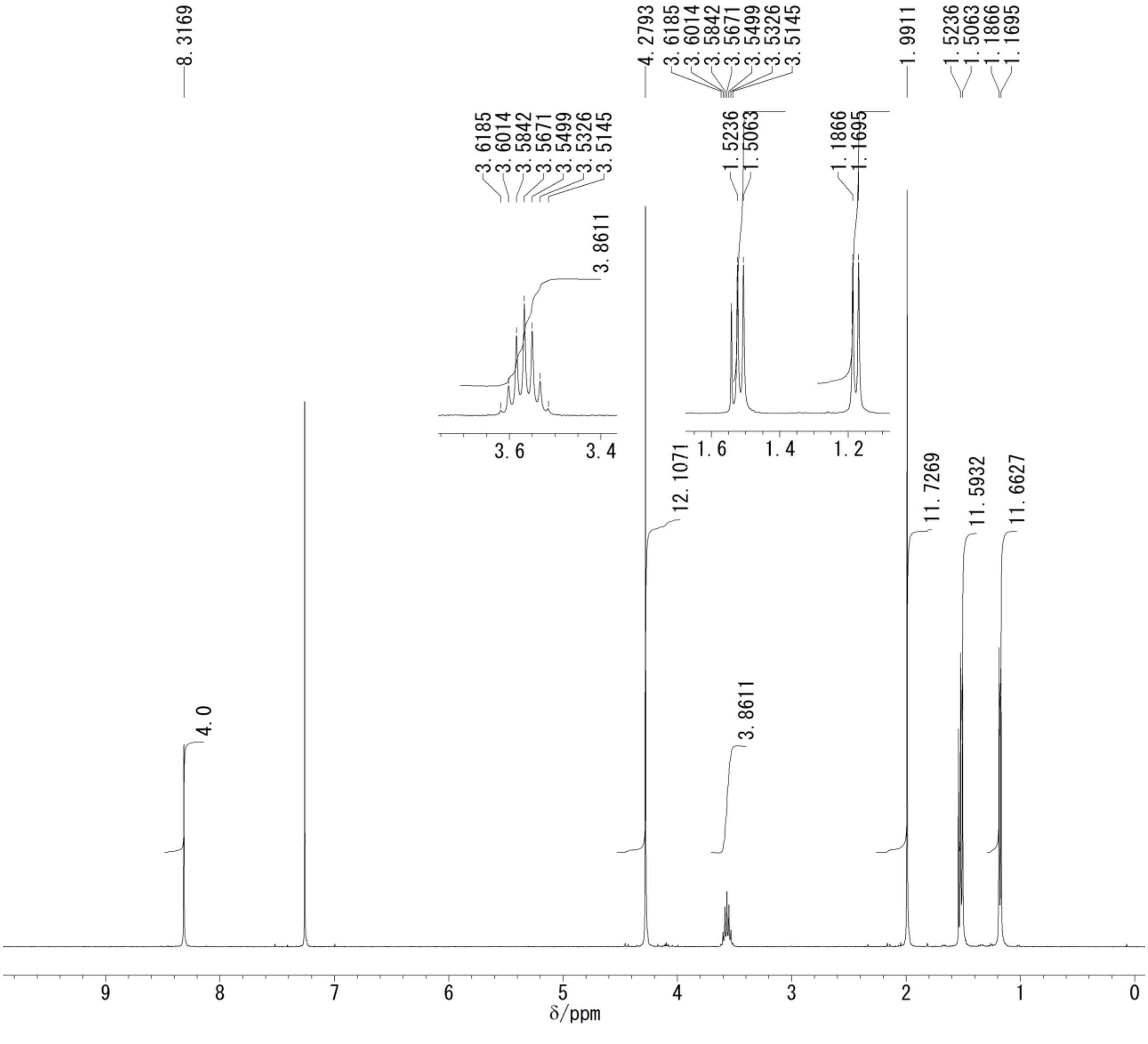
Compound **9** (^{13}C NMR spectrum in $CDCl_3$)



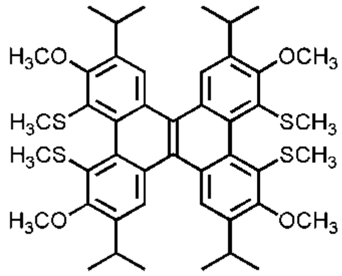


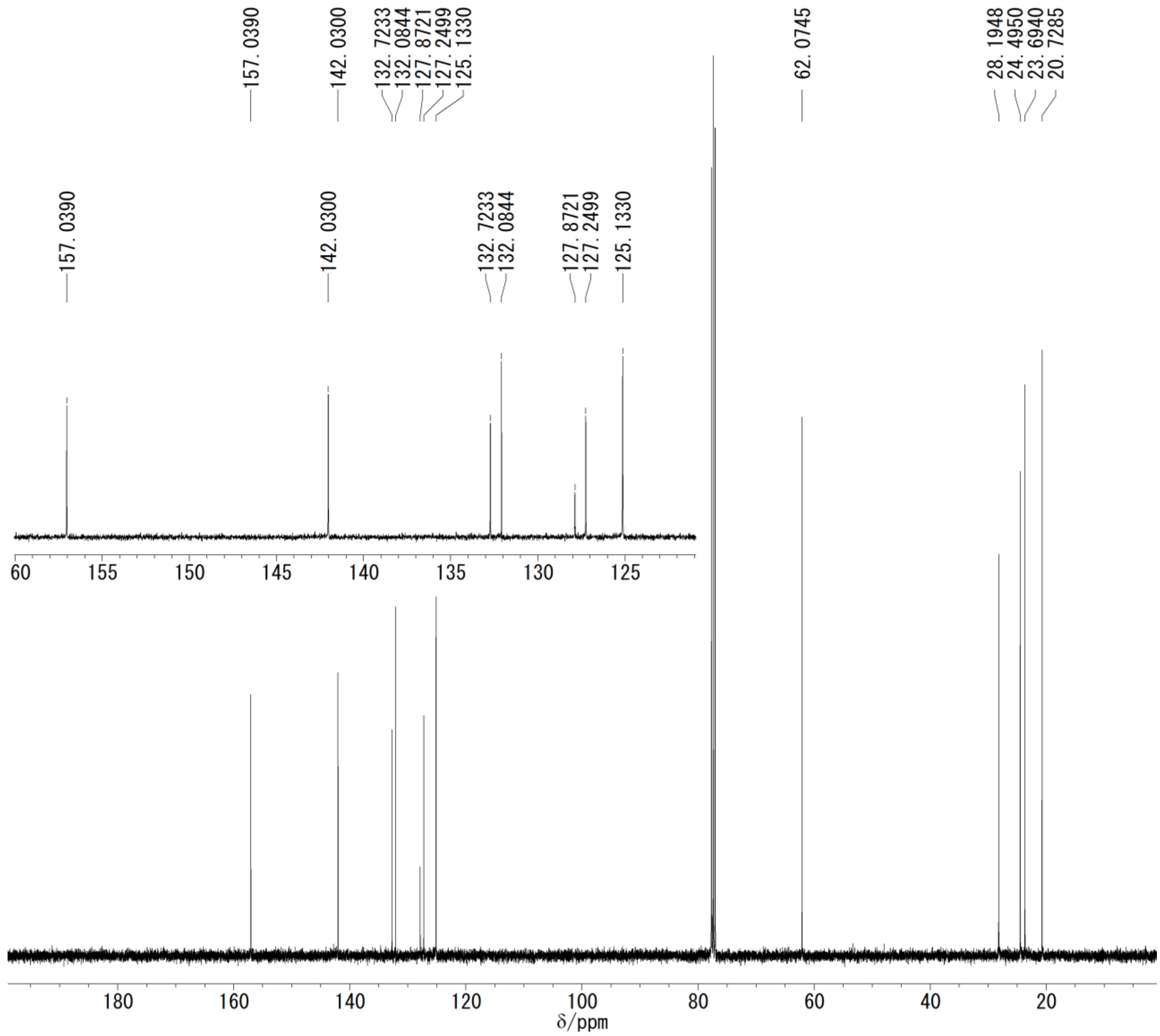
Compound **10** (^1H NMR spectrum in $CDCl_3$)



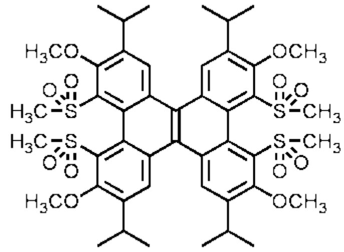


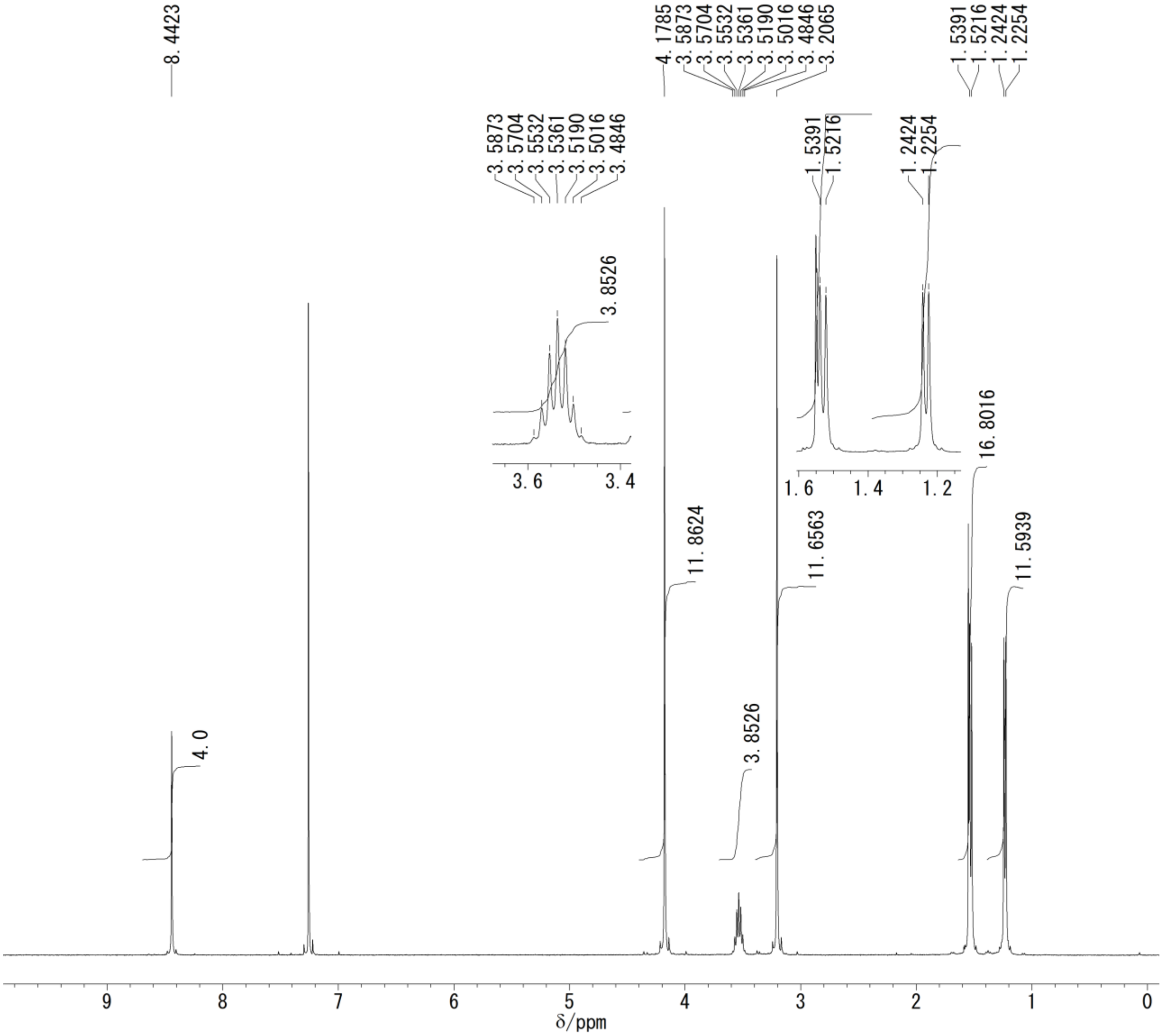
Compound **10** (^{13}C NMR spectrum in $CDCl_3$)



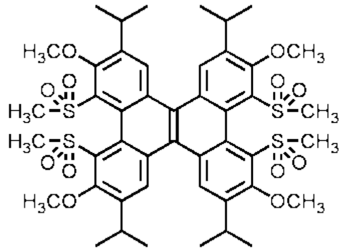


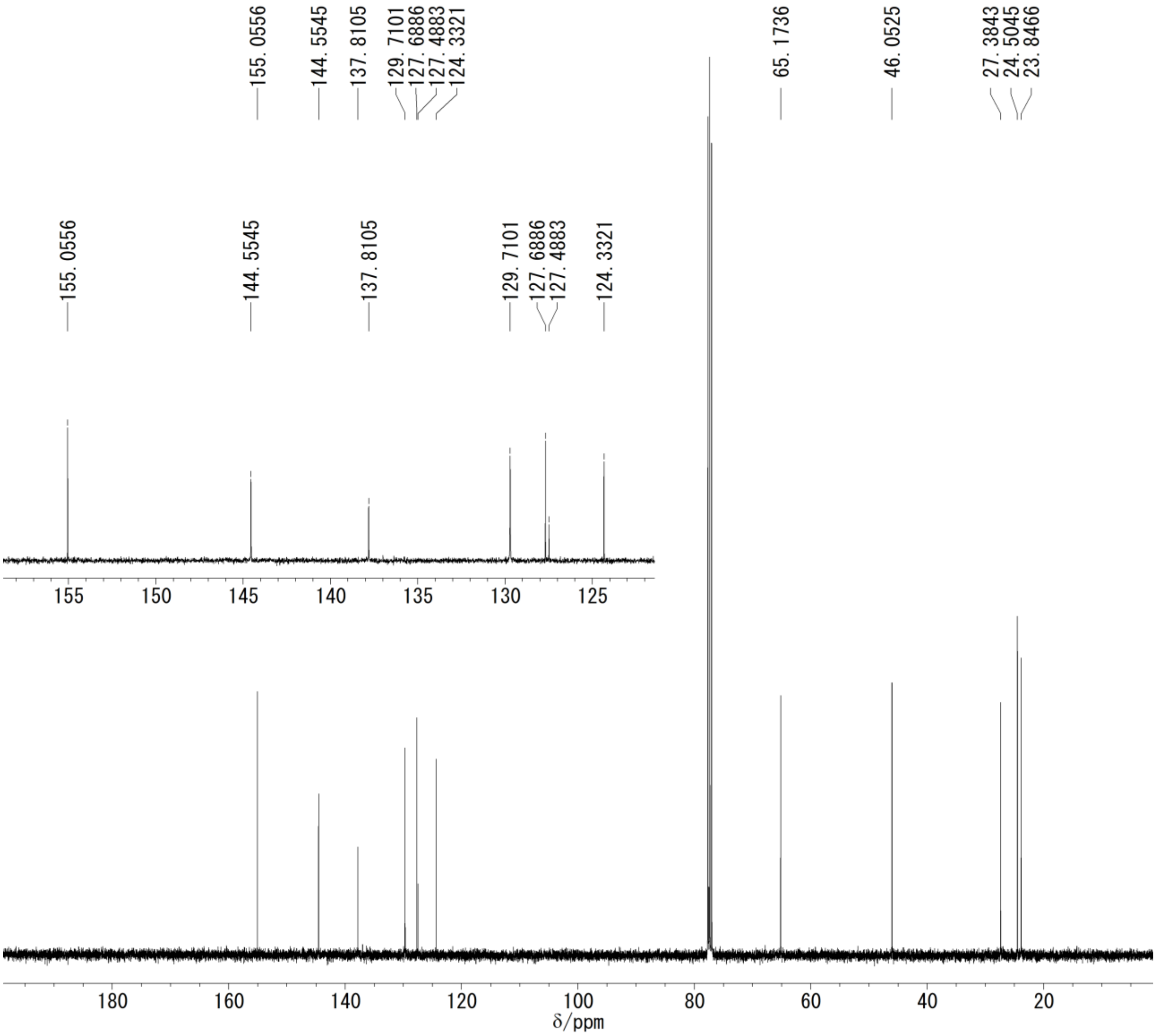
Compound **11** (^{1}H NMR spectrum in $CDCl_3$)



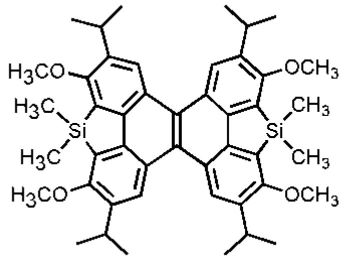


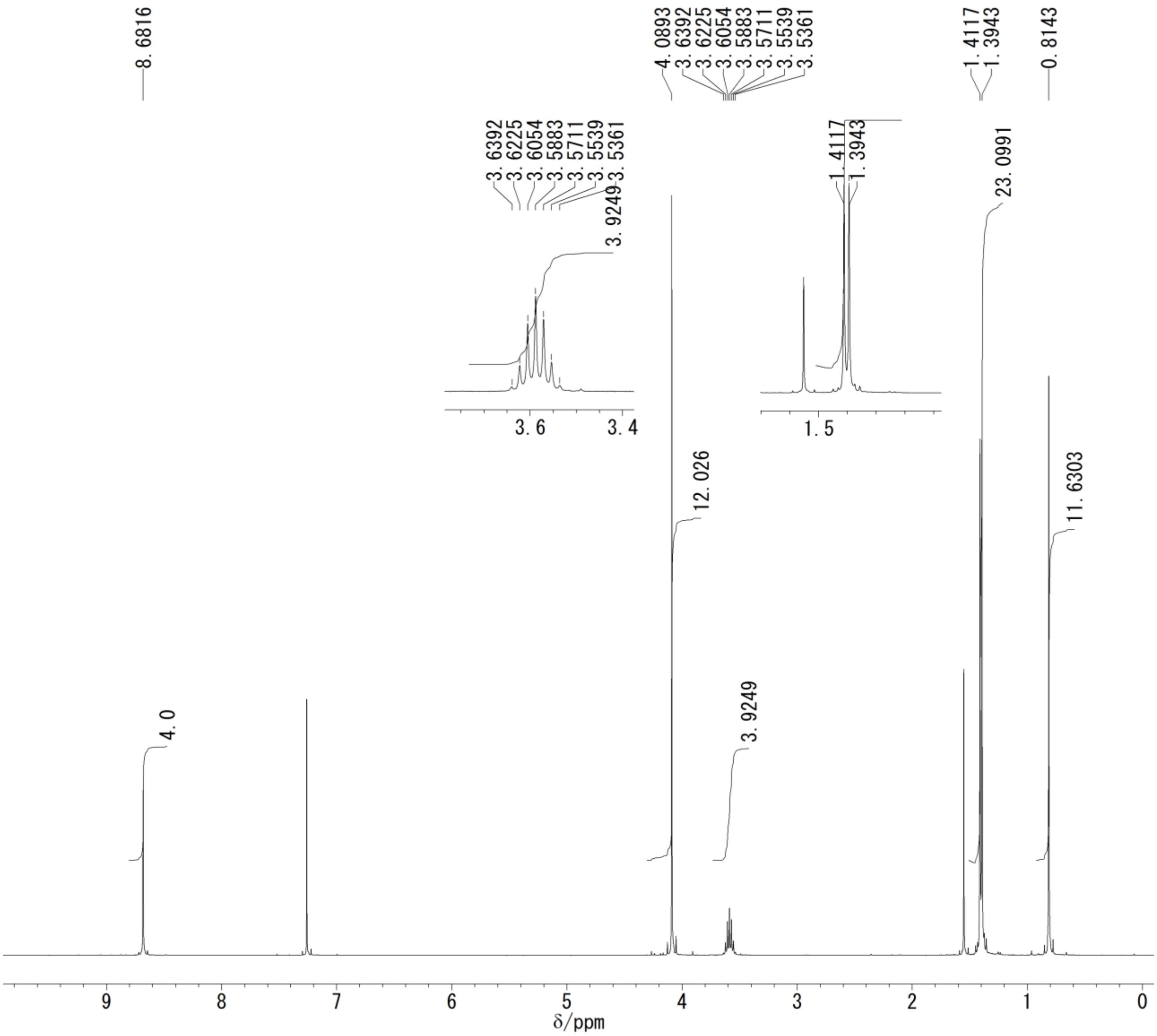
Compound **11** (^{13}C NMR spectrum in $CDCl_3$)



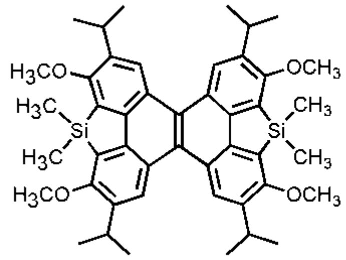


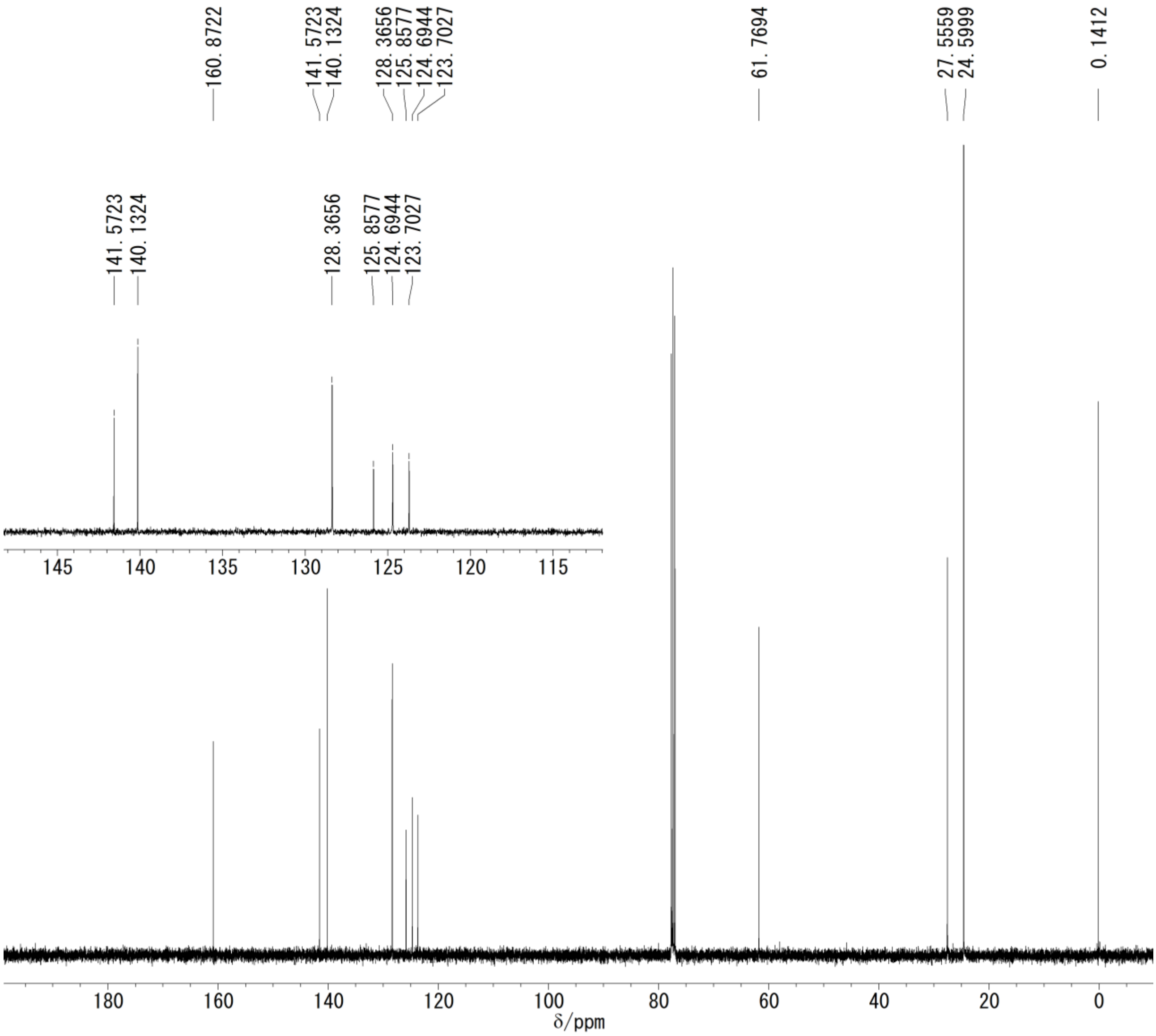
Compound **12** ([1]H NMR spectrum in $CDCl_3$)





Compound **12** (^{13}C NMR spectrum in $CDCl_3$)





14. Absorption and emission spectra for **12**

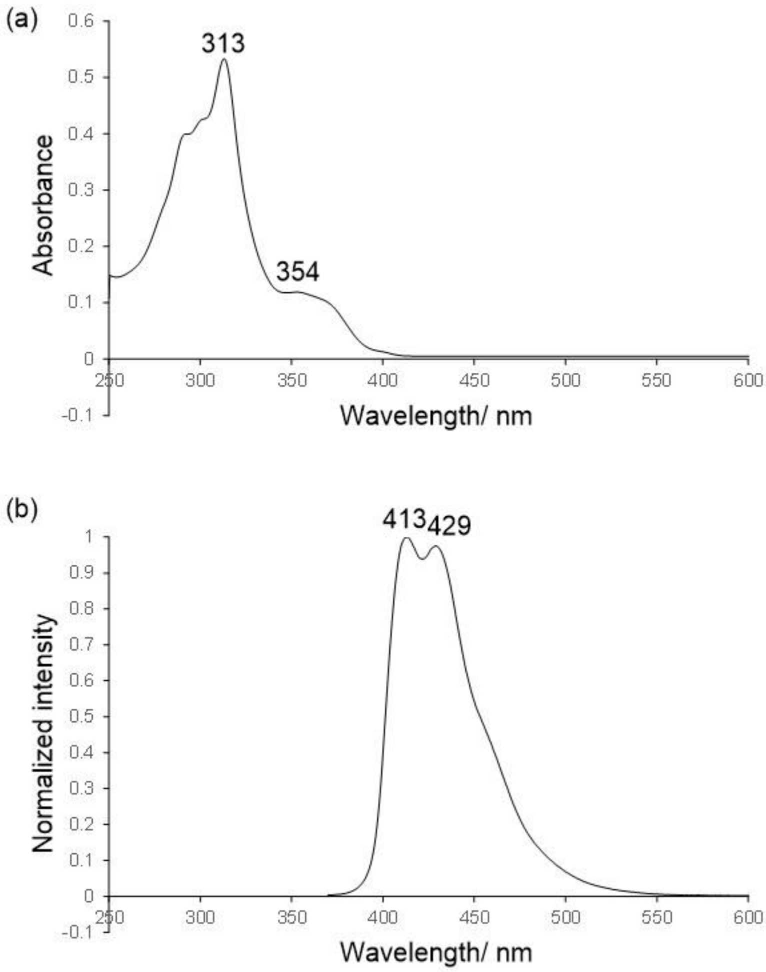


Fig. S1. (a) Absorption and (b) emission spectra (excited at 357 nm) for **12** in (298 K, 1.0×10^{-5} M in CH_2Cl_2).

15. Geometrically optimized structures and orbital drawings of HOMO and LUMO calculated using the DFT method (Fig. S2-S5).

DFT calculation: All calculations were conducted using a Gaussian 16 suite program (G16RevC.01). Optimization was performed at the B3LYP/6-31G(d,p) level of theory. Harmonic vibration frequency analysis was conducted with the optimized structures at the same level of theory to verify all stationary points as local minima (with no imaginary frequency).

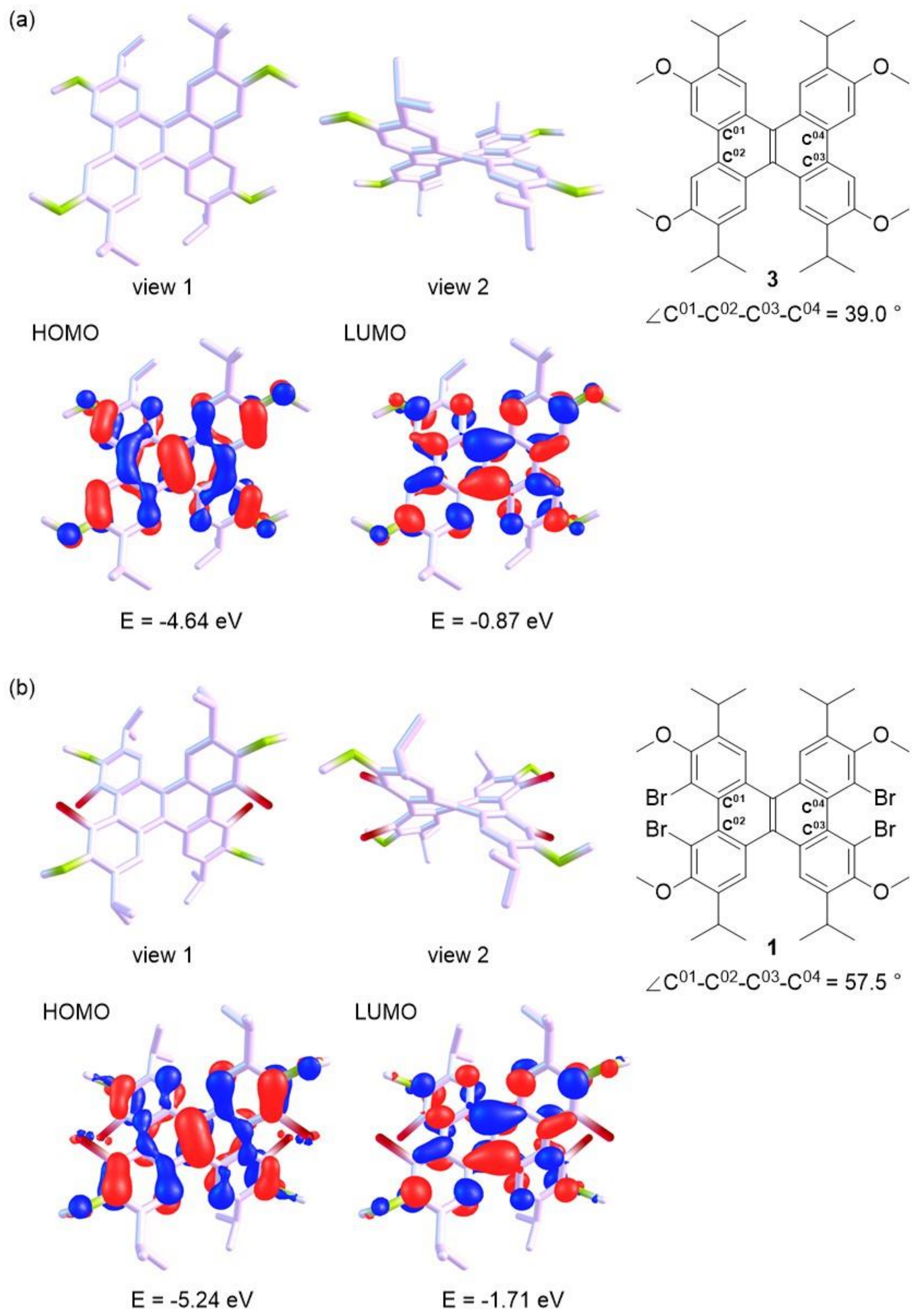


Fig. S2. Optimized structures, torsion angles, and orbital drawings of HOMO and LUMO for (a) **3** and (b) **1** calculated at B3LYP/6-31G(d,p).

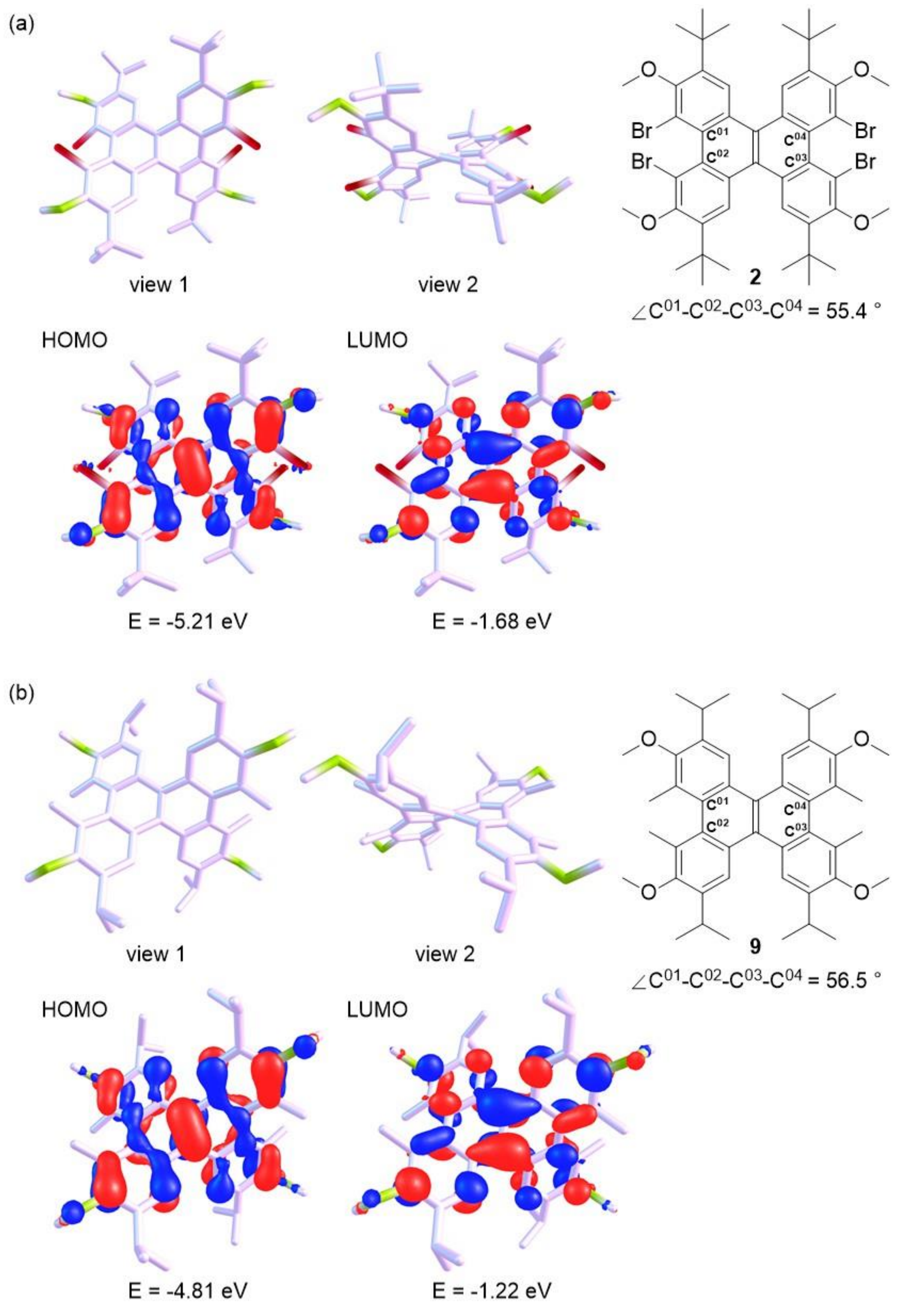


Fig. S3. Optimized structures, torsion angles, and orbital drawings of HOMO and LUMO for (a) **2** and (b) **9** calculated at B3LYP/6-31G(d,p).

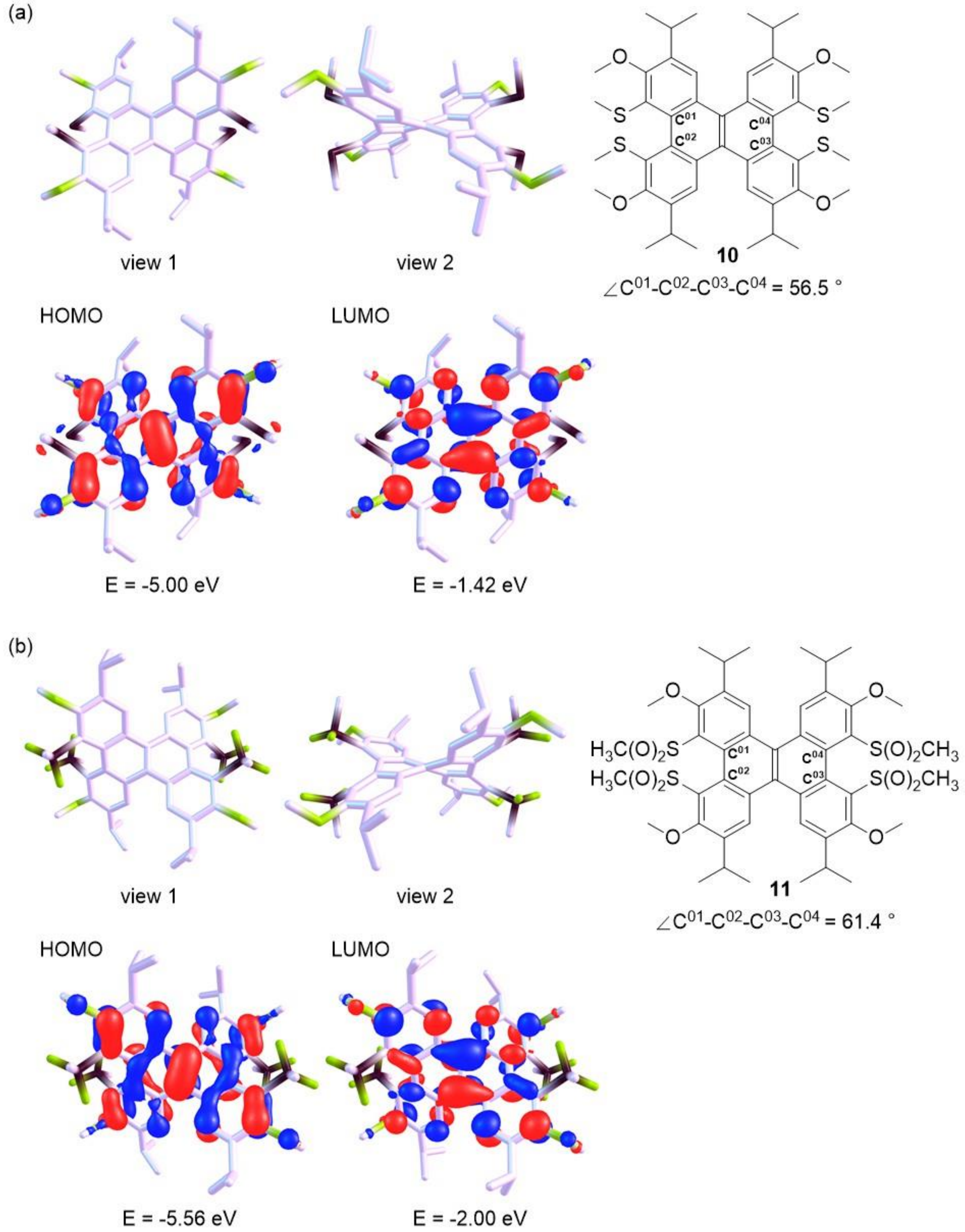


Fig. S4. Optimized structures, torsion angles, and orbital drawings of HOMO and LUMO for (a) **10** and (b) **11** calculated at B3LYP/6-31G(d,p).

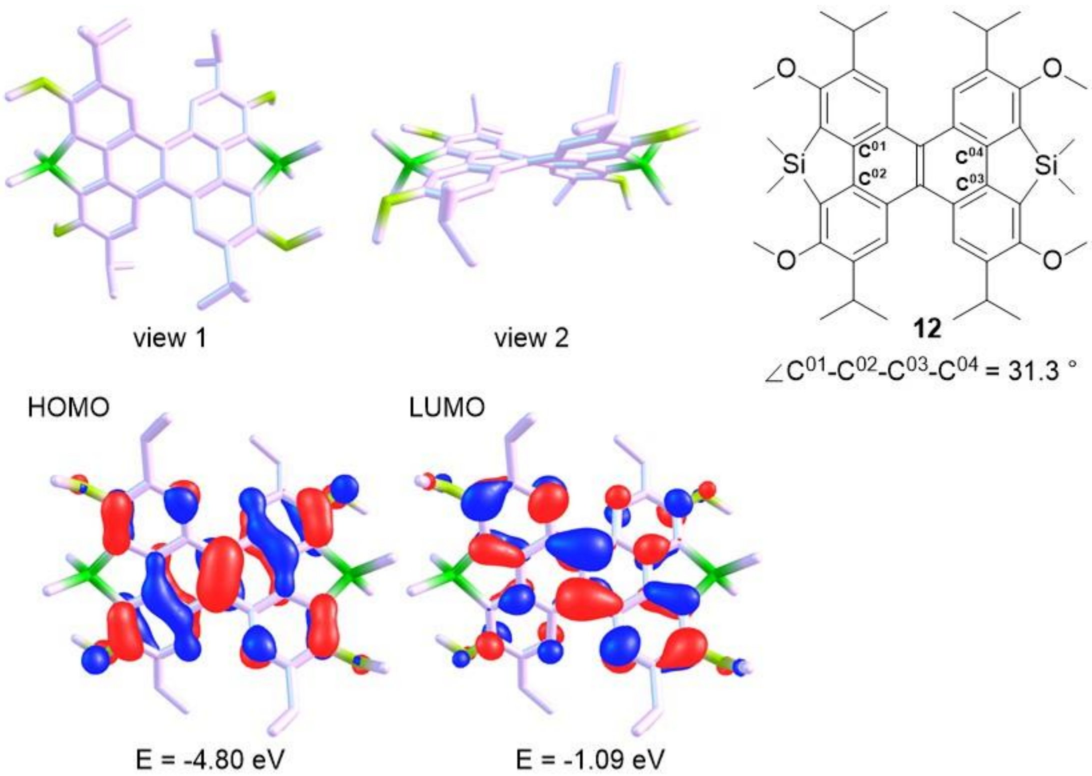


Fig. S5. Optimized structure, torsion angle, and orbital drawings of HOMO and LUMO for **12** calculated at B3LYP/6-31G(d,p).

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **3**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
8	-1.595189	4.766051	-3.281498
8	1.595189	-4.766051	-3.281498
8	-1.595189	-4.766051	3.281498
8	1.595189	4.766051	3.281498
6	0.865408	-1.270541	-2.696124
6	-0.243867	-2.478929	0.684872
6	-0.865408	-1.270541	2.696124
6	-0.312307	-1.249115	1.388521
6	0.243867	-2.478929	-0.684872
6	0.312307	-1.249115	-1.388521
6	0	0	0.700941
6	0	0	-0.700941
6	1.296745	-2.42458	-3.327602

6	0.660248	-3.665063	-1.327574
6	-1.162437	-3.647569	2.617398
6	-1.296745	-2.42458	3.327602
6	1.162437	-3.647569	-2.617398
6	-0.660248	3.665063	-1.327574
6	0.243867	2.478929	0.684872
6	-0.660248	-3.665063	1.327574
6	-1.162437	3.647569	-2.617398
6	-0.312307	1.249115	-1.388521
6	-0.243867	2.478929	-0.684872
6	-0.865408	1.270541	-2.696124
6	1.162437	3.647569	2.617398
6	0.865408	1.270541	2.696124
6	0.312307	1.249115	1.388521
6	1.967631	-2.428515	-4.696281
6	0.660248	3.665063	1.327574
6	1.296745	2.42458	3.327602
6	-3.500992	-2.529253	4.549358
6	-1.967631	-2.428515	4.696281
6	-1.296745	2.42458	-3.327602
6	3.500992	-2.529253	-4.549358
6	-1.967631	2.428515	-4.696281
6	1.967631	2.428515	4.696281
6	-1.484217	6.022757	-2.636505
6	1.484217	-6.022757	-2.636505
6	1.587611	-1.236584	-5.584063
6	-1.484217	-6.022757	2.636505
6	-1.587611	-1.236584	5.584063
6	1.587611	1.236584	5.584063
6	1.484217	6.022757	2.636505
6	3.500992	2.529253	4.549358
6	-1.587611	1.236584	-5.584063
6	-3.500992	2.529253	-4.549358
1	1.01055	-0.326909	-3.204405
1	-1.01055	-0.326909	3.204405
1	-1.01055	0.326909	-3.204405
1	1.01055	0.326909	3.204405
1	1.633578	-3.340065	-5.205796
1	-3.979331	-2.596207	5.533058
1	-3.783536	-3.413865	3.973291

1	-3.899205	-1.645579	4.038382
1	-1.633578	-3.340065	5.205796
1	3.979331	-2.596207	-5.533058
1	3.783536	-3.413865	-3.973291
1	3.899205	-1.645579	-4.038382
1	-1.633578	3.340065	-5.205796
1	1.633578	3.340065	5.205796
1	-2.097458	6.068234	-1.727141
1	-1.848945	6.762253	-3.351146
1	-0.442929	6.253375	-2.376662
1	0.442929	-6.253375	-2.376662
1	2.097458	-6.068234	-1.727141
1	1.848945	-6.762253	-3.351146
1	1.969355	-0.289683	-5.186235
1	0.503072	-1.144946	-5.69426
1	2.019478	-1.363138	-6.582218
1	-1.848945	-6.762253	3.351146
1	-0.442929	-6.253375	2.376662
1	-2.097458	-6.068234	1.727141
1	-1.969355	-0.289683	5.186235
1	-0.503072	-1.144946	5.69426
1	-2.019478	-1.363138	6.582218
1	0.503072	1.144946	5.69426
1	2.019478	1.363138	6.582218
1	1.969355	0.289683	5.186235
1	2.097458	6.068234	1.727141
1	1.848945	6.762253	3.351146
1	0.442929	6.253375	2.376662
1	3.899205	1.645579	4.038382
1	3.979331	2.596207	5.533058
1	3.783536	3.413865	3.973291
1	-0.503072	1.144946	-5.69426
1	-2.019478	1.363138	-6.582218
1	-1.969355	0.289683	-5.186235
1	-3.899205	1.645579	-4.038382
1	-3.979331	2.596207	-5.533058
1	-3.783536	3.413865	-3.973291
1	-0.632574	-4.596208	0.778501
1	0.632574	-4.596208	-0.778501
1	-0.632574	4.596208	-0.778501

1	0.632574	4.596208	0.778501

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **1**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
35	4.976621	0.01687	1.640613
35	-4.976621	-0.01687	1.640613
35	4.975706	-0.013105	-1.689241
35	-4.975706	0.013105	-1.689241
8	-4.554056	-2.914518	2.386822
8	4.563753	-2.902157	-2.43409
8	4.554056	2.914518	2.386822
8	-4.563753	2.902157	-2.43409
6	1.219803	-2.646391	-1.001015
6	2.45955	0.639678	0.329118
6	1.216796	2.648007	0.954999
6	1.239747	1.376888	0.344916
6	2.460011	-0.637748	-0.378339
6	1.239747	-1.376902	-0.391487
6	0.0001	0.697057	-0.023444
6	-0.0001	-0.697057	-0.023444
6	2.336949	-3.211394	-1.605357
6	3.533461	-1.146295	-1.138852
6	3.505392	2.430757	1.643053
6	2.333482	3.213679	1.5564
6	3.507546	-2.428994	-1.694556
6	-3.534598	-1.149737	1.088641
6	-2.460011	0.637748	-0.378339
6	3.534598	1.149737	1.088641
6	-3.505392	-2.430757	1.643053
6	-1.239747	-1.376888	0.344916
6	-2.45955	-0.639678	0.329118
6	-1.216796	-2.648007	0.954999
6	-3.507546	2.428994	-1.694556
6	-1.219803	2.646391	-1.001015
6	-1.239747	1.376902	-0.391487
6	2.268972	-4.584391	-2.263594

6	-3.533461	1.146295	-1.138852
6	-2.336949	3.211394	-1.605357
6	1.95145	4.411645	3.73996
6	2.29056	4.573702	2.243882
6	-2.333482	-3.213679	1.5564
6	1.388664	-4.551756	-3.52803
6	-2.29056	-4.573702	2.243882
6	-2.268972	4.584391	-2.263594
6	-5.714005	-3.301081	1.637477
6	5.711766	-3.302003	-1.674345
6	1.797642	-5.673834	-1.284405
6	5.714005	3.301081	1.637477
6	1.342275	5.574383	1.567551
6	-1.797642	5.673834	-1.284405
6	-5.711766	3.302003	-1.674345
6	-1.388664	4.551756	-3.52803
6	-1.342275	-5.574383	1.567551
6	-1.95145	-4.411645	3.73996
1	0.279287	-3.179889	-1.058062
1	0.275118	3.177547	1.009385
1	-0.275118	-3.177547	1.009385
1	-0.279287	3.179889	-1.058062
1	3.284448	-4.833501	-2.582505
1	1.966168	5.383522	4.245475
1	2.674414	3.757926	4.23447
1	0.953289	3.978368	3.867866
1	3.30347	4.98643	2.189447
1	1.387631	-5.530727	-4.019564
1	1.756614	-3.811561	-4.244473
1	0.35059	-4.298357	-3.28594
1	-3.30347	-4.98643	2.189447
1	-3.284448	4.833501	-2.582505
1	-6.128228	-2.454527	1.082363
1	-6.44494	-3.646436	2.37062
1	-5.476352	-4.117525	0.944772
1	5.467028	-4.13925	-1.009333
1	6.109562	-2.468499	-1.087844
1	6.459177	-3.621628	-2.402571
1	0.768006	-5.503403	-0.952129
1	2.43336	-5.713346	-0.394099

1	1.828256	-6.65691	-1.766288
1	6.44494	3.646436	2.37062
1	5.476352	4.117525	0.944772
1	6.128228	2.454527	1.082363
1	0.291912	5.280954	1.668577
1	1.563384	5.681384	0.500609
1	1.445594	6.559426	2.033911
1	-2.43336	5.713346	-0.394099
1	-1.828256	6.65691	-1.766288
1	-0.768006	5.503403	-0.952129
1	-6.109562	2.468499	-1.087844
1	-6.459177	3.621628	-2.402571
1	-5.467028	4.13925	-1.009333
1	-0.35059	4.298357	-3.28594
1	-1.387631	5.530727	-4.019564
1	-1.756614	3.811561	-4.244473
1	-1.563384	-5.681384	0.500609
1	-1.445594	-6.559426	2.033911
1	-0.291912	-5.280954	1.668577
1	-0.953289	-3.978368	3.867866
1	-1.966168	-5.383522	4.245475
1	-2.674414	-3.757926	4.23447

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **2**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
35	4.960673	1.664559	-0.036028
35	-4.960673	1.664559	0.036028
35	4.960673	-1.664559	0.036028
35	-4.960673	-1.664559	-0.036028
8	-4.628082	2.239784	2.982502
8	4.628082	-2.239784	2.982502
8	4.628082	2.239784	-2.982502
8	-4.628082	-2.239784	-2.982502
6	1.2137	-0.985303	2.64183
1	0.258663	-1.054294	3.139334
6	2.459406	0.34147	-0.644761

6	1.2137	0.985303	-2.64183
1	0.258663	1.054294	-3.139334
6	1.240751	0.362992	-1.376588
6	2.459406	-0.34147	0.644761
6	1.240751	-0.362992	1.376588
6	0	0	-0.696993
6	0	0	0.696993
6	2.324432	-1.570922	3.241407
6	3.537291	-1.076622	1.180664
6	3.523703	1.594254	-2.480323
6	2.324432	1.570922	-3.241407
6	3.523703	-1.594254	2.480323
6	-3.537291	1.076622	1.180664
6	-2.459406	-0.34147	-0.644761
6	3.537291	1.076622	-1.180664
6	-3.523703	1.594254	2.480323
6	-1.240751	0.362992	1.376588
6	-2.459406	0.34147	0.644761
6	-1.2137	0.985303	2.64183
1	-0.258663	1.054294	3.139334
6	-3.523703	-1.594254	-2.480323
6	-1.2137	-0.985303	-2.64183
1	-0.258663	-1.054294	-3.139334
6	-1.240751	-0.362992	-1.376588
6	2.214817	-2.270418	4.616154
6	-3.537291	-1.076622	-1.180664
6	-2.324432	-1.570922	-3.241407
6	2.509111	3.783145	-4.461122
1	2.422976	4.279973	-5.434246
1	3.512044	3.959302	-4.071499
1	1.787454	4.248988	-3.781852
6	2.214817	2.270418	-4.616154
6	-2.324432	1.570922	3.241407
6	0.800248	-2.134825	5.216853
1	0.776672	-2.637286	6.188674
1	0.035334	-2.60384	4.590241
1	0.519841	-1.089119	5.380923
6	-2.214817	2.270418	4.616154
6	-2.214817	-2.270418	-4.616154
6	-5.786103	1.423203	3.215641

1	-6.140622	0.953677	2.295354
1	-6.553754	2.099928	3.594983
1	-5.572646	0.653618	3.965835
6	5.786103	-1.423203	3.215641
1	5.572646	-0.653618	3.965835
1	6.140622	-0.953677	2.295354
1	6.553754	-2.099928	3.594983
6	3.202653	-1.644415	5.629134
1	3.04141	-0.564897	5.720906
1	4.239296	-1.818813	5.343616
1	3.05016	-2.090416	6.618213
6	5.786103	1.423203	-3.215641
1	6.553754	2.099928	-3.594983
1	5.572646	0.653618	-3.965835
1	6.140622	0.953677	-2.295354
6	0.800248	2.134825	-5.216853
1	0.035334	2.60384	-4.590241
1	0.519841	1.089119	-5.380923
1	0.776672	2.637286	-6.188674
6	-3.202653	-1.644415	-5.629134
1	-4.239296	-1.818813	-5.343616
1	-3.05016	-2.090416	-6.618213
1	-3.04141	-0.564897	-5.720906
6	-5.786103	-1.423203	-3.215641
1	-6.140622	-0.953677	-2.295354
1	-6.553754	-2.099928	-3.594983
1	-5.572646	-0.653618	-3.965835
6	-0.800248	-2.134825	-5.216853
1	-0.519841	-1.089119	-5.380923
1	-0.776672	-2.637286	-6.188674
1	-0.035334	-2.60384	-4.590241
6	-0.800248	2.134825	5.216853
1	-0.519841	1.089119	5.380923
1	-0.776672	2.637286	6.188674
1	-0.035334	2.60384	4.590241
6	-2.509111	3.783145	4.461122
1	-1.787454	4.248988	3.781852
1	-2.422976	4.279973	5.434246
1	-3.512044	3.959302	4.071499
6	2.509111	-3.783145	4.461122

1	1.787454	-4.248988	3.781852
1	3.512044	-3.959302	4.071499
1	2.422976	-4.279973	5.434246
6	-3.202653	1.644415	5.629134
1	-4.239296	1.818813	5.343616
1	-3.04141	0.564897	5.720906
1	-3.05016	2.090416	6.618213
6	-2.509111	-3.783145	-4.461122
1	-1.787454	-4.248988	-3.781852
1	-3.512044	-3.959302	-4.071499
1	-2.422976	-4.279973	-5.434246
6	3.202653	1.644415	-5.629134
1	4.239296	1.818813	-5.343616
1	3.04141	0.564897	-5.720906
1	3.05016	2.090416	-6.618213

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **9**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
8	-4.30071	3.293755	2.339243
8	-1.178654	-5.290919	-2.410931
8	4.30071	-3.293755	2.339243
8	1.178654	5.290919	-2.410931
6	-2.071712	-2.034231	-1.015251
6	1.44964	-2.103084	0.309289
6	2.893045	-0.2331	0.944182
6	1.713714	-0.699953	0.330153
6	0.236611	-2.542357	-0.391006
6	-0.867833	-1.635046	-0.404754
6	0.654164	0.236975	-0.036892
6	-0.654164	-0.236975	-0.036892
6	-2.230133	-3.273841	-1.62498
6	0.134556	-3.752955	-1.126453
6	3.483482	-2.452032	1.595125
6	3.810781	-1.084537	1.546361
6	-1.103971	-4.113907	-1.677323
6	-2.304489	2.970005	1.04325

6	-0.236611	2.542357	-0.391006
6	2.304489	-2.970005	1.04325
6	-3.483482	2.452032	1.595125
6	-1.713714	0.699953	0.330153
6	-1.44964	2.103084	0.309289
6	-2.893045	0.2331	0.944182
6	1.103971	4.113907	-1.677323
6	2.071712	2.034231	-1.015251
6	0.867833	1.635046	-0.404754
6	-3.540818	-3.658647	-2.300433
6	-0.134556	3.752955	-1.126453
6	2.230133	3.273841	-1.62498
6	4.733495	-0.278293	3.747593
6	5.050655	-0.565282	2.265705
6	-3.810781	1.084537	1.546361
6	-3.881516	-2.708419	-3.464174
6	-5.050655	0.565282	2.265705
6	3.540818	3.658647	-2.300433
6	-5.217866	4.069602	1.570612
6	-1.44964	-6.456386	-1.635765
6	-4.702625	-3.735815	-1.292611
6	5.217866	-4.069602	1.570612
6	5.685302	0.659732	1.590119
6	4.702625	3.735815	-1.292611
6	1.44964	6.456386	-1.635765
6	3.881516	2.708419	-3.464174
6	-5.685302	-0.659732	1.590119
6	-4.733495	0.278293	3.747593
1	-2.884135	-1.320567	-1.076457
1	3.053605	0.835072	1.008631
1	-3.053605	-0.835072	1.008631
1	2.884135	1.320567	-1.076457
1	-3.39806	-4.654316	-2.729558
1	5.632395	0.053435	4.279553
1	4.353911	-1.17551	4.24363
1	3.976355	0.508483	3.838115
1	5.792418	-1.370555	2.251056
1	-4.794456	-3.03752	-3.972787
1	-3.072604	-2.681614	-4.200253
1	-4.048567	-1.684478	-3.112668

1	-5.792418	1.370555	2.251056
1	3.39806	4.654316	-2.729558
1	-4.703051	4.715877	0.849504
1	-5.770725	4.691802	2.277919
1	-5.923283	3.429653	1.024651
1	-2.439045	-6.401508	-1.163027
1	-0.696456	-6.609482	-0.852823
1	-1.428025	-7.303478	-2.325095
1	-4.908588	-2.757915	-0.843975
1	-4.480464	-4.433303	-0.478337
1	-5.620123	-4.073453	-1.787215
1	5.770725	-4.691802	2.277919
1	5.923283	-3.429653	1.024651
1	4.703051	-4.715877	0.849504
1	5.040954	1.54324	1.650998
1	5.89869	0.470251	0.533048
1	6.628117	0.915387	2.084974
1	4.480464	4.433303	-0.478337
1	5.620123	4.073453	-1.787215
1	4.908588	2.757915	-0.843975
1	0.696456	6.609482	-0.852823
1	1.428025	7.303478	-2.325095
1	2.439045	6.401508	-1.163027
1	4.048567	1.684478	-3.112668
1	4.794456	3.03752	-3.972787
1	3.072604	2.681614	-4.200253
1	-5.89869	-0.470251	0.533048
1	-6.628117	-0.915387	2.084974
1	-5.040954	-1.54324	1.650998
1	-3.976355	-0.508483	3.838115
1	-5.632395	-0.053435	4.279553
1	-4.353911	1.17551	4.24363
6	1.916722	-4.378884	1.438702
1	2.464519	-5.153263	0.892808
1	2.144439	-4.52381	2.498065
1	0.851742	-4.552914	1.280455
6	1.332377	-4.58932	-1.523186
1	2.265321	-4.05475	-1.34201
1	1.387511	-5.547461	-0.996804
1	1.262228	-4.824449	-2.58847

6	-1.916722	4.378884	1.438702
1	-0.851742	4.552914	1.280455
1	-2.464519	5.153263	0.892808
1	-2.144439	4.52381	2.498065
6	-1.332377	4.58932	-1.523186
1	-1.387511	5.547461	-0.996804
1	-1.262228	4.824449	-2.58847
1	-2.265321	4.05475	-1.34201

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **10**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
8	4.556699	2.344496	-2.980907
8	-4.556699	-2.344496	-2.980907
8	-4.556699	2.344496	2.980907
8	4.556699	-2.344496	2.980907
6	-1.200024	-0.984724	-2.637991
6	-2.469793	0.34951	0.64348
6	-1.200024	0.984724	2.637991
6	-1.241338	0.368907	1.369711
6	-2.469793	-0.34951	-0.64348
6	-1.241338	-0.368907	-1.369711
6	0	0	0.695234
6	0	0	-0.695234
6	-2.308934	-1.581606	-3.2193
6	-3.571798	-1.078814	-1.171584
6	-3.496866	1.627261	2.459975
6	-2.308934	1.581606	3.2193
6	-3.496866	-1.627261	-2.459975
6	3.571798	1.078814	-1.171584
6	2.469793	-0.34951	0.64348
6	-3.571798	1.078814	1.171584
6	3.496866	1.627261	-2.459975
6	1.241338	0.368907	-1.369711
6	2.469793	0.34951	-0.64348
6	1.200024	0.984724	-2.637991
6	3.496866	-1.627261	2.459975

6	1.200024	-0.984724	2.637991
6	1.241338	-0.368907	1.369711
6	-2.244654	-2.286981	-4.569948
6	3.571798	-1.078814	1.171584
6	2.308934	-1.581606	3.2193
6	-1.995685	3.797513	4.379802
6	-2.244654	2.286981	4.569948
6	2.308934	1.581606	-3.2193
6	-1.995685	-3.797513	-4.379802
6	2.244654	2.286981	-4.569948
6	2.244654	-2.286981	4.569948
6	5.624073	1.546367	-3.508279
6	-5.624073	-1.546367	-3.508279
6	-1.217037	-1.680412	-5.536267
6	-5.624073	1.546367	3.508279
6	-1.217037	1.680412	5.536267
6	1.217037	-1.680412	5.536267
6	5.624073	-1.546367	3.508279
6	1.995685	-3.797513	4.379802
6	1.217037	1.680412	-5.536267
6	1.995685	3.797513	-4.379802
1	-0.248228	-1.046248	-3.148552
1	-0.248228	1.046248	3.148552
1	0.248228	1.046248	-3.148552
1	0.248228	-1.046248	3.148552
1	-3.233058	-2.183307	-5.030444
1	-1.992373	4.313119	5.346672
1	-2.774552	4.244683	3.757122
1	-1.026961	3.973721	3.899003
1	-3.233058	2.183307	5.030444
1	-1.992373	-4.313119	-5.346672
1	-2.774552	-4.244683	-3.757122
1	-1.026961	-3.973721	-3.899003
1	3.233058	2.183307	-5.030444
1	3.233058	-2.183307	5.030444
1	6.058623	0.907705	-2.734062
1	6.379318	2.247075	-3.869841
1	5.27204	0.928355	-4.343902
1	-5.27204	-0.928355	-4.343902
1	-6.058623	-0.907705	-2.734062

1	-6.379318	-2.247075	-3.869841
1	-0.188052	-1.843584	-5.197619
1	-1.364258	-0.602972	-5.660179
1	-1.308517	-2.150211	-6.520955
1	-6.379318	2.247075	3.869841
1	-5.27204	0.928355	4.343902
1	-6.058623	0.907705	2.734062
1	-0.188052	1.843584	5.197619
1	-1.364258	0.602972	5.660179
1	-1.308517	2.150211	6.520955
1	1.364258	-0.602972	5.660179
1	1.308517	-2.150211	6.520955
1	0.188052	-1.843584	5.197619
1	6.058623	-0.907705	2.734062
1	6.379318	-2.247075	3.869841
1	5.27204	-0.928355	4.343902
1	1.026961	-3.973721	3.899003
1	1.992373	-4.313119	5.346672
1	2.774552	-4.244683	3.757122
1	1.364258	0.602972	-5.660179
1	1.308517	2.150211	-6.520955
1	0.188052	1.843584	-5.197619
1	1.026961	3.973721	-3.899003
1	1.992373	4.313119	-5.346672
1	2.774552	4.244683	-3.757122
16	-5.00172	1.511076	0.162761
16	5.00172	1.511076	-0.162761
16	-5.00172	-1.511076	-0.162761
16	5.00172	-1.511076	0.162761
6	-4.717098	3.315504	-0.011812
1	-5.525995	3.688321	-0.645197
1	-4.761501	3.801588	0.963253
1	-3.759876	3.512186	-0.498389
6	-4.717098	-3.315504	0.011812
1	-5.525995	-3.688321	0.645197
1	-4.761501	-3.801588	-0.963253
1	-3.759876	-3.512186	0.498389
6	4.717098	3.315504	0.011812
1	5.525995	3.688321	0.645197
1	4.761501	3.801588	-0.963253

1	3.759876	3.512186	0.498389
6	4.717098	-3.315504	-0.011812
1	5.525995	-3.688321	-0.645197
1	4.761501	-3.801588	0.963253
1	3.759876	-3.512186	-0.498389

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **11**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
16	-1.060361	5.090441	0.080136
16	2.522342	4.553156	-0.054822
16	1.060361	-5.090441	0.080136
16	-2.522342	-4.553156	-0.054822
8	2.996942	4.180527	-2.92823
8	-1.62348	4.87305	2.967451
8	-2.996942	-4.180527	-2.92823
8	2.437829	5.90857	-0.612201
8	2.130221	4.317143	1.345738
8	0.754819	-4.744302	-1.318987
8	-0.754819	4.744302	-1.318987
8	0.588317	-6.366908	0.630456
8	1.62348	-4.87305	2.967451
8	-0.588317	6.366908	0.630456
8	-2.130221	-4.317143	1.345738
8	-2.437829	-5.90857	-0.612201
6	0	2.488502	0.643283
6	2.152481	3.215292	-2.430289
6	-0.563385	-1.167075	-1.35122
6	-0.788507	1.343507	2.656263
1	-0.987342	0.416241	3.177802
6	-0.588579	3.673145	1.15668
6	-0.190225	1.281761	1.380679
6	-0.744406	-2.375395	-0.611585
6	1.096014	-3.70773	2.459881
6	0	0	-0.681485
6	0	-2.488502	0.643283
6	-1.658541	-3.329691	-1.124959

6	0.563385	1.167075	-1.35122
6	-2.152481	-3.215292	-2.430289
6	0.190225	-1.281761	1.380679
6	1.150282	1.051681	-2.626833
1	1.06377	0.108811	-3.152576
6	-1.193289	2.534462	3.23947
6	1.658541	3.329691	-1.124959
6	2.493609	1.913856	-4.602071
1	3.099707	2.804939	-4.785186
6	0.788507	-1.343507	2.656263
1	0.987342	-0.416241	3.177802
6	-1.096014	3.70773	2.459881
6	0	0	0.7107
6	0.744406	2.375395	-0.611585
6	-1.894634	-2.067469	-3.209493
6	0.588579	-3.673145	1.15668
6	1.193289	-2.534462	3.23947
6	1.894634	2.067469	-3.209493
6	-1.866116	2.582215	4.606501
1	-1.714262	3.590185	5.003073
6	-1.150282	-1.051681	-2.626833
1	-1.06377	-0.108811	-3.152576
6	-2.493609	-1.913856	-4.602071
1	-3.099707	-2.804939	-4.785186
6	1.398079	1.852141	-5.683053
1	0.772478	0.960294	-5.564163
1	1.846382	1.81136	-6.681429
1	0.741693	2.726719	-5.640009
6	4.241003	3.991607	-0.181273
1	4.570349	4.070497	-1.21515
1	4.303841	2.970261	0.195412
1	4.803609	4.669339	0.464066
6	1.866116	-2.582215	4.606501
1	1.714262	-3.590185	5.003073
6	-0.648948	5.760408	3.56365
1	-1.196172	6.665106	3.830495
1	0.14006	5.999627	2.850193
1	-0.225677	5.302947	4.465443
6	-2.867759	5.051835	0.209349
1	-3.211019	5.85811	-0.442096

1	-3.157723	5.231914	1.242399
1	-3.22496	4.089347	-0.15806
6	-1.398079	-1.852141	-5.683053
1	-0.772478	-0.960294	-5.564163
1	-1.846382	-1.81136	-6.681429
1	-0.741693	-2.726719	-5.640009
6	3.431755	0.695759	-4.693586
1	4.229274	0.752263	-3.946596
1	3.897326	0.650014	-5.683695
1	2.893431	-0.245771	-4.539904
6	-4.241003	-3.991607	-0.181273
1	-4.803609	-4.669339	0.464066
1	-4.570349	-4.070497	-1.21515
1	-4.303841	-2.970261	0.195412
6	2.324977	5.299452	-3.549395
1	1.833602	4.976233	-4.474478
1	3.106299	6.024197	-3.780312
1	1.60035	5.741076	-2.864244
6	2.867759	-5.051835	0.209349
1	3.211019	-5.85811	-0.442096
1	3.157723	-5.231914	1.242399
1	3.22496	-4.089347	-0.15806
6	-2.324977	-5.299452	-3.549395
1	-3.106299	-6.024197	-3.780312
1	-1.60035	-5.741076	-2.864244
1	-1.833602	-4.976233	-4.474478
6	0.648948	-5.760408	3.56365
1	0.225677	-5.302947	4.465443
1	1.196172	-6.665106	3.830495
1	-0.14006	-5.999627	2.850193
6	-3.431755	-0.695759	-4.693586
1	-4.229274	-0.752263	-3.946596
1	-3.897326	-0.650014	-5.683695
1	-2.893431	0.245771	-4.539904
6	-3.388864	2.381309	4.463845
1	-3.823026	3.13831	3.804889
1	-3.880228	2.458045	5.439762
1	-3.616329	1.393587	4.047613
6	3.388864	-2.381309	4.463845
1	3.823026	-3.13831	3.804889

1	3.880228	-2.458045	5.439762
1	3.616329	-1.393587	4.047613
6	1.269595	-1.589813	5.615771
1	1.466514	-0.549134	5.337104
1	1.716135	-1.747616	6.602708
1	0.186531	-1.715455	5.710764
6	-1.269595	1.589813	5.615771
1	-1.466514	0.549134	5.337104
1	-1.716135	1.747616	6.602708
1	-0.186531	1.715455	5.710764

Cartesian Coordinates of Optimized Structures: Cartesian coordinates for **12**, optimized at the B3LYP/6-31G(d,p) level of theory.

	Coordinates (Angstroms)		
Atomic Type	X	Y	Z
14	-0.050677	5.051741	0.106085
8	-3.400307	4.864068	-1.164304
8	3.114022	5.015941	1.193444
6	0.706715	0.001824	-0.039229
6	2.732772	1.380078	0.697454
1	3.319933	0.481694	0.838242
6	-2.75392	1.327687	-0.78345
1	-3.291264	0.412425	-0.989189
6	1.395993	1.263049	0.240809
6	1.225671	3.722359	0.492147
6	-1.421845	1.248881	-0.301185
6	2.543871	3.777824	0.913705
6	-2.655149	3.747619	-0.876437
6	3.32197	2.597893	1.033983
6	-1.333437	3.745998	-0.437509
6	0.658126	2.465589	0.188158
6	-3.374308	2.529082	-1.080763
6	-0.731347	2.470712	-0.20201
6	4.777782	2.663096	1.487088
1	4.977379	3.698022	1.777443
6	-4.777782	2.591199	-1.679518
1	-5.260264	3.481168	-1.262231
6	0.642735	6.233748	-1.198658

1	1.61911	6.586125	-0.84927
1	0.011248	7.108798	-1.376718
1	0.799272	5.721339	-2.152905
6	-5.66278	1.386252	-1.333924
1	-5.308964	0.463752	-1.807101
1	-6.682867	1.558508	-1.692541
1	-5.710744	1.218258	-0.253201
6	-0.622164	6.017038	1.633224
1	-0.888302	5.332435	2.444603
1	-1.498149	6.641012	1.428201
1	0.174163	6.678088	1.991471
6	-4.707837	2.787459	-3.208576
1	-4.13504	3.682162	-3.465292
1	-5.713041	2.894851	-3.631772
1	-4.228836	1.926505	-3.688075
6	-2.762289	6.082016	-1.500911
1	-3.544746	6.73124	-1.900058
1	-1.991241	5.931118	-2.264162
1	-2.318501	6.574532	-0.629383
6	5.058878	1.767605	2.707058
1	4.394949	2.009735	3.543206
1	6.092917	1.895257	3.045596
1	4.91977	0.706958	2.471711
6	5.73899	2.339054	0.327314
1	5.609035	1.30993	-0.021847
1	6.781014	2.454982	0.646129
1	5.567517	3.006528	-0.52261
6	3.028898	5.410069	2.56308
1	1.988179	5.440983	2.905979
1	3.462999	6.41044	2.628036
1	3.592435	4.731504	3.216341
14	0.050677	-5.051741	0.106085
8	3.400307	-4.864068	-1.164304
8	-3.114022	-5.015941	1.193444
6	-0.706715	-0.001824	-0.039229
6	-2.732772	-1.380078	0.697454
1	-3.319933	-0.481694	0.838242
6	2.75392	-1.327687	-0.78345
1	3.291264	-0.412425	-0.989189
6	-1.395993	-1.263049	0.240809

6	-1.225671	-3.722359	0.492147
6	1.421845	-1.248881	-0.301185
6	-2.543871	-3.777824	0.913705
6	2.655149	-3.747619	-0.876437
6	-3.32197	-2.597893	1.033983
6	1.333437	-3.745998	-0.437509
6	-0.658126	-2.465589	0.188158
6	3.374308	-2.529082	-1.080763
6	0.731347	-2.470712	-0.20201
6	-4.777782	-2.663096	1.487088
1	-4.977379	-3.698022	1.777443
6	4.777782	-2.591199	-1.679518
1	5.260264	-3.481168	-1.262231
6	-0.642735	-6.233748	-1.198658
1	-1.61911	-6.586125	-0.84927
1	-0.011248	-7.108798	-1.376718
1	-0.799272	-5.721339	-2.152905
6	5.66278	-1.386252	-1.333924
1	5.308964	-0.463752	-1.807101
1	6.682867	-1.558508	-1.692541
1	5.710744	-1.218258	-0.253201
6	0.622164	-6.017038	1.633224
1	0.888302	-5.332435	2.444603
1	1.498149	-6.641012	1.428201
1	-0.174163	-6.678088	1.991471
6	4.707837	-2.787459	-3.208576
1	4.13504	-3.682162	-3.465292
1	5.713041	-2.894851	-3.631772
1	4.228836	-1.926505	-3.688075
6	2.762289	-6.082016	-1.500911
1	3.544746	-6.73124	-1.900058
1	1.991241	-5.931118	-2.264162
1	2.318501	-6.574532	-0.629383
6	-5.058878	-1.767605	2.707058
1	-4.394949	-2.009735	3.543206
1	-6.092917	-1.895257	3.045596
1	-4.91977	-0.706958	2.471711
6	-5.73899	-2.339054	0.327314
1	-5.609035	-1.30993	-0.021847
1	-6.781014	-2.454982	0.646129

1	-5.567517	-3.006528	-0.52261
6	-3.028898	-5.410069	2.56308
1	-1.988179	-5.440983	2.905979
1	-3.462999	-6.41044	2.628036
1	-3.592435	-4.731504	3.216341