

Supporting Information

Thiophene-backbone Arcuate Graphene Nanoribbons with : Shotgun Synthesis and Length-dependent Properties

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Table of Contents

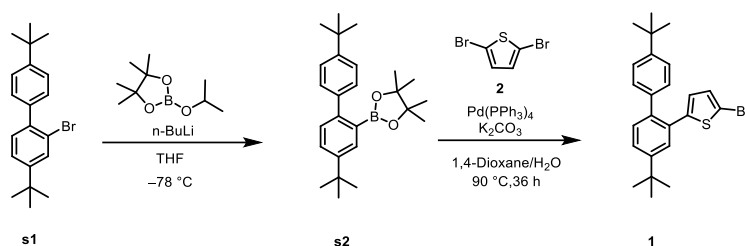
1. General.....	3
2. Synthetic Procedures.....	4
2.1 Synthesis of 2-bromo-5-(4,4'-di-tert-butyl-[1,1'-biphenyl]-2-yl)thiophene (1)	4
2.2 Synthesis of 1,3-Bis(4-chlorophenyl)ferrocene (3)	5
2.3 Synthesis of 4a , 4b , 4c , and 4d	6
2.4 The optimization of Shotgun Synthetic Route of 4a , 4b , 4c , and 4d	8
2.5 Syntheses of the thiophene-fused arcuate graphene nanoribbons.....	12
2.6 Syntheses of the thiophene-dioxides fused arcuate graphene nanoribbons	15
3. X-Ray Crystallography	17
3.1 Experimental details on crystal growth.....	17
3.2 Single-crystal Structure and Packing of AR-11 and ARO-11	18
4. Electrochemistry	20
5. The photophysical properties	22
6. Mass Spectra	25
7. Calculated details	28
7.1 Calculated molecular geometries	28
7.2 Lengths and the arc-shaped of AR-<i>n</i> and ARO-<i>n</i>	30
7.3 Source code of the program for the measurement of lengths and arc-shaped.	33
7.4 Stereoisomers of AR-11	35
7.5 Electronic structures and molecular aromaticity of AR-11 , ARO-11	40
7.6 TD-DFT calculation.....	41
7.7 Frontier Molecular Orbitals	47
8. NMR Spectra	51
9. Cartesian coordinates of optimized structures	78
10. References.....	96

1. General

All reagents and solvents were obtained from commercial suppliers and used without further purification unless noted otherwise. The silica-gel column chromatography was performed using silica gel (200-300 mesh). All reactions were run under argon atmosphere unless otherwise stated. Nuclear magnetic resonance (NMR) spectra were recorded on a JEOL JNM-ECZ500R (^1H 600 MHz, ^{13}C 151 MHz) spectrometer. Chemical shifts are expressed in parts per million (ppm) relative to tetramethylsilane (δ 0.00 ppm). ^1H and ^{13}C NMR spectra are referenced against the residual solvent peak (CDCl_3 $\delta_{\text{H}} = 7.26$ ppm, CDCl_3 $\delta_{\text{C}} = 77.16$ ppm). The high-resolution mass spectra (HRMS) were conducted on Thermo fisher scientific exactive plus LC-MS (ESI) and LC-MS (APCI) mass spectrometer. Fourier transform ion cyclotron resonance ultra high resolution mass spectrometer (FTICR-MS) by matrix-assisted laser desorption/ionization (MALDI) were performed JEOL Spiral TOF instrument. UV-vis-NIR spectra were recorded on SHIMADZU UV-2700 spectrophotometer in dichloromethane. Single-crystal X-ray data were collected on a Supernova single-crystal diffractometer equipped with graphite-monochromatized $\text{Ga-K}\alpha$ ($\lambda = 1.34050$) at 100 K or on a Bruker Apex diffractometer and 1.5 kW graphite monochromated $\text{Mo-K}\alpha$ ($\lambda = 0.71073$) and $\text{Cu-K}\alpha$ radiation ($\lambda = 1.54184$ Å) at 298 K. Absorption corrections were applied using SADABS. The structures were solved by the direct method and refined by full-matrix least-squares on F^2 using SHELXTL and OLEX2.¹ The diffused electron densities resulting from these residual cations and solvent molecules were removed from the data set using the SQUEEZE routine of PLATON and refined further using the data generated.²

2. Synthetic Procedures

2.1 Synthesis of 2-bromo-5-(4,4'-di-tert-butyl-[1,1'-biphenyl]-2-yl)thiophene (1)

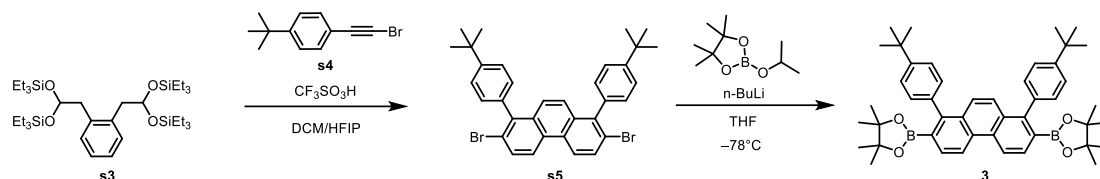


Scheme S1. Synthetic Route of end block 1

Compound s2: 2-(4,4'-di-tert-butyl-[1,1'-biphenyl]-2-pinacol ester) **s2** was prepared according to previous literature.³

Compound 1: compound **s2** (784 mg, 2.00 mmol, 1.00 equiv.), 2,5-dibromothiophene **2** (2.42 g, 10.0 mmol, 5.00 equiv.), Pd(PPh₃)₄ (231 mg, 0.200 mmol, 0.100 equiv.) and K₂CO₃ (1.38 g, 10.0 mmol, 5.00 equiv.) were added to a 250 mL dry round-bottom flask equipped with a stir bar. After the flask was evacuated and refilled with argon 3 times, degassed 1,4-dioxane (100 mL) and water (20 mL) were transferred to the flask via syringe. The mixture was stirred at 90°C for 36 h. After cooling down to room temperature, the aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na₂SO₄, filtered and concentrated under reduced pressure. The residue was then purified by silica gel column chromatography with petroleum ether to afford the compound **1** as a white powder solid (516 mg, 1.21 mmol, 60.4%). ¹H NMR (600 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 2.0 Hz, 1H), 7.41 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.31 (dd, *J* = 10.4, 8.2 Hz, 3H), 7.16 (d, *J* = 8.3 Hz, 2H), 6.81 (d, *J* = 3.8 Hz, 1H), 6.44 (d, *J* = 3.8 Hz, 1H), 1.38 (s, 9H), 1.34 (s, 9H). ¹³C NMR {¹H} (151 MHz, Chloroform-*d*) δ 150.8, 150.4, 146.0, 138.3, 138.2, 132.2, 130.1, 130.1, 129.6, 127.7, 127.3, 125.6, 125.4, 111.9, 34.9, 34.9, 31.8, 31.7. HRMS analysis (ESI): calculated for C₂₄H₂₇BrS [M+H]⁺: 429.1069, found: 429.1081.

2.2 Synthesis of 1,3-Bis(4-chlorophenyl)ferrocene (3)



Scheme S2. Synthetic Route of link building block **3**

Compound s3 (1,2-bis(2,2-bis((triethylsilyl)oxy)ethyl)benzene): **s3** was prepared according to previous literature.⁴

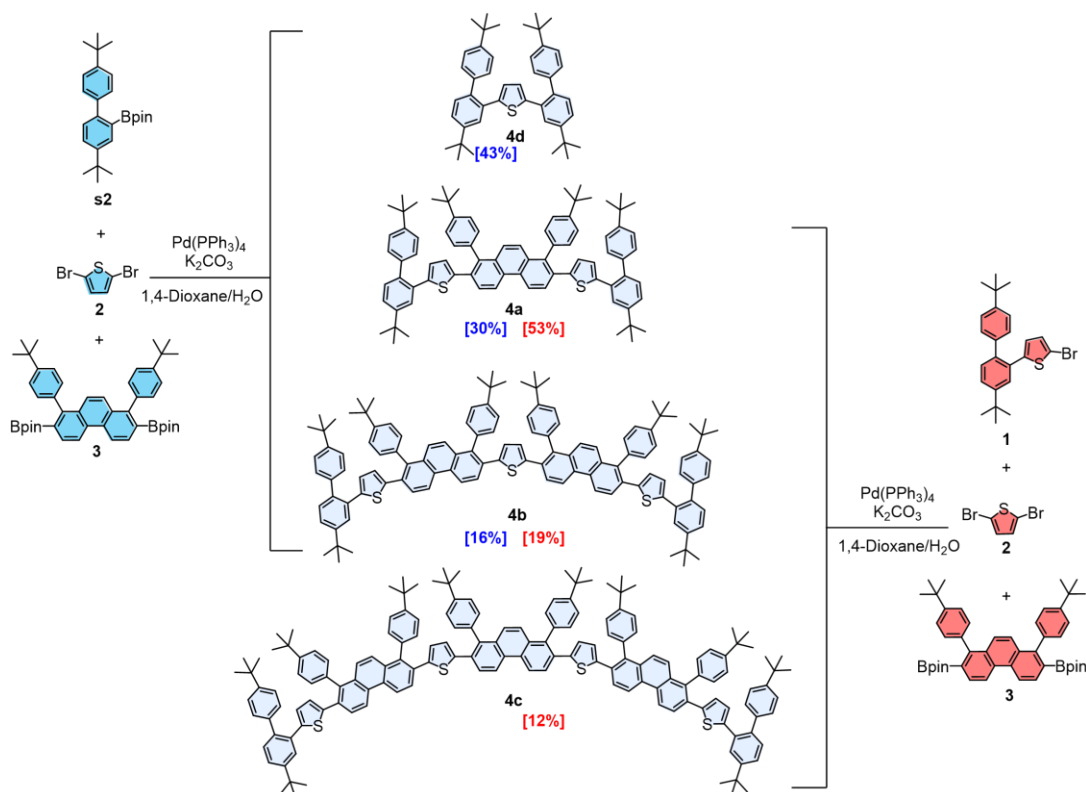
Compound s4 (1-(bromoethynyl)-4-(tert-butyl)benzene): **s4** was prepared according to previous literature.⁵

Compound s5: A dry Schlenk tube equipped with a magnetic stir bar and a septum was charged with compound **s4** (5.69 g, 24.0 mmol, 4.00 equiv.) and compound **s3** (3.93 g, 6.00 mmol, 1.00 equiv.) under air. CF_3Ph (150 mL) and hexafluoroisopropanol (HFIP) (15 mL) were then added under argon atmosphere. Subsequently, the reaction mixture was cooled to -30°C . After 30 minutes, the freshly prepared solution of $\text{CF}_3\text{SO}_3\text{H}$ (0.5 M in HFIP, 18 mL, 9.00 mmol, 1.50 equiv.) was added dropwise. After stirring at -30°C for 12 h, After return to room temperature, the aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was then purified by silica gel column chromatography with (DCM/petroleum ether = 1/10) to afforded the compound **s5** as a white powder solid (1.43 g, 2.38 mmol, 39%). ^1H NMR (600 MHz, Chloroform-*d*) δ 8.58 (d, J = 9.0 Hz, 2H), 7.92 (d, J = 8.9 Hz, 2H), 7.47 (d, J = 8.3 Hz, 4H), 7.28 (s, 2H), 7.19 (d, J = 8.4 Hz, 4H), 1.38 (s, 18H). ^{13}C NMR $\{^1\text{H}\}$ (151 MHz, Chloroform-*d*) δ 151.0, 141.1, 136.8, 132.4, 131.0, 130.0, 129.4, 126.4, 125.5, 123.8, 123.3, 35.0, 31.8. HRMS analysis (ESI): calculated for $\text{C}_{34}\text{H}_{32}\text{Br}_2$ $[\text{M}]^+$: 600.0845, found: 600.0853.

Compound 3: To 2,7-dibromo-1,8-bis(4-(tert-butyl)phenyl) phenanthrene **s5** (1.80 g, 3.00 mmol, 1.00 equiv.) in dry THF (42 mL) at -80°C was carefully added a solution of 1.6 M *n*-butyllithium in hexanes (7.50 mL, 12.0 mmol, 4.00 equiv.). After stirring for 90 min at -80°C , 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (3.67 mL, 18.0 mmol, 6.00 equiv.) was slowly added and the clear and transparent solution is agitated for 5 h at room temperature to become a white turbid liquid. Quench the reaction with diluted HCl solution. The aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was then purified by silica gel column chromatography with (petroleum ether/DCM/ethyl acetate = 10/1/1) to afforded the compound **3** as a white powder solid (1.76 g, 2.5 mmol, 85%). ^1H NMR (600 MHz, Chloroform-*d*) δ 8.75 (d, J = 8.4 Hz, 2H), 7.90 (d, J = 8.3 Hz, 2H), 7.52 (s, 2H), 7.40–7.37 (m, 4H), 7.27–7.24 (m, 4H), 1.36 (s, 18H), 1.12 (s, 24H). ^{13}C NMR $\{^1\text{H}\}$ (151 MHz, Chloroform-*d*) δ 150.0, 147.0, 138.9, 131.8, 130.8, 130.5, 130.4, 125.3, 124.7, 121.8, 83.9, 34.9, 31.8, 24.9. HRMS

analysis (ESI): calculated for $C_{46}H_{56}B_2O_4$ $[M+H]^+$: 695.4437, found: 695.4455.

2.3 Synthesis of 4a, 4b, 4c, and 4d



Scheme S3. Shotgun Synthetic Route of the precursor of GNRs.

Compound 4d, 4a and 4b: Compound **3** (69.5 mg, 0.100 mmol, 1.00 equiv.), compound **2** (36.3 mg, 0.150 mmol, 1.50 equiv.), compound **s2** (39.2 mg, 0.100 mmol, 1.00 equiv.), $Pd(PPh_3)_4$ (28.9 mg, 0.025 mmol, 0.250 equiv.) and K_2CO_3 (173 mg, 1.25 mmol, 12.5 equiv.) were added to a 25 mL round-bottom flask equipped with a stir bar. After the flask was evacuated and refilled with argon 3 times, degassed 1,4-dioxane (4.0 mL) and water (0.5 mL) were transferred to the flask via syringe. The mixture was stirred at 90°C for 36 h. After cooling down to room temperature, the aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na_2SO_4 , filtered and concentrated under reduced pressure. The residue was then purified by silica gel column chromatography with (petroleum ether/DCM = 20/1 to petroleum ether/DCM = 3/1) afforded the compound **4d** (13.1 mg, 0.021 mmol, 43%) as a white powder solid, **4a** (16.7 mg, 0.0150 mmol, 30%) as a yellow powder solid, **4b** (14.2 mg, 0.008 mmol, 16%) as a yellow powder solid. Isolated yields were based on the amount of **s2**.

Compound 4a, 4b and 4c: Compound **3** (695 mg, 1.00 mmol, 2.00 equiv.), compound **2** (120 mg, 0.500 mmol, 1.00 equiv.), compound **1** (512 mg, 1.20 mmol, 2.40 equiv.), $Pd(PPh_3)_4$ (288 mg, 0.250 mmol, 0.500 equiv.) and K_2CO_3 (1.73 g, 12.5 mmol, 25.0 equiv.) were added to a 250 mL round-bottom flask equipped with a stir bar. After the flask was evacuated and refilled with argon 3 times, degassed 1,4-dioxane (40 mL) and water (5 mL) were transferred to the flask via syringe. The mixture was stirred at 90°C for 36 h. After cooling down to room temperature, the aqueous layer was extracted with

dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na₂SO₄, filtered and concentrated under reduced pressure. The residue was then purified by silica gel column chromatography with (petroleum ether / DCM = 30/1 to petroleum ether / DCM = 2/1) afforded the compound **4a** (362 mg, 0.320 mmol, 53%) as a white powder solid, **4b** (189 mg, 0.114 mmol, 19%) as a yellow powder solid and **4c** (150 mg, 0.069 mmol, 12%) as a yellow powder solid. Isolated yields were based on the amount of **1**.

4a: ¹H NMR (600 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 8.9 Hz, 2H), 7.90 (d, *J* = 8.8 Hz, 2H), 7.43 (d, *J* = 2.1 Hz, 2H), 7.39 (d, *J* = 8.3 Hz, 4H), 7.35 (dd, *J* = 8.1, 2.1 Hz, 2H), δ 7.30 (d, *J* = 8.4 Hz, 4H), 7.28 (d, *J* = 4.1 Hz, 4H), 7.15 (d, *J* = 8.3 Hz, 4H), 7.12 (d, *J* = 8.5 Hz, 4H), 6.60 (d, *J* = 3.8 Hz, 2H), 6.42 (d, *J* = 3.8 Hz, 2H), 1.36 (s, 18H), 1.35 (s, 18H), 1.35 (s, 18H). ¹³C NMR {¹H} (151 MHz, Chloroform-*d*) δ 150.9, 150.4, 149.9, 144.7, 143.4, 138.7, 138.2, 137.9, 136.5, 133.0, 131.9, 131.7, 131.0, 130.9, 129.6, 129.4, 127.8, 127.5, 127.3, 127.2, 126.0, 125.6, 125.2, 125.1, 122.7, 35.0, 34.9, 34.9, 31.9, 31.8, 31.7. HRMS analysis (ESI): calculated for C₈₂H₈₆S₂ [M+H]⁺: 1135.6244, found: 1135.6284.

4b: ¹H NMR (600 MHz, Chloroform-*d*) δ 8.73–8.64 (m, 4H), 7.91 (d, *J* = 8.8 Hz, 2H), 7.83 (d, *J* = 8.8 Hz, 2H), 7.44–7.39 (m, 10H), 7.37–7.33 (m, 3H), 7.33–7.27 (m, 9H), 7.14 (dd, *J* = 15.2, 8.2 Hz, 12H), 6.60 (d, *J* = 3.8 Hz, 2H), 6.58 (s, 2H), 6.42 (d, *J* = 3.8 Hz, 2H), 1.40 (s, 18H), 1.37–1.35 (m, 54H). ¹³C {¹H} NMR (151 MHz, Chloroform-*d*) δ 150.7, 150.2, 149.7, 144.5, 144.1, 143.2, 138.5, 137.9, 137.7, 136.2, 132.7, 131.7, 131.5, 131.4, 130.8, 130.7, 129.4, 129.2, 127.6, 127.5, 127.3, 127.0, 127.0, 127.0, 125.8, 125.5, 125.4, 125.0, 124.9, 124.8, 122.4, 34.8, 34.8, 34.7, 34.6, 31.7, 31.6, 31.5. HRMS analysis (APCI): calculated for C₁₂₀H₁₂₀S₃ [M+H]⁺: 1658.8658, found: 1658.8680.

4c: ¹H NMR (600 MHz, Chloroform-*d*) δ 8.71–8.64 (m, 6H), 7.90 (d, *J* = 8.8 Hz, 2H), 7.87–7.82 (m, 4H), 7.43–7.39 (m, 14H), 7.35 (dd, *J* = 8.1, 2.1 Hz, 2H), 7.32–7.27 (m, 12H), 7.16–7.11 (m, 16H), 6.60 (d, *J* = 3.8 Hz, 2H), 6.61–6.56 (m, 4H), 6.42 (d, *J* = 3.8 Hz, 2H), 1.39 (s, 36H), 1.37–1.34 (m, 54H). ¹³C {¹H} NMR (151 MHz, Chloroform-*d*) δ 150.7, 150.7, 150.2, 149.7, 144.1, 144.1, 138.5, 138.0, 137.7, 136.3, 132.7, 131.7, 131.4, 131.4, 130.8, 130.7, 129.4, 129.3, 127.6, 127.5, 127.3, 127.0, 127.0, 127.0, 125.8, 125.7, 125.5, 125.4, 125.0, 124.8, 122.5, 122.4, 34.8, 34.8, 34.7, 34.6, 31.7, 31.6, 31.5. HRMS analysis (APCI): calculated for C₁₅₈H₁₅₄S₄ [M]⁺: 2180.0961, found: 2180.0938.

4d: ¹H NMR (600 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 2.1 Hz, 2H), 7.36 (dd, *J* = 8.0, 2.1 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 4H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 4H), 6.42 (s, 2H), 1.36 (s, 18H), 1.33 (s, 18H). ¹³C NMR {¹H} (151 MHz, Chloroform-*d*) δ 150.4, 150.0, 143.8, 138.8, 138.2, 133.0, 131.0, 130.0, 127.7, 127.3, 125.1, 125.1, 34.9, 34.8, 31.8, 31.7. HRMS analysis (ESI): calculated for C₄₄H₅₂S [M+H]⁺: 613.3862, found: 613.3875.

2.4 The optimization of Shotgun Synthetic Route of 4a, 4b, 4c, and 4d

Table S1. Compound **s2** acts as an end block

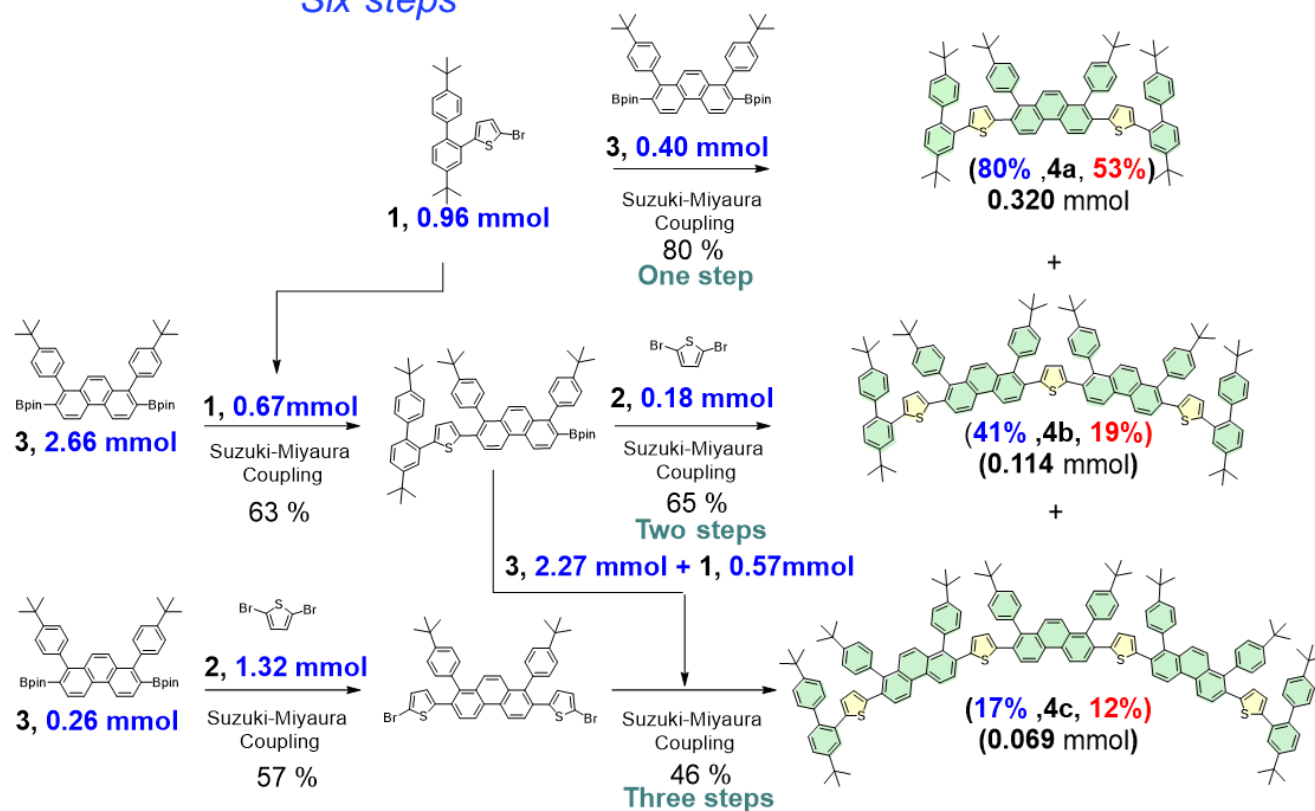
	3 (mmol)	3 (equiv.)	2 (equiv.)	s2 (equiv.)	1,4-Dioxane (mmol/mL)	H₂O (mmol/mL)	temp.(°C)/ time(h)	4d (mmol/%)	4a (mmol/%)	4b (mmol/%)
1	0.100	2.00	3.00	2.00	0.025	0.014	90/36	0.021/43	0.015/30	0.008/16
2	0.100	1.00	1.00	1.00	0.025	0.014	90/36	0.011/22	0.016/32	0.009/18
3	0.100	2.00	3.00	4.00	0.007	0.030	90/24	0.045/45	0.015/15	0.014/14
4	0.100	1.00	1.00	3.00	0.007	0.030	90/24	0.055/37	0.028/19	0.007/5
Pd(PPh ₃) ₄ (0.5 equiv.), K ₂ CO ₃ (25 equiv.). Yield: 4d = (2 × 4d mmol ÷ s2 mmol)%, 4a = (2 × 4a mmol ÷ s2 mmol)%, 4b = (2 × 4b mmol ÷ s2 mmol)%										

Table S2. Compound **1** acts as an end block

	3 (mmol)	3 (equiv.)	2 (equiv.)	1 (equiv.)	1,4-Dioxane (mmol/mL)	H₂O (mmol/mL)	temp.(°C)/ time(h)	4a (mmol/%)	4b (mmol/%)	4c (mmol/%)
1	0.100	2.00	1.00	2.40	0.010	0.050	90/36	0.032/54	0.012/24	0.008/13
2	0.100	3.00	2.00	2.40	0.010	0.050	90/36	0.018/45	0.009/23	0.005/11
3	0.100	2.00	1.00	5.00	0.020	0.100	90/24	0.023/18	0.017/14	0.004/3
4	0.100	2.00	1.00	2.00	0.020	0.100	90/24	0.030/60	0.005/10	0.008/17
5	1.00	2.00	1.00	2.40	0.025	0.500	90/24	0.320/53	0.114/19	0.069/12
6	1.00	2.00	1.00	2.40	0.020	0.100	90/36	0.260/43	0.150/25	0.034/6
Pd(PPh ₃) ₄ (0.5 equiv.), K ₂ CO ₃ (25 equiv.). Yield: 4a = (2 × 4a mmol ÷ 1 mmol)%, 4b = (2 × 4b mmol ÷ 1 mmol)%, 4c = (2 × 4c mmol ÷ 1 mmol)%										

Iterative synthesis

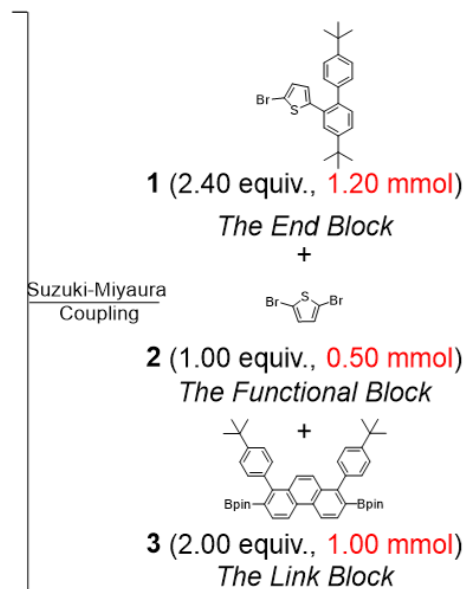
Six steps



VS

Shotgun synthesis

One step



	Com. 4a	Com. 4b	Com. 4c	Total
<i>Iterative synthesis</i>	80%, one step 0.320 mmol	41%, two steps 0.114 mmol	17%, three steps 0.069 mmol	Six steps: 216 h Com.1: 2.20 mmol Com.2: 1.50 mmol Com.3: 5.59 mmol
<i>Shotgun synthesis</i>	53% 0.320 mmol	19% 0.114 mmol	12% 0.069 mmol	One step: 36 h Com.1: 1.20 mmol Com.2: 0.50 mmol Com.3: 1.00 mmol

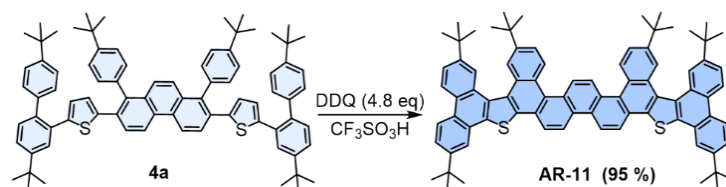
Scheme S4. Comparison of the raw material consumption and time required for iterative synthesis and Shotgun synthesis to achieve the same amount of compounds **4a**, **4b**, and **4c**.

2.5 Syntheses of the thiophene-fused arcuate graphene nanoribbons

General procedure 1 (GP1) for the Scholl cyclization:

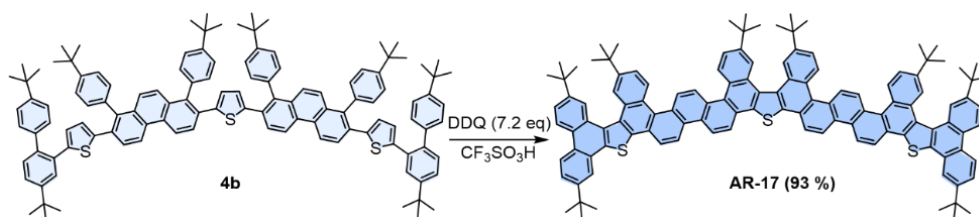
A 100 mL Schlenk flask charged with the precursors and 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) was purged with argon for ten minutes. Dry DCM was added to make a clear solution. The mixture was then cooled down to -10°C under argon atmosphere. After stirring at -10°C for 30 minutes, trifluoromethanesulfonic acid (TfOH) was added at -10°C . The mixture immediately turned black upon the addition of TfOH. The mixture was stirred at -10°C for 60 minutes and then quenched by pouring it into sat. aq. NaHCO_3 (30 mL). After stirring vigorously for 15 minutes, the aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na_2SO_4 , filtered and concentrated under reduced pressure. the crude product mixture was purified by silica gel column chromatography gave **AR**.

AR-11



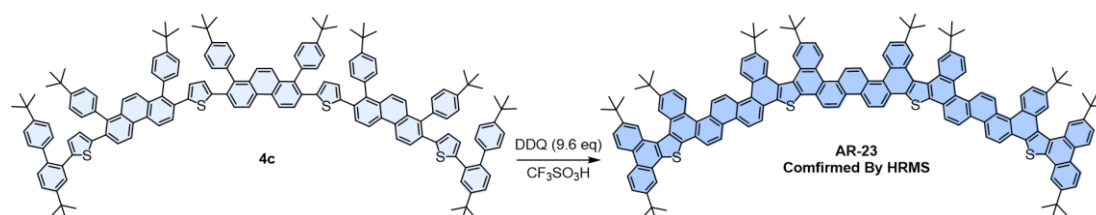
According to GP1, compound **4a** (56.0 mg, 50 μmol , 1.0 equiv.) and DDQ (54.0 mg, 240 μmol , 4.8 equiv.) in DCM/TfOH (55 mL/1.1 mL) were used to setup the reaction. The product was obtained after workup, Purification by silica gel chromatography (DCM/petroleum ether = 1/50 to 1/10) gave **AR-11**, then recrystallization from $\text{CHCl}_3/\text{CH}_3\text{OH}$, and drying in vacuum as a yellow solid (53.6 mg, 47.5 μmol , 95%). ^1H NMR (600 MHz, Chloroform-*d*) δ 9.28 (d, J = 8.7 Hz, 2H), 9.21 (s, 2H), 9.12 (d, J = 9.8 Hz, 2H), 8.82 (d, J = 2.0 Hz, 2H), 8.76 (d, J = 2.1 Hz, 2H), 8.69 (dd, J = 14.3, 8.7 Hz, 4H), 8.51 (dd, J = 8.6, 1.1 Hz, 2H), 8.26 (d, J = 1.9 Hz, 2H), 7.84 (dd, J = 8.7, 2.1 Hz, 2H), 7.80–7.76 (m, 4H), 1.57 (s, 18H), 1.41 (s, 18H), 1.40 (s, 18H). ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, Chloroform-*d*) δ 162.9, 150.5, 148.4, 148.2, 138.4, 137.2, 132.9, 132.0, 131.0, 130.4, 129.3, 128.6, 128.5, 128.3, 128.1, 128.1, 127.9, 127.1, 126.8, 125.6, 125.2, 125.0, 124.1, 123.5, 123.2, 123.0, 122.6, 122.0, 120.7, 35.5, 35.5, 35.4, 31.8, 31.7. HRMS analysis (APCI): calculated for $\text{C}_{82}\text{H}_{78}\text{S}_2$ $[\text{M}+\text{H}]^+$: 1127.5618, found: 1127.5637.

AR-17



According to GP1, compound **4b** (33.2 mg, 20 μ mol) and DDQ (32.7 mg, 144 μ mol, 7.2 equiv.) in DCM/TfOH (70 mL/1.4 mL) were used to setup the reaction. The product was obtained after workup, purification by silica gel chromatography (DCM/ petroleum ether = 1/20 to 1/5) gave **AR-17**, then recrystallization from CHCl₃/ CH₃OH, and drying in vacuum as a dark yellow solid (30.6 mg, 18.6 μ mol, 93%). ¹H NMR (600 MHz, Chloroform-*d*) δ 9.32 (d, *J* = 8.5 Hz, 2H), 9.27 (d, *J* = 8.5 Hz, 2H), 9.23–9.16 (m, 4H), 9.01 (s, 2H), 8.98 (s, 4H), 8.81 (s, 2H), 8.77 (s, 2H), 8.62 (dd, *J* = 19.4, 8.5 Hz, 4H), 8.40 (s, 4H), 8.21 (s, 2H), 7.90 (d, *J* = 7.9 Hz, 2H), 7.85 (d, *J* = 9.7 Hz, 2H), 7.74 (d, *J* = 6.7 Hz, 4H), 1.58 (s, 18H), 1.51 (s, 18H), 1.45 (s, 18H), 1.44 (s, 18H). ¹³C NMR spectra (600 MHz, 9 hours) could not be recorded because of its high aggregation in solution, (Figure S45). HRMS analysis (APCI): calculated for C₁₂₀H₁₀₈S₃ [M+H]⁺: 1646.7719, found: 1646.7776.

AR-23



According to GP1, compound **4c** (5.5 mg, 2.5 μ mol) and DDQ (5.5 mg, 24 μ mol, 9.6 equiv.) in DCM/TfOH (20 mL/0.4 mL) were used to setup the reaction. The product was obtained after workup. Purification by silica gel chromatography (DCM/ petroleum ether = 1/20 to 1/5) gave **AR-23**, then recrystallization from CHCl₃/ CH₃OH, and drying in vacuum as a dark yellow solid (4.5 mg). Well-resolved ¹H and ¹³C NMR spectra could not be recorded because of its high aggregation in solution (Figure S51). MALDI HRMS (CHCA) (*m/z*): calculated for C₁₅₈H₁₃₈S₄ [M]⁺: 2163.9709, found: 2163.9706.

General procedure for the flow electrolysis

The flow electrolysis cell is assembled using two aluminum bodies (① and ⑤, 75*75*15 mm) with a groove (50*50*3 mm). The anode (④), which is made of graphite (C, 49*49*5 mm), is insulated from the aluminum body by PTFE or silicone film. The cathode (②) is a Ni plate (49*49*3 mm). The anode and cathode are held apart by a fluorinated ethylene propylene (FEP) foil (③) of 250 μm thickness. A rectangular reaction channel (total length: 313 mm, width: 3.2 mm) is cut in the FEP foil to give an overall channel volume of 250 μL . The whole device is held together by steel screws. The inside view of the device is shown in Figure S2 A. The reaction setups are shown in Figure S2 B.

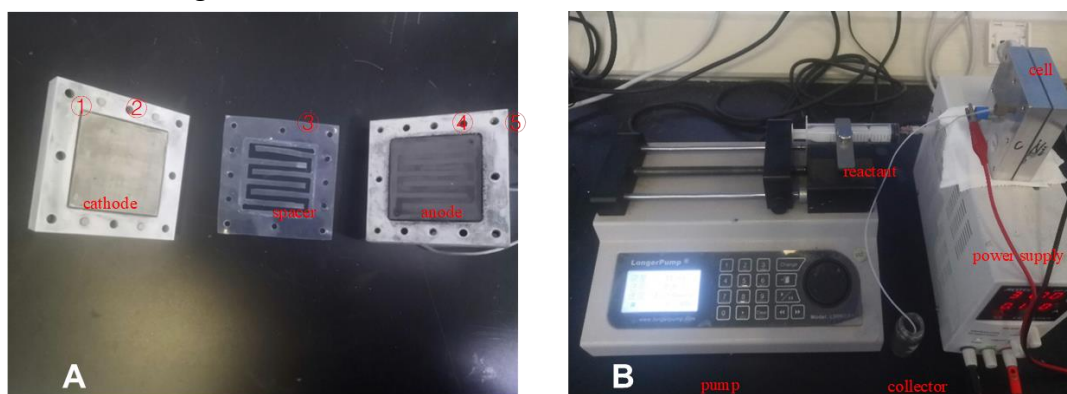
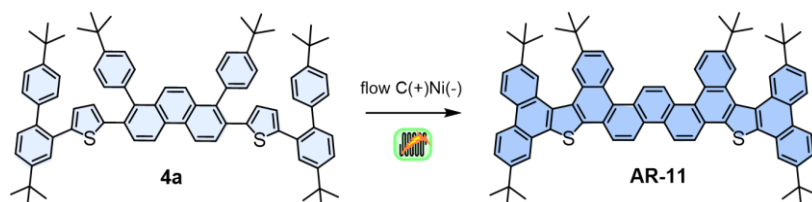


Figure S1. Setups for the flow electrolysis. Details of the reactor have been reported.¹



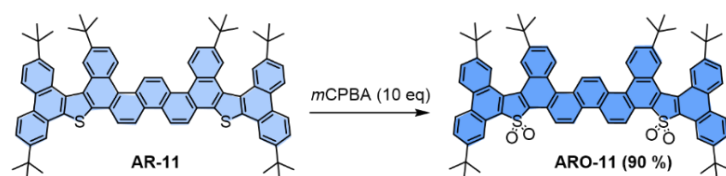
The electrolysis was conducted with a constant voltage of 1.65 V using a flow electrolytic cell, which was equipped with a graphite anode and a Ni cathode with a surface area of 10 cm^2 and an interelectrode distance of 250 μm . The precursor 4a (0.1 mmol, 113.6 mg), the electrolyte $n\text{Bu}_4\text{NBF}_4$ (20 mmol, 6.5 g), dissolving in DCM/TFA (135/15 mL) were pushed using a syringe pump to pass through the flow electrolytic cell with a flow rate of 0.10 mL min^{-1} (residence time = 2.5 min, total time spent = 25 h). The reaction mixture is evaporated under vacuum to obtain the crude residue. The crude residue was washed with methanol and crude residue was subjected to flash column chromatography on silica gel to yield the desired product. purification by silica gel chromatography (DCM/petroleum ether = 1/50 to 1/10) gave **AR-11**.

2.6 Syntheses of the thiophene-dioxides fused arcuate graphene nanoribbons

General procedure 2 (GP2) for the oxidation:

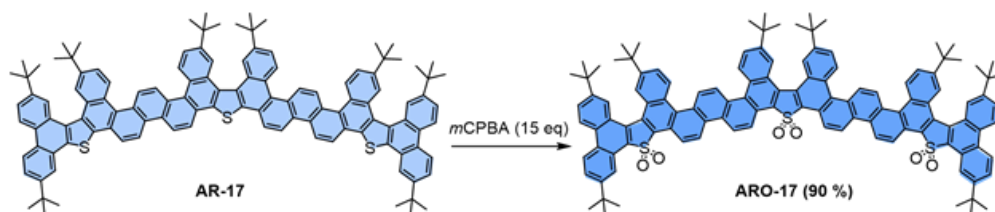
A 25 mL Schlenk flask charged with **AR** was purged with argon for ten minutes. Dry DCM was added to make a clear solution. The mixture stirring at room temperature for 20 minutes. meta-Chloroperoxybenzoic acid (*m*CPBA) was added in one portion at room temperature under argon atmosphere. The mixture was stirred at room temperature for 60 minutes and then quenched by pouring it into sat. aq. sodium thiosulfate (30 mL). After stirring vigorously for 15 minutes, the aqueous layer was extracted with dichloromethane (DCM) for three times. The combined organic layers were washed with brine and dried with Na₂SO₄, filtered and concentrated under reduced pressure. the crude product mixture was purified by silica gel column chromatography gave **ARO**.

ARO-11



According to GP2, compound **AR-11** (56.4 mg, 50 μ mol) and *m*CPBA (86.3 mg, 500 μ mol, 10 equiv.) in DCM (70 mL) were used to setup the reaction. The product was obtained after workup, Purification by silica gel chromatography (DCM/ethyl acetate/petroleum ether = 1/1/20) gave **ARO-11**, then recrystallization from CHCl₃/ CH₃OH, and drying in vacuum as an orange yellow solid. (53.6 mg, 45 μ mol, 90%). ¹H NMR (600 MHz, Chloroform-*d*) δ 9.35 (d, *J* = 8.8 Hz, 2H), 9.22 (s, 2H), 9.18 (s, 2H), 8.90 (d, *J* = 8.8 Hz, 2H), 8.77 (d, *J* = 9.0 Hz, 2H), 8.72 (d, *J* = 8.8 Hz, 2H), 8.64 (d, *J* = 1.9 Hz, 2H), 8.40 (d, *J* = 2.0 Hz, 2H), 8.34 (d, *J* = 2.1 Hz, 2H), 8.01 (dd, *J* = 8.9, 2.1 Hz, 2H), 7.92 (ddd, *J* = 18.5, 8.7, 1.9 Hz, 4H), 1.56 (s, 18H), 1.38 (s, 18H), 1.35 (s, 18H). ¹³C {¹H} NMR (151 MHz, Chloroform-*d*) δ 151.5, 149.0, 148.7, 134.1, 133.4, 132.2, 131.7, 130.7, 130.7, 130.6, 130.0, 129.8, 129.7, 128.4, 128.2, 127.9, 127.8, 127.2, 126.6, 126.0, 124.1, 123.9, 123.8, 123.3, 123.1, 123.0, 121.7, 119.8, 35.2, 35.1, 35.1, 31.2, 31.1, 31.0. HRMS analysis (ESI): calculated for C₈₂H₇₈O₄S₂ [M+Na]⁺: 1213.5234, found: 1213.5258.

ARO-17



According to GP2, compound **AR-17** (4.9 mg, 3 μ mol) and *m*CPBA (7.8 mg, 45 μ mol, 15 equiv.) in CH_2Cl_2 (10 mL) were used to setup the reaction. The product was obtained after workup, Purification by silica gel chromatography (DCM/ethyl acetate/ petroleum ether / = 1/2/20) gave **ARO-17**, then recrystallization from $\text{CHCl}_3/\text{CH}_3\text{OH}$, and drying in vacuum as an orange yellow solid. (4.7 mg, 2.7 mmol, 90%). ^1H NMR (600 MHz, Chloroform-*d*) δ 9.40 (dd, $J = 23.9, 8.7$ Hz, 4H), 9.27 (s, 4H), 9.23 (s, 4H), 8.97 (dd, $J = 26.8, 8.6$ Hz, 4H), 8.77 (dd, $J = 25.5, 8.8$ Hz, 4H), 8.64 (d, $J = 25.7$ Hz, 4H), 8.40 (d, $J = 27.7$ Hz, 4H), 8.07 (dd, $J = 32.1, 8.7$ Hz, 4H), 7.94 (t, $J = 10.8$ Hz, 4H), 1.46 (s, 18H), 1.39 (d, $J = 8.3$ Hz, 54H). ^{13}C $\{^1\text{H}\}$ NMR (151 MHz, Tetrachloroethane-*d*₂) δ 152.0, 149.9, 149.6, 149.5, 149.2, 149.2, 133.8, 133.8, 133.5, 133.4, 133.2, 132.3, 132.3, 131.8, 131.2, 131.1, 130.9, 130.9, 130.8, 130.5, 130.3, 128.7, 128.6, 128.5, 128.2, 128.0, 127.7, 127.0, 127.0, 126.1, 123.9, 123.5, 123.2, 122.0, 119.7, 35.5, 35.4, 35.3, 35.3, 31.5, 31.4, 31.3, 31.2. HRMS analysis (APCI): calculated for $\text{C}_{120}\text{H}_{108}\text{O}_6\text{S}_3$ $[\text{M}]^+$: 1741.7336, found: 1741.7382.

3. X-Ray Crystallography

3.1 Experimental details on crystal growth

Single crystals of **AR-11** (Colorless transparent prismatic) obtained by slowly evaporating CDCl₃-CS₂-Acetone, **ARO-11** (clear light yellow sheet) obtained by slowly evaporating CHCl₃-MeOH (1:1, v/v) solutions at room temperature,

Table S3. Crystallographic data and structure refinement details for **AR-11**, **ARO-11**.

Compound	AR-11	ARO-11
CCDC Deposition number	2303699	2303698
Empirical formula	C ₈₂ H ₇₈ S ₂	C ₈₂ H ₇₈ O ₄ S ₂
Formula weight	1126.55	1190.53
Temperature/K	100.0(9)	100.0(4)
Crystal system	monoclinic	monoclinic
Space group	P21/c	I2/a
a/Å	10.3995(2)	25.5478(5)
b/Å	16.4712(2)	20.7666(2)
c/Å	40.5773(5)	31.3909(5)
α/°	90	90
β/°	91.4480(10)	110.188(2)
γ/°	90	90
Volume/Å ³	6948.36(18)	15631.0(5)
Z	4	8
ρ _{calc} g/cm ³	1.078	1.216
μ/mm ⁻¹	0.652	1.903
F(000)	2408	6000
Crystal size/mm ³	0.03 × 0.01 × 0.01	0.02 × 0.01 × 0.005
Radiation	micro-focus metaljet (λ = 1.3405)	micro-focus metaljet (λ = 1.3405)
2θ range for data collection/°	3.788 to 105.86	4.526 to 105.864
Index ranges	-12 ≤ h ≤ 12, -19 ≤ k ≤ 19, -45 ≤ l ≤ 48	-30 ≤ h ≤ 30, -24 ≤ k ≤ 24, -37 ≤ l ≤ 24
Reflections collected	68565	79840
	12265	13676
Independent reflections	[R _{int} = 0.0822, R _{sigma} = 0.0491]	[R _{int} = 0.0438, R _{sigma} = 0.0288]
Data/restraints/parameters	12265/13/775	13676/18/883
Final R indexes [I >= 2σ (I)]	1.047	1.034
Final R indexes [all data]	R ₁ = 0.0791, wR ₂ = 0.2132	R ₁ = 0.0842, wR ₂ = 0.2435
Largest diff. peak/hole / e Å ⁻³	R ₁ = 0.0897, wR ₂ = 0.2214	R ₁ = 0.0950, wR ₂ = 0.2535

These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

3.2 Single-crystal Structure and Packing of AR-11 and ARO-11

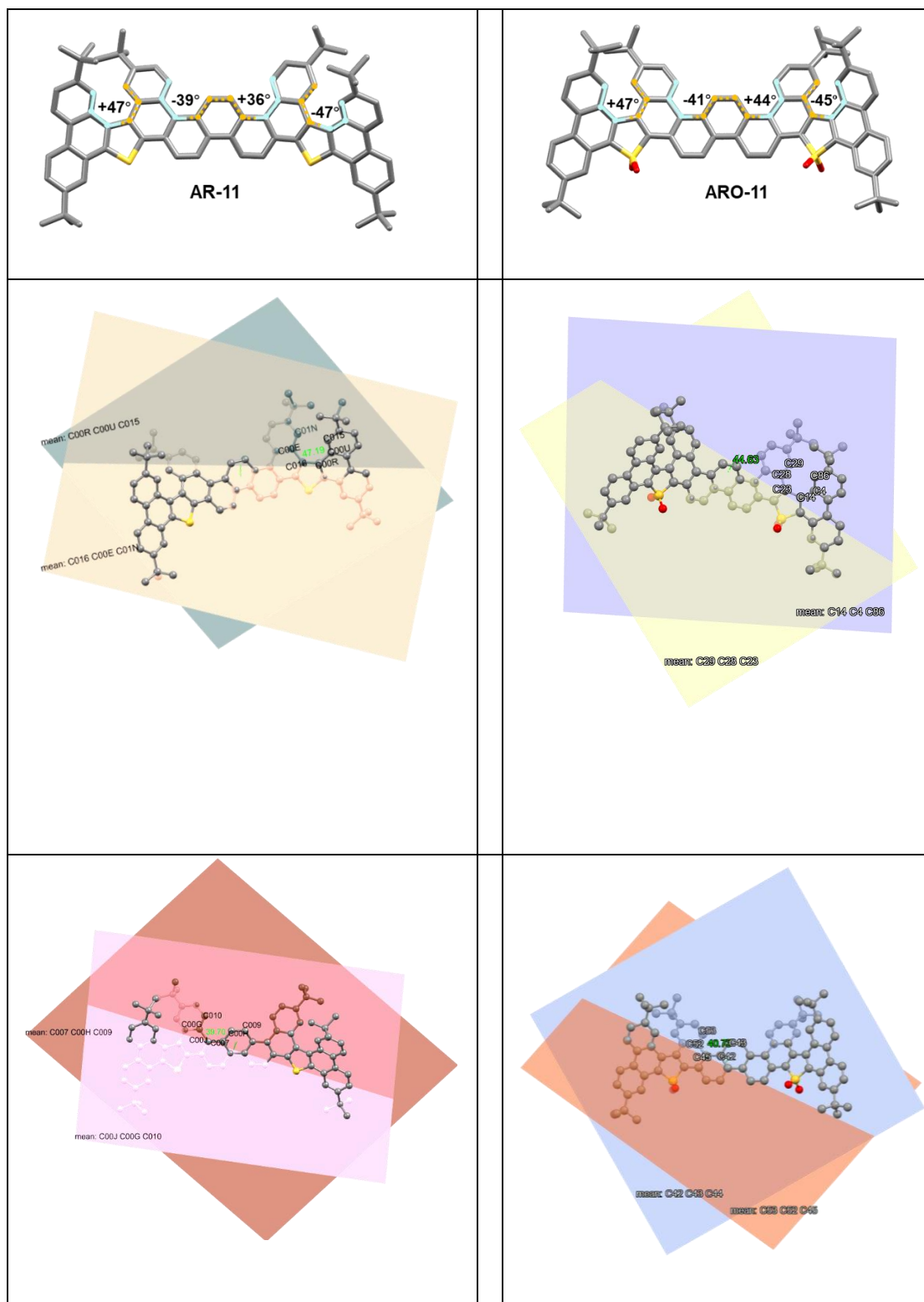


Figure S2 (a). cove edges angle diagram of X-ray crystallographic structures of **AR-11** and **ARO-11** (thermal ellipsoids shown at 50% probability, hydrogen atoms were omitted for clarity).

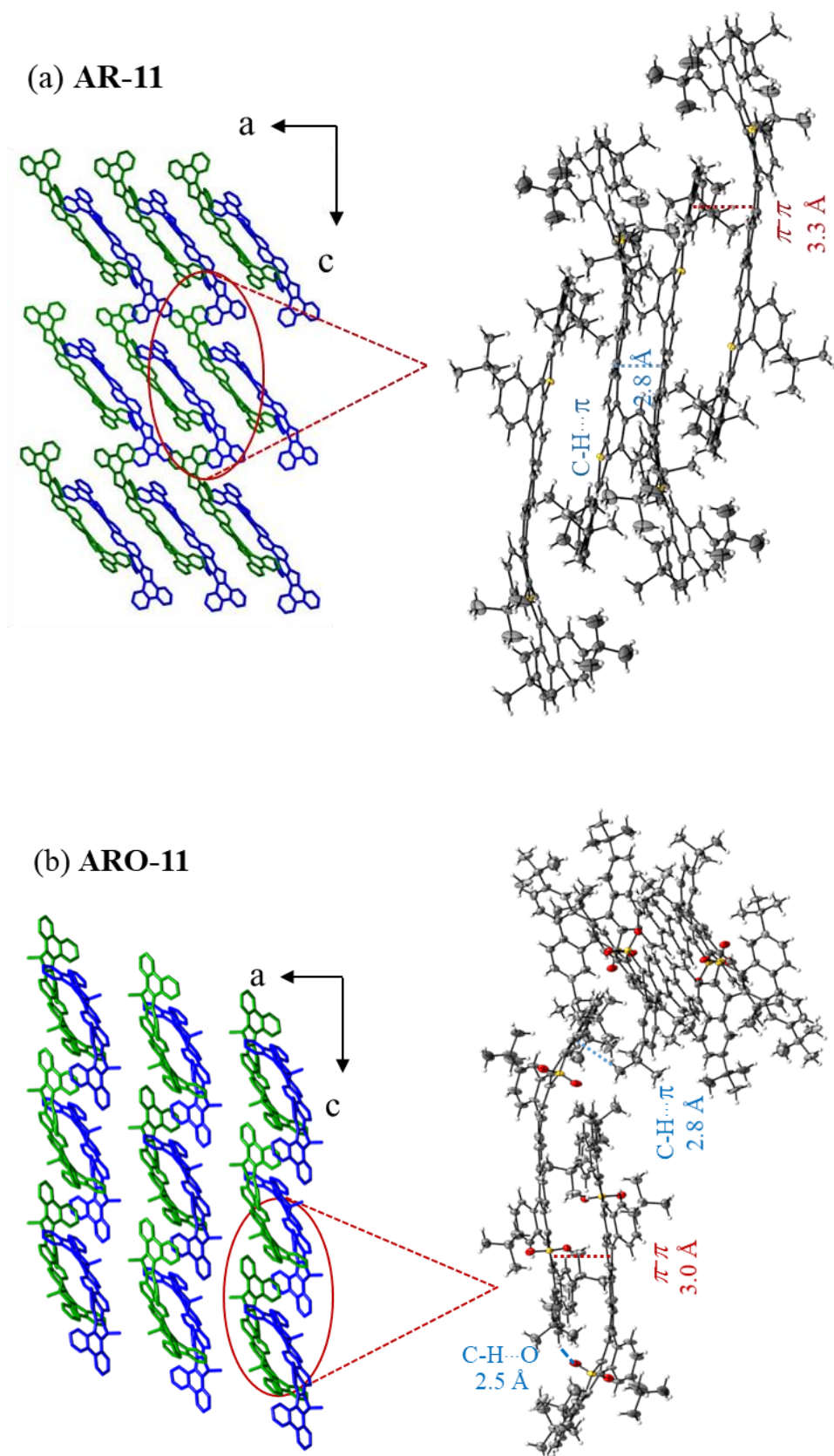


Figure S2(b). The packing structure of (a). AR-11 and (b). ARO-11.

4. Electrochemistry

Electrochemical measurements were carried out with Metrohm Autolab PGSTAT204 electricity workstation at room temperature. Cyclic voltammograms (CV) and differential pulse voltammogram (DPV) were carried out using a conventional three-electrode system equipped with a glassy carbon working electrode (1.5 mm diameter), a platinum counter electrode, and Ag/AgCl (3 mol L⁻¹ KCl) reference electrode. The commercial electrolytes Na[BArF₂₄] and [*n*-Bu₄N][PF₆] were purified by recrystallisation. [*n*-Bu₄N][BArF] was synthesized as previously reported.⁶ Analyte solutions were between 0.1-1 mM.

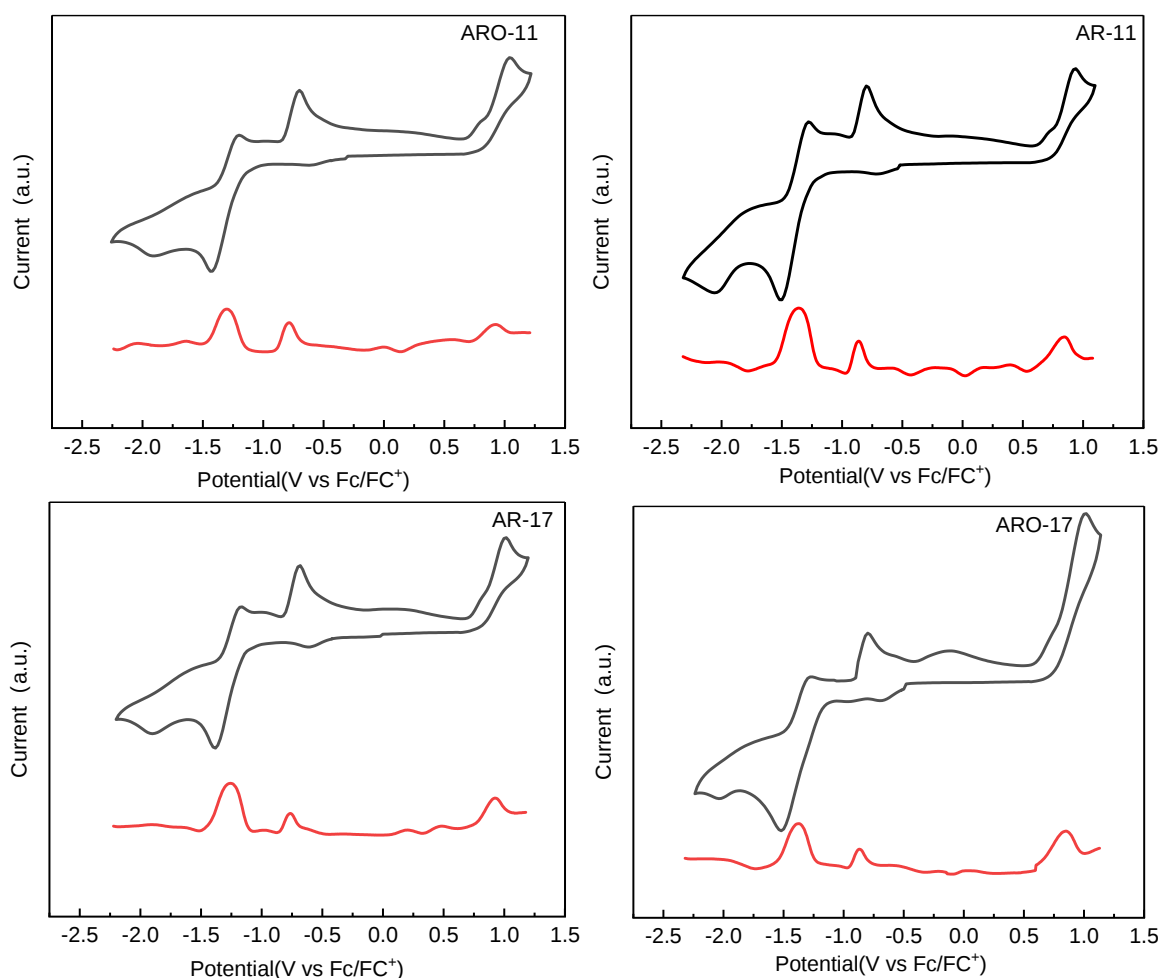


Figure S3(a). CV and DPV of AR-11, ARO-11 and AR-17, ARO-17 in THF solution containing 0.1M Bu₄NPF₆ at room temperature at a scan rate of 0.1 V/s. (1.0×10^{-5} mol/L in THF for CV and DPV).

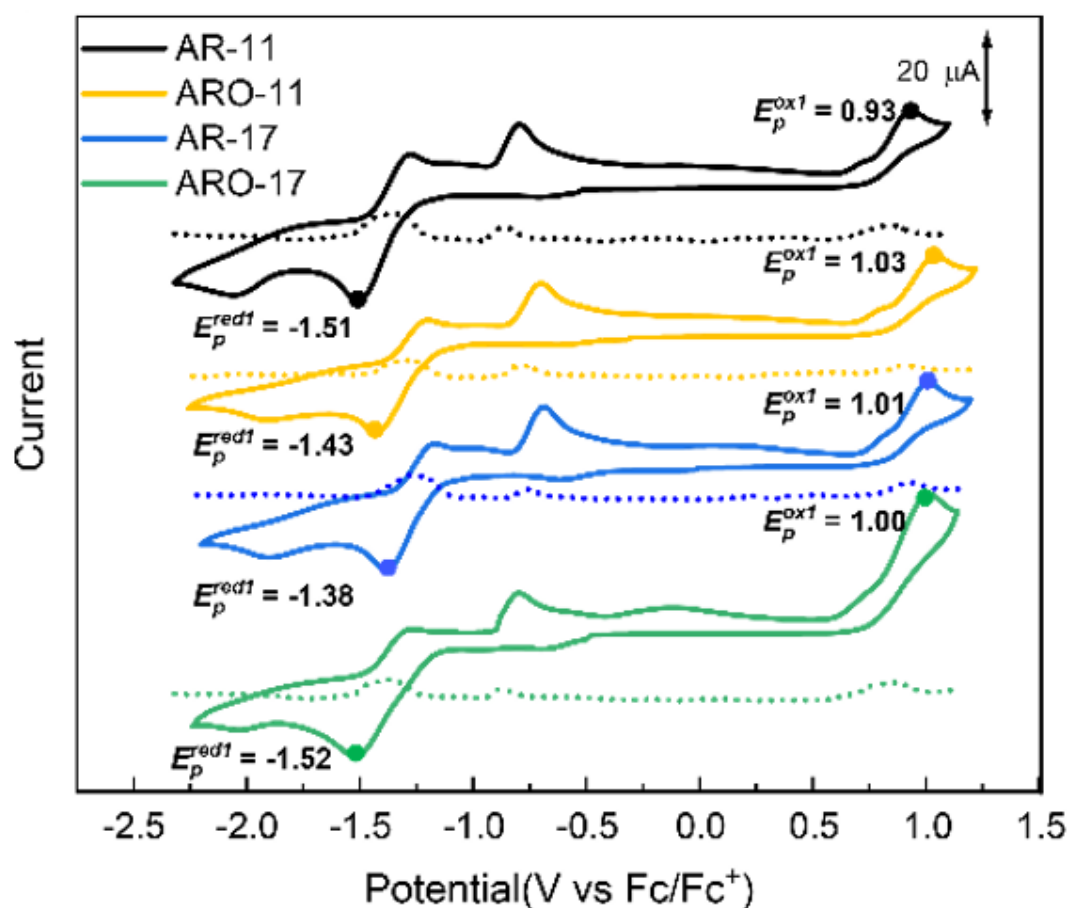


Figure S3(b). CV and DPV of AR-11, ARO-11 and AR-17, ARO-17 in THF solution containing 0.1 M Bu₄NPF₆ at room temperature at a scan rate of 0.1 V/s. (1.0×10^{-5} mol/L in THF for CV and DPV).

5. The photophysical properties

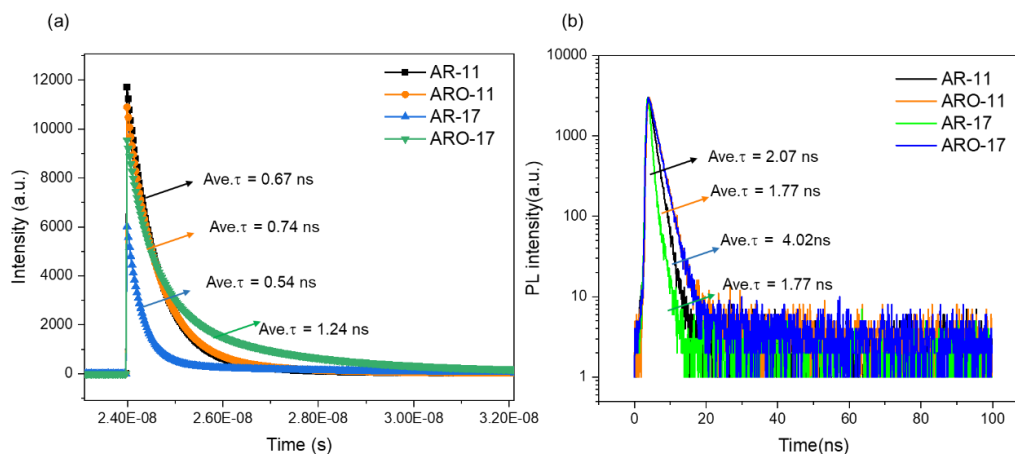


Figure S4. a) Fluorescence lifetime in solid state. b) Fluorescence lifetime in liquid state (1.0×10^{-5} M).

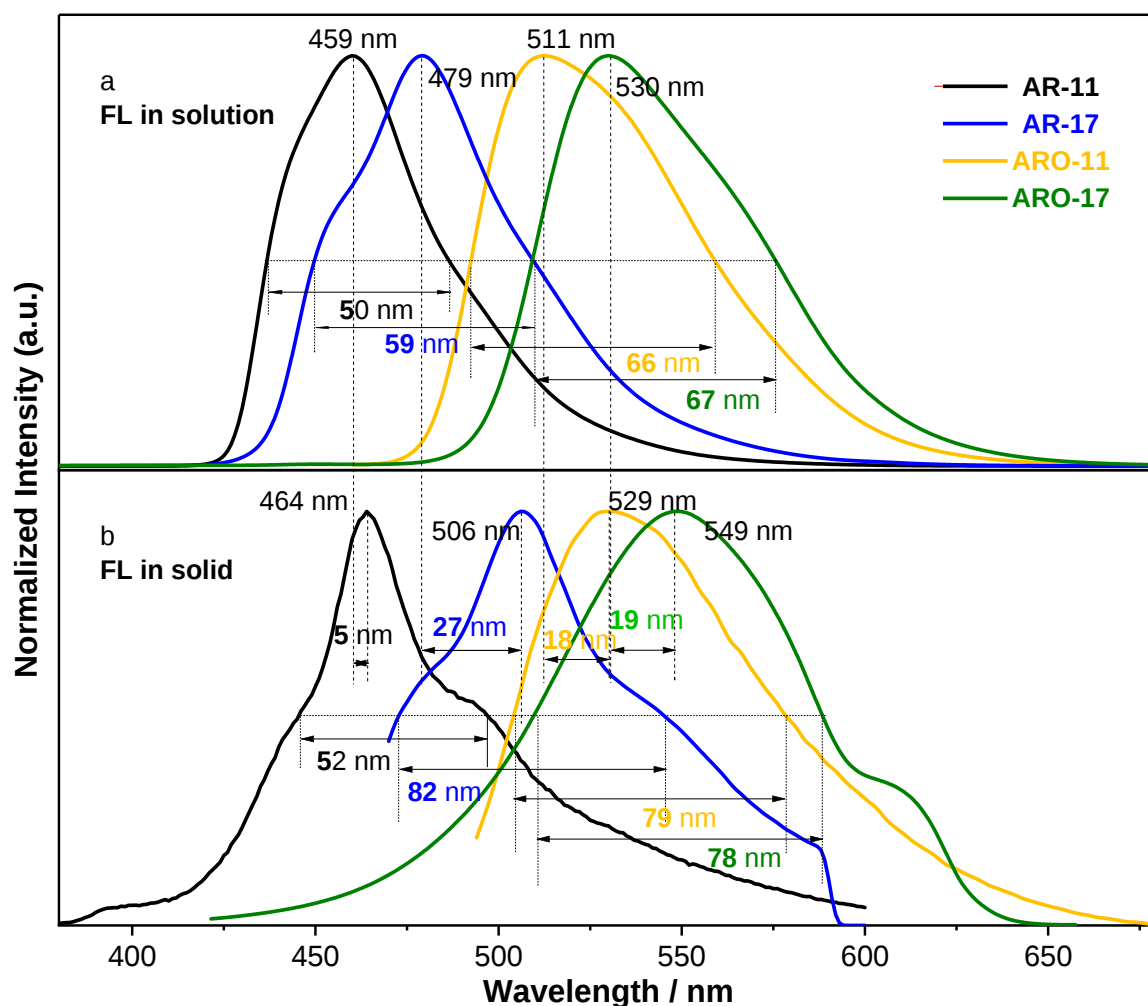


Figure S5. Contrast of shift and broadening of solid and liquid fluorescence emission spectra.

FT-IR spectra

A comparison of the FTIR spectra of precursor **4c** and **AR-23** revealed the strong attenuation of the signal triad from aromatic C-H stretching vibrations at 3026, and 3076 cm^{-1} , as well as the disappearance of out-of-plane C-H deformation bands at 800 and 839 cm^{-1} , which are characteristic for mono- and disubstituted benzene rings. Moreover, the band appearing at 909 and 953 cm^{-1} could be assigned to the out-of-plane band from the aromatic C-H moiety at the cove position. The **4b** and **AR-17** show the same trend.

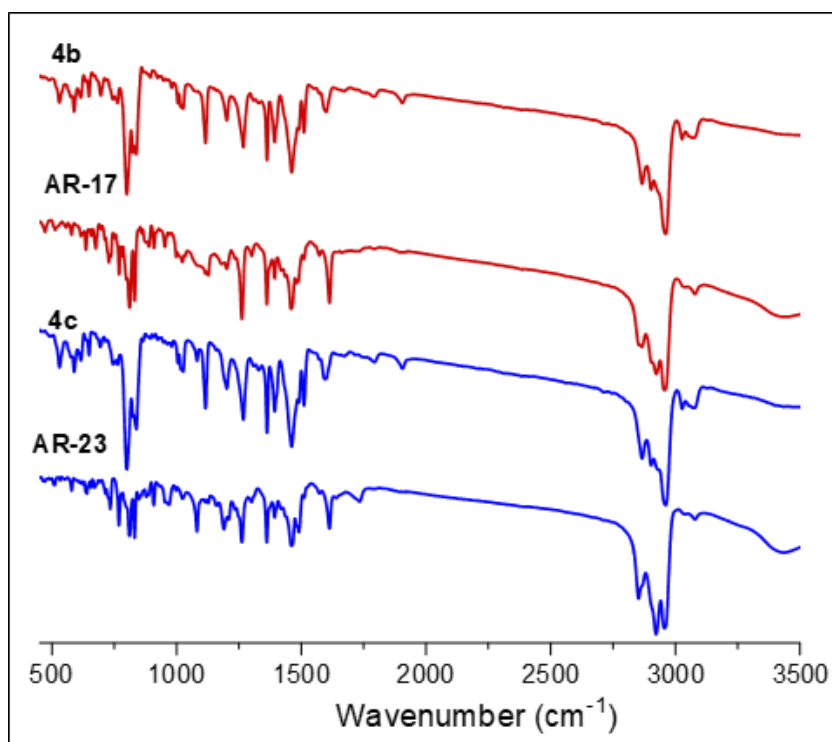


Figure S6 a). FT-IR spectra of **4b**, **AR-17**, and **4c**, **AR-23** measured on powder samples

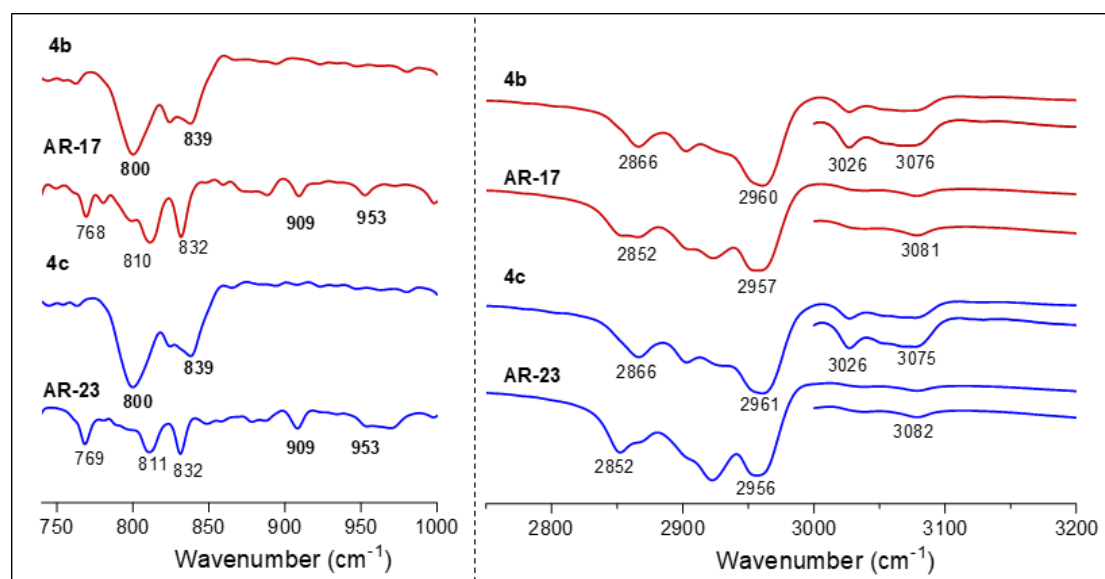


Figure S6 b). Locally amplified FT-IR spectra of **4b**, **AR-17** and **4c**, **AR-23**.

Raman spectra

Raman spectrum of a powder sample of **4c** and **AR-23** was measured at 785 nm, and showed first-order D band (disorder band) and G band (graphite band) at 1343 and 1417 cm^{-1} , respectively, consistent with literature values for GNRs. The Raman spectrum of the **4c** exhibits a multi-component D band at 1300 cm^{-1} and G band at 1597 cm^{-1} , which can be attributed to the nonplanar nature and defects of **4c**. In addition, the D and G bands split into several components of **AR-23** and **AR-17**, possibly due to resonant effects associated with their unique structure.

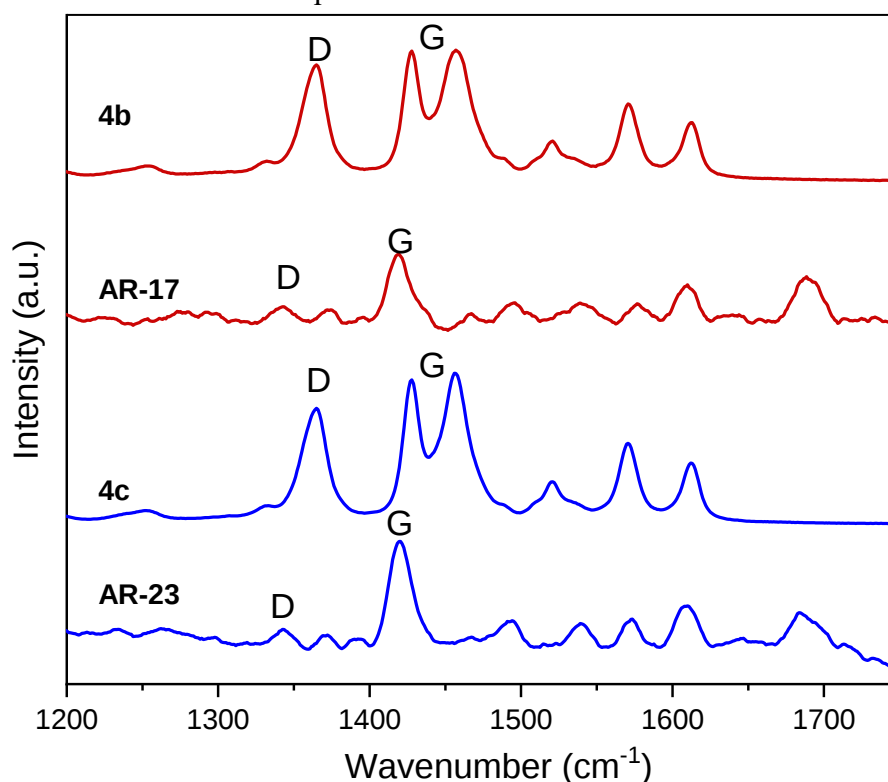


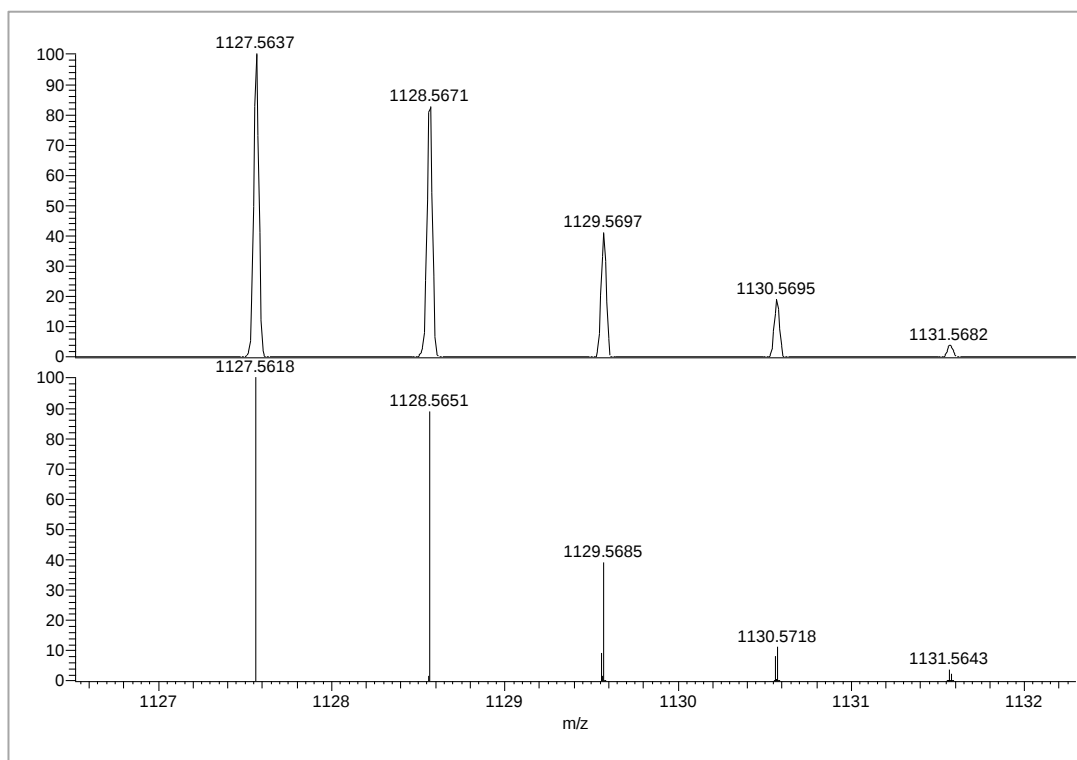
Figure S7. Raman spectrum of **4b**, **AR-17**, and **4c**, **AR-23** recorded with a 785 nm excitation laser (baseline subtraction was carried out because of the strong fluorescence background of **4b**, **AR-17**, and **4c**, **AR-23**).

Table S4. Spectroscopic Characterizations of **AR-11**, **AR-17** and **ARO-11**, **ARO-17**.

compound	λ_{abs} [nm] ^a	ϵ_{max} [10 ⁵ M ⁻¹ cm ⁻¹] ^a	λ_{em} [nm] ^a	Φ [%] ^{a,c}	τ [ns] ^{a,d}	λ_{em} [nm] ^b	Φ [%] ^{b,c}	τ [ns] ^{b,d}	λ_{broaden} [nm]
AR-11	415/392	1.19/1.01	459	15	2.07	464	4.74	0.67	5
AR-17	434/410	1.74/1.56	479	37	4.02	506	0.18	0.54	27
ARO-11	466/441	0.65/0.56	511	65	1.77	529	5.85	0.74	18
ARO-17	486/463	1.04/0.92	530	71	1.77	549	1.50	1.24	19

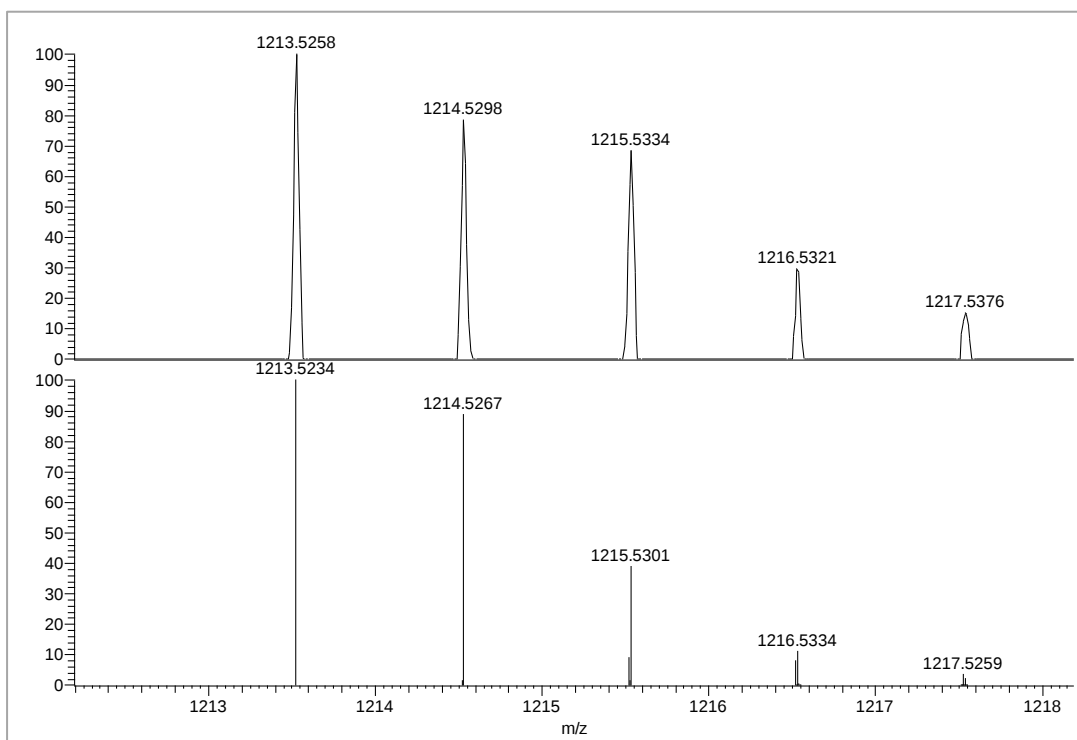
^aMeasured in CH₂Cl₂ solution (1.0 × 10⁻⁵ M). ^bMeasured in solid state. ^cFluorescence quantum yield. ^dFluorescence lifetime.

6. Mass Spectra



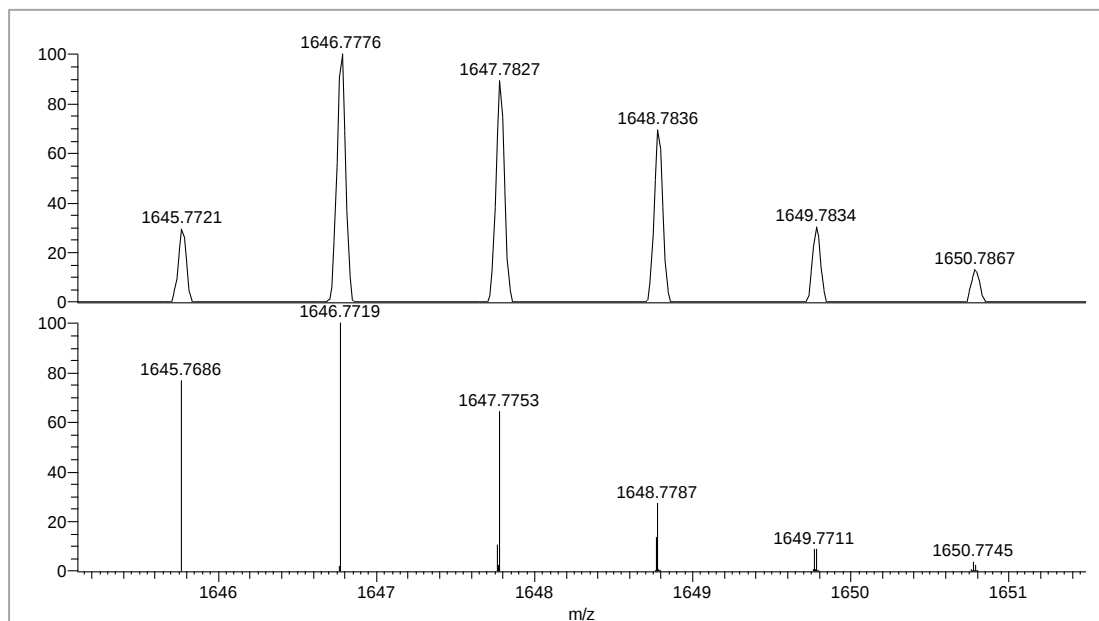
HRMS analysis (APCI) of AR-11

Calculated for $C_{82}H_{78}S_2$ $[M+H]^+$: 1127.5618, found: 1127.5637.



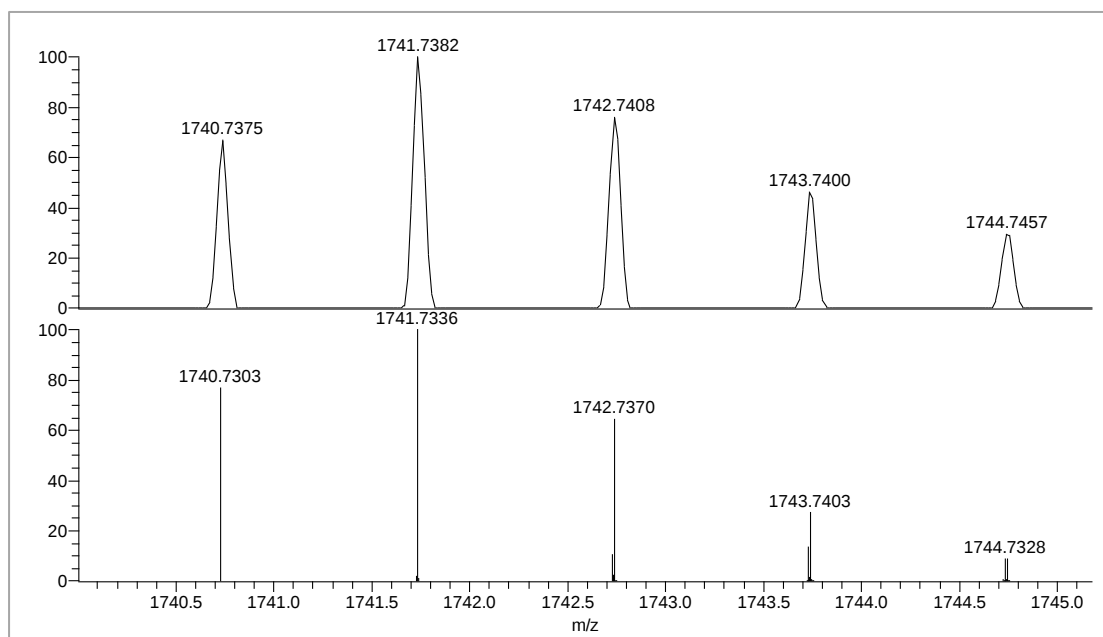
HRMS analysis (ESI) of ARO-11

Calculated for $C_{82}H_{78}O_4S_2$ $[M+Na]^+$: 1213.5234, found: 1213.5258.



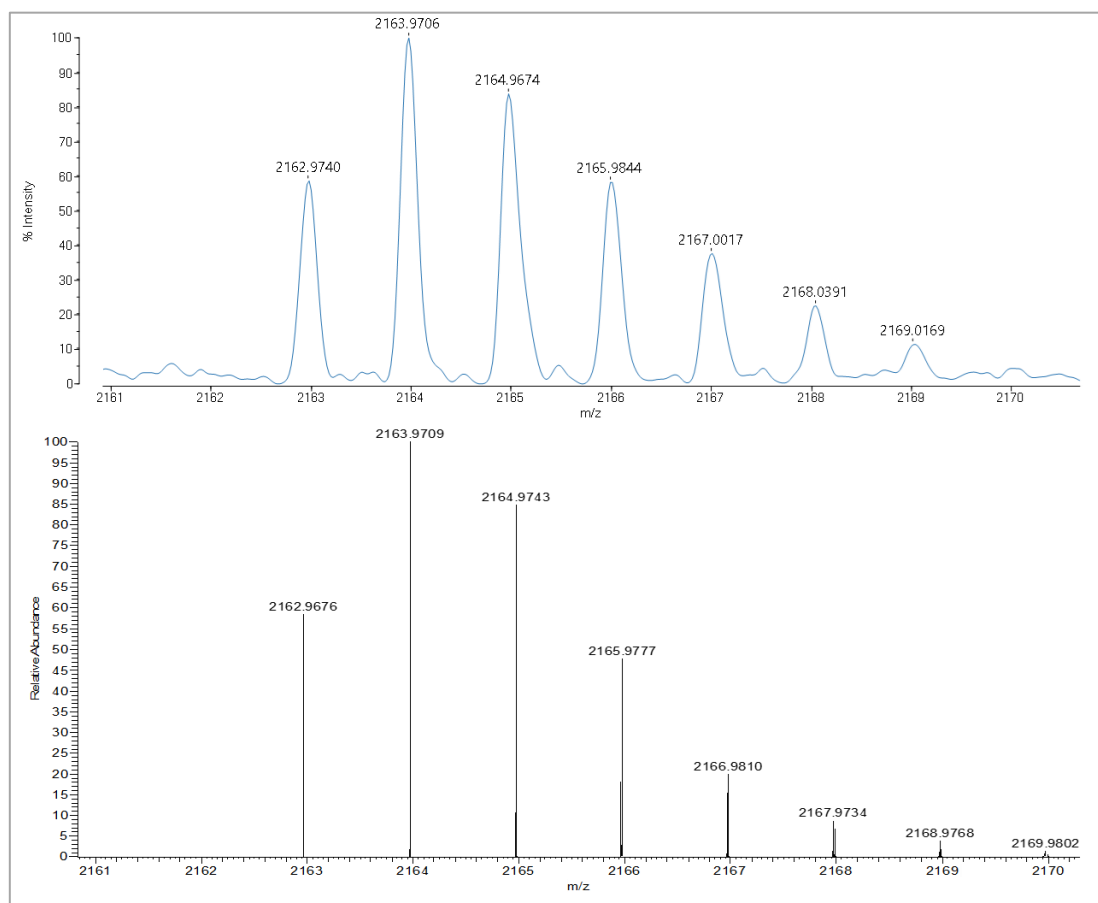
HRMS analysis (APCI) of AR-17

Calculated for $C_{120}H_{108}S_3$ $[M+H]^+$: 1646.7719, found: 1646.7776.



HRMS analysis (APCI) of ARO-17

Calculated for $C_{120}H_{108}O_6S_3$ $[M]^+$: 1741.7336, found: 1741.7382.



MALDI HRMS (CHCA) of AR-23

Calculated for $C_{158}H_{138}S_4 [M]^+$: 2163.9709, found: 2163.9706.

Figure S8. Mass spectrum information of AR-11, ARO-11, AR-17, ARO-17, AR-23.

7. Calculated details

Geometry optimizations were performed by Gaussian 16 C.01 package⁷ at the ω B97XD/6-31G(d,p) level of theory⁸. Solvation effects of dichloromethane (CH_2Cl_2) were included using the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) with a standard state of 1 M⁹. Energy minima and transition states were verified through vibrational analysis. Frequency calculations were performed at the same theoretical level as for geometry optimizations to verify the stationary points as either minima or first-order saddle points on the potential energy surface, as well as to obtain thermal Gibbs free energy corrections at 298 K. Intrinsic reaction coordinate (IRC) computations were used to ensure that each transition state connected the correct two minima.

Highly accurate electronic energies were computed by ORCA 5.0.4 package¹⁰ at the RI- ω B97M-V/Def2-TZVP, Def2/J level of theory¹¹. Solvation effects were included using the solvation model based on density (SMD) with a standard state of 1 M¹². Geometrical counterpoise correction (gCP) were included to remove artificial overbinding effects from BSSE¹³. Grimme's quasiharmonic correction¹⁴ were applied by using Shermo 2.4 package¹⁵. Optimized structures were illustrated using VMD 1.9.3¹⁶.

TDDFT calculations were benchmarked across a range of functionals, including B3LYP-D3(BJ), PBE0-D3(BJ), PBE38, CAM-B3LYP, ω B97XD, M06-2X¹⁷, with the 6-31G(d,p) basis set by Gaussian 16 C.01 package. Solvation effects were included using the Polarizable Continuum Model (PCM) using the integral equation formalism variant (IEFPCM) with a standard state of 1 M. Benchmark results demonstrate that calculations under PBE0-D3(BJ) exhibit the closest agreement with experimental data.

7.1 Calculated molecular geometries

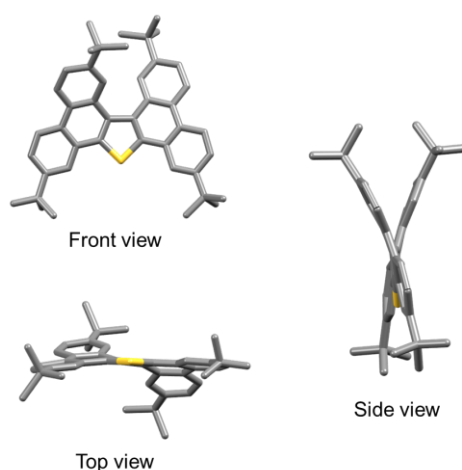


Figure S9 a). molecular geometry of AR-5 optimized by DFT calculation

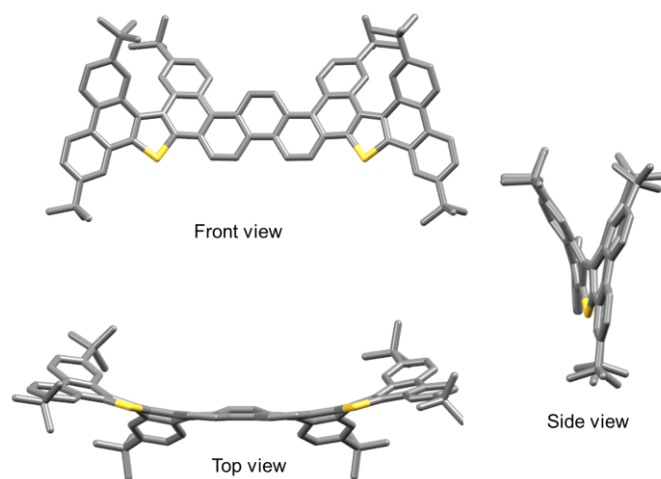


Figure S9 b). molecular geometry of AR-11 optimized by DFT calculation

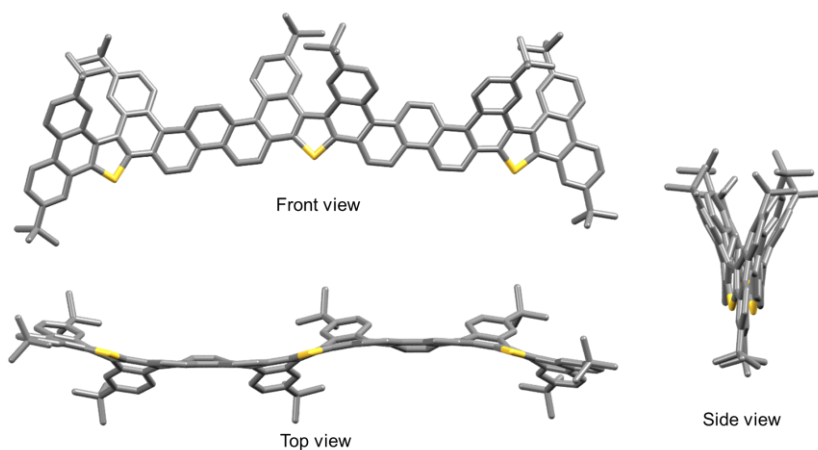


Figure S9 c). molecular geometry of AR-17 optimized by DFT calculation

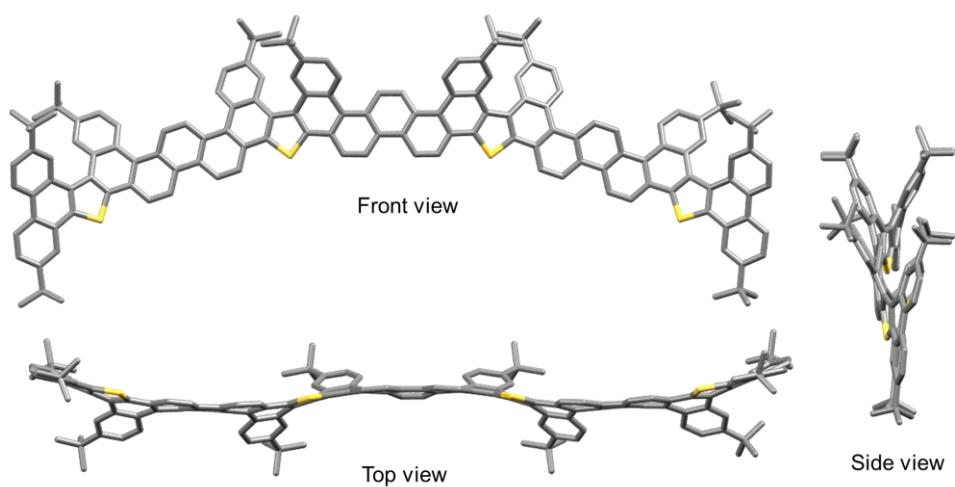


Figure S9 d). molecular geometry of AR-23 optimized by DFT calculation

7.2 Lengths and the arc-shaped of AR- n and ARO- n

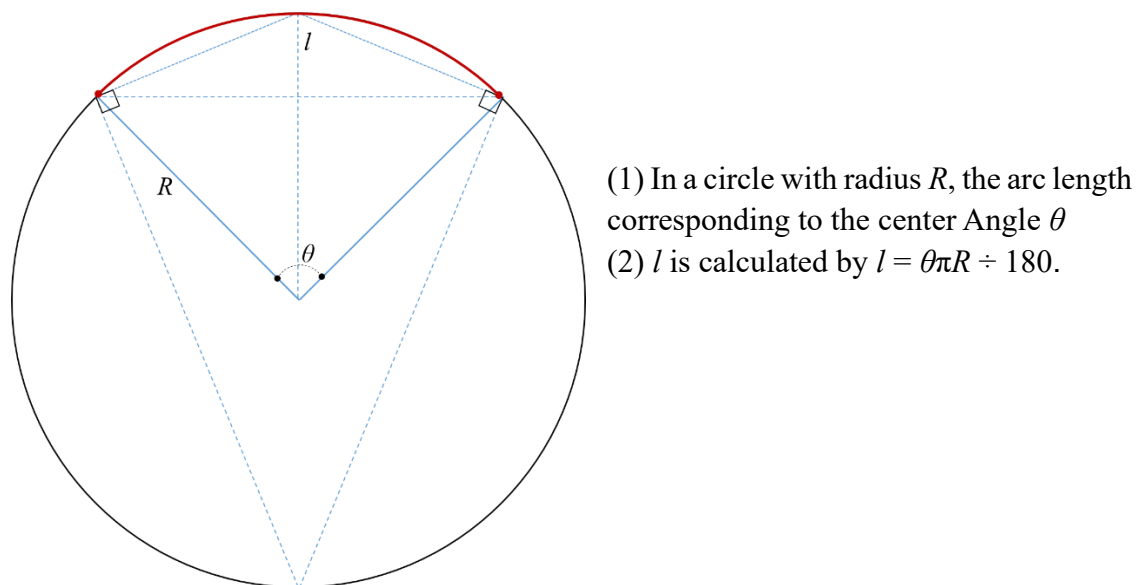


Figure S10. The calculating formula and schematic diagram of arc length and radian.

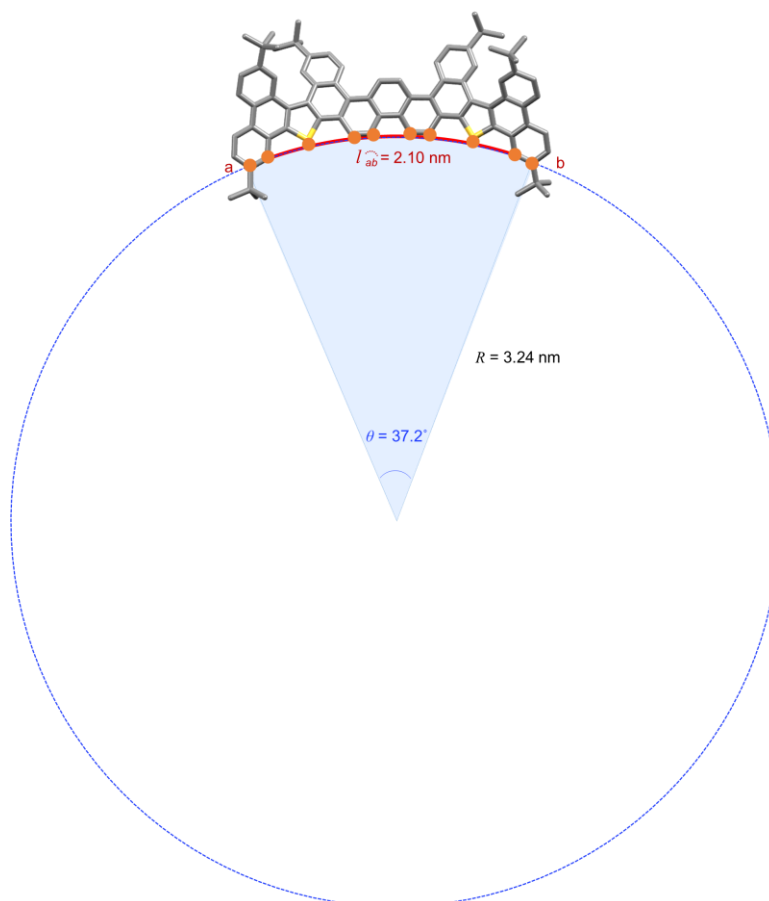


Figure S11. The arc lengths and arc-shaped of AR-11. (Orange atoms are used for fitting)

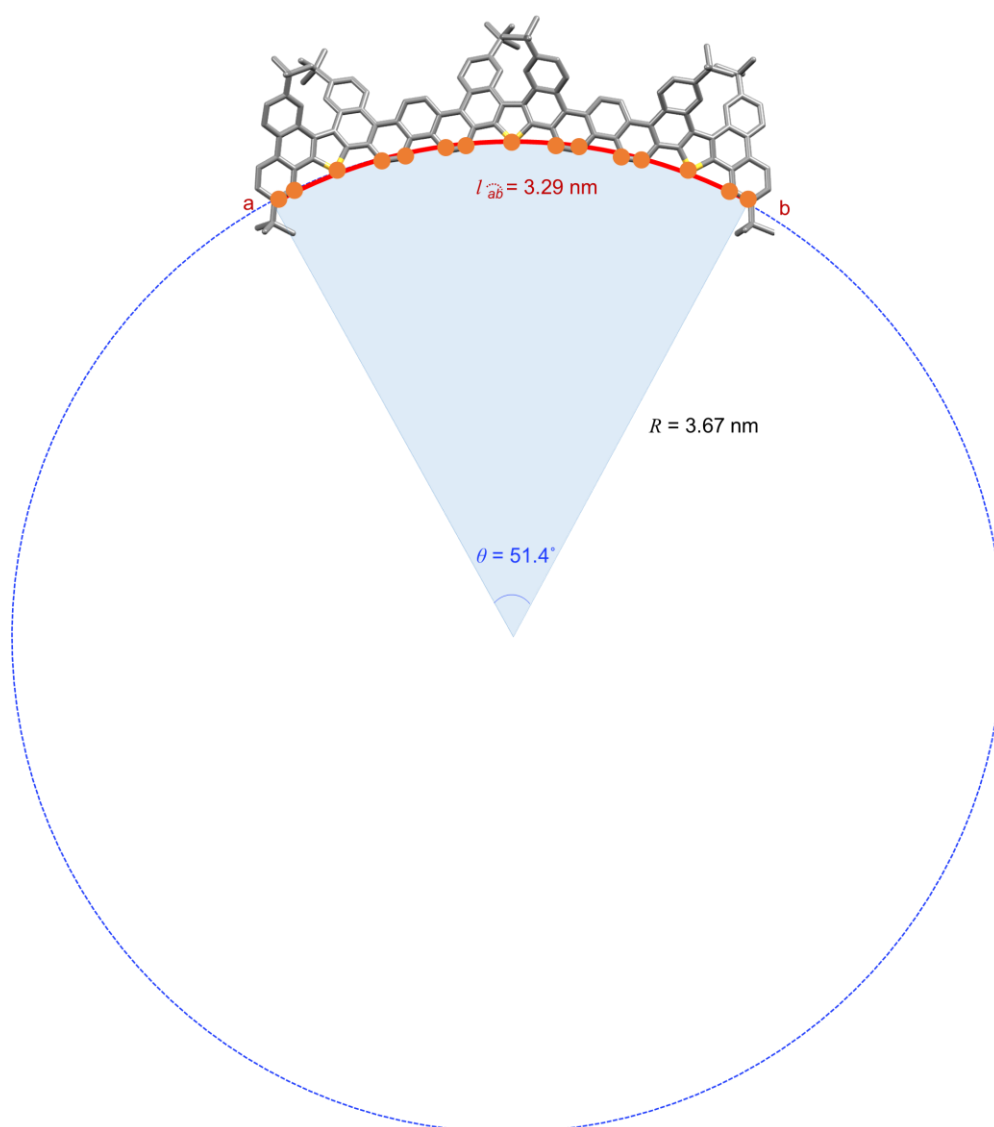


Figure S12. The arc lengths and arc-shaped of AR-17 (Orange atoms are used for fitting).

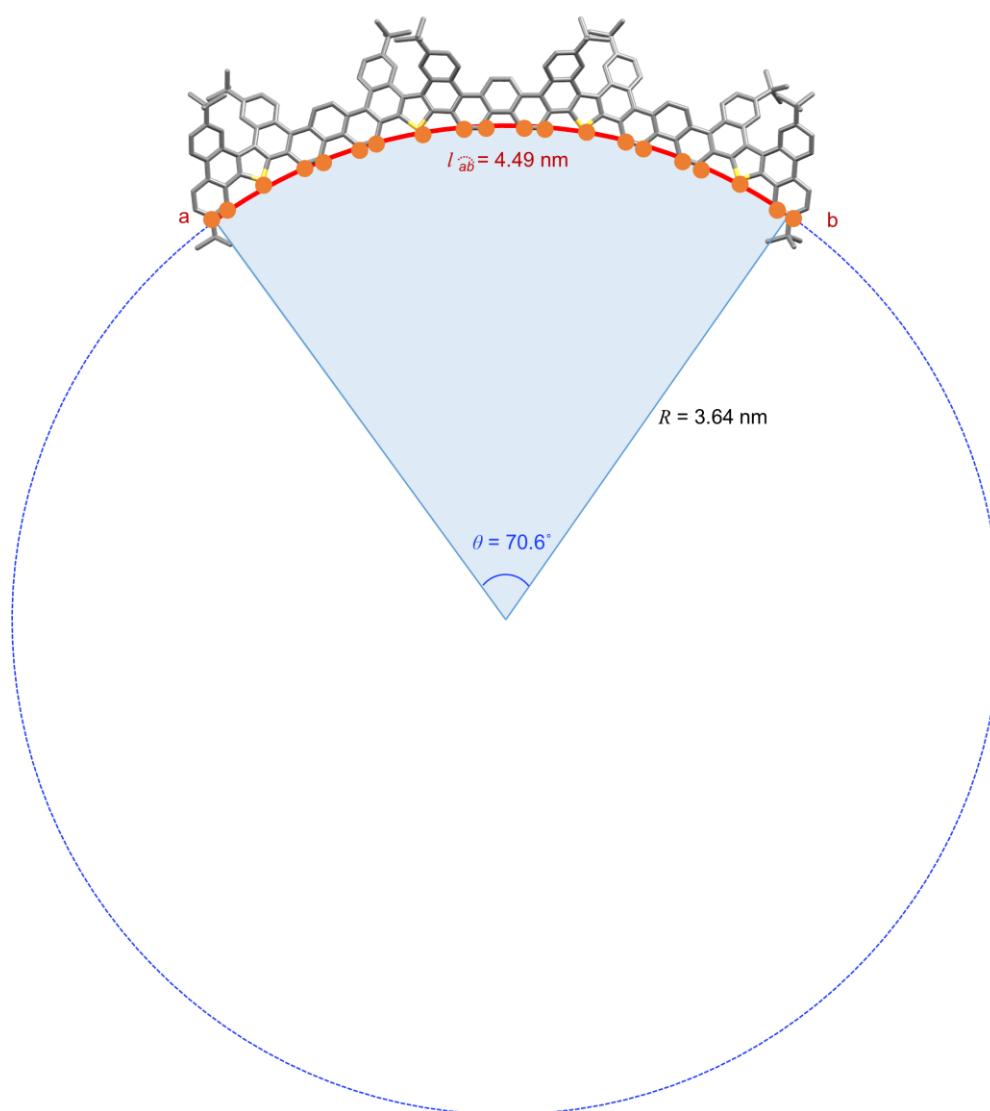


Figure S13. The arc lengths and arc-shaped of AR-23 (Orange atoms are used for fitting).

7.3 Source code of the program for the measurement of lengths and arc-shaped.

Table S5. Source code of the program for the measurement of lengths and the arc-shaped.

```
""" Measure_Arc

This program is designed to measure the arc length and radians of curved molecules.
Author: Xinyu Chen
"""

import numpy as np
import os
from re import split as re_split
from scipy.optimize import leastsq
from typing import Tuple

def read_geometry(__path: str) -> list[tuple[float, float, float]]:
    __geometry = []
    with open(__path) as __fi:
        ext = os.path.splitext(__path)[1]
        if ext == ".xyz":
            for _ in range(2):
                __fi.__next__()
            for line in __fi:
                line = line.strip()
                if line:
                    __, __x, __y, __z = re_split(r'[\t]+', line)
                    __geometry.append((float(__x), float(__y), float(__z)))
        elif ext == ".gjf":
            read = False
            for line in __fi:
                line = line.strip()
                if read and line:
                    __, __x, __y, __z = re_split(r'[\t]+', line)
                    __geometry.append((float(__x), float(__y), float(__z)))
                elif not read and not line:
                    read = True
                    for _ in range(3):
                        __fi.__next__()
        elif ext == ".out":
            read = False
            for line in __fi:
                if "Number          Number          Type          X          Y"
Z" in line:
                    read = True
                    __geometry = []
                    continue
                elif "Rotational constants (GHZ)" in line or "Distance matrix
(angstroms):" in line:
                    read = False
                    continue
                if read and "-----" not in line:
                    __, __, __, __x, __y, __z = re_split(r'[\t]+', line.strip())
                    __geometry.append((float(__x), float(__y), float(__z)))
    return __geometry

def generate_i_tuple(__indexes: str) -> tuple[int, ...]:
    __i_list = []
    for term in __indexes.split(","):
        if "-" in term:
            start, stop = term.split("-")
            __i_list.extend(iter(range(start, stop + 1)))
        else:
            __i_list.append(term)
    __i_tuple = tuple(map(int, __i_list))
    return __i_tuple

def normalize(__vector: np.ndarray) -> np.ndarray:
    norm = np.linalg.norm(__vector)
    if norm == 0:
        return __vector
    else:
```

```

        return __vector / norm

if __name__ == '__main__':
    path = input("Input the path of the file containing the geometry: ")
    i_plane_atoms = input("Input the atom indexes used to fit a plane(e.g. 1-5,8;
input 'a' to select all): ")
    i_arc_atoms = generate_i_tuple(input("Input the atom indexes used to fit an
arc(e.g. 1-5,8)"
                                     ", beginning and ending with the end-side
atoms: "))
    starting_estimate = input("Input the starting estimate for the plane
fitting(e.g. 1,1,1,0; "
                              "press ENTER to use the default value 1,1,1,0): ") or
"1,1,1,0"
    starting_estimate = tuple(map(float, starting_estimate.split(",")))
    geometry = read_geometry(path)

    # Fit a plane
    def error1(__p: np.ndarray) -> np.ndarray:
        __n = __p[:3]
        __error = ((__n * np.array(plane_atoms)).sum(axis=1) + __p[3]) /
np.linalg.norm(__n)
        return __error

    if i_plane_atoms == "a":
        plane_atoms = geometry
    else:
        i_plane_atoms = generate_i_tuple(i_plane_atoms)
        plane_atoms = [geometry[i-1] for i in i_plane_atoms]
    result1 = leastsq(error1, np.array(starting_estimate))
    a, b, c, d = result1[0] # Plane: ax + by + cz + d = 0

    # Choose origin, x base, y base in the plane
    arc_atoms = [geometry[i-1] for i in i_arc_atoms]
    unit_normal_vector = normalize(np.array([a, b, c]))
    projected_vector = np.array(arc_atoms[0]) - np.array([-d/a, c, -b])
    proj = np.vdot(unit_normal_vector, projected_vector)
    origin = np.array(arc_atoms[0]) - proj * unit_normal_vector
    x1, y1, z1 = (b-c)/a, (c-a)/b, (a-b)/c
    A = np.array([[b, c], [y1, z1]])
    B = np.array([[a], [x1]])
    x_base = normalize(np.array([x1, y1, z1]))
    y_base = normalize(np.insert(-np.linalg.solve(A, B).T, 0, 1.))

    # Project
    atom_projections = [np.zeros(2)]
    for atom in arc_atoms[1:]:
        atom_vector = np.array(atom) - origin
        x_p = np.vdot(x_base, atom_vector)
        y_p = np.vdot(y_base, atom_vector)
        atom_projections.append([x_p, y_p])

    # Fit the arc
    a2d = np.array(atom_projections)
    def error2(__p: np.ndarray) -> np.ndarray:
        __r, __a, __b = __p
        __error = __r ** 2 - ((a2d - np.array([__a, __b])) ** 2).sum(axis=1)
        return __error

    c_0 = (a2d[0] + a2d[-1]) / 2
    r_0 = np.linalg.norm(a2d[0]-a2d[-1]) / 2
    result2 = leastsq(error2, np.insert(c_0, 0, r_0))
    r, a, b = result2[0] # Circle: (x - a) ** 2 + (y - b) ** 2 = r ** 2
    center = np.array([a, b])
    start_vector = a2d[0] - center
    end_vector = a2d[-1] - center
    angle_radian = (
        np.arccos(np.vdot(start_vector, end_vector) / (np.linalg.norm(start_vector)
* np.linalg.norm(end_vector))))
    angle_degree = angle_radian * 180 / np.pi
    arc_length = r * angle_radian

    print(f"angle: {angle_degree:.1f}(degree)/{angle_radian:.3f}(rad), arc_length:
{arc_length:.1f}, radius: {r:.2f}")

```

7.4 Stereoisomers of AR-11

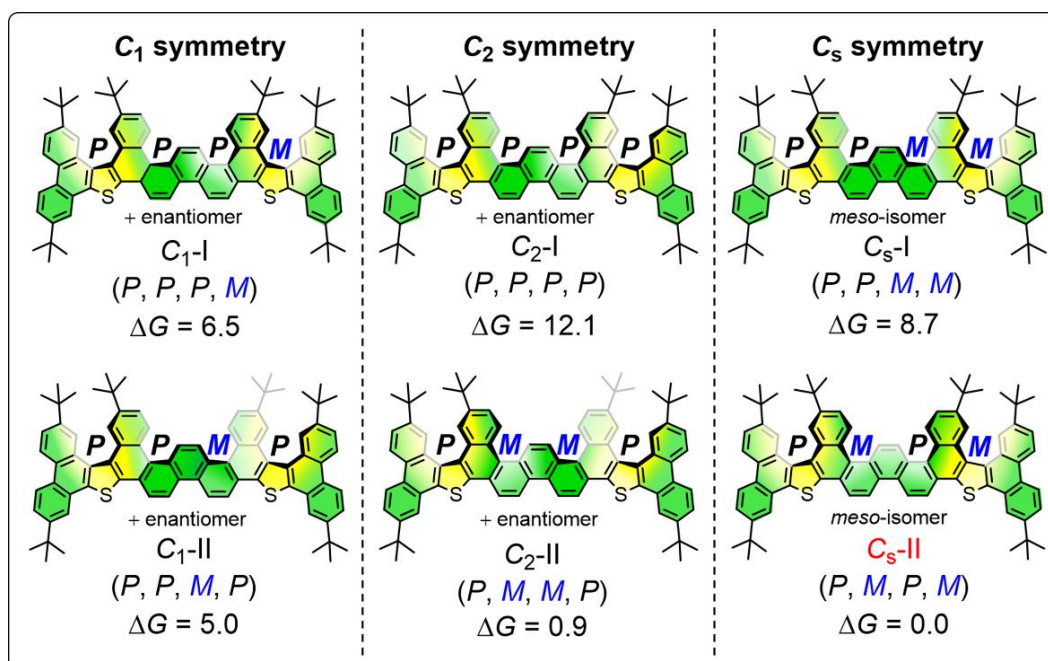


Figure S14. Stereoisomers of AR-11 and their relative Gibbs free energies (Unit, $\text{kcal}\cdot\text{mol}^{-1}$).

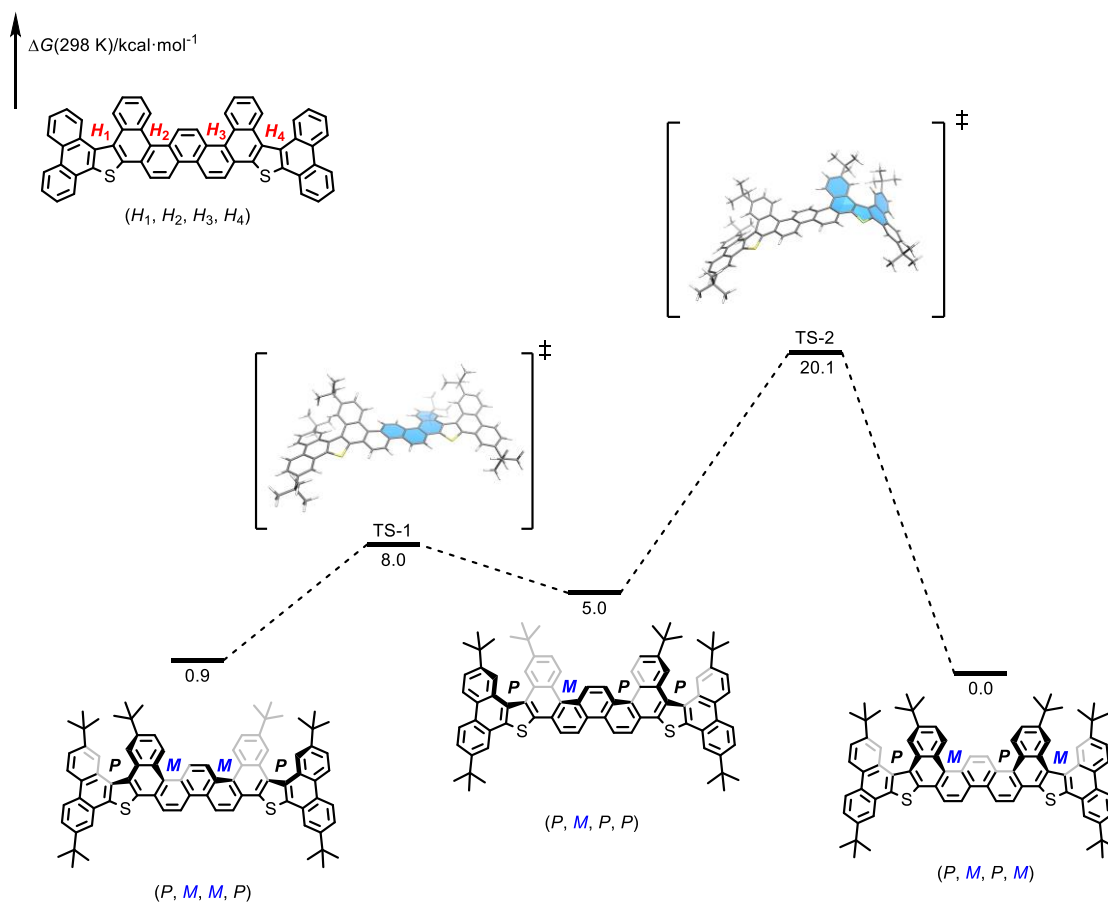
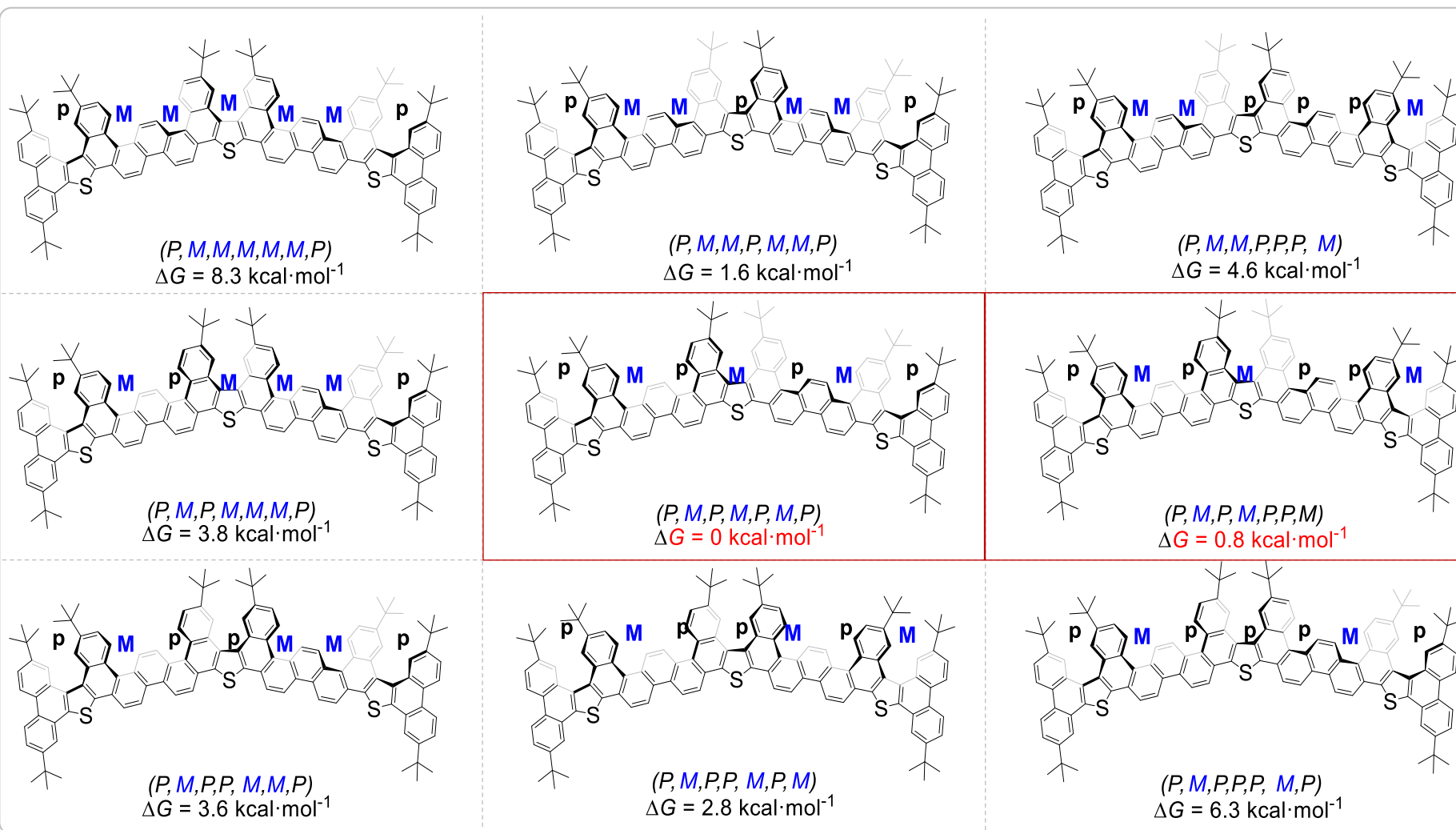
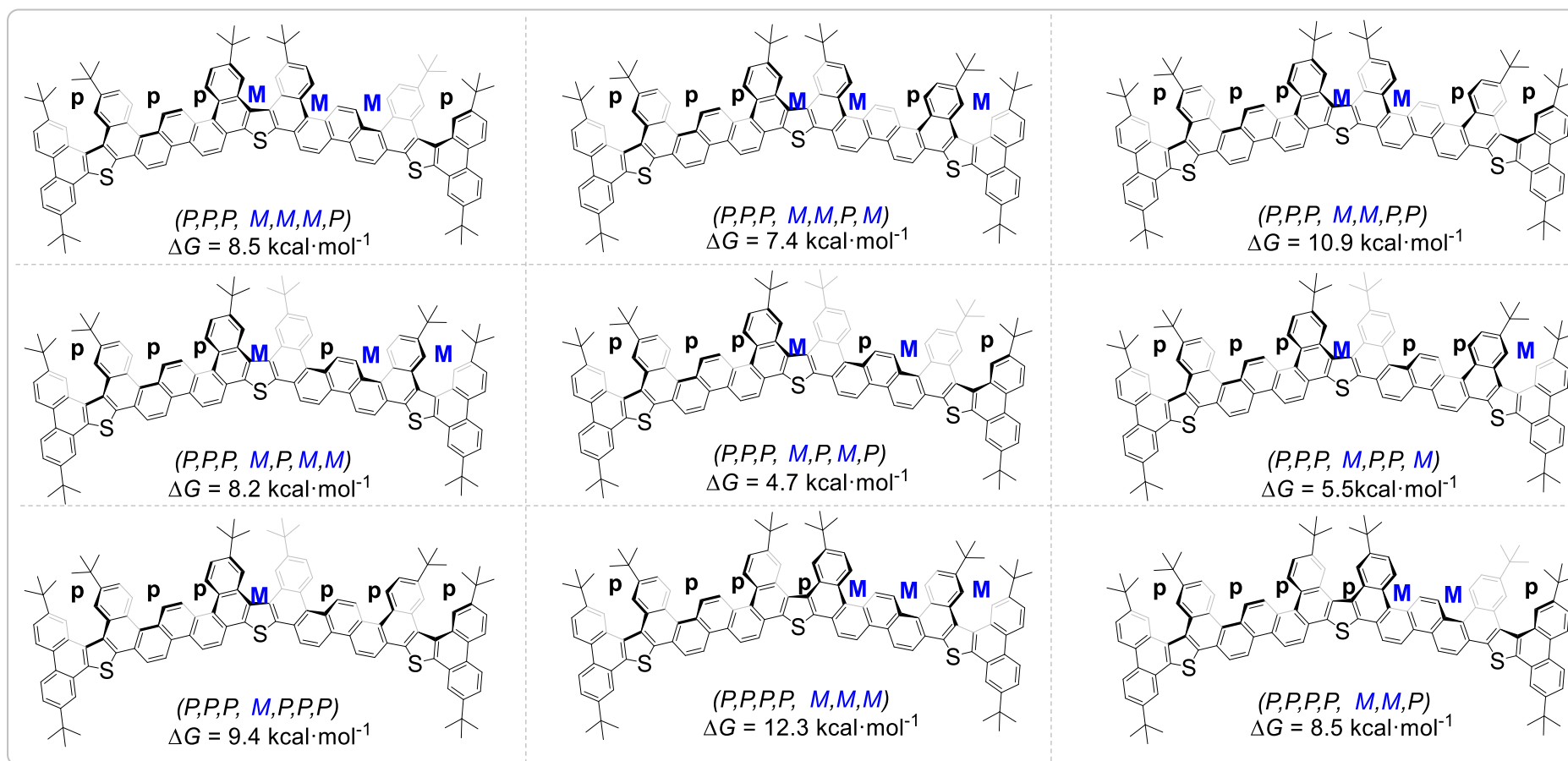
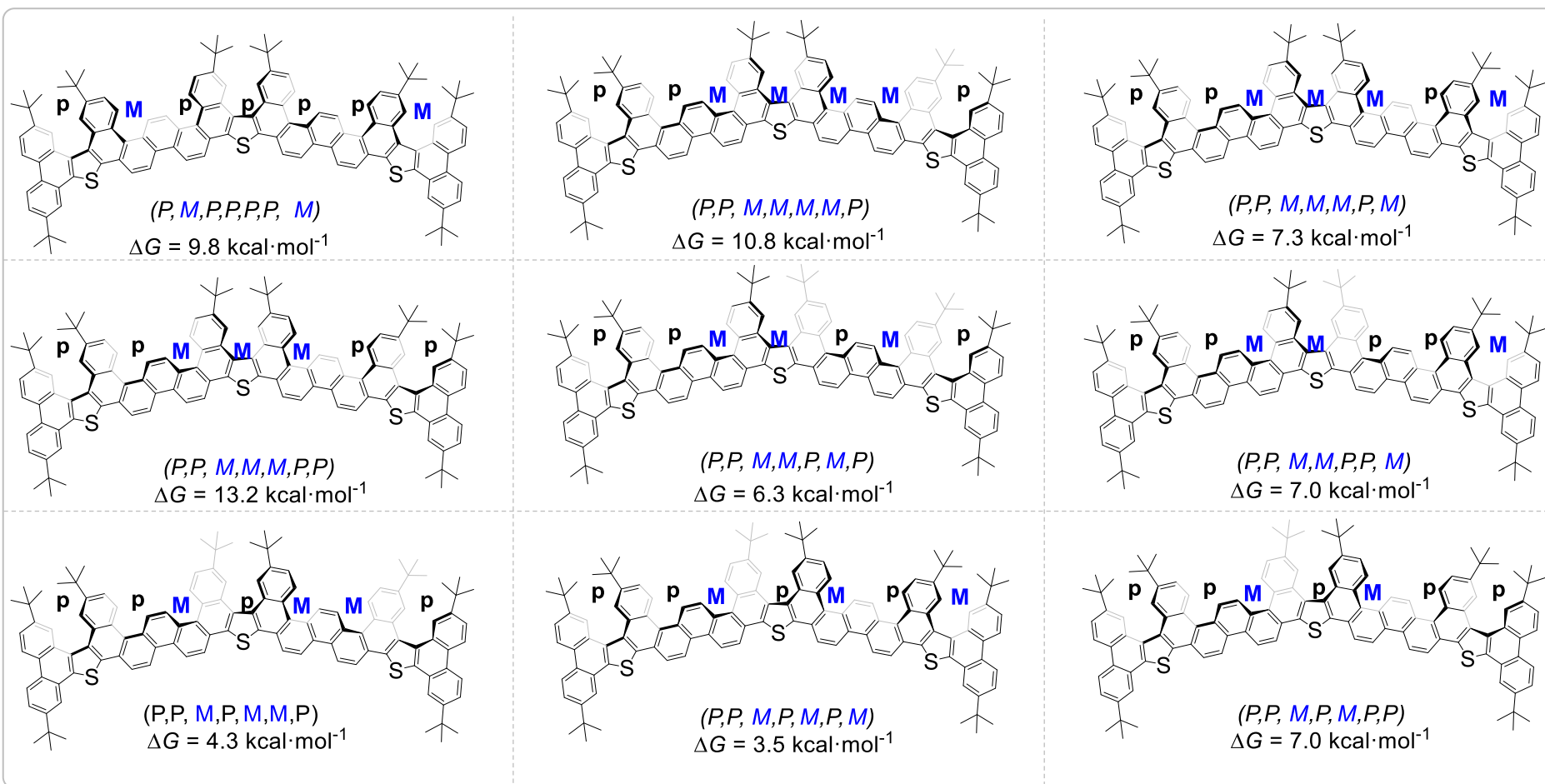


Figure S15. Calculated Gibbs free energies of AR-11 for the conversion from the (P,M,M,P) to the (P,M,P,M).







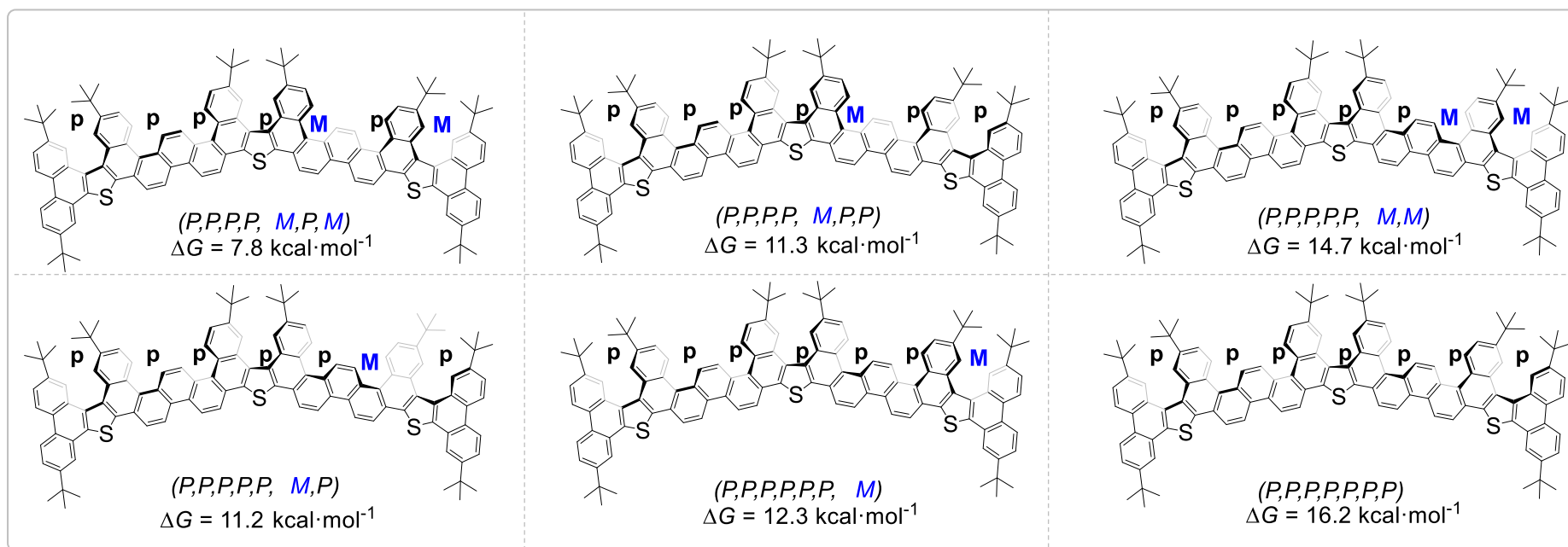


Figure S16. 36 types of AR-17 isomers with varying free energies based on the calculations at the PM7 level of theory.

7.5 Electronic structures and molecular aromaticity of AR-11, ARO-11.

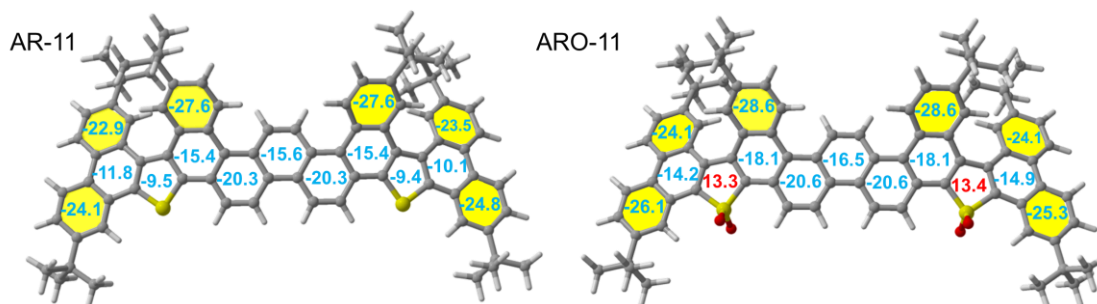


Figure S17. Nucleus-independent chemical shifts (NICS)(1)_{zz} calculation are conducted at the B3LYP/6-31G (d,p).

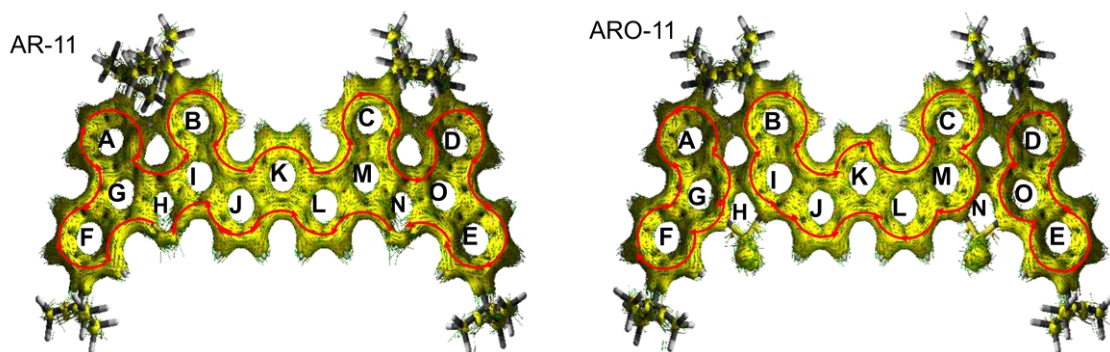


Figure S18. Anisotropy of the induced current densities (ACID) calculation are conducted at the B3LYP/6-31G (d).

7.6 TD-DFT calculation

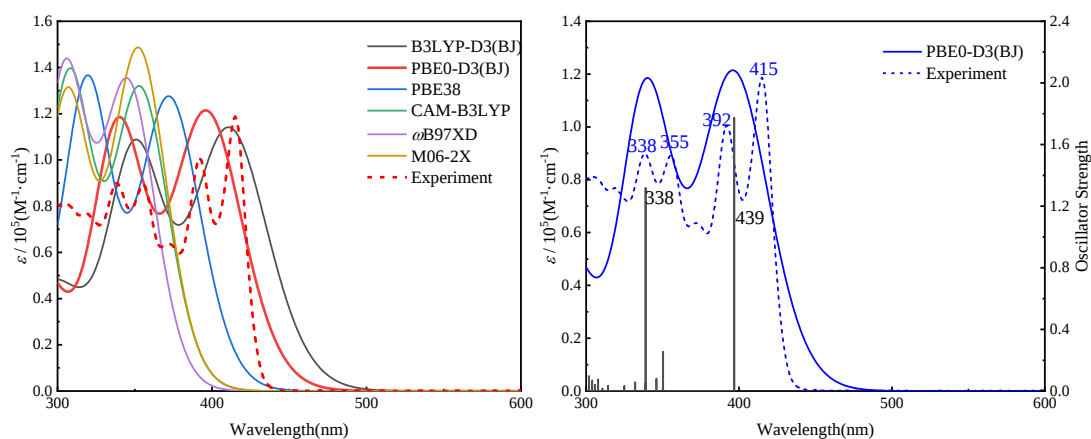


Table S6. Major electronic transitions for **AR-11** by TD-DFT method using PBE0-D3(BJ)/6-31G(d,p).

Transition	Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
S1	3.1243	396.84	1.7739	H → L: 95.1%;
S2	3.2373	382.99	0.0019	H-2 → L: 7.7%; H-1 → L: 40.6%; H → L+1: 41.9%;
S3	3.5388	350.35	0.2543	H-2 → L: 28.5%; H-1 → L: 36.5%; H → L+1: 18.8%; H → L+2: 9.2%;
S4	3.5839	345.95	0.0808	H-3 → L: 54.9%; H-2 → L+1: 12.2%; H → L+3: 6.8%
S5	3.6580	338.94	0.0493	H-4 → L: 32.0%; H-3 → L+2: 6.4%; H-2 → L: 15.7%; H-1 → L: 7.5%; H → L+1: 8.8%; H → L+2: 14.8%;
S6	3.6589	338.86	1.3190	H-2 → L+1: 7.5%; H-1 → L+1: 77.2%;
S7	3.7334	332.09	0.0568	H-4 → L: 25.6%; H-2 → L: 34.6%; H → L+1: 26.5%;
S8	3.7725	328.66	0.0007	H-7 → L: 10.1%; H-3 → L: 11.8%; H-2 → L+1: 26.1%; H → L+5: 18.5%;

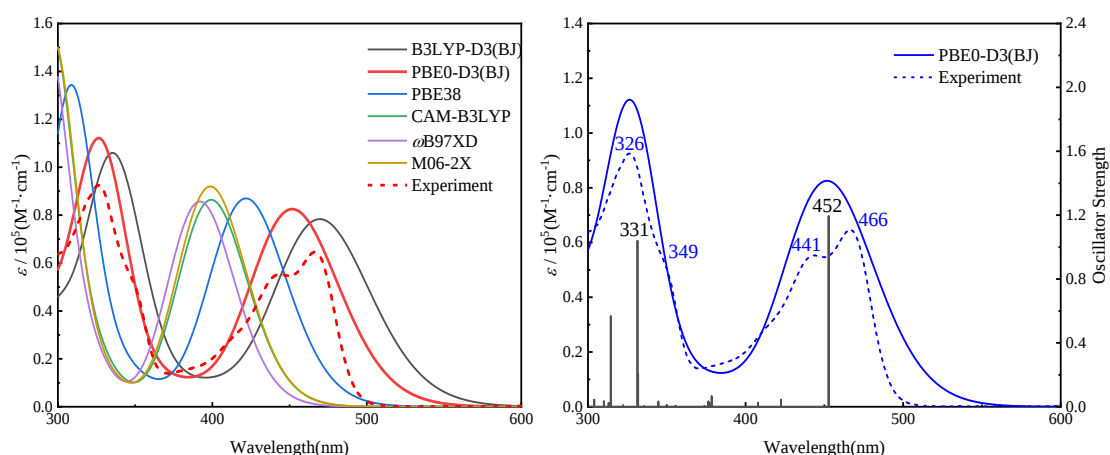


Table S7. Major electronic transitions for **ARO-11** by TD-DFT method using PBE0-D3(BJ)/6-31G(d,p).

Transition	Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
S1	2.7389	452.68	1.1940	H-2 $\rightarrow$ L+1: 5.3%; H $\rightarrow$ L: 92.2%;
S2	2.9348	422.46	0.0456	H-1 $\rightarrow$ L: 81.0%; H $\rightarrow$ L+1: 9.6%; H $\rightarrow$ L+2: 5.4%;
S3	3.0403	407.80	0.0266	H-2 $\rightarrow$ L: 42.8%; H $\rightarrow$ L+1: 48.6%;
S4	3.2762	378.44	0.0668	H-1 $\rightarrow$ L+1: 72.6%;
S5	3.2857	377.35	0.0209	H-4 $\rightarrow$ L: 45.3%; H-3 $\rightarrow$ L+1: 17.3%; H-2 $\rightarrow$ L: 18.6%; H $\rightarrow$ L+1: 11.5%;
S12	3.7364	331.83	0.2047	H-7 $\rightarrow$ L: 54.8%; H-5 $\rightarrow$ L+1: 18.2%; H $\rightarrow$ L+2: 12.7%;
S13	3.7415	331.37	1.0396	H-2 $\rightarrow$ L+2: 7.5%; H-1 $\rightarrow$ L+2: 74.7%;
S14	3.8472	322.27	0.0047	H-4 $\rightarrow$ L: 28.2%; H-3 $\rightarrow$ L+1: 64.0%;
S15	3.8476	322.24	0.0093	H-4 $\rightarrow$ L+1: 62.8%; H-3 $\rightarrow$ L: 27.9%;
S16	3.9432	314.43	0.5671	H-2 $\rightarrow$ L+2: 10.1%; H $\rightarrow$ L+3: 68.5%;
S17	3.9600	313.09	0.0242	H-8 $\rightarrow$ L: 12.1%; H-6 $\rightarrow$ L+1: 34.4%; H-5 $\rightarrow$ L+1: 36.4%; H-1 $\rightarrow$ L+3: 5.3%;

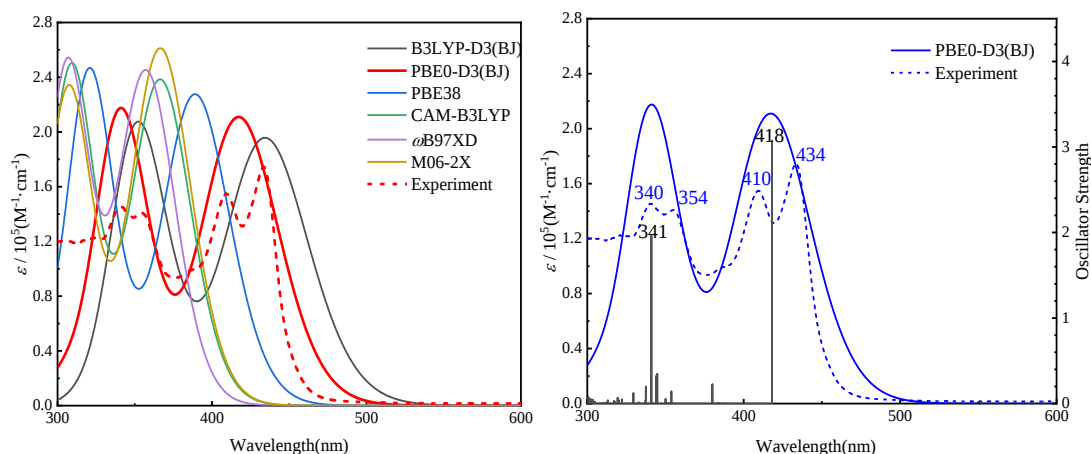


Table S8. Major electronic transitions for **AR-17** by TD-DFT method using PBE0-D3(BJ)/6-31G(d,p).

Transition	Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
S1	2.9656	418.07	3.0739	H-1 $\rightarrow$ L+1: 5.3%; H $\rightarrow$ L: 90.3%;
S2	3.2044	386.91	0.0021	H-3 $\rightarrow$ L+1: 7.0%; H-2 $\rightarrow$ L: 46.0%; H-1 $\rightarrow$ L+2: 6.4%; H $\rightarrow$ L+1: 6.2%; H $\rightarrow$ L+3: 24.8%;
S3	3.2310	383.73	0.0078	H-3 $\rightarrow$ L: 34.7%; H-2 $\rightarrow$ L+1: 10.2%; H-1 $\rightarrow$ L+3: 7.4%; H $\rightarrow$ L+2: 34.2%;
S4	3.2631	379.96	0.2255	H-1 $\rightarrow$ L: 55.1%; H $\rightarrow$ L+1: 34.4%;
S5	3.5050	353.73	0.1432	H-4 $\rightarrow$ L: 16.3%; H-3 $\rightarrow$ L: 29.4%; H-1 $\rightarrow$ L+1: 24.5%; H $\rightarrow$ L+2: 18.4%;
S8	3.5963	344.76	0.3486	H-6 $\rightarrow$ L: 21.4%; H-5 $\rightarrow$ L+1: 11.9%; H-4 $\rightarrow$ L: 9.4%; H-2 $\rightarrow$ L+1: 8.6%; H $\rightarrow$ L+2: 6.0%;
S9	3.6061	343.82	0.3200	H-5 $\rightarrow$ L: 9.8%; H-2 $\rightarrow$ L: 30.8%; H $\rightarrow$ L+3: 37.4%;
S10	3.6362	340.98	1.9566	H-3 $\rightarrow$ L+2: 34.6%; H-2 $\rightarrow$ L+1: 6.5%; H-2 $\rightarrow$ L+3: 36.9%;
S11	3.6749	337.38	0.1993	H-6 $\rightarrow$ L: 20.5%; H-4 $\rightarrow$ L: 11.6%; H-3 $\rightarrow$ L: 11.7%; H-1 $\rightarrow$ L+1: 9.7%; H-1 $\rightarrow$ L+3: 5.3%; H $\rightarrow$ L+2: 23.2%;
S12	3.6762	337.27	0.0430	H-3 $\rightarrow$ L+3: 27.6%; H-2 $\rightarrow$ L+2: 36.1%;

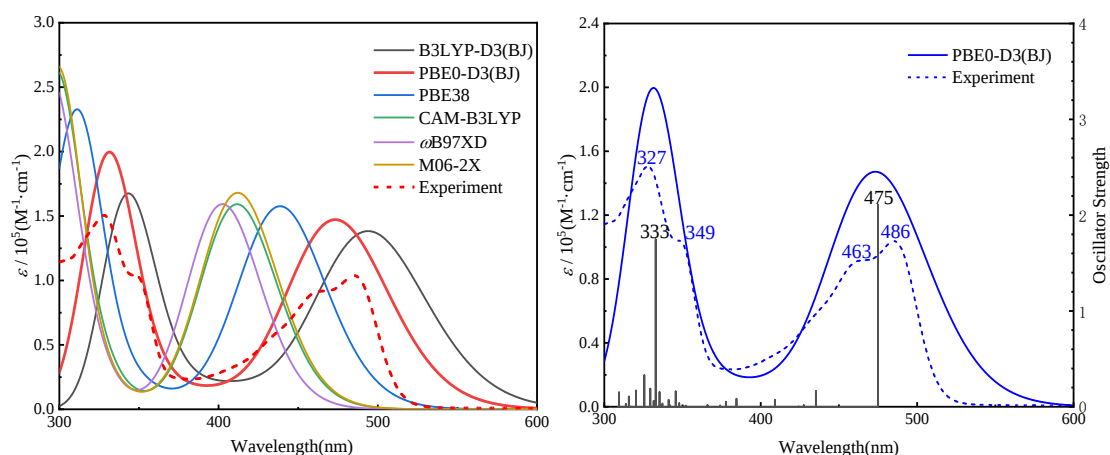


Table S9. Major electronic transitions for **ARO-17** by TD-DFT method using PBE0-D3(BJ)/6-31G(d,p).

Transition	Energy (eV)	Wavelength (nm)	Osc. Strength	Major contributions
S1	2.6108	474.88	2.1103	H-1 $\rightarrow$ L+1: 6.3%; H $\rightarrow$ L: 87.4%;
S2	2.8487	435.23	0.1664	H-1 $\rightarrow$ L: 46.5%; H-1 $\rightarrow$ L+2: 5.9%; H $\rightarrow$ L+1: 38.2%;
S3	2.9002	427.50	0.0168	H-3 $\rightarrow$ L+1: 5.9%; H-2 $\rightarrow$ L: 72.8%; H-1 $\rightarrow$ L+1: 6.9%; H $\rightarrow$ L+2: 5.3%;
S4	2.9229	424.18	0.0036	H-3 $\rightarrow$ L: 76.6%; H-2 $\rightarrow$ L+1: 7.2%;
S5	3.0314	409.00	0.0738	H-4 $\rightarrow$ L: 22.5%; H-1 $\rightarrow$ L+1: 27.9%; H $\rightarrow$ L+2: 34.2%;
S23	3.6979	335.28	0.1548	H-6 $\rightarrow$ L: 51.0%; H-6 $\rightarrow$ L+2: 13.5%; H-5 $\rightarrow$ L+1: 25.7%;
S24	3.7017	334.94	0.0078	H-6 $\rightarrow$ L+1: 23.9%; H-5 $\rightarrow$ L: 44.2%; H-5 $\rightarrow$ L+2: 11.8%;
S25	3.7253	332.82	1.7472	H-3 $\rightarrow$ L+4: 29.9%; H-2 $\rightarrow$ L+3: 35.0%;
S26	3.7401	331.50	0.0623	H-11 $\rightarrow$ L: 18.5%; H-3 $\rightarrow$ L+3: 14.0%; H-2 $\rightarrow$ L+4: 10.2%; H-1 $\rightarrow$ L+2: 6.9%;
S27	3.7638	329.41	0.1896	H-11 $\rightarrow$ L: 14.7%; H-4 $\rightarrow$ L+1: 12.0%; H-3 $\rightarrow$ L+3: 24.1%; H-2 $\rightarrow$ L+4: 25.7%;

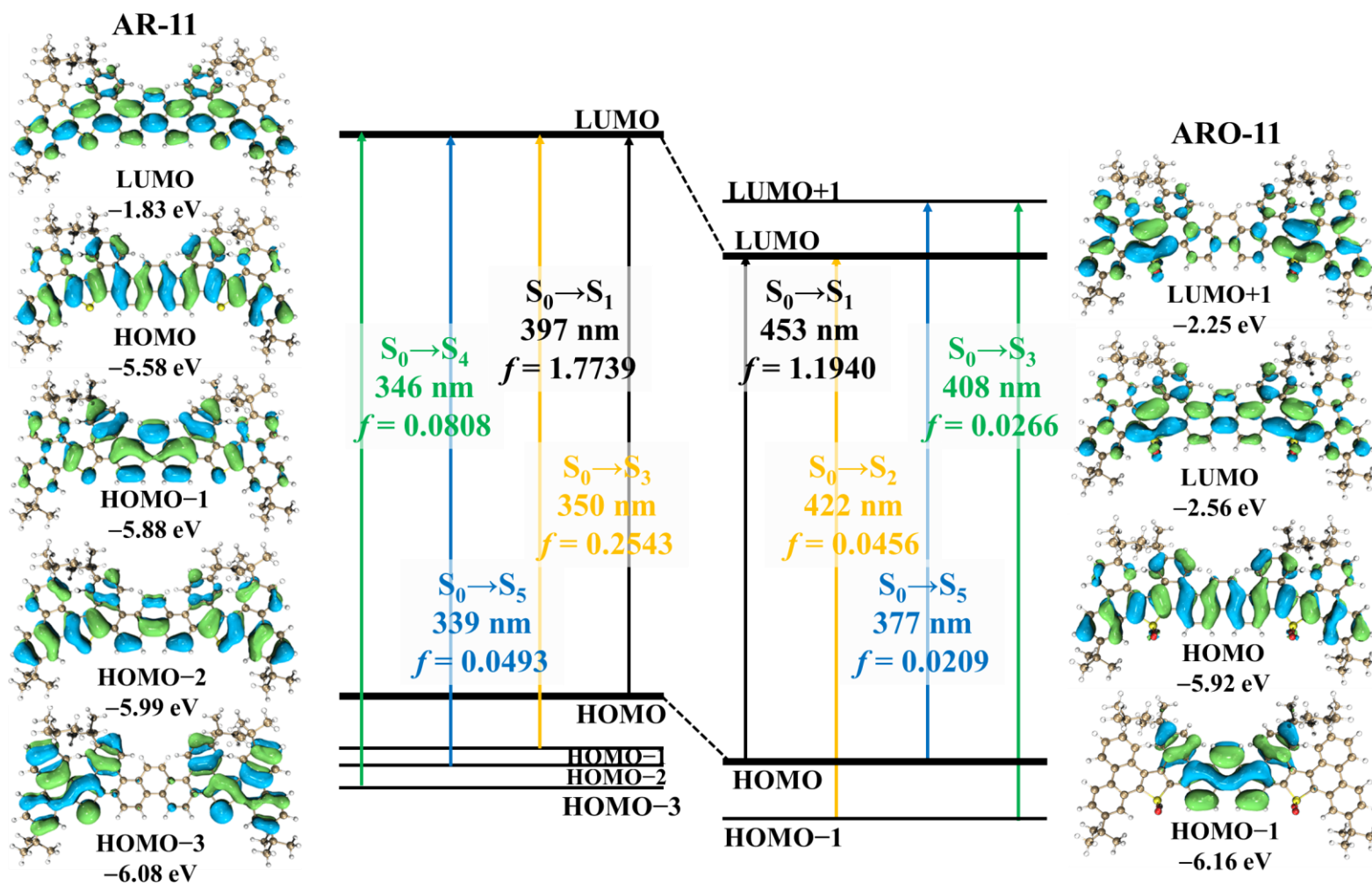


Figure S19. Energy diagrams and frontier molecular orbitals of **AR-11** and **ARO-11** calculated at the PBE0-D3(BJ)/6-31G(d,p) level of theory.

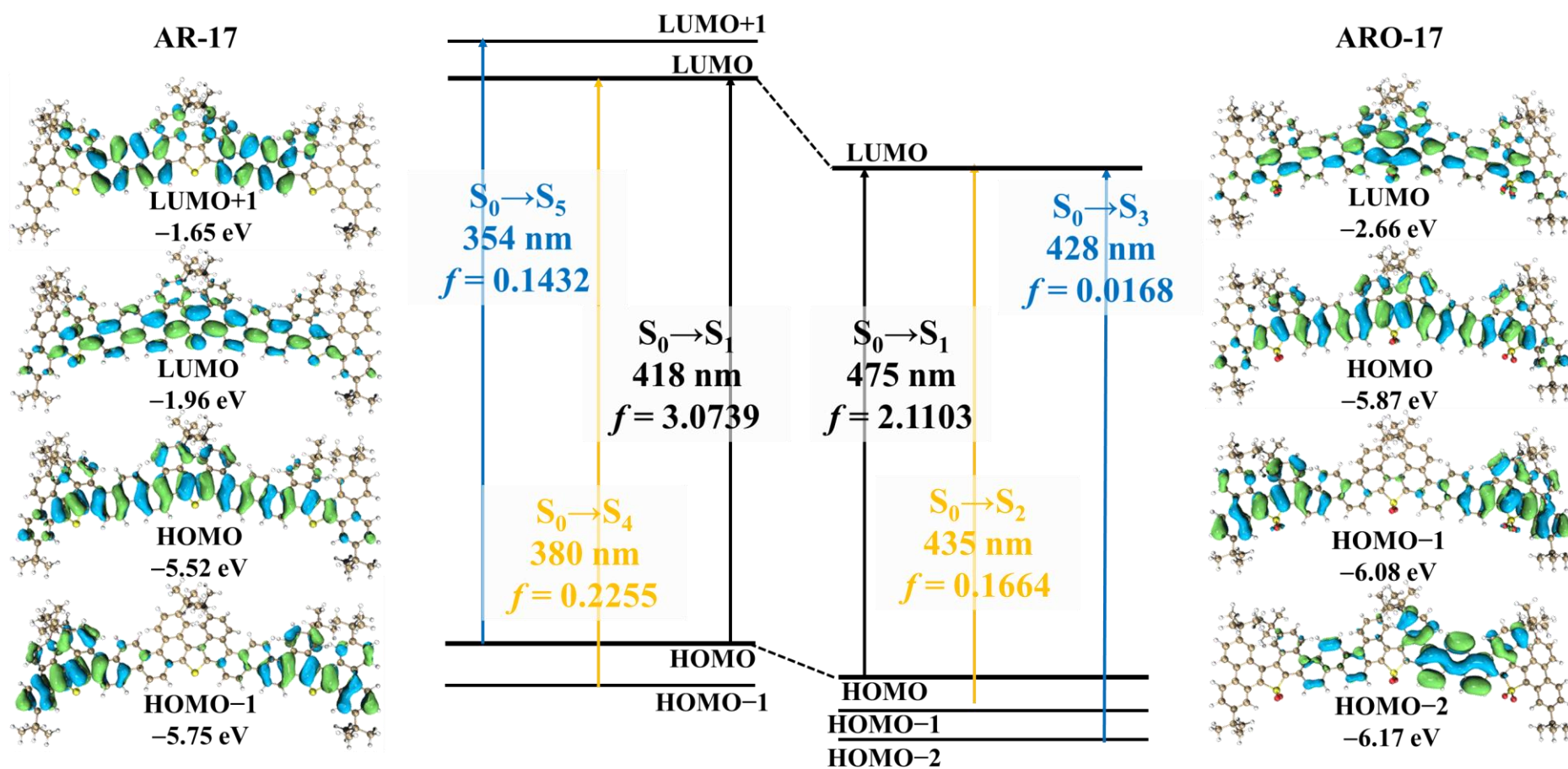


Figure S20. Energy diagrams and frontier molecular orbitals of **AR-17** and **ARO-17** calculated at the PBE0-D3(BJ)/6-31G(d,p) level of theory.

7.7 Frontier Molecular Orbitals

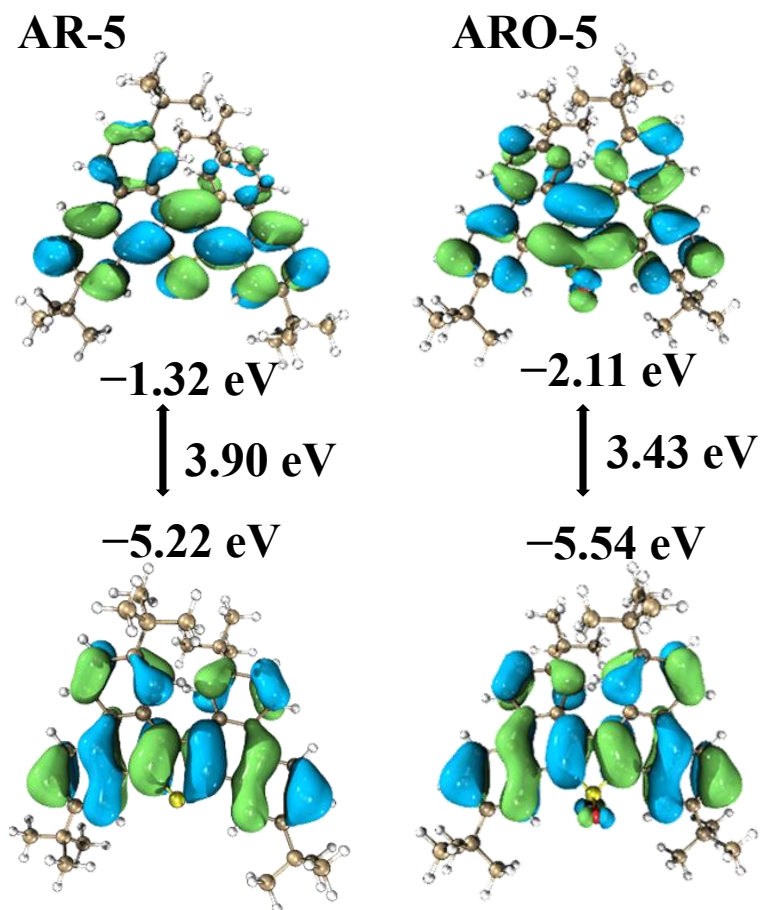


Figure S21. The frontier molecular orbitals of AR-5 and ARO-5 calculated at the B3LYP/6-31G(d) level of theory.

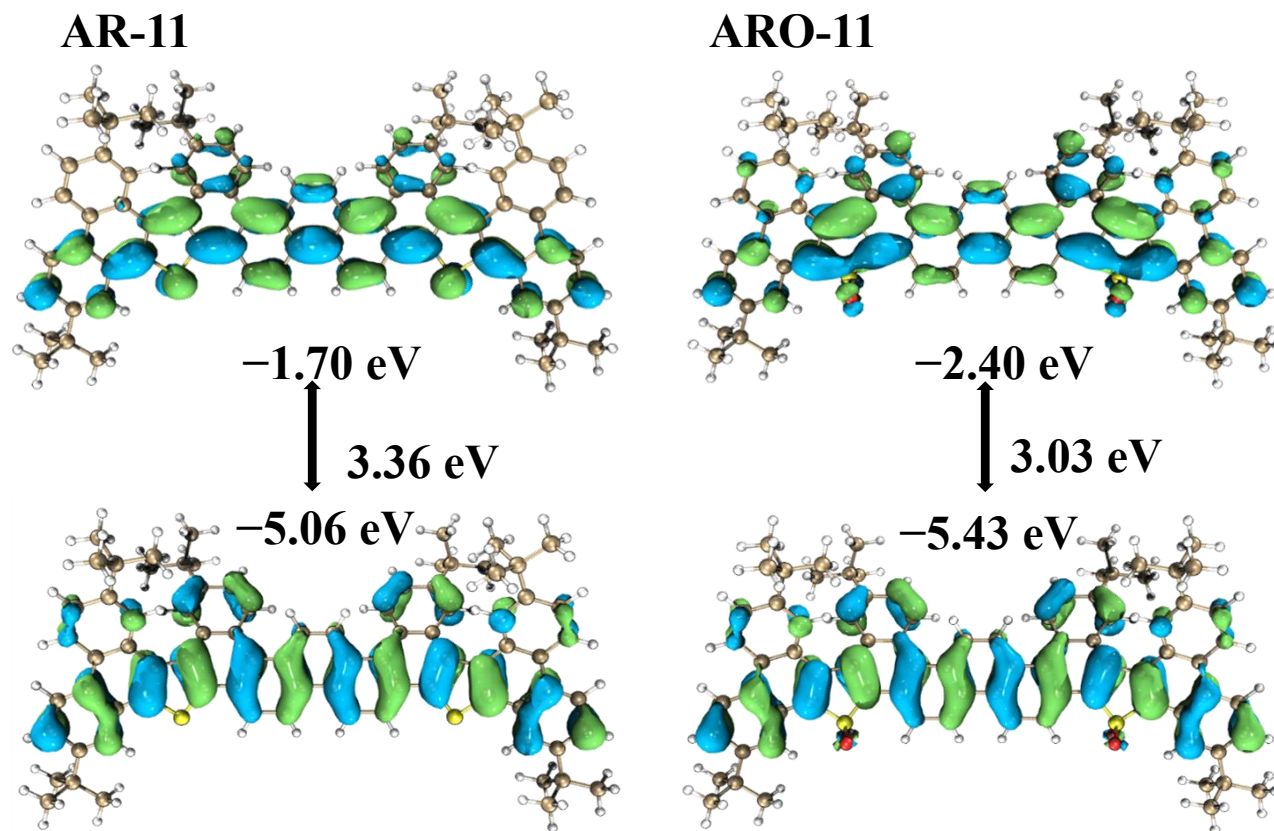


Figure S22. The frontier molecular orbitals of AR-11 and ARO-11 calculated at the B3LYP/6-31G(d) level of theory.

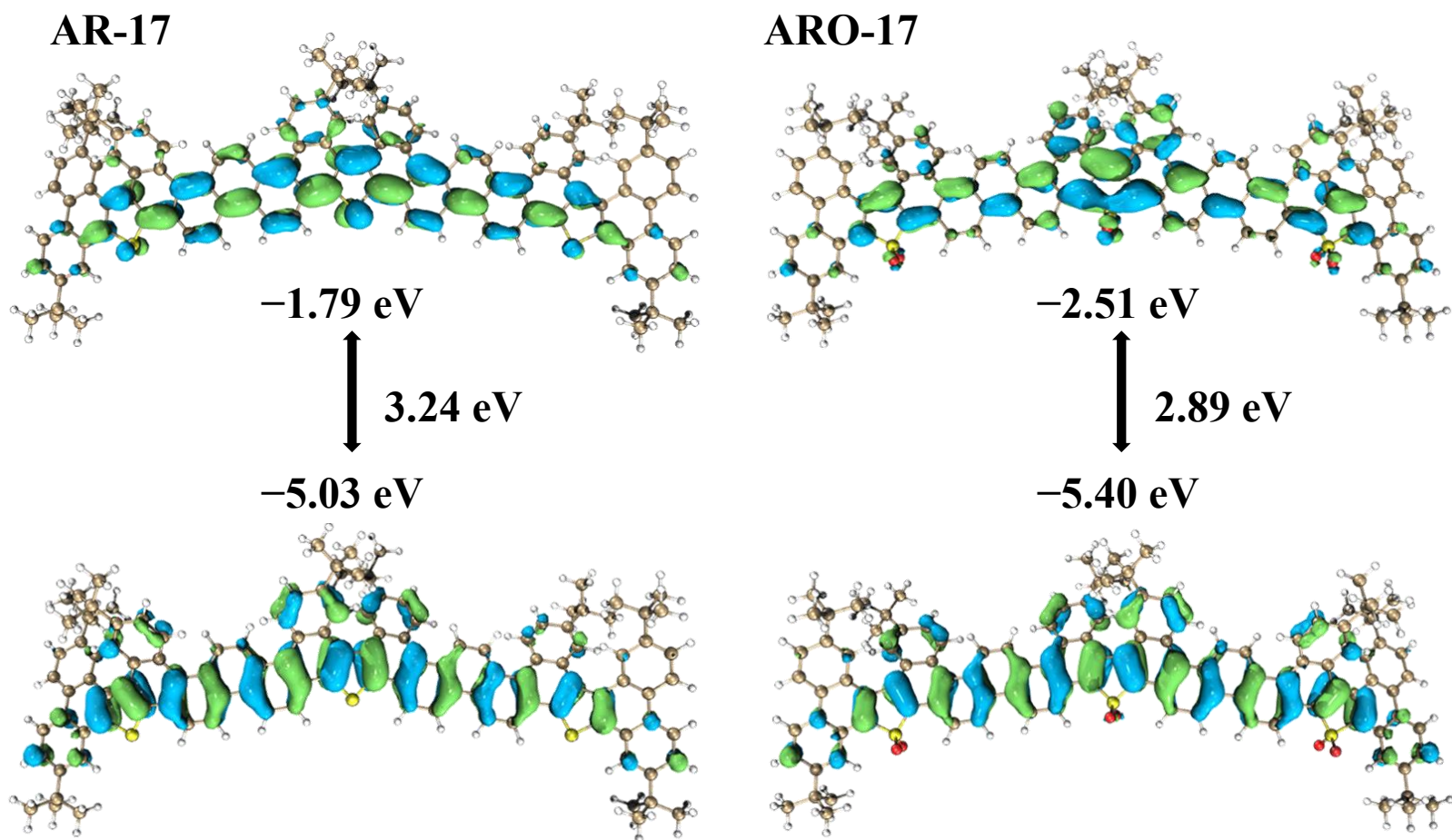


Figure S23. The frontier molecular orbitals of AR-17 and ARO-17 calculated at the B3LYP/6-31G(d) level of theory.

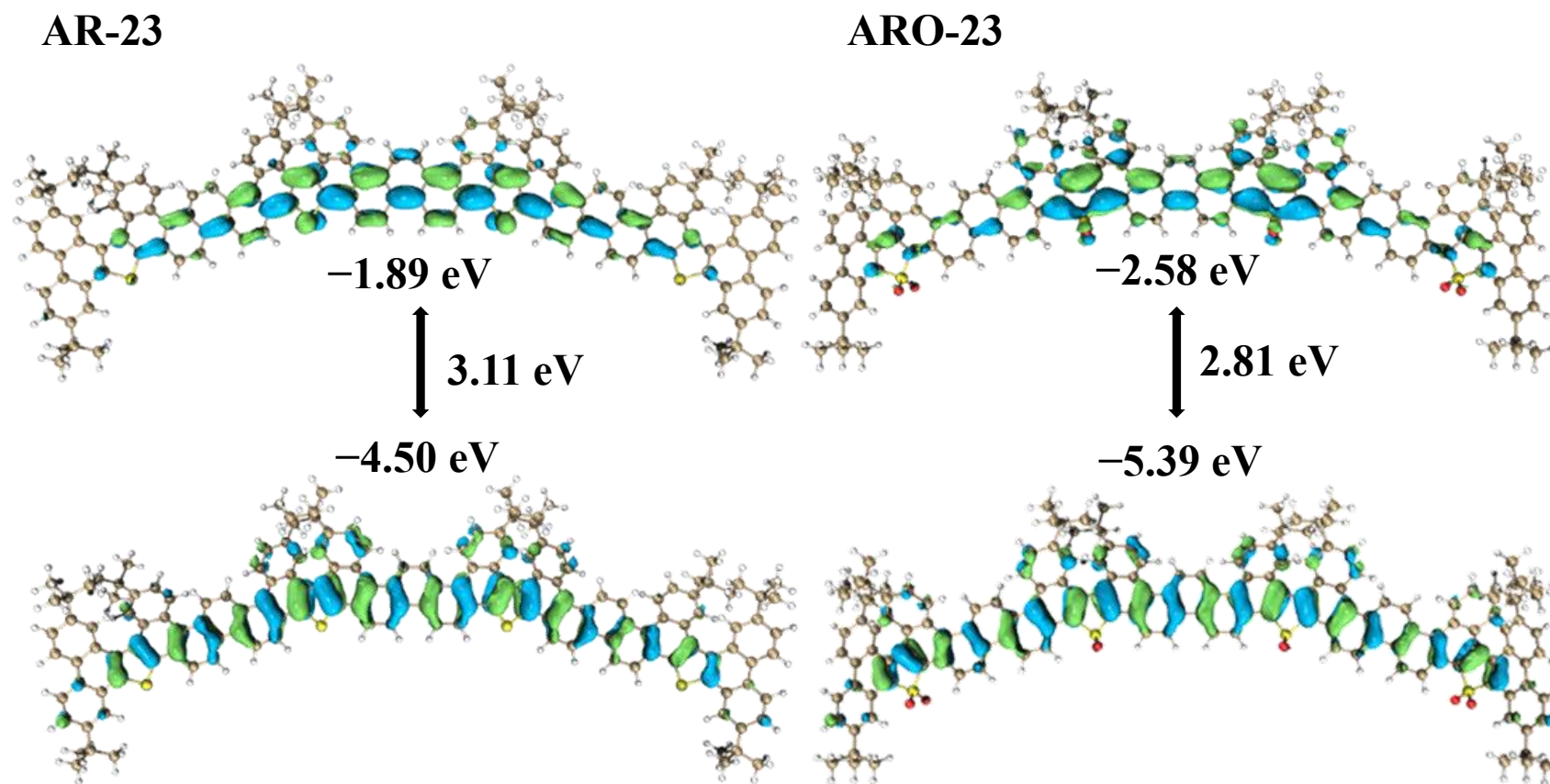


Figure S24. The frontier molecular orbitals of **AR-23** and **ARO-23** calculated at the B3LYP/6-31G(d) level of theory.

8. NMR Spectra

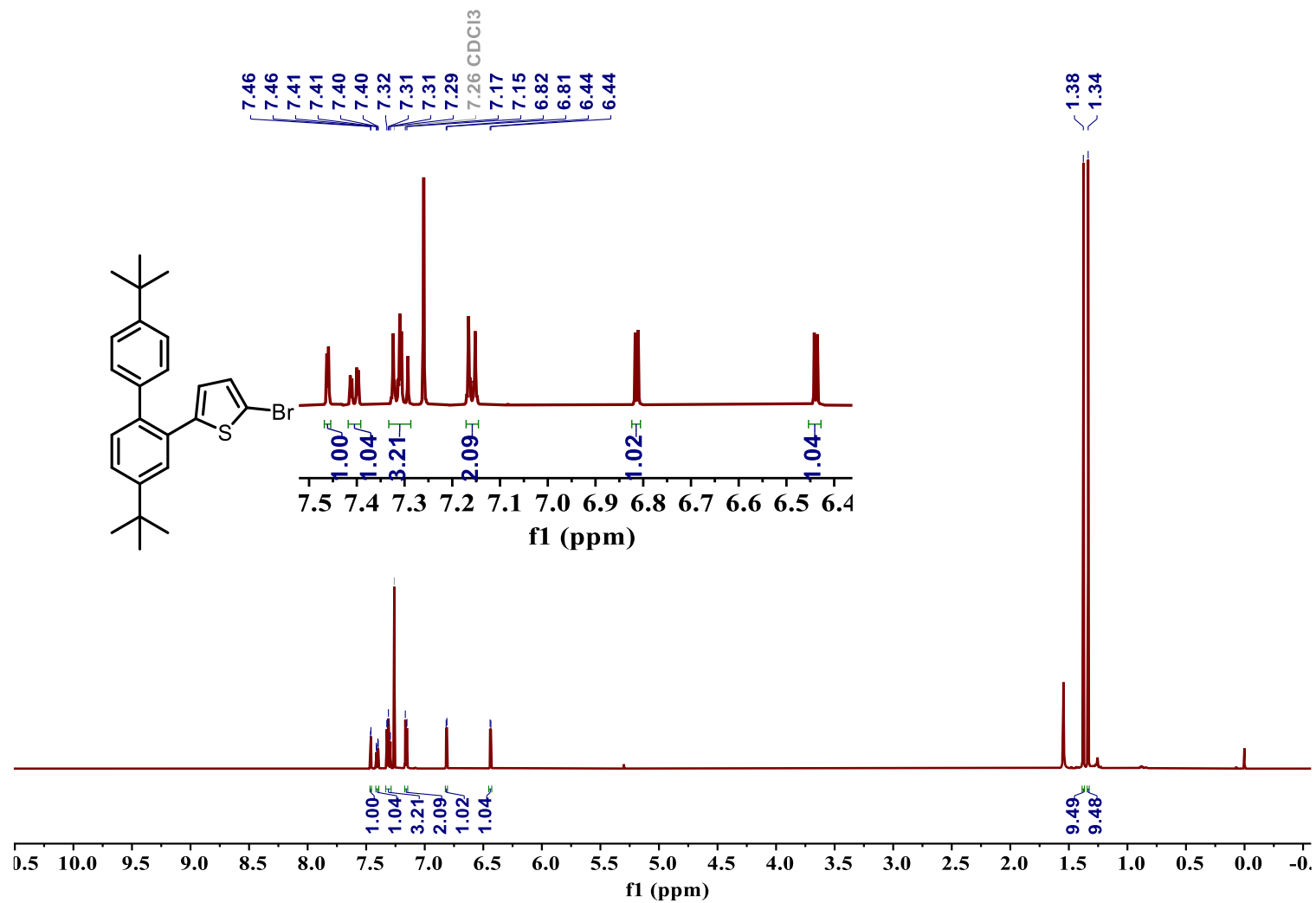


Figure S25. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of **1**.

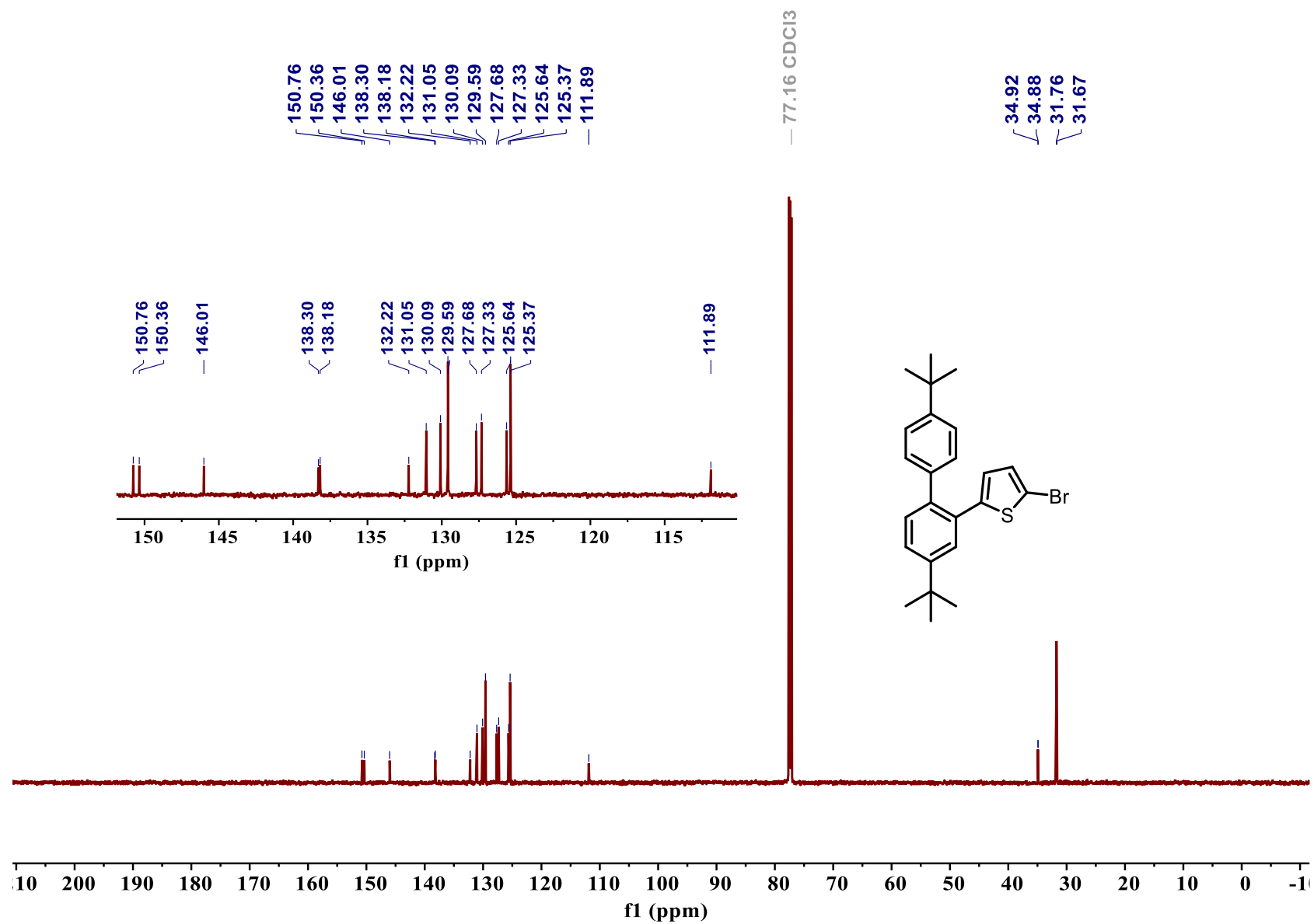


Figure S26. ¹³C NMR spectrum (151 MHz, Chloroform-*d*) of 1.

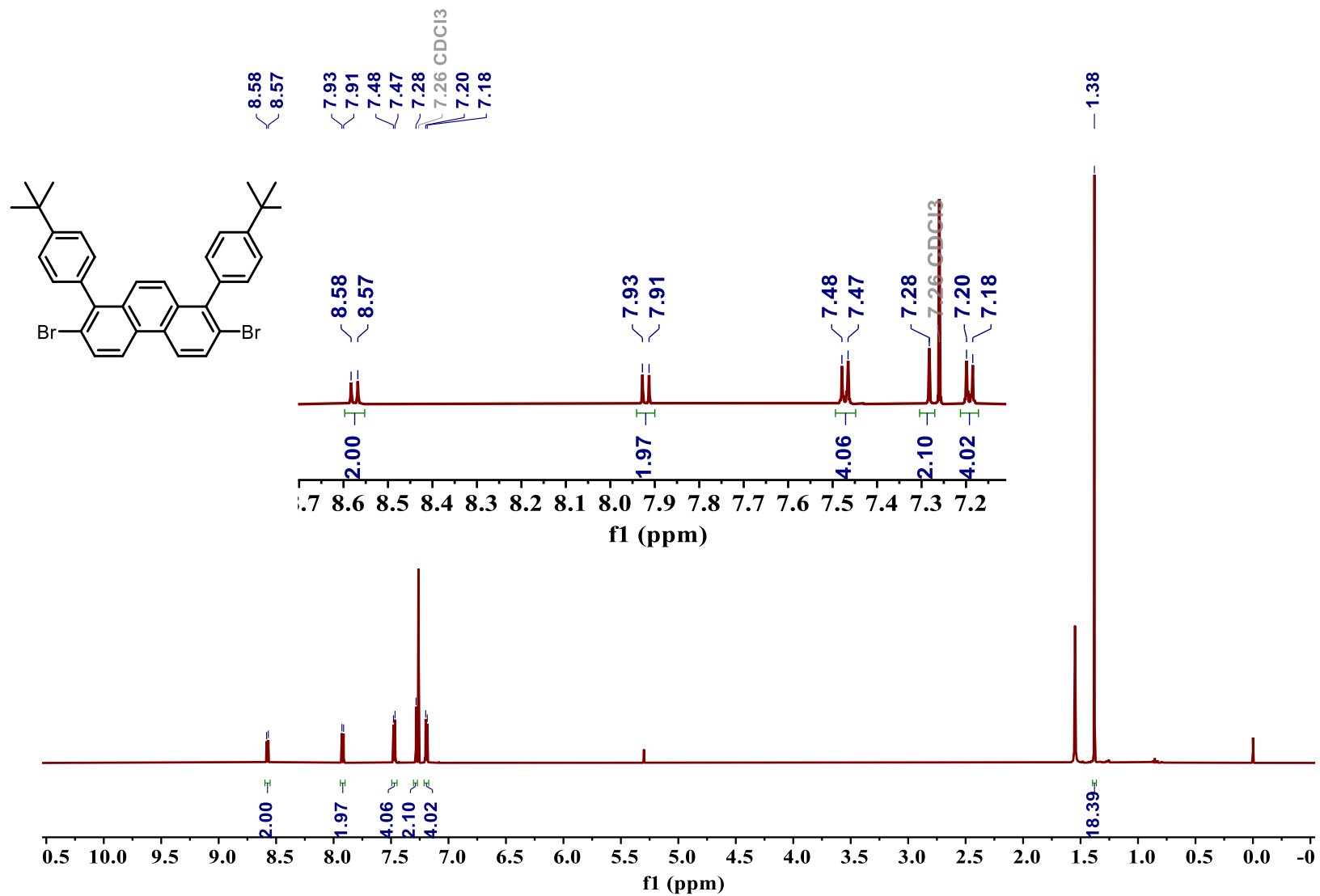


Figure S27. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of **s5**.

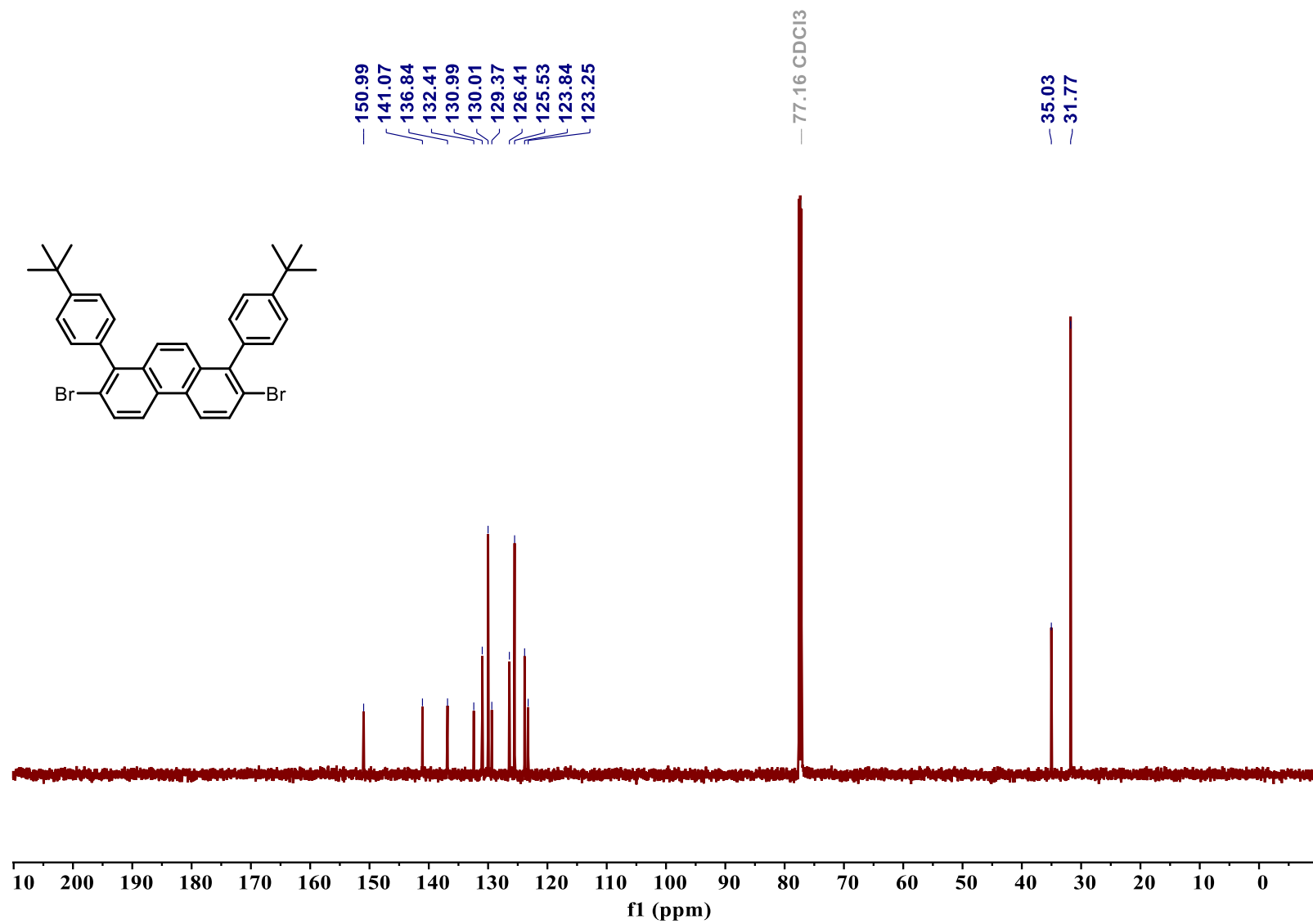


Figure S28. ^{13}C NMR spectrum (151 MHz, Chloroform-*d*) of **s5**.

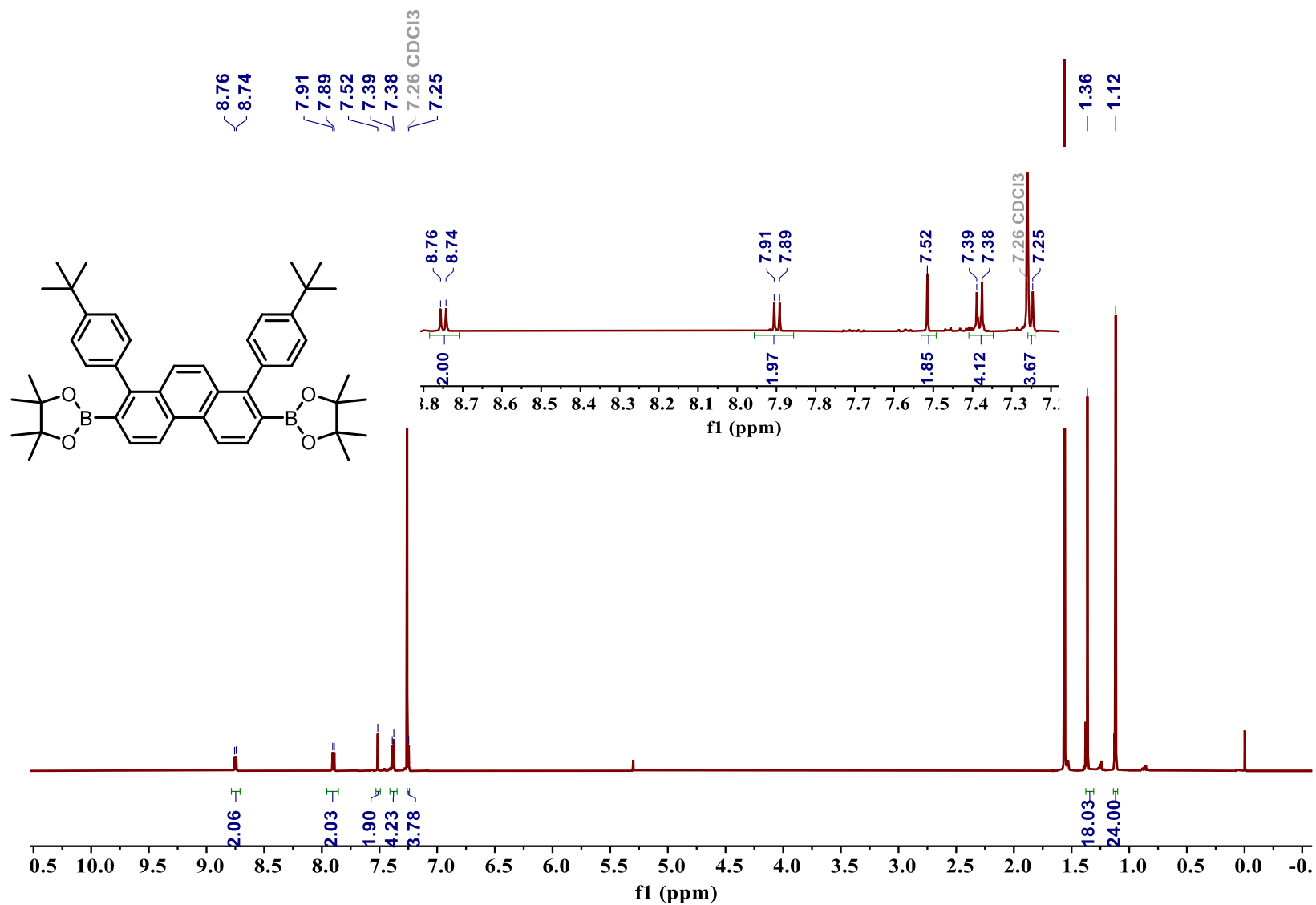


Figure S29. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of 3.

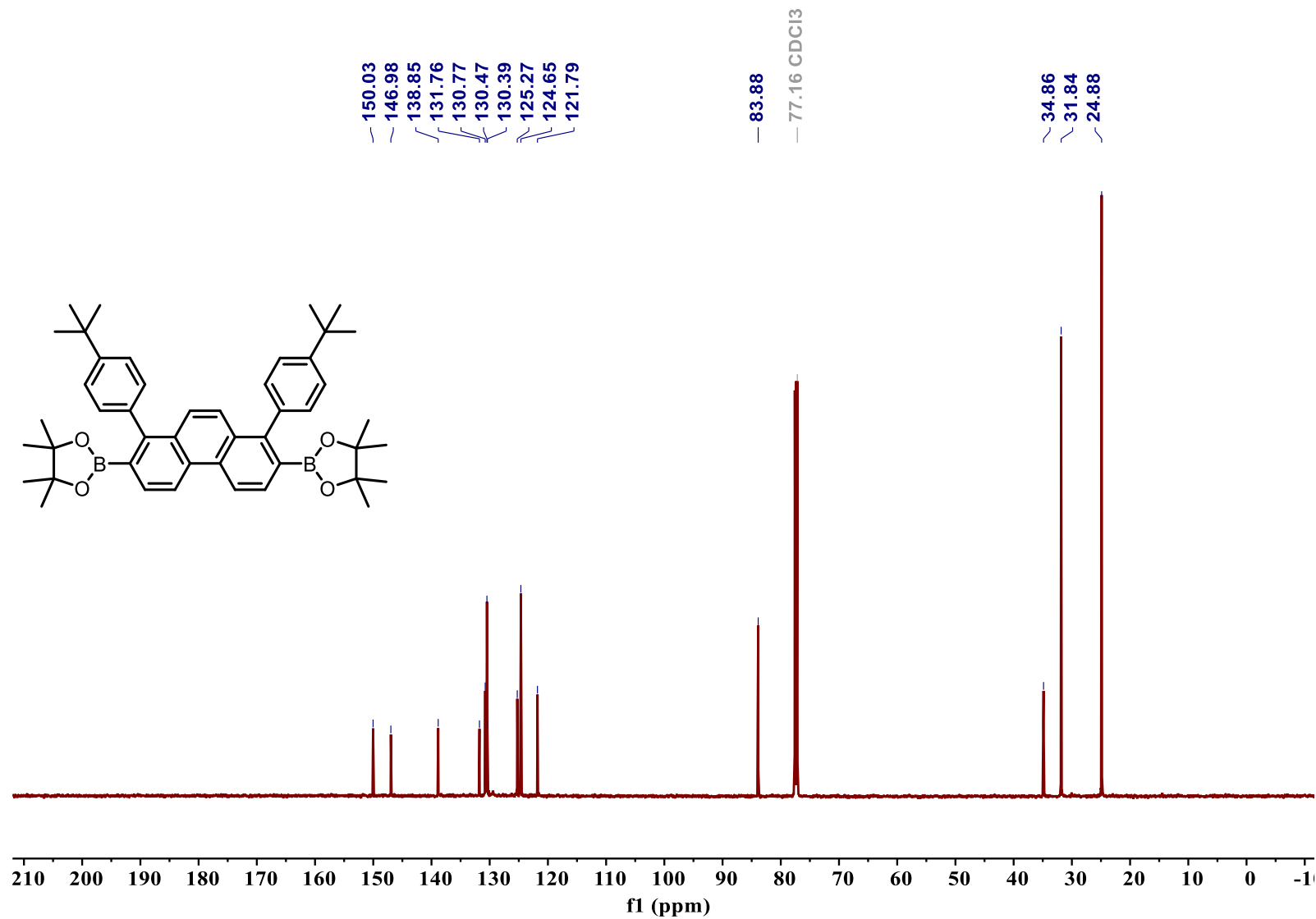


Figure S30. ^{13}C NMR spectrum (151 MHz, Chloroform-*d*) of **3**.

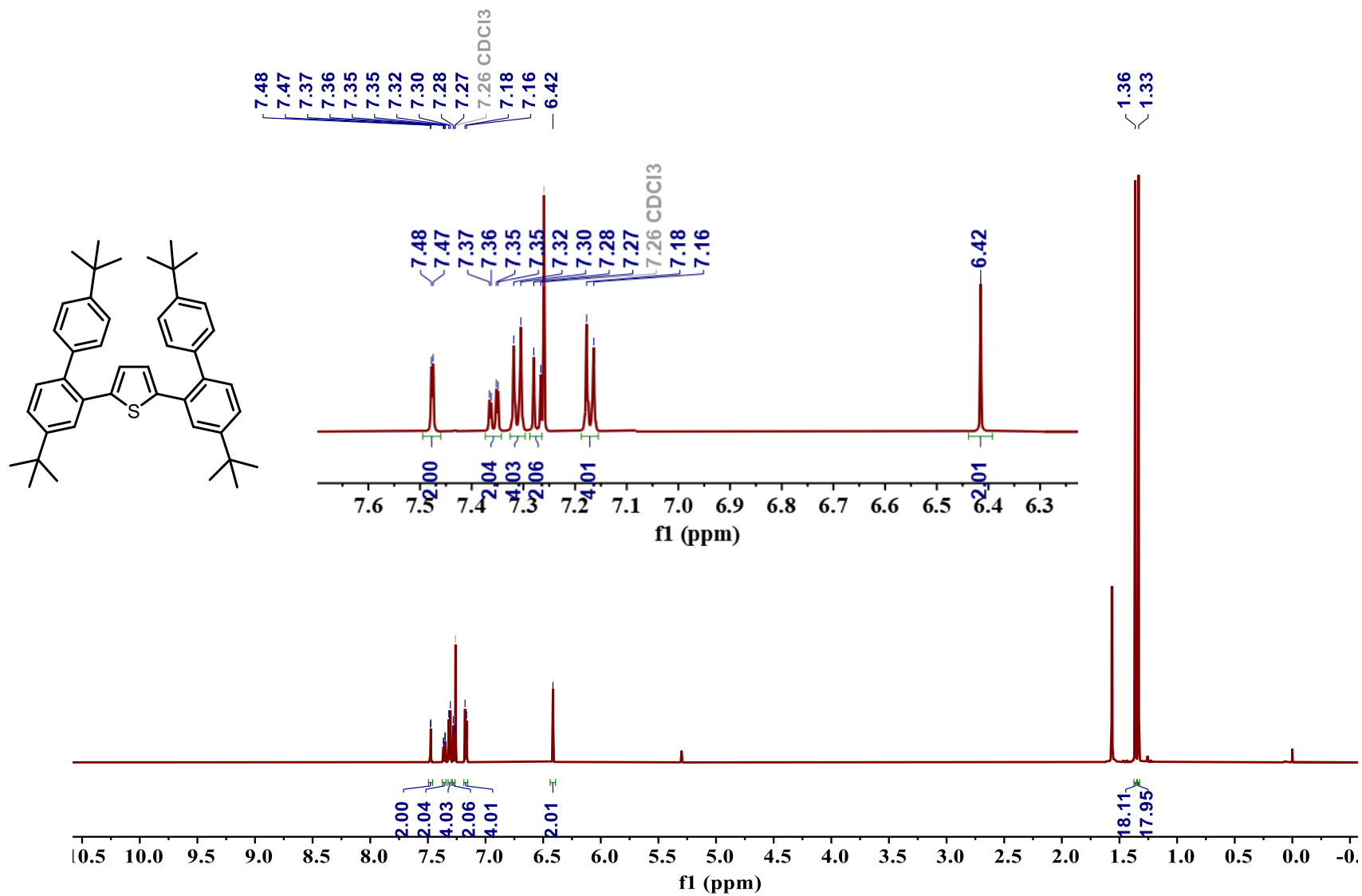


Figure S31. ^1H NMR spectrum (600 MHz, $\text{Chloroform-}d$) of **4d**.

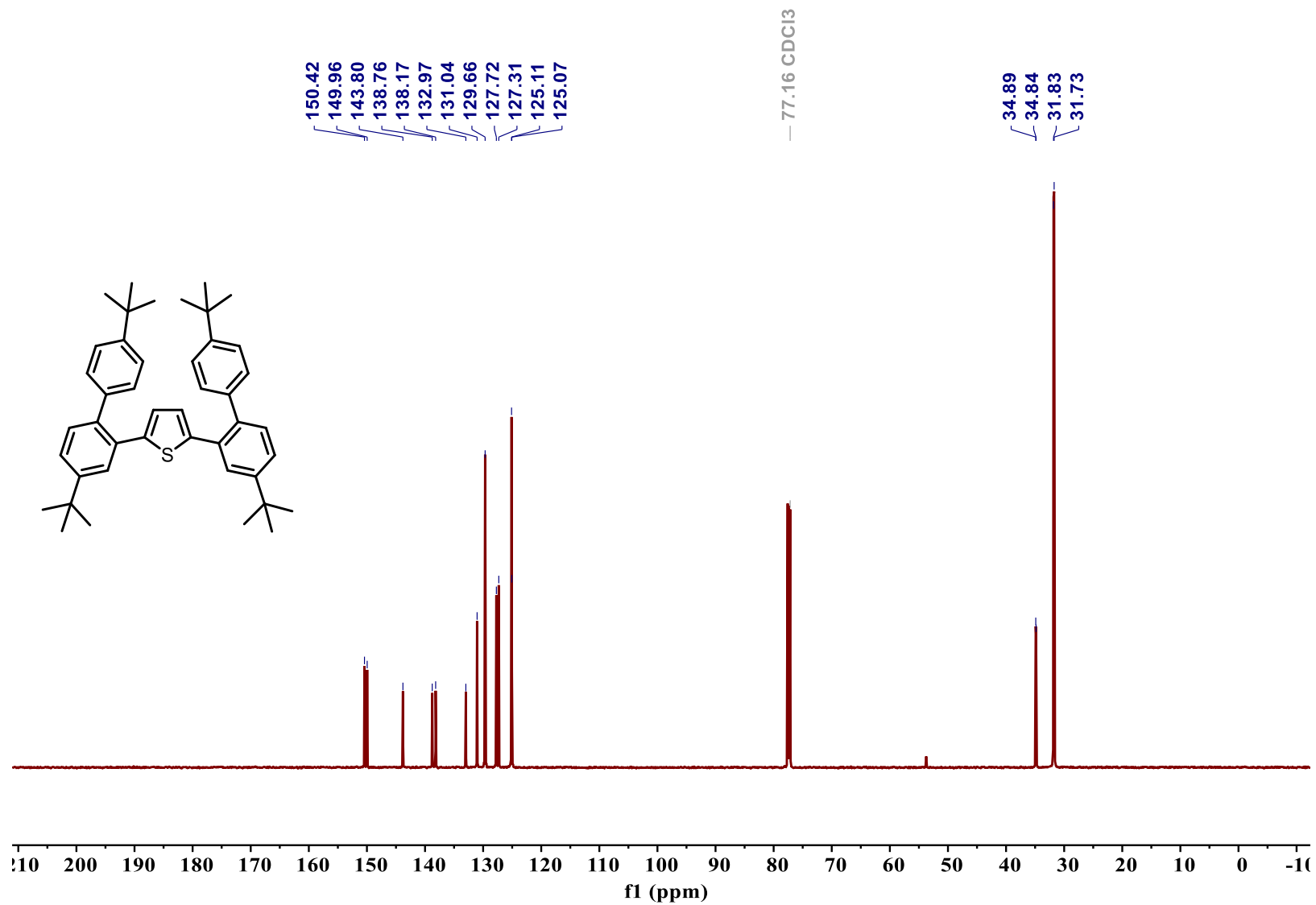


Figure S32. ¹³C NMR spectrum (151 MHz, Chloroform-*d*) of 4d.

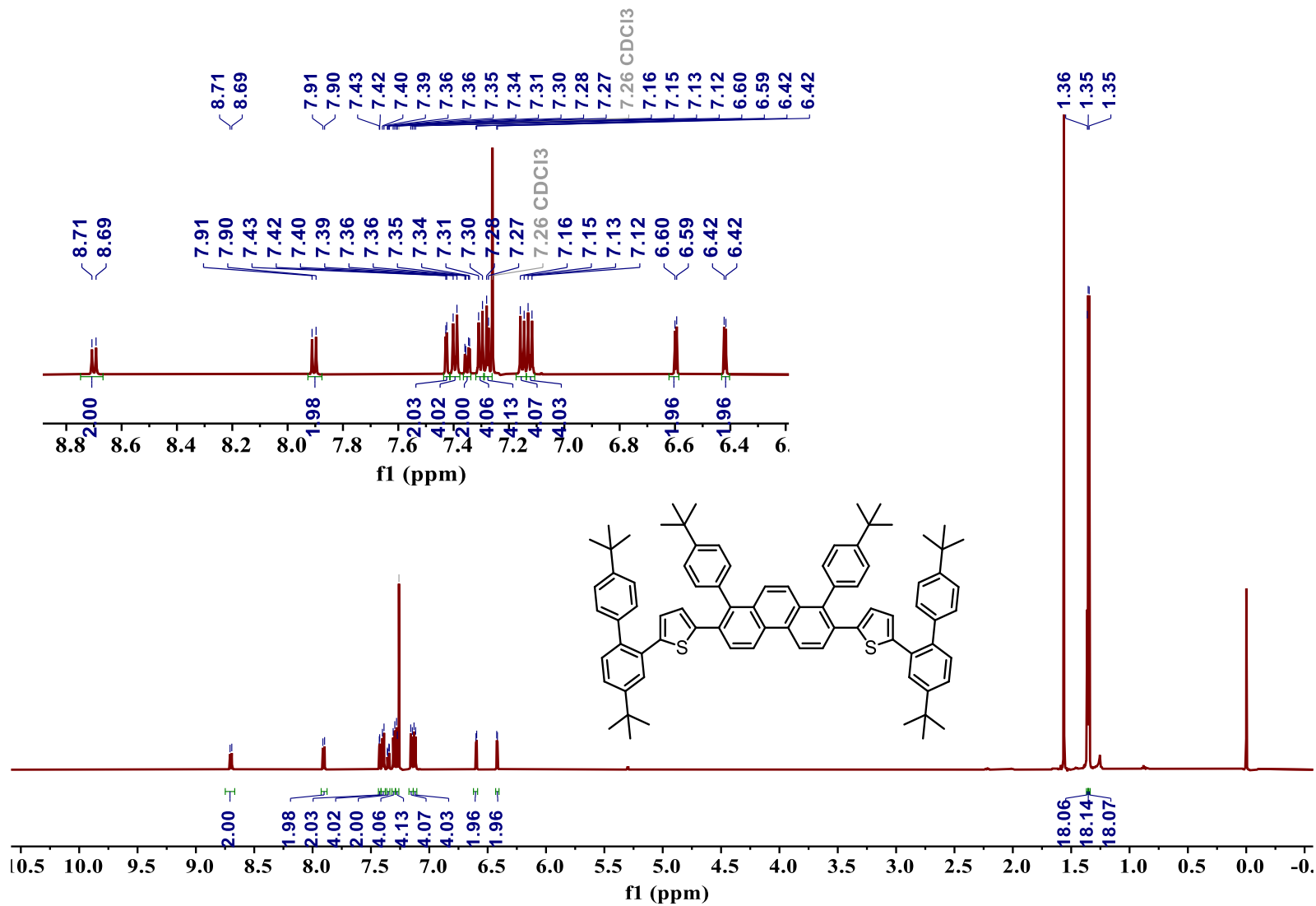


Figure S33. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of **4a**.

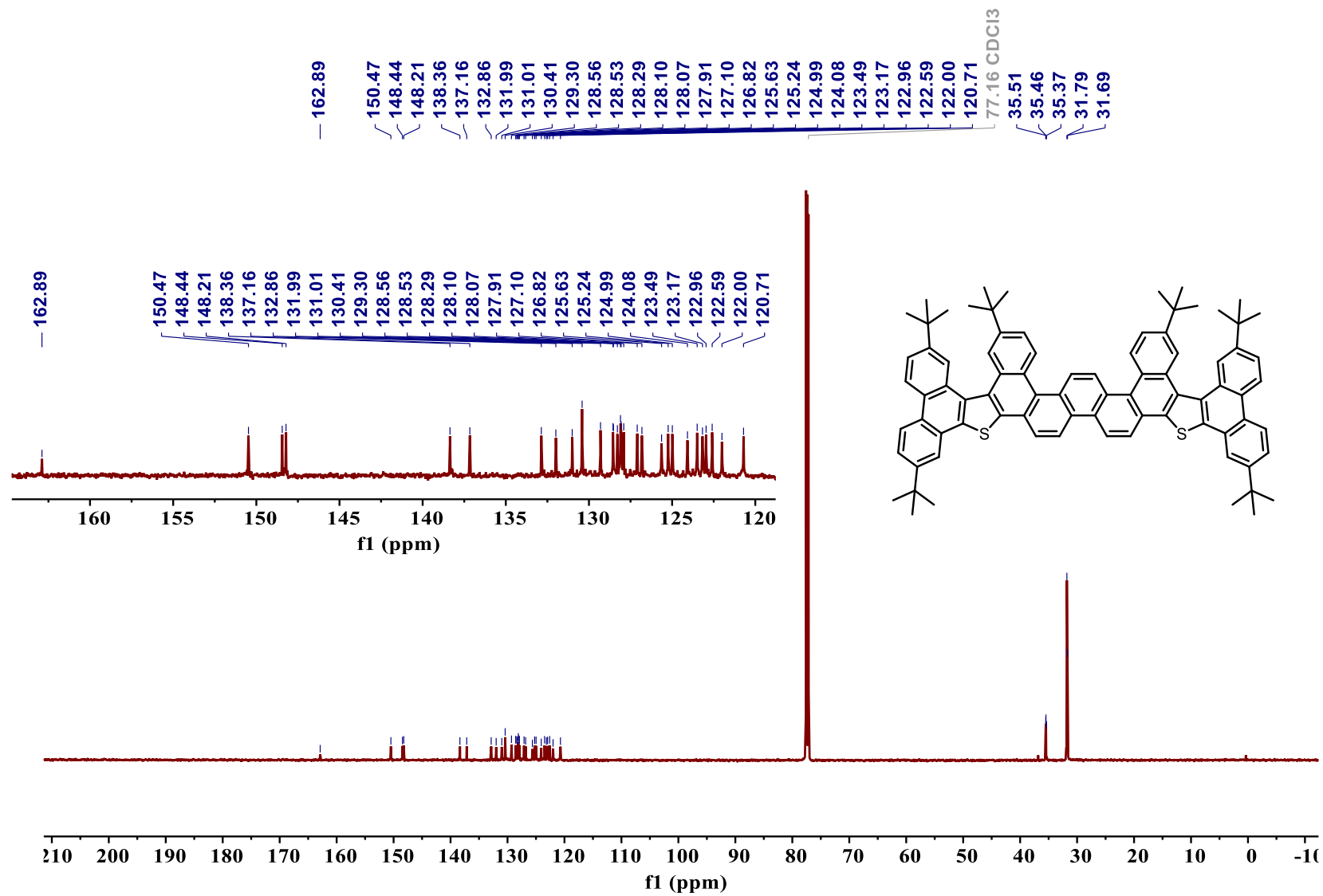


Figure S36. ¹³C NMR spectrum (151 MHz, Chloroform-*d*) of AR-11.

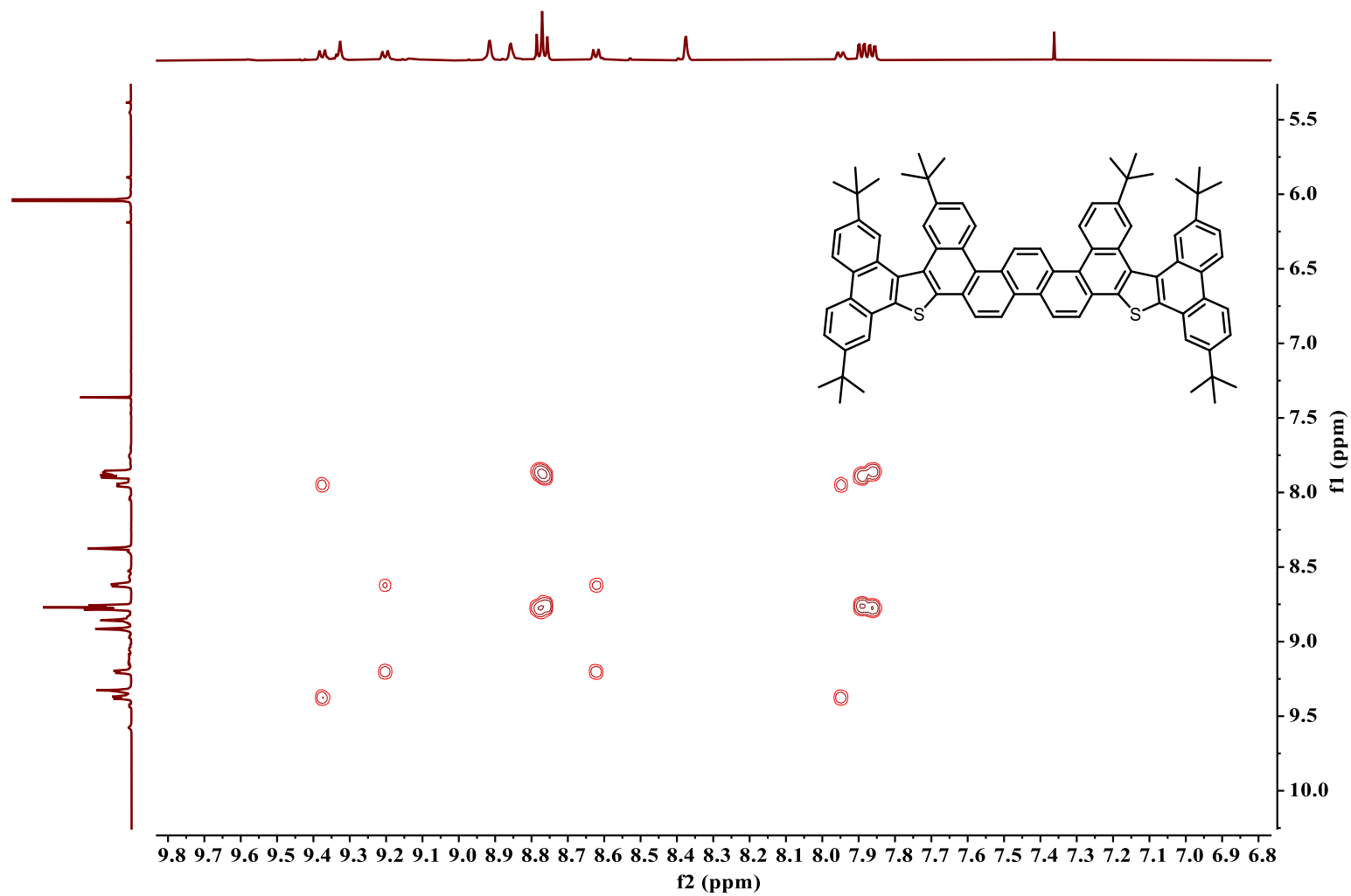


Figure S37. ^1H - ^1H COSY NMR spectrum (600/600 MHz, Chloroform-*d*, 298 K) of **AR-11**.

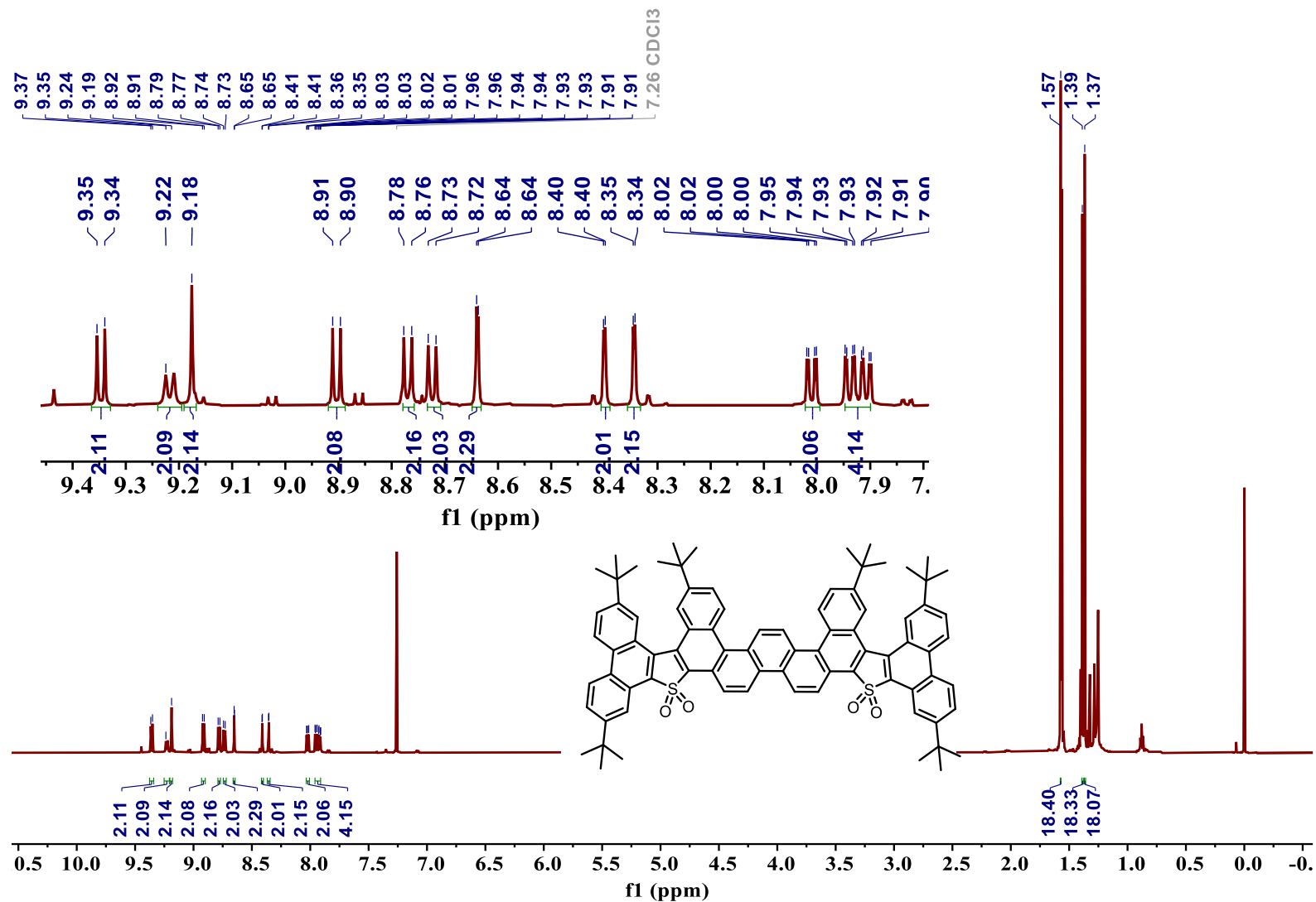


Figure S38. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of ARO-11.

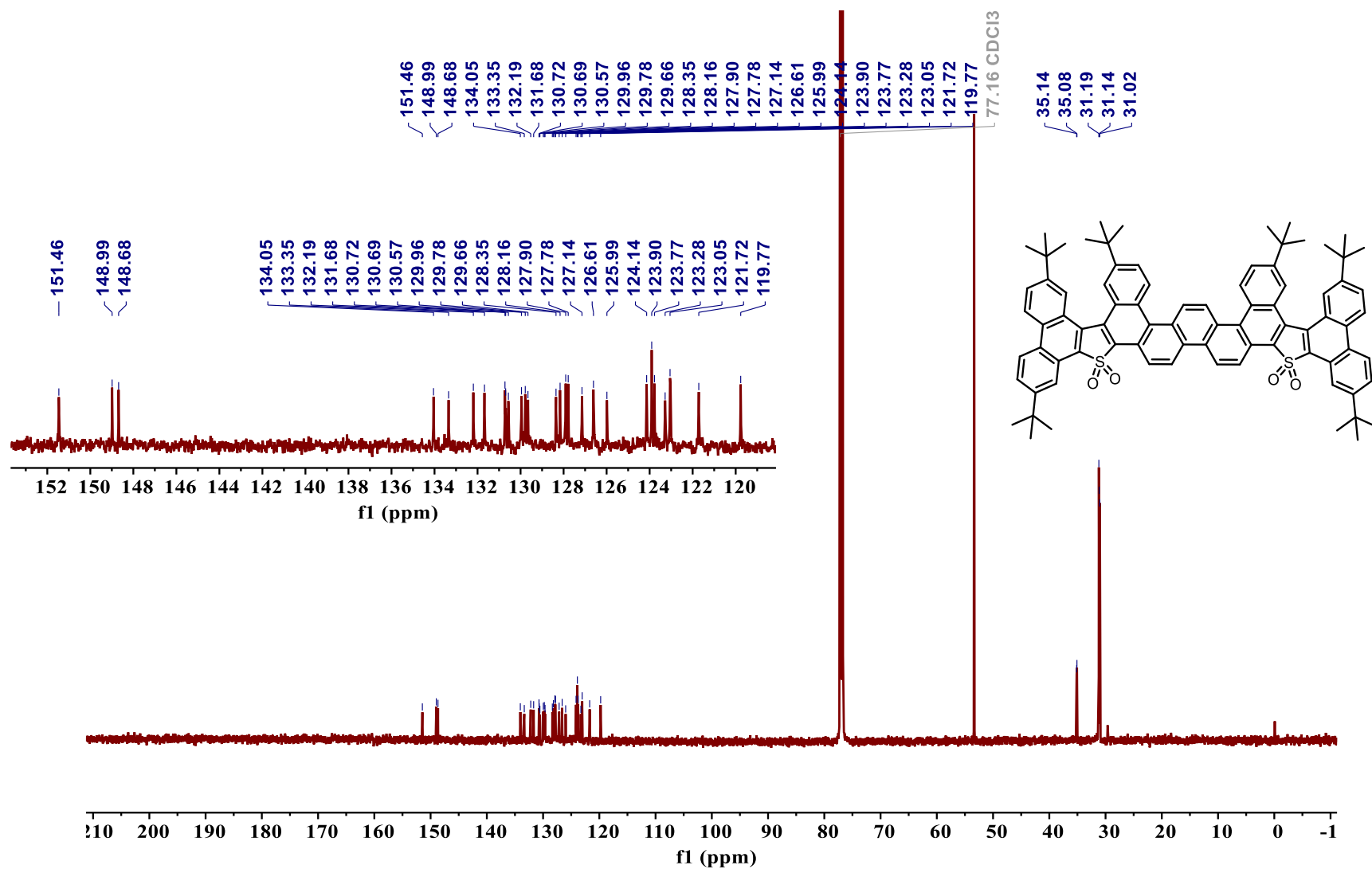


Figure S39. ¹³C NMR spectrum (151 MHz, Chloroform-*d*) of ARO-11.

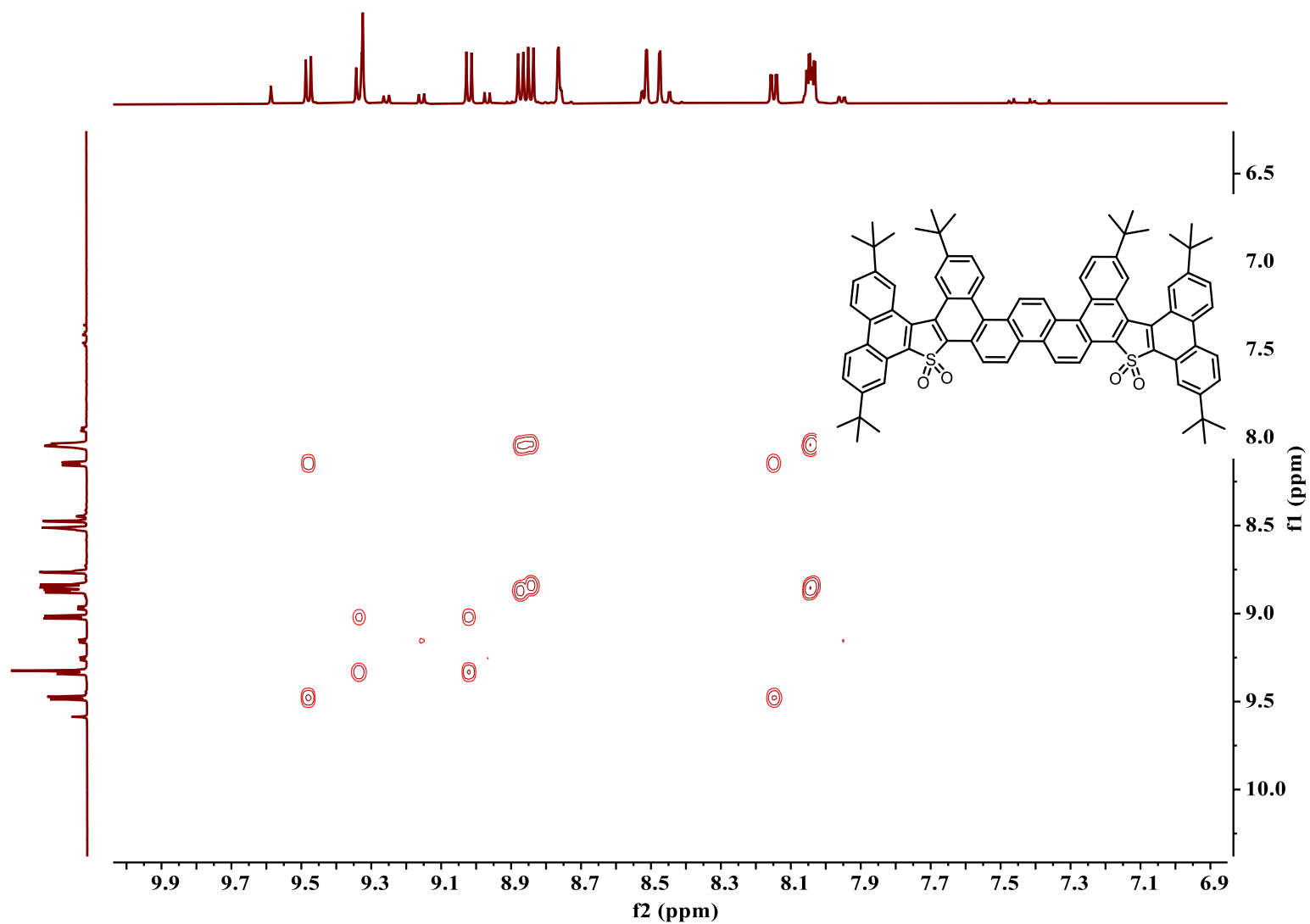
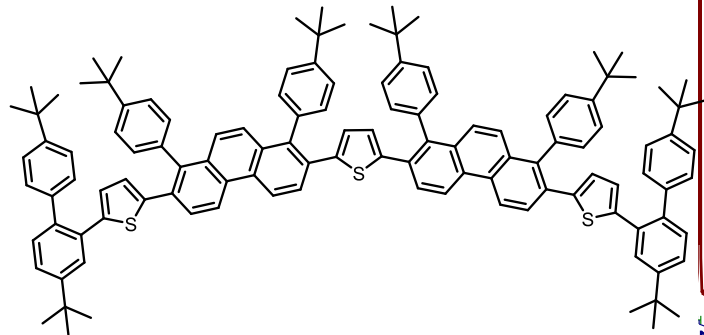


Figure S40. ^1H - ^1H COSY NMR spectrum (600/600 MHz, Chloroform- d , 298 K) of **ARO-11**.



S67

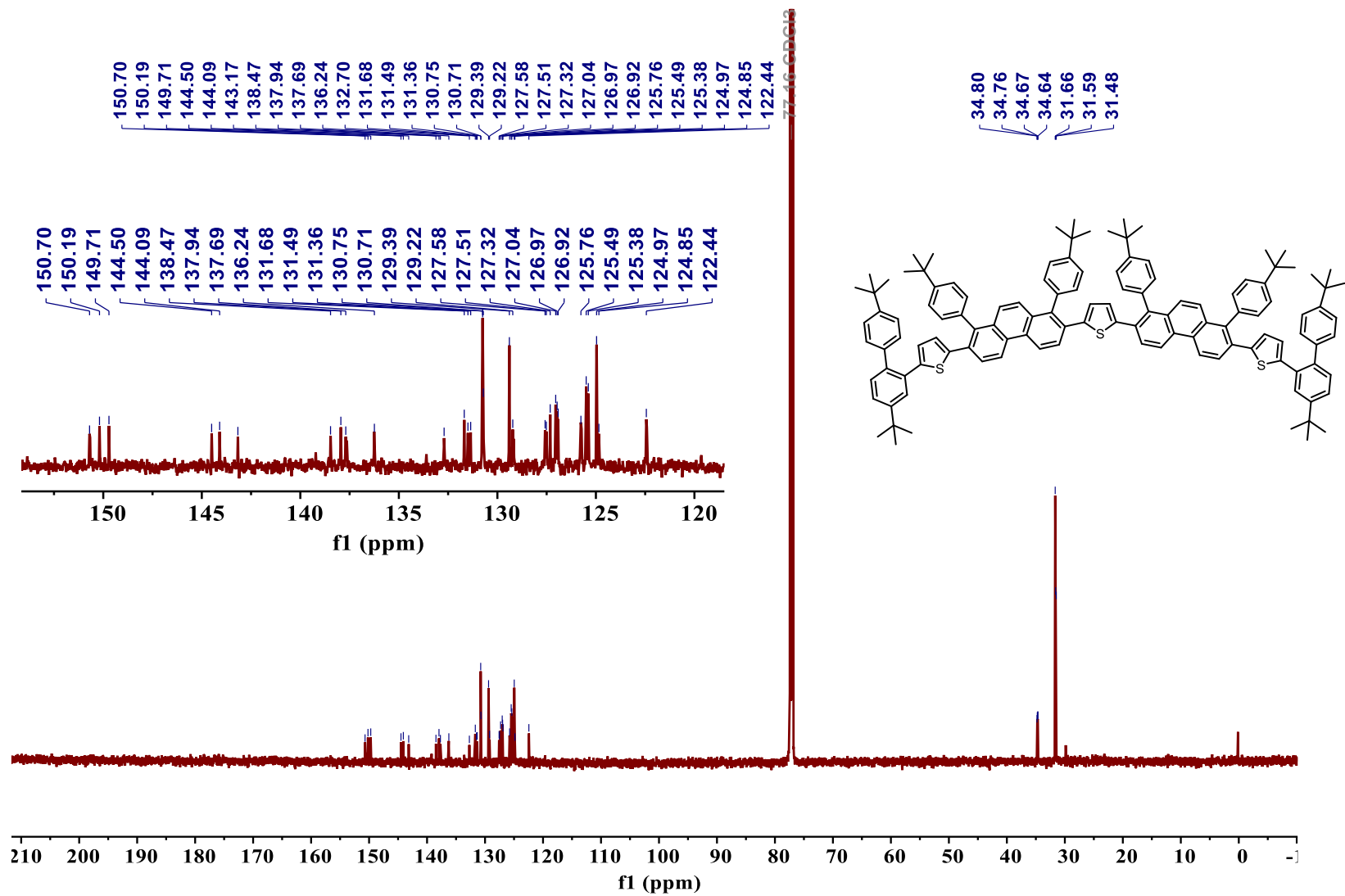


Figure S42. ^{13}C NMR spectrum (151 MHz, $\text{Chloroform-}d$) of **4b**

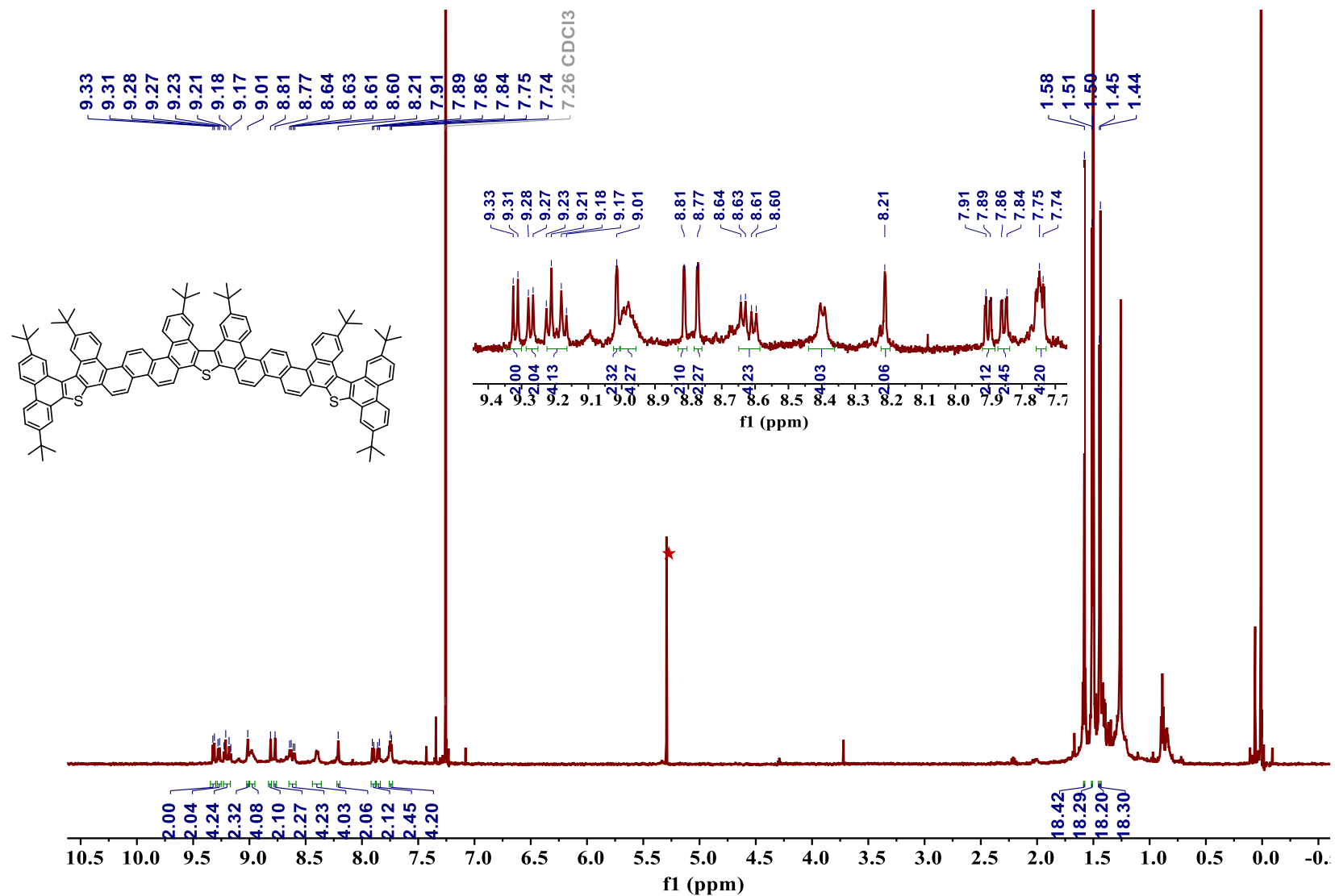


Figure S43. ¹H NMR spectrum (600 MHz, Chloroform-*d*) of AR-17 (The star is dichloromethane)

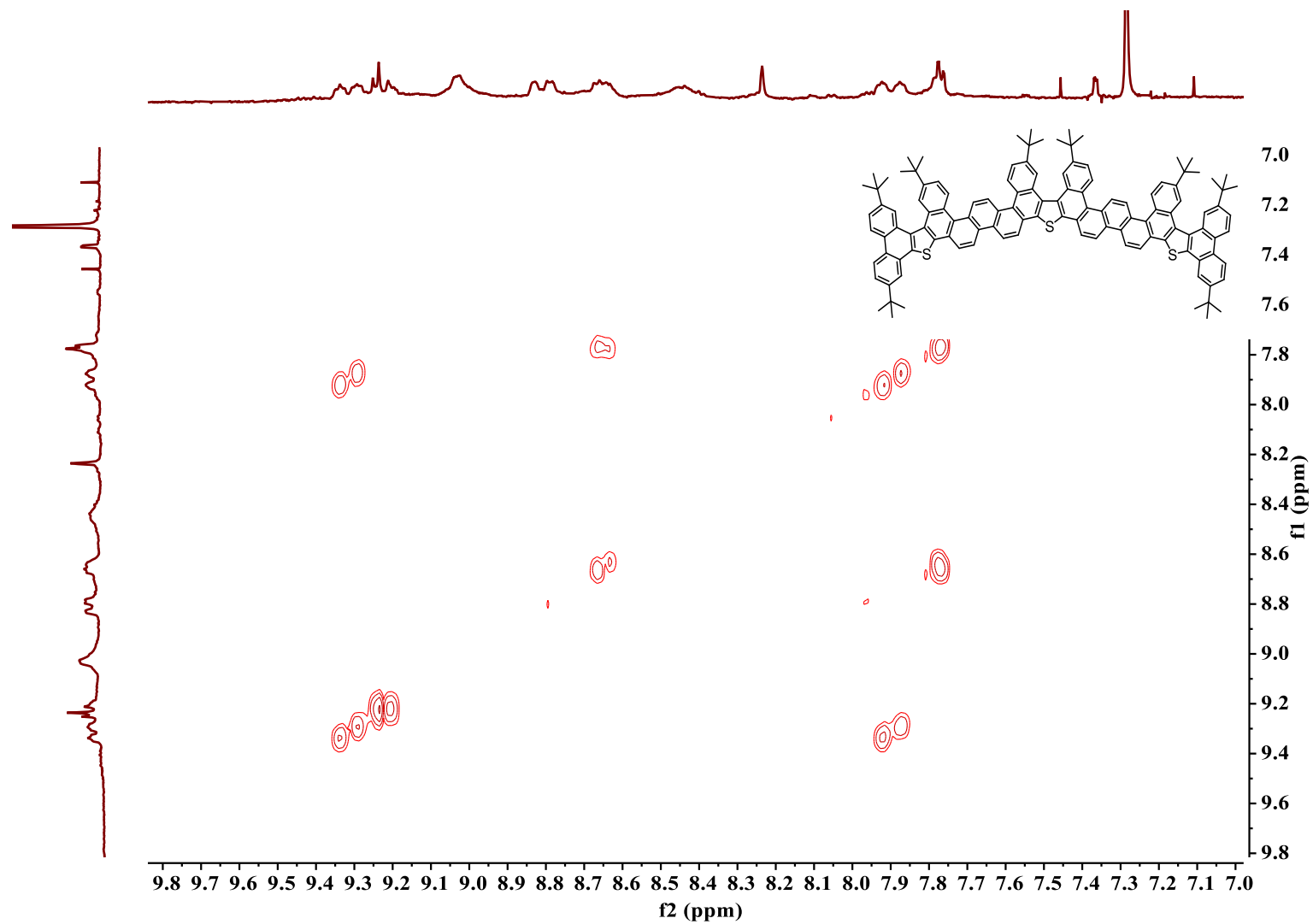


Figure S44. ^1H - ^1H COSY NMR spectrum (600/600 MHz, Chloroform- d , 298 K) of **AR-17**

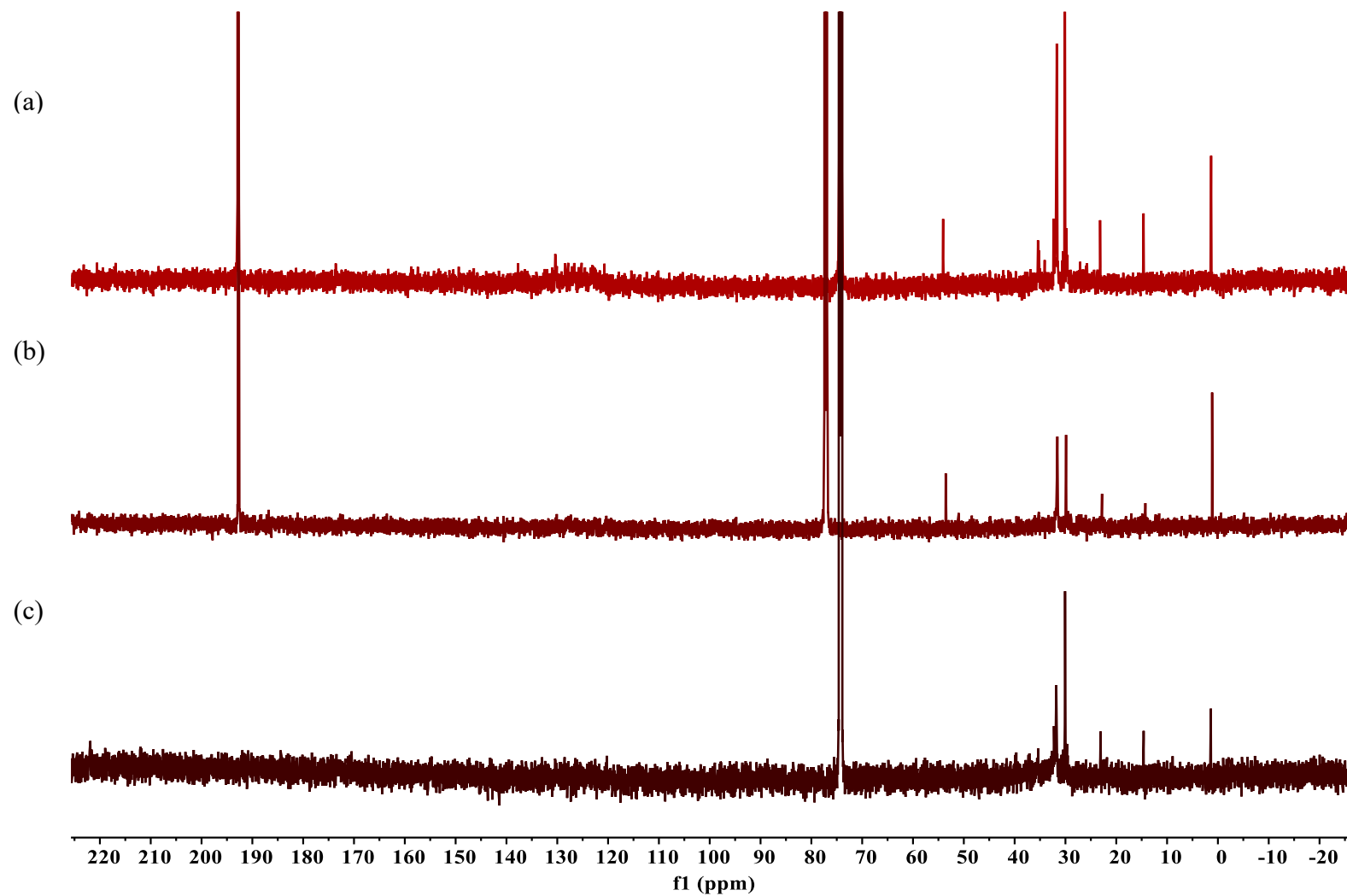


Figure S45. ^{13}C NMR spectrum of AR-17. (a): 151 MHz, 298k, 9 hours, Tetrachloroethane- d_2 and CS_2 . $V_{\text{C}_2\text{D}_2\text{Cl}_4} : V_{\text{CS}_2} = 2 : 1$.
(b): 151 MHz, 298k, 9 hours, Chloroform- d and CS_2 . $V_{\text{CDCl}_3} : V_{\text{CS}_2} = 2 : 1$.
(c): 151 MHz, 298k, 9 hours, Tetrachloroethane- d_2 .

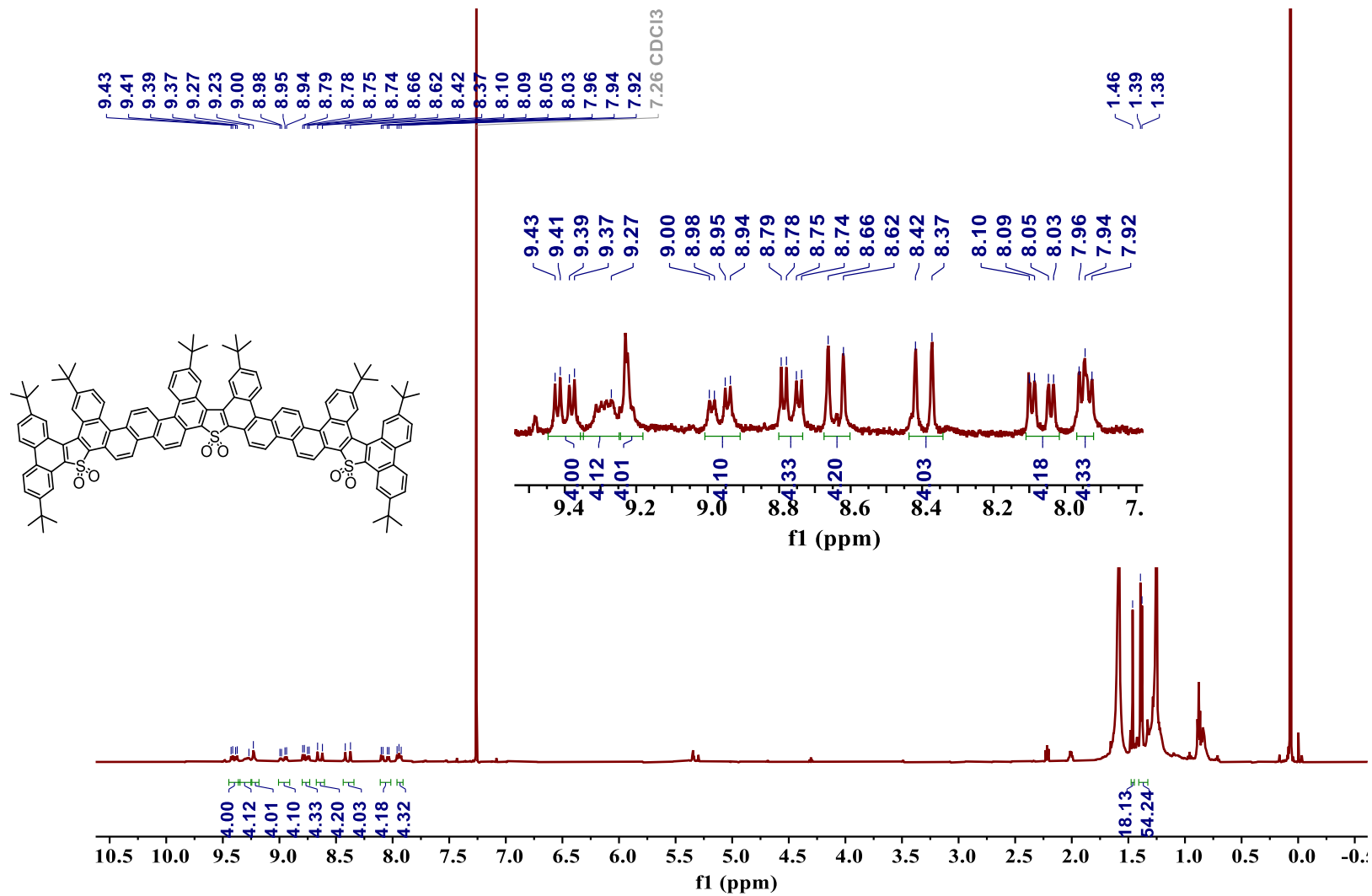


Figure S46. ^1H NMR spectrum (600 MHz, $\text{Chloroform-}d$) of ARO-17

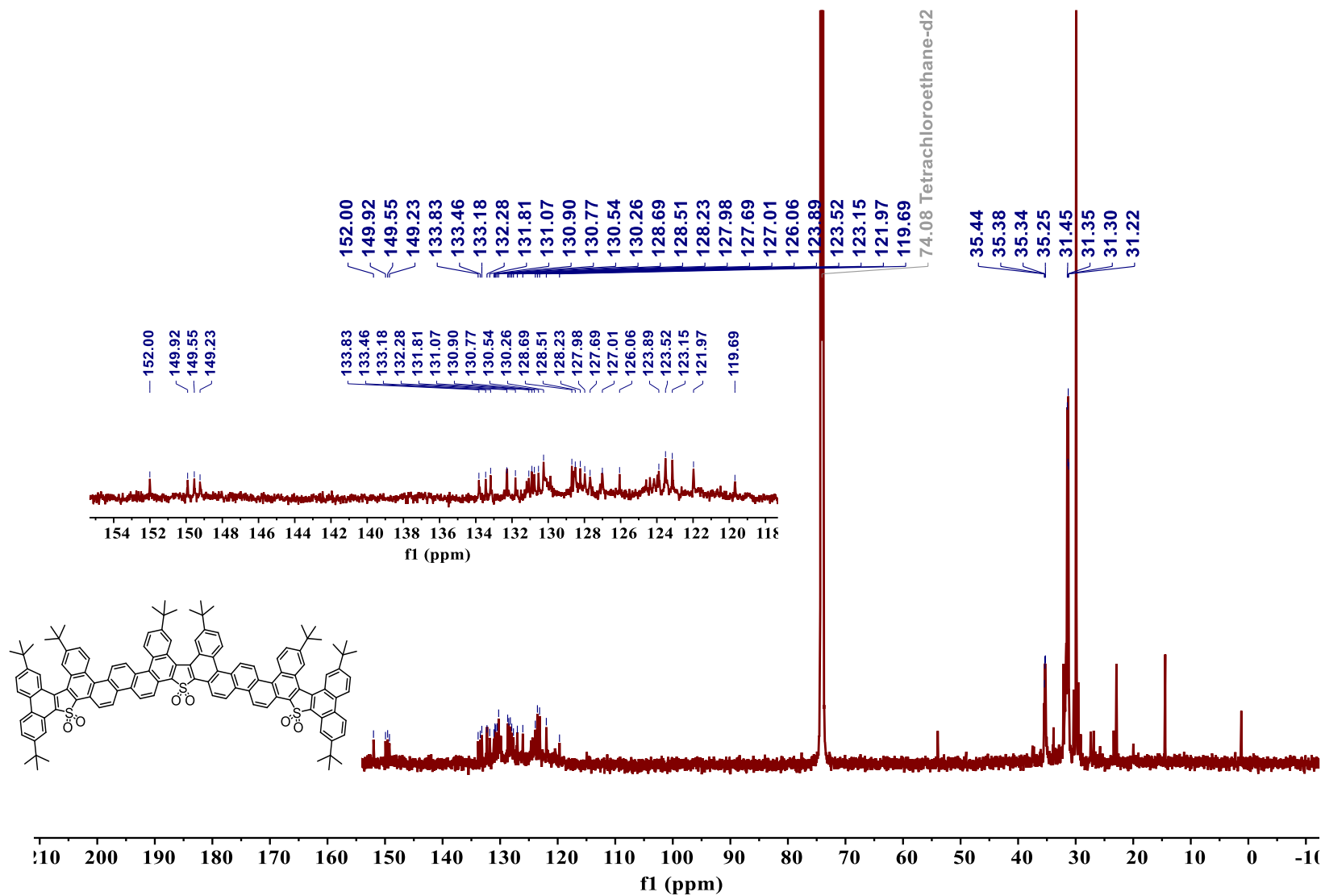


Figure S47. ^{13}C NMR spectrum (151 MHz, Tetrachloroethane- d_2) of ARO-17

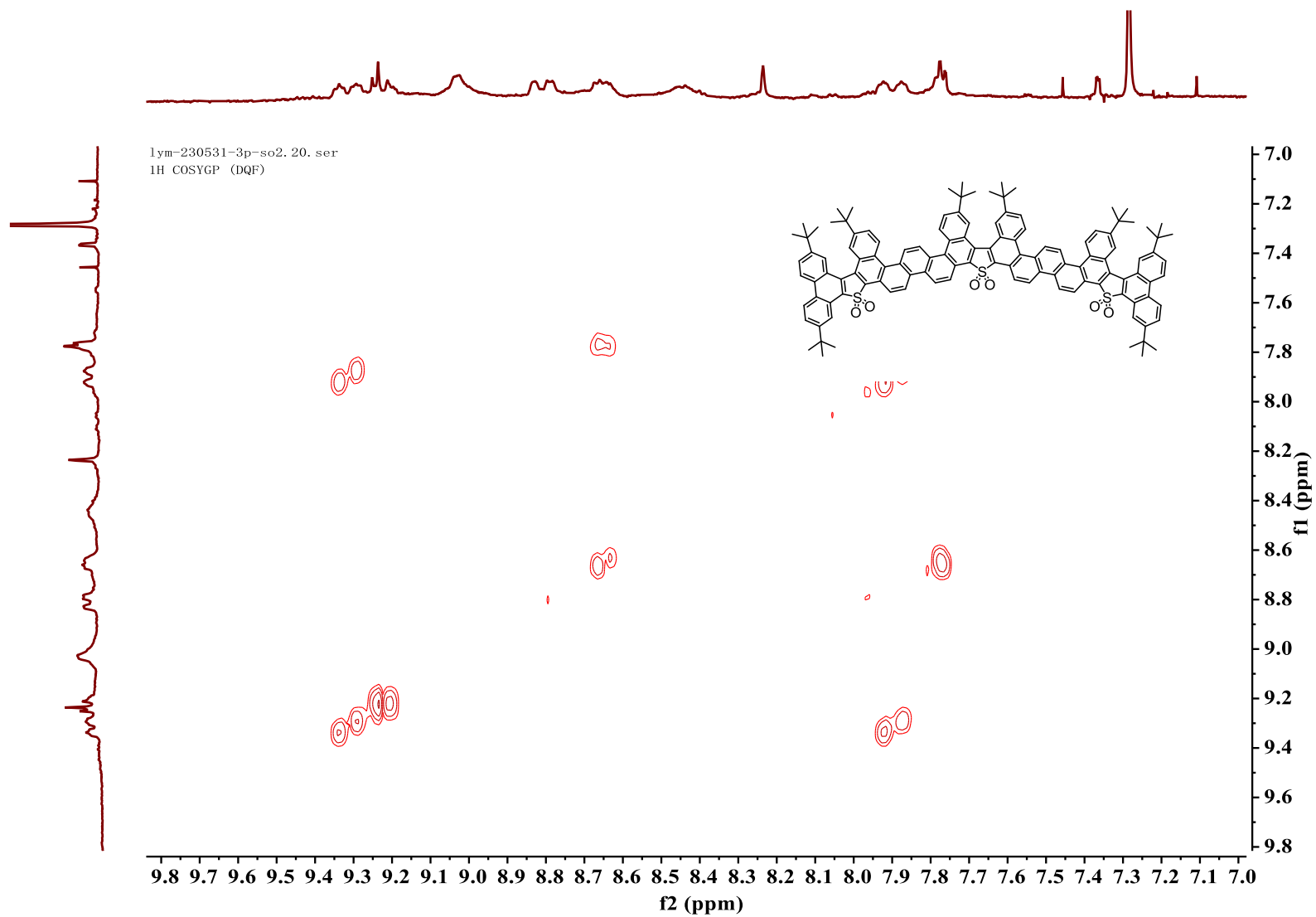
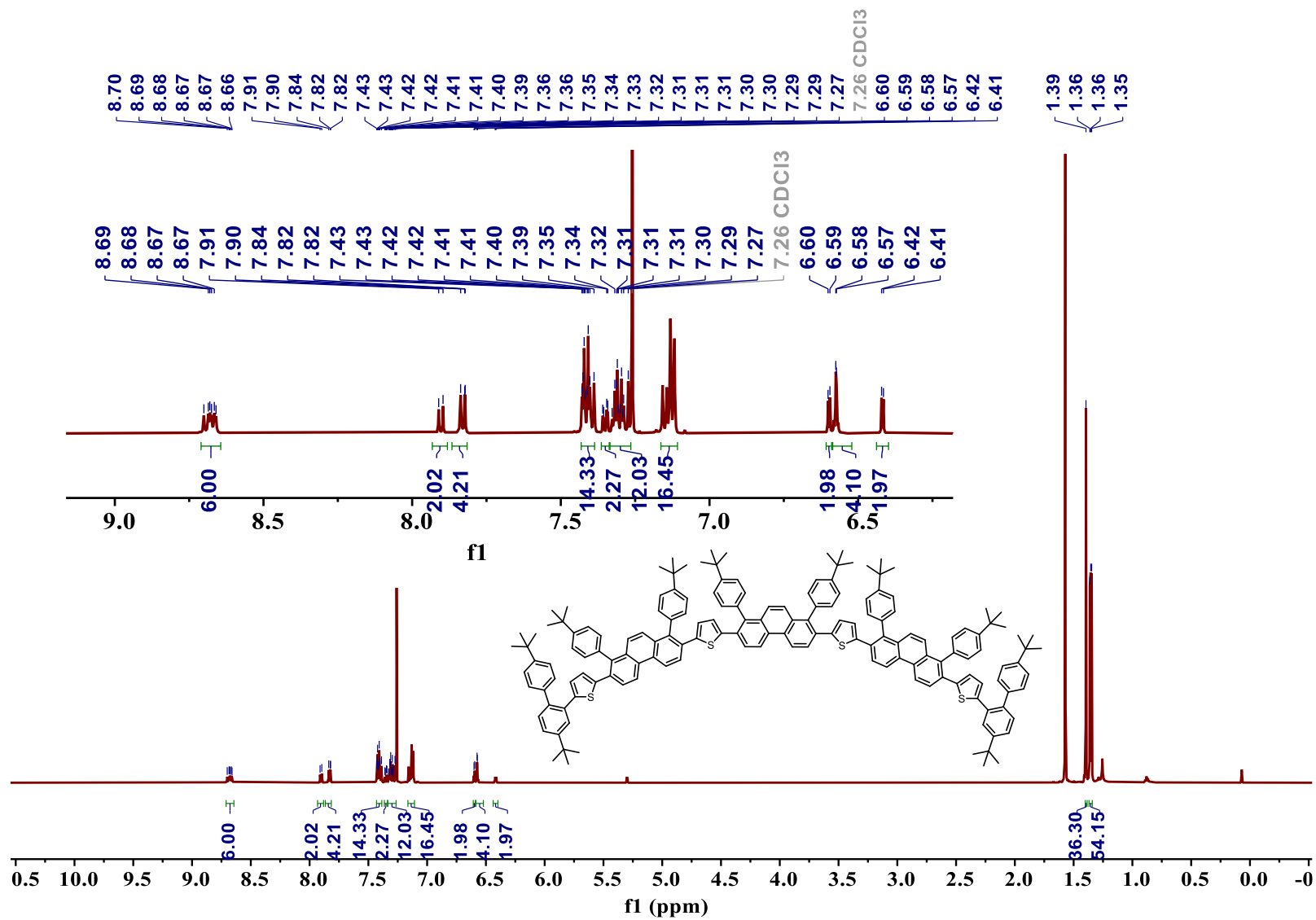


Figure S48. ^1H - ^1H COSY NMR spectrum (600/600 MHz, Chloroform- d , 298 K) of **ARO-17**



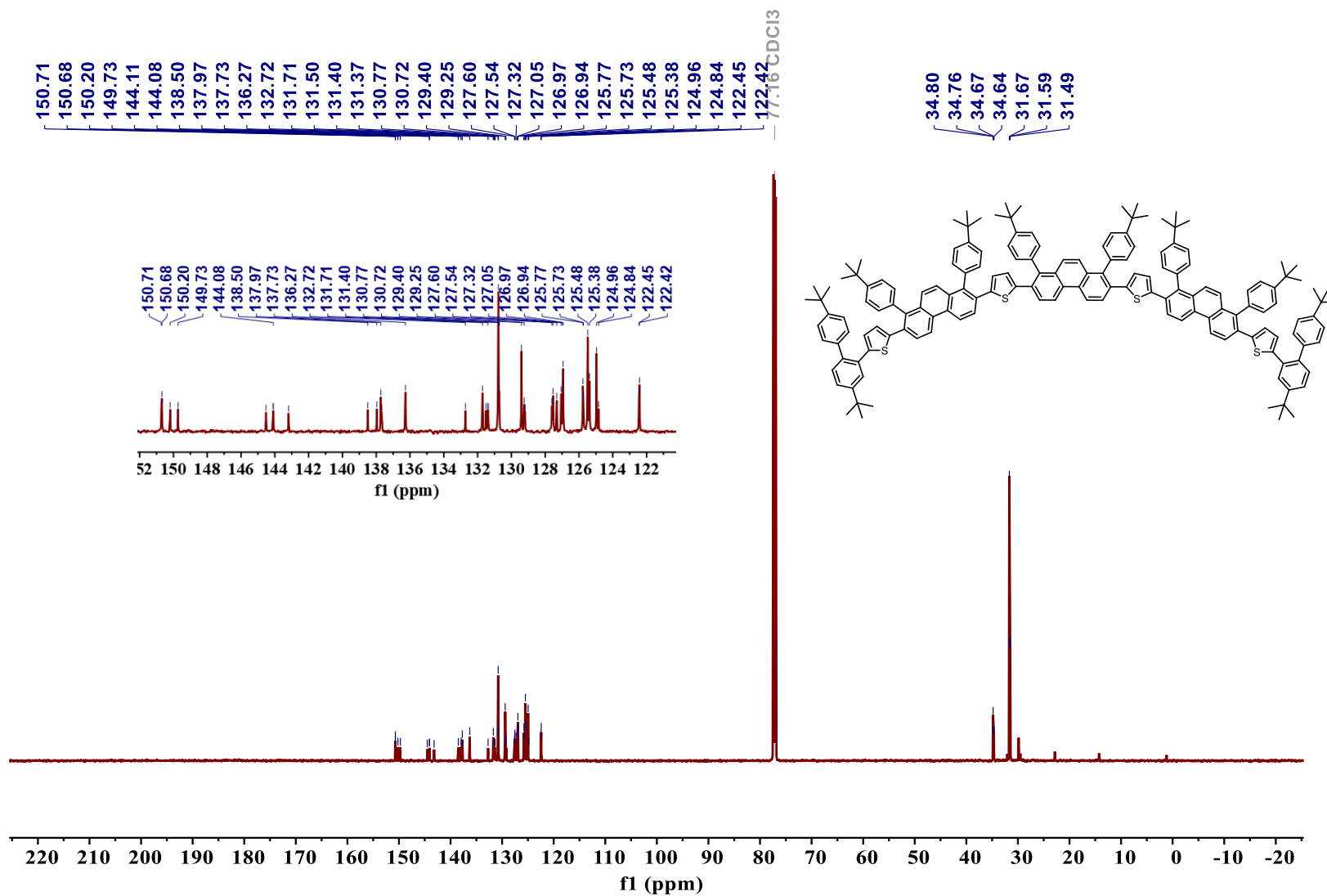


Figure S50. ^{13}C NMR spectrum (151 MHz, Chloroform- d) of **4c**

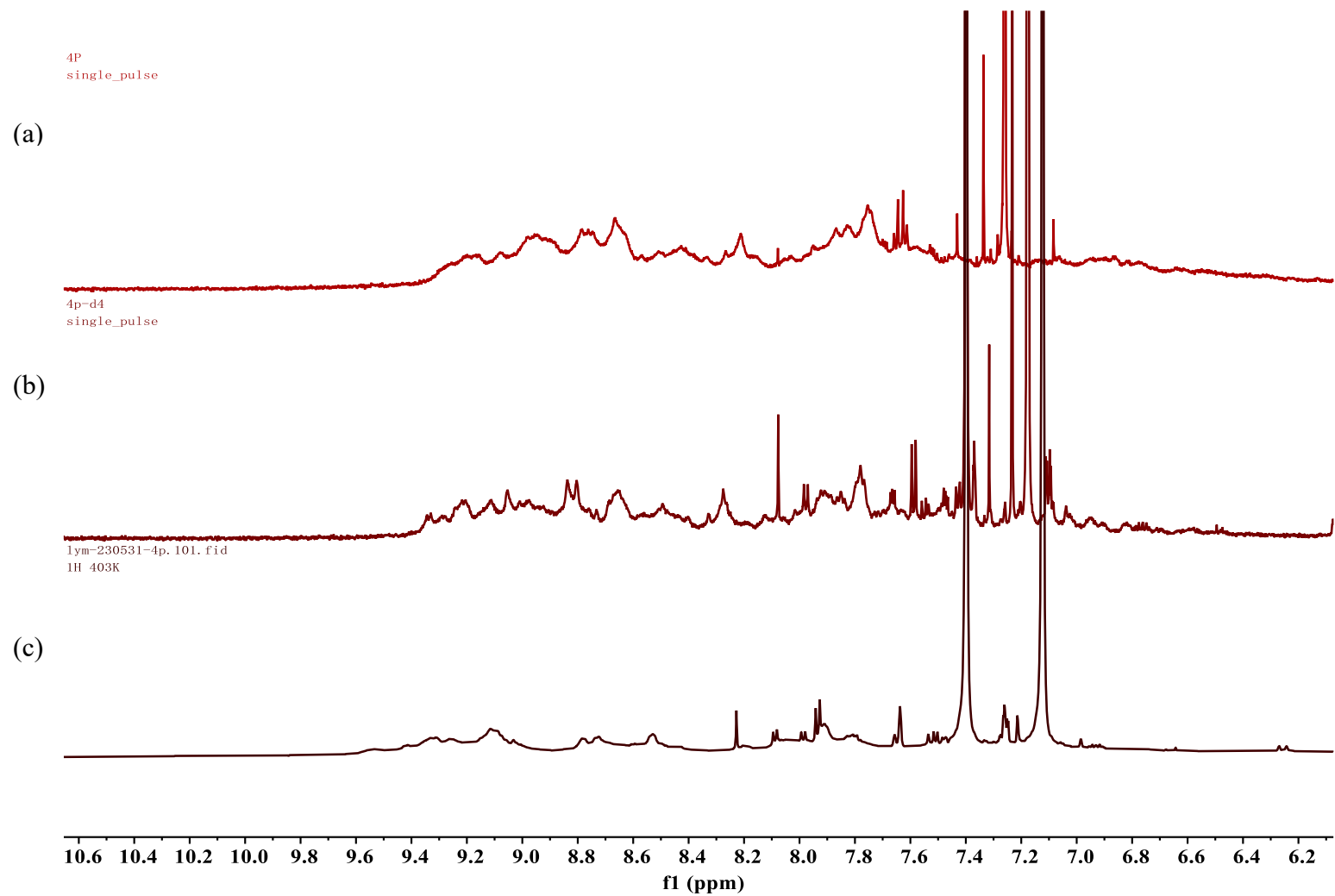


Figure S51. ^1H NMR spectrum (600 MHz,) of **AR-23**. (a): 298k, Chloroform- d and CS_2 . $V_{\text{CDCl}_3} : V_{\text{CS}_2} = 1 : 1$.
(b): 298k, 1,2-Dichlorobenzene- d_4 and CS_2 . $V_{\text{C}_6\text{D}_4\text{Cl}_2} : V_{\text{CS}_2} = 2 : 1$.
(c): 403k, 1,2-Dichlorobenzene- d_4 .

9 Cartesian coordinates of optimized structures

AR-5

C	-3.02773200	-4.48910100	-0.50272400	C	-5.34193200	-4.56020400	0.45906100
C	-2.76542500	-3.13989100	-0.32314800	C	-5.01473700	-4.30374200	-2.02218900
C	-1.46715000	-2.64944200	-0.10461600	C	-4.55362600	-6.48713500	-0.91146000
C	-0.37383900	-3.54394500	-0.03732000	H	-4.96914300	-5.01525100	1.38202000
C	-1.92871000	-5.36628000	-0.46719500	H	-5.36141600	-3.47576300	0.60073100
C	0.95076500	-3.03205800	0.30604300	H	-6.37276100	-4.89560800	0.30367100
C	1.17343700	-1.63977500	0.40115300	H	-4.40403500	-4.57143200	-2.89010600
C	2.37937300	-1.17649500	0.96872100	H	-6.04065200	-4.63834300	-2.20878800
H	2.47703300	-0.11438900	1.14069700	H	-5.02855000	-3.21295400	-1.94203800
C	3.40230000	-2.02454300	1.34896700	H	-5.59646400	-6.77627100	-1.07275600
C	3.20649200	-3.40491800	1.14075300	H	-3.97686500	-6.83390400	-1.77481200
H	-3.58460300	-2.42727400	-0.37014000	H	-4.19684500	-7.01520100	-0.02142400
H	-2.07418800	-6.42920500	-0.61884300	C	-4.46658200	4.96417800	0.74269000
H	3.98581200	-4.11150400	1.40962600	C	-5.34189200	4.56025000	-0.45906100
C	-1.18700600	-1.24107200	-0.00733000	C	-5.01470100	4.30378100	2.02218800
C	0.09048100	-0.72495900	0.06410800	C	-4.55357100	6.48717200	0.91146300
S	-2.40926600	0.00001000	-0.00000200	H	-4.96909800	5.01529700	-1.38201900
C	-1.18699600	1.24108100	0.00732700	H	-5.36138400	3.47581000	-0.60073500
C	-1.46712800	2.64945400	0.10461400	H	-6.37271800	4.89566200	-0.30367200
C	0.09048700	0.72495800	-0.06411100	H	-4.40399800	4.57146400	2.89010600
C	-2.76539800	3.13991400	0.32314700	H	-6.04061400	4.63839100	2.20878700
C	-0.37380900	3.54394700	0.03732000	H	-5.02852300	3.21299300	1.94203500
C	1.17345100	1.63976400	-0.40115400	H	-5.59640600	6.77631600	1.07276100
C	-3.02769400	4.48912500	0.50272500	H	-3.97680600	6.83393500	1.77481500
H	-3.58458200	2.42730400	0.37013600	H	-4.19678600	7.01523700	0.02142700
C	0.95079100	3.03205000	-0.30604300	C	-2.01402200	-3.89031100	0.65404000
C	2.37938300	1.17647500	-0.96872200	H	1.88841200	-4.96442900	0.57998200
C	-1.92866400	5.36629500	0.46719800	C	-0.64575500	-4.90764000	-0.24013300
H	2.47703400	0.11436800	-1.14069900	H	0.16187100	-5.63066500	-0.22679000
C	3.40231900	2.02451500	-1.34896700	C	2.01405600	3.89029400	-0.65403800
H	-2.07413200	6.42922200	0.61884700	H	1.88845500	4.96441300	-0.57997900
C	3.20652200	3.40489100	-1.14075100	C	-0.64571200	4.90764400	0.24013500
H	3.98584800	4.11147100	-1.40962200	H	0.16192000	5.63066300	0.22679400
C	4.68381200	-1.52312800	2.02382900				
C	5.91389600	-1.96102800	1.20686500				
C	4.70380900	0.00554700	2.15526100				
C	4.77340500	-2.13194200	3.43694700				
H	5.96311200	-3.04798700	1.09543000				
H	5.90289100	-1.51917700	0.20617000				
H	6.83092600	-1.63618200	1.70950100				
H	3.90397500	0.36594800	2.80998600				
H	5.65661600	0.32505300	2.58818600				
H	4.59340600	0.49852900	1.18426300				
H	5.67354800	-1.77196100	3.94644800				
H	3.90323900	-1.84850800	4.03721300				
H	4.82115600	-3.22440200	3.40423900				
C	4.68382600	1.52309000	-2.02382900				
C	5.91391400	1.96097800	-1.20686300				
C	4.70381100	-0.00558500	-2.15526400				
C	4.77342700	2.13190600	-3.43694500				
H	5.96313800	3.04793600	-1.09542300				
H	5.90290500	1.51912400	-0.20616800				
H	6.83094100	1.63612700	-1.70949900				
H	3.90397500	-0.36597800	-2.80999100				
H	5.65661500	-0.32509800	-2.58818900				
H	4.59340200	-0.49856800	-1.18426800				
H	5.67356700	1.77191900	-3.94644600				
H	3.90325900	1.84848100	-4.03721300				
H	4.82118600	3.22436600	-3.40423400				
C	-4.46662500	-4.96414100	-0.74269000				

AR-11(PPPM)

-3966.801358 Hartree

C	10.23762300	-3.90842500	-1.66773800
C	8.95695400	-3.47070400	-1.37275600
C	8.67905000	-2.14027800	-1.01911600
C	9.72211500	-1.18673500	-0.97461900
C	11.27187700	-2.95910000	-1.59161600
C	9.40549400	0.21354600	-0.70591800
C	8.09232400	0.58967300	-0.34590100
C	7.75708500	1.95921100	-0.30575100
H	6.72116200	2.21730600	-0.14031600
C	8.68491000	2.96245600	-0.50732000
C	10.01282900	2.56932300	-0.76718500
H	8.13277400	-4.17864500	-1.39582500
H	12.29528200	-3.25009300	-1.79682800
H	10.78079600	3.32070800	-0.92465700
C	7.36054400	-1.71056700	-0.63744600
C	7.08462600	-0.44451500	-0.16477700
S	5.94791400	-2.72846300	-0.68951100
C	4.97640400	-1.46128800	0.00534500
C	3.55158200	-1.52113600	0.16203200
C	5.72064000	-0.34327800	0.32391200
C	2.79795400	-2.63898300	-0.27834800
C	2.89393200	-0.40232400	0.69811200
C	5.10808000	0.60994600	1.23163400
H	3.31566200	-3.51039900	-0.66770300
C	3.70448700	0.57589700	1.41943900
C	5.90153200	1.41873000	2.07219400

H	6.97403200	1.35177700	1.96160500	H	-3.41107400	-3.47902200	0.19715600
C	5.36873900	2.22493700	3.05795900	C	-5.70694900	-0.13942400	-0.13745800
C	3.97152500	2.18743300	3.23151700	S	-5.96466400	-2.65202800	0.49804000
H	3.50690200	2.76436700	4.02549600	C	-5.66564000	2.35730100	-0.10424300
C	8.30808300	4.44792500	-0.50610900	C	-3.68138700	3.52477900	-0.68315100
C	6.82469200	4.66527500	-0.17779400	H	-1.95382100	2.35537600	-1.02459800
C	9.15320500	5.20206600	0.53757100	C	-7.13452300	-0.42508400	-0.17015100
C	8.58683200	5.03495300	-1.90333100	C	-7.40582300	-1.69972700	0.27989800
H	6.17262700	4.23000700	-0.94155400	H	-6.71421200	2.33057400	0.15507100
H	6.55225300	4.22661300	0.78747200	C	-5.03387200	3.56981800	-0.28047500
H	6.61074700	5.73765400	-0.13253300	H	-3.16476200	4.43723700	-0.96495200
H	10.22500500	5.10409500	0.34284500	C	-8.23772100	0.33045400	-0.74873300
H	8.90871000	6.26947700	0.51850900	C	-8.73684500	-2.16898300	0.56156600
H	8.96025700	4.82887400	1.54755600	C	-5.72536400	4.91330300	-0.03037500
H	8.30860000	6.09400600	-1.93287200	C	-9.56324900	-0.07738200	-0.48227900
H	9.64524900	4.95932000	-2.16951600	C	-8.01295500	1.33472200	-1.71356800
H	8.00919600	4.50669500	-2.66788500	C	-8.97740800	-3.41067100	1.17123700
C	6.23820600	3.07823900	3.98698800	C	-9.81570500	-1.30217600	0.27178500
C	7.73133800	2.94876900	3.65753900	C	-5.66485500	5.80083000	-1.28708100
C	5.83289200	4.55795300	3.85044800	C	-7.19507900	4.73399700	0.37198900
C	6.02470200	2.62467400	5.44395700	C	-4.98892500	5.62557100	1.12162500
H	8.09584200	1.93024100	3.82415400	C	-10.60652400	0.66539000	-1.07047700
H	7.94423000	3.21610800	2.61790700	H	-6.99022500	1.53232200	-2.00010200
H	8.31034000	3.61754300	4.30198500	C	-9.04023000	2.01468400	-2.33900600
H	4.77636600	4.71233700	4.08835900	C	-10.24921500	-3.82526900	1.53266000
H	6.42342700	5.17574700	4.53544300	H	-8.12649300	-4.05283600	1.38236000
H	6.00442300	4.92158000	2.83282100	C	-11.09817300	-1.72004900	0.66182800
H	6.65710300	3.21117700	6.11903300	H	-4.63698100	5.97248700	-1.61917000
H	4.98676200	2.75504900	5.76343800	H	-6.21677200	5.35343600	-2.11799400
H	6.28343700	1.56820400	5.56286100	H	-6.11056000	6.77843700	-1.07481700
C	10.47796700	-5.37666300	-2.04172300	H	-7.29026600	4.19584400	1.32031700
C	10.03788200	-6.27898500	-0.87323900	H	-7.66596700	5.71387600	0.49808600
C	9.65554700	-5.72327000	-3.29729900	H	-7.76113800	4.18333100	-0.38573700
C	11.95553200	-5.66448000	-2.34108100	H	-5.47190200	6.58245500	1.34747400
H	10.60396100	-6.04463200	0.03345400	H	-5.00108300	5.01225100	2.02774300
H	8.97504300	-6.15826700	-0.64533200	H	-3.94441500	5.82751300	0.86587600
H	10.20883000	-7.33184500	-1.12216900	C	-10.35622000	1.69128400	-1.95251000
H	9.94732400	-5.08978000	-4.14050600	H	-11.63790300	0.39803800	-0.87017900
H	9.81889700	-6.76859800	-3.58060200	C	-8.79479600	3.03648300	-3.45499700
H	8.58333600	-5.58654100	-3.13066900	C	-11.30982600	-2.93966700	1.27370100
H	12.07610200	-6.71869200	-2.60835900	C	-10.44788000	-5.19189200	2.20064500
H	12.32337000	-5.06617800	-3.18077200	H	-11.95319100	-1.07597800	0.48949600
H	12.59159600	-5.46977500	-1.47169300	H	-11.19738100	2.21659500	-2.39484700
C	10.35385700	1.24137000	-0.88087400	C	-9.34143400	4.41362900	-3.03585800
H	11.37506200	0.99390600	-1.14708300	C	-7.30291800	3.17728700	-3.78495200
C	11.02006500	-1.64359100	-1.25735400	C	-9.52407100	2.57110900	-4.73064900
H	11.85851900	-0.95809800	-1.21018400	H	-12.32223000	-3.20575600	1.55370500
C	3.17525100	1.37599300	2.45741600	C	-9.93419900	-6.29769400	1.25918300
H	2.12505800	1.29911400	2.70779400	C	-9.65771200	-5.23363800	3.52242400
C	1.43694600	-2.63410900	-0.22019200	C	-11.92349700	-5.47518600	2.51351300
H	0.89746500	-3.50906600	-0.56168500	H	-10.40666400	4.36922500	-2.79040600
C	1.46371700	-0.32143700	0.54791100	H	-8.81132500	4.80087400	-2.16110000
C	0.73755800	0.89954300	0.70020300	H	-9.21680000	5.13319800	-3.85225900
C	0.72832300	-1.46176900	0.15926100	H	-6.88838300	2.24317400	-4.17706500
C	-0.60149600	0.97724700	0.47904700	H	-7.16482700	3.94900300	-4.54868500
H	1.26912300	1.80880700	0.94634200	H	-6.71412100	3.46361900	-2.90858000
H	-1.08400500	1.92865800	0.64573500	H	-9.33280700	3.27065900	-5.55147700
C	-1.39008300	-0.16537700	0.12990800	H	-9.17609600	1.57987000	-5.03659200
C	-2.82447300	-0.11340100	-0.07202100	H	-10.60673400	2.51750000	-4.58459600
C	-0.71828100	-1.40783200	0.09345500	H	-10.47832200	-6.28404000	0.30985900
C	-3.53656400	-1.31871600	0.05882400	H	-8.86981200	-6.17961300	1.03722800
C	-3.57930600	1.1153400	-0.31172300	H	-10.07205200	-7.28181500	1.71976600
C	-2.84382500	-2.55574000	0.13234400	H	-10.00035500	-4.45003400	4.20507700
C	-4.96668600	-1.28204100	0.08651100	H	-9.79446400	-6.20219200	4.01527100
C	-4.99424200	1.11751400	-0.21589700	H	-8.58579000	-5.09066400	3.35915500
C	-2.98303800	2.34206900	-0.69291100	H	-12.01618200	-6.46157200	2.97806400

H	-12.33896700	-4.74162200	3.21178200	C	-10.11400300	5.60074800	-2.80493100
H	-12.53719900	-5.47734000	1.60701000	C	-12.08821200	5.87906400	-1.31004900
C	-1.48650300	-2.60329200	0.06898200	H	-10.15366200	6.47871000	0.56035400
H	-0.99402300	-3.56754100	0.09381300	H	-8.75094700	6.34952500	-0.50859700

AR-11(PPMP)

-3966.803815 Hartree

C	-10.33925000	4.09567000	-0.81113000	H	-12.22241600	6.89565200	-1.69201000
C	-9.04608400	3.60168600	-0.76141800	H	-12.68763600	5.21000300	-1.93564100
C	-8.75037200	2.31349600	-0.28660200	H	-12.48860400	5.85279000	-0.29154700
C	-9.78833300	1.47639800	0.18335300	C	-10.40832300	-0.58768300	1.47085100
C	-11.36720100	3.24389100	-0.37007400	H	-11.44063300	-0.25996300	1.51426900
C	-9.45667200	0.18112900	0.77112000	C	-11.09837700	1.97832600	0.11140300
C	-8.12842200	-0.29839300	0.73323200	H	-11.93233900	1.36513700	0.43341200
C	-7.78735800	-1.43551100	1.49511600	C	-3.09409500	-2.42011600	-0.93558700
H	-6.74447600	-1.71363000	1.54129100	H	-2.03104500	-2.47673700	-1.13228800
C	-8.71945000	-2.16731100	2.20497200	C	-1.48112500	2.44896700	-1.00415900
C	-10.05852000	-1.73254900	2.14871000	H	-0.96655900	3.36821000	-1.25253300
H	-8.22512100	4.21881000	-1.11661000	C	-1.46858400	0.10364200	-0.36071800
H	-12.39916400	3.57282300	-0.40207400	C	-0.74288900	-0.96968300	0.24255200
H	-10.83006800	-2.27911000	2.68261200	C	-0.74727400	1.28444500	-0.64777900
C	-7.41588100	1.77749700	-0.31200000	C	0.61246300	-0.96472600	0.31634200
C	-7.11702700	0.47439200	0.02720600	H	-1.29198100	-1.77209200	0.71990400
S	-6.00931400	2.68246900	-0.79857500	H	1.10273400	-1.75875900	0.86267800
C	-5.00660700	1.26991800	-0.62142300	C	1.39870400	0.11541600	-0.19901300
C	-3.57787700	1.26620000	-0.74336300	C	2.84487900	0.08921600	-0.22487700
C	-5.73353300	0.14885300	-0.27390800	C	0.69907400	1.29666700	-0.53977700
C	-2.84350900	2.45122600	-1.00119800	C	3.51409900	1.32417100	-0.26755300
C	-2.89496100	0.05734600	-0.53811000	C	3.64212200	-1.12948900	-0.13483800
C	-5.08114600	-1.13545900	-0.45435500	C	2.78791700	2.51928300	-0.50818200
H	-3.37770800	3.37284200	-1.21177500	C	4.93471300	1.35068100	-0.10147000
C	-3.67091000	-1.17883600	-0.58280400	C	5.04098600	-1.05871300	0.09092900
C	-5.83604400	-2.30160700	-0.70023800	C	3.10342300	-2.43241600	-0.28324800
H	-6.91243500	-2.21127300	-0.68585200	H	3.32470100	3.45985600	-0.58417200
C	-5.25921800	-3.51499600	-1.01746200	C	5.71671600	0.21618100	-0.02548400
C	-3.85505700	-3.55018100	-1.12333900	S	5.85898200	2.81345000	0.11479900
H	-3.35508700	-4.46999700	-1.41164300	C	5.72372100	-2.22159500	0.51625400
C	-8.33809900	-3.37411000	3.06926700	C	3.82120000	-3.55921400	0.03623500
C	-9.13409200	-4.61361100	2.61952600	H	2.10362200	-2.55283000	-0.67797000
C	-6.84106000	-3.69889600	2.97604500	C	7.13447200	0.54652500	0.01333600
C	-8.67603300	-3.06134800	4.53983700	C	7.33424900	1.89496500	0.22057100
H	-10.21375500	-4.45166400	2.68575200	H	6.74364100	-2.10197400	0.85236500
H	-8.89785400	-4.88201100	1.58574300	C	5.13433200	-3.46780000	0.54587000
H	-8.88731300	-5.46973600	3.25642700	H	3.34783400	-4.52918600	-0.08206300
H	-6.22458500	-2.88616500	3.37271500	C	8.30409900	-0.26433400	-0.29867200
H	-6.62153200	-4.59670800	3.56217700	C	8.62169600	2.46402600	0.52002500
H	-6.52836000	-3.88595300	1.94381500	C	5.82896600	-4.70285800	1.12726700
H	-8.39653700	-3.90403600	5.18139600	C	9.58900900	0.24207400	-0.00336600
H	-8.13365800	-2.17472000	4.88188400	C	8.19451900	-1.45098500	-1.05354300
H	-9.74525000	-2.87554300	4.67800300	C	8.77571600	3.81045200	0.88714400
C	-6.08597800	-4.76952000	-1.31743100	C	9.74182800	1.60144200	0.50770000
C	-5.68808400	-5.89208100	-0.34075100	C	5.88758600	-5.83641800	0.08688100
C	-7.59247000	-4.51293900	-1.17817200	C	7.25761200	-4.39008200	1.59114600
C	-5.80638500	-5.22908900	-2.76132500	C	5.01558300	-5.18299300	2.34570200
H	-4.62200800	-6.12826800	-0.40682900	C	10.69976200	-0.55977700	-0.33389500
H	-5.90598100	-5.61063200	0.69382800	H	7.20842100	-1.74424900	-1.38332500
H	-6.24728300	-6.80588200	-0.56848000	C	9.29143200	-2.20106500	-1.43182800
H	-7.94878100	-3.78471100	-1.91350100	C	9.99768800	4.33937400	1.27065300
H	-8.14180600	-5.44523000	-1.34213300	H	7.89466400	4.44665800	0.88797500
H	-7.85243600	-4.14017300	-0.18262900	C	10.97176000	2.13975200	0.91890400
H	-6.40761800	-6.11293400	-3.00009400	H	4.89311800	-6.11446400	-0.27362500
H	-6.05898800	-4.43926900	-3.47518600	H	6.49204100	-5.55255400	-0.77873500
H	-4.75493400	-5.49212400	-2.90862200	H	6.33780400	-6.72924600	0.53359100
C	-10.59883200	5.51003600	-1.34549400	H	7.26554900	-3.66304600	2.40926800
C	-9.82949000	6.52896500	-0.48359300	H	7.73650300	-5.30423200	1.95553900

H	7.87132300	-3.98886100	0.77863400	C	3.70869200	1.09537500	0.66838300
H	5.49664600	-6.05330400	2.80508100	C	5.82724700	2.29826400	0.54517700
H	4.94291200	-4.39300400	3.09933500	H	6.85472500	2.29136800	0.21088200
H	3.99911400	-5.47104400	2.06106800	C	5.25978200	3.47248000	0.99193700
C	10.55734600	-1.75161700	-1.00636100	C	3.93564100	3.39026800	1.47493900
H	11.70128500	-0.21518200	-0.10254800	H	3.47714800	4.24638300	1.96046000
C	9.17625500	-3.43785400	-2.32995500	C	9.19520600	2.23356600	3.72904900
C	11.09734700	3.46374700	1.29025400	C	9.77973100	3.64562100	3.54071000
C	10.10146200	5.81775100	1.66703200	C	7.73438400	2.36061600	4.18085700
H	11.85312200	1.50938500	0.95656400	C	9.97779500	1.50751900	4.84085000
H	11.44820700	-2.31984300	-1.25667500	H	10.82483400	3.61212200	3.21892400
C	9.72746900	-4.67408500	-1.59576100	H	9.21645400	4.21133300	2.79313800
C	7.72395500	-3.71514300	-2.73998400	H	9.73894700	4.19950500	4.48481500
C	9.99910200	-3.20396800	-3.61213100	H	7.30084100	1.38410100	4.41878000
H	12.07234100	3.82046200	1.60065600	H	7.67916200	2.97774600	5.08309600
C	9.65760800	6.69492700	0.48106300	H	7.10788000	2.82819900	3.41566000
C	9.18667000	6.08716400	2.87690900	H	9.87037900	2.04332900	5.79010300
C	11.53352200	6.21624700	2.04917400	H	9.60226600	0.48891500	4.97746800
H	10.76588900	-4.53045700	-1.28288400	H	11.04575100	1.44480100	4.61299000
H	9.13677800	-4.90171600	-0.70388800	C	5.98922000	4.81850000	0.94997200
H	9.69567900	-5.54868400	-2.25441100	C	6.04068400	5.45631800	2.35039800
H	7.31606200	-2.90272900	-3.34967700	C	7.42358100	4.67539200	0.42444600
H	7.67688400	-4.63281500	-3.33463000	C	5.21414400	5.75482700	0.00165400
H	7.07061600	-3.84352700	-1.87198800	H	5.04262800	5.59381300	2.77602400
H	9.90402600	-4.06351700	-4.28434300	H	6.62189100	4.84505400	3.04588800
H	9.64700600	-2.31361000	-4.14178400	H	6.51338800	6.44257500	2.29339100
H	11.06228000	-3.06744600	-3.39426600	H	7.43976100	4.32379700	-0.61194500
H	10.29044100	6.51574700	-0.39351500	H	7.92638100	5.64709600	0.45267300
H	8.62209500	6.49362400	0.19247300	H	8.01037300	3.97478100	1.02669200
H	9.73021700	7.75520900	0.74594000	H	5.72061700	6.72311600	-0.07454600
H	9.47840800	5.46763300	3.73043500	H	5.14700800	5.32226900	-1.00121000
H	9.25452500	7.13844600	3.17671500	H	4.19587200	5.93435100	0.35960900
H	8.13877200	5.87210600	2.64938300	C	10.12284200	-4.79794700	-3.49473100
H	11.55939100	7.27735400	2.31512900	C	9.62222000	-6.05056600	-2.75094100
H	11.89560900	5.65076500	2.91372600	C	9.24811500	-4.55485900	-4.73937600
H	12.23161400	6.06595600	1.21944300	C	11.56112500	-5.06001400	-3.96194100
C	1.44263900	2.49686000	-0.70661300	H	10.22624200	-6.24040600	-1.85841900
H	0.94053400	3.42582400	-0.94351500	H	8.58055200	-5.94563200	-2.43468500

AR-11(PPPP)

-3966.792469 Hartree

C	10.02820900	-3.58319800	-2.56252900	H	11.57945900	-5.93795400	-4.61479400
C	8.80183800	-3.20948700	-2.03670400	H	11.96311500	-4.21658300	-4.53232300
C	8.65510500	-2.10324900	-1.18465200	H	12.23124100	-5.25984400	-3.11969900
C	9.78655300	-1.34107000	-0.81336500	C	10.74599700	0.30614700	0.81878500
C	11.14057800	-2.79672300	-2.21551300	H	11.74993200	0.05046800	0.49932800
C	9.63598500	-0.27757800	0.17597600	C	11.02176300	-1.71342300	-1.36749700
C	8.34904800	0.11158600	0.60835200	H	11.91320700	-1.14074100	-1.13734200
C	8.23025400	0.91977900	1.75845400	C	3.19055500	2.24808200	1.31149200
H	7.23723400	1.09133000	2.14795200	H	2.18714200	2.22704700	1.71395200
C	9.32401700	1.43593100	2.42641200	C	1.44148900	-2.41598600	-0.26361100
C	10.59738700	1.15132000	1.89427800	H	0.90775600	-3.34206500	-0.43880500
H	7.91209300	-3.77296700	-2.30473600	C	1.44321100	-0.00934600	0.14306100
H	12.12056900	-3.03247600	-2.61321800	C	0.67544800	1.19498700	0.08045000
H	11.48712300	1.55588900	2.36740000	C	0.72436500	-1.21499600	-0.01027000
C	7.36654800	-1.65847500	-0.72318100	C	-0.67545700	1.19498400	-0.08056500
C	7.17931300	-0.48634700	-0.02181700	H	1.17584900	2.15138000	0.09016600
S	5.87547200	-2.50963700	-1.01247300	H	-1.17586300	2.15137400	-0.09027200
C	4.96517500	-1.21562800	-0.27819100	C	-1.44321200	-0.00935400	-0.14318800
C	3.53961700	-1.21570700	-0.15525600	C	-2.88875300	-0.03761200	-0.25115100
C	5.76591900	-0.15874900	0.10338800	C	-0.72435800	-1.21500100	0.01011900
C	2.79274700	-2.39588800	-0.41185800	C	-3.53960700	-1.21573100	0.15513700
C	2.88875000	-0.03759800	0.25104100	C	-3.70870600	1.09536400	-0.66845800
C	5.11311400	1.07985100	0.46875100	C	-2.79272800	-2.39591300	0.41170400
H	3.31609100	-3.30514600	-0.69072800	C	-4.96516300	-1.21565700	0.27810300

C	-5.11312400	1.07983400	-0.46879500	H	-8.19616700	-4.41369400	4.47493100
C	-3.19058500	2.24808100	-1.31156300	H	-11.57931200	-5.93803500	4.61485200
H	-3.31606300	-3.30518000	0.69056200	H	-11.96295800	-4.21665900	4.53242600
C	-5.76591800	-0.15877200	-0.10343600	H	-12.23115000	-5.25989400	3.11979500
S	-5.87543900	-2.50968000	1.01238700	C	-1.44147100	-2.41600100	0.26344100
C	-5.82726000	2.29824800	-0.54518600	H	-0.90773100	-3.34208000	0.43861100
C	-3.93567700	3.39026800	-1.47497600	AR-11(PMMP) -3966.8103947 Hartree			
H	-2.18718100	2.22705200	-1.71404400				
C	-7.17930900	-0.48637200	0.02180500	C	-0.04523400	10.39329600	4.02450800
C	-7.36652300	-1.65851300	0.72315500	C	0.00215700	9.08325600	3.57703500
H	-6.85473000	2.29134600	-0.21086700	C	0.05772300	8.75573900	2.21246600
C	-5.25980600	3.47247200	-0.99194200	C	0.04523400	9.77970900	1.23752200
H	-3.47719600	4.24639100	-1.96049600	C	-0.02698400	11.40461800	3.04798900
C	-8.34906300	0.11157200	-0.60831700	C	-0.00016600	9.42426200	-0.17837200
C	-8.65506600	-2.10329200	1.18466200	C	0.11827200	8.07438300	-0.57730200
C	-5.98924500	4.81849000	-0.94994000	C	-0.14629500	7.72923000	-1.91919000
C	-9.63598700	-0.27759500	-0.17590300	H	-0.16120200	6.67926700	-2.17315400
C	-8.23030500	0.91978100	-1.75841100	C	-0.42148200	8.66960400	-2.89288300
C	-8.80177300	-3.20954300	2.03670000	C	-0.43702200	10.02172100	-2.49664700
C	-9.78652300	-1.34110200	0.81342600	H	0.01495400	8.27256900	4.30065800
C	-6.04074800	5.45632500	-2.35035700	H	-0.04620200	12.44707500	3.34325300
C	-7.42359100	4.67537500	-0.42437600	H	-0.64040800	10.79944000	-3.22666800
C	-5.21414400	5.75480700	-0.00163200	C	0.18690200	7.39754400	1.75707100
C	-10.74601800	0.30614200	-0.81866700	C	0.37079700	7.05780800	0.43295300
H	-7.23729500	1.09133500	-2.14793800	S	0.16040000	6.00795600	2.80725800
C	-9.32408800	1.43594600	-2.42632500	C	0.47704200	4.95055800	1.46039800
C	-10.02812700	-3.58325600	2.56256400	C	0.46998000	3.51763400	1.53116900
H	-7.91202100	-3.77303100	2.30469100	C	0.66245100	5.64320300	0.28095800
C	-11.02171500	-1.71345800	1.36759700	C	0.16784500	2.82990800	2.73377600
H	-5.04270400	5.59382500	-2.77601000	C	0.69712600	2.79235900	0.35037200
H	-6.62197400	4.84506900	-3.04583800	C	1.28925900	4.91760500	-0.80918900
H	-6.51345000	6.44258100	-2.29332500	H	0.02084400	3.39592500	3.64866000
H	-7.43974100	4.32376600	0.61201100	C	1.30851400	3.50179100	-0.77095700
H	-7.92639200	5.64707900	-0.45257700	C	2.04863200	5.59602600	-1.78552500
H	-8.01039900	3.97477000	-1.02661400	H	2.08398800	6.67427200	-1.72945100
H	-5.72061500	6.72309400	0.07459400	C	2.78843900	4.94035500	-2.74906500
H	-5.14697900	5.32223700	1.00122400	C	2.79446700	3.53257400	-2.70554800
H	-4.19588200	5.93433700	-0.35961400	H	3.39970500	2.96981900	-3.40992300
C	-10.59744100	1.15133000	-1.89415300	C	-0.75072900	8.28784900	-4.34015200
H	-11.74994300	0.05046200	-0.49918000	C	0.22445400	8.99148400	-5.30256000
C	-9.19531900	2.23359800	-3.72895600	C	-0.65351900	6.77390000	-4.57253300
C	-11.14050400	-2.79677100	2.21560100	C	-2.18983000	8.73649000	-4.65990700
C	-10.12273100	-4.79802100	3.49474800	H	0.18406300	10.07976000	-5.20117800
H	-11.91316500	-1.14076800	1.13748400	H	1.25602500	8.67569400	-5.12160900
H	-11.48719200	1.55590900	-2.36723900	H	-0.02813000	8.74527400	-6.33941700
C	-9.77983500	3.64565100	-3.54057900	H	-1.39328600	6.22488900	-3.98152400
C	-7.73451200	2.36065100	-4.18081100	H	-0.84114000	6.55029700	-5.62733500
C	-9.97794600	1.50756600	-4.84074100	H	0.33746600	6.38522800	-4.31706500
H	-12.12048200	-3.03252500	2.61333800	H	-2.45524600	8.45897100	-5.68576500
C	-9.62215000	-6.05063100	2.75091700	H	-2.90382000	8.26180500	-3.98008300
C	-9.24795300	-4.55496100	4.73936200	H	-2.30545800	9.82028400	-4.56573900
C	-11.56099800	-5.06008300	3.96201300	C	3.63481800	5.68297500	-3.78798900
H	-10.82492800	3.61214900	-3.21875900	C	3.16892300	5.29034500	-5.20263900
H	-9.21653200	4.21135200	-2.79301900	C	3.51971100	7.20615000	-3.64142600
H	-9.73908200	4.19954700	-4.48467900	C	5.11488400	5.29204700	-3.61308700
H	-7.30097900	1.38413800	-4.41876200	H	3.24262300	4.21163000	-5.36883200
H	-7.67931800	2.97779300	-5.08304400	H	2.12902400	5.58568500	-5.37164600
H	-7.10798100	2.82822300	-3.41562900	H	3.78938800	5.78763100	-5.95586900
H	-9.87056000	2.04338900	-5.78999000	H	3.92223000	7.55231900	-2.68426700
H	-9.60242300	0.48896300	-4.97738400	H	4.08848400	7.69710100	-4.43720900
H	-11.04589500	1.44484800	-4.61284600	H	2.48155800	7.54522500	-3.71173600
H	-10.22621100	-6.24045000	1.85841600	H	5.73655900	5.83270900	-4.33479500
H	-8.58049400	-5.94569900	2.43461800	H	5.46458900	5.53911200	-2.60616900
H	-9.68635300	-6.92895400	3.40211000	H	5.27527100	4.22181600	-3.77193400
H	-9.58031900	-3.66355100	5.28008900				
H	-9.30952200	-5.41162100	5.41910700				

C	-0.09907600	10.68732800	5.52911100	H	-3.92223000	-7.55231900	-2.68426700
C	-1.35594000	10.03111800	6.13131100	H	-4.08848400	-7.69710100	-4.43720900
C	1.15786900	10.10955800	6.20694600	H	-2.48155800	-7.54522500	-3.71173600
C	-0.15523200	12.19250200	5.82388400	H	-5.73655900	-5.83270900	-4.33479500
H	-2.26275200	10.42279000	5.66042000	H	-5.46458900	-5.53911200	-2.60616900
H	-1.35080900	8.94568800	5.99739500	H	-5.27527100	-4.22181600	-3.77193400
H	-1.41179000	10.23479200	7.20604700	C	0.43702200	-10.02172100	-2.49664700
H	2.06518200	10.55571300	5.78838400	H	0.33916000	-11.42930400	-0.91840300
H	1.13789800	10.31699200	7.28223700	C	0.75072900	-8.28784900	-4.34015200
H	1.22689000	9.02577300	6.07742600	C	0.02698400	-11.40461800	3.04798900
H	-0.19978400	12.35204900	6.90551000	C	0.09907600	-10.68732800	5.52911100
H	0.73219500	12.71313400	5.45007500	H	-0.03203900	-11.92720900	0.99406900
H	-1.04226900	12.65935700	5.38394500	H	0.64040800	-10.79944000	-3.22666800
C	-0.25185200	10.38146800	-1.18175100	C	-0.22445400	-8.99148400	-5.30256000
H	-0.33916000	11.42930400	-0.91840300	C	0.65351900	-6.77390000	-4.57253300
C	0.01558800	11.10550100	1.70099900	C	2.18983000	-8.73649000	-4.65990700
H	0.03203900	11.92720900	0.99406900	H	0.04620200	-12.44707500	3.34325300
C	2.10031500	2.84305500	-1.73886400	C	1.35594000	-10.03111800	6.13131100
H	2.22994600	1.76993100	-1.68149300	C	-1.15786900	-10.10955800	6.20694600
C	0.06160600	1.47183300	2.75719000	C	0.15523200	-12.19250200	5.82388400
H	-0.16113400	0.98343100	3.69784900	H	-0.18406300	-10.07976000	-5.20117800
C	0.36565800	1.39103000	0.34072200	H	-1.25602500	-8.67569400	-5.12160900
C	0.18432700	0.65372500	-0.87174000	H	0.02813000	-8.74527400	-6.33941700
C	0.12100000	0.71455400	1.55611000	H	1.39328600	-6.22488900	-3.98152400
C	-0.18432700	-0.65372500	-0.87174000	H	0.84114000	-6.55029700	-5.62733500
H	0.28771600	1.16074900	-1.82178400	H	-0.33746600	-6.38522800	-4.31706500
H	-0.28771600	-1.16074900	-1.82178400	H	2.45524600	-8.45897100	-5.68576500
C	-0.36565800	-1.39103000	0.34072200	H	2.90382000	-8.26180500	-3.98008300
C	-0.69712600	-2.79235900	0.35037200	H	2.30545800	-9.82028400	-4.56573900
C	-0.12100000	-0.71455400	1.55611000	H	2.26275200	-10.02172100	5.66042000
C	-0.46998000	-3.51763400	1.53116900	H	1.35080900	-8.94568800	5.99739500
C	-1.30851400	-3.50179100	-0.77095700	H	1.41179000	-10.23479200	7.20604700
C	-0.16784500	-2.82990800	2.73377600	H	-2.06518200	-10.55571300	5.78838400
C	-0.47704200	-4.95055800	1.46039800	H	-1.13789800	-10.31699200	7.28223700
C	-1.28925900	-4.91760500	-0.80918900	H	-1.22689000	-9.02577300	6.07742600
C	-2.10031500	-2.84305500	-1.73886400	H	0.19978400	-12.35204900	6.90551000
H	-0.02084400	-3.39592500	3.64866000	H	-0.73219500	-12.71313400	5.45007500
C	-0.66245100	-5.64320300	0.28095800	H	1.04226900	-12.65935700	5.38394500
S	-0.16040000	-6.00795600	2.80725800	C	-0.06160600	-1.47183300	2.75719000
C	-2.04863200	-5.59602600	-1.78552500	H	0.16113400	-0.98343100	3.69784900
C	-2.79446700	-3.53257400	-2.70554800				
H	-2.22994600	-1.76993100	-1.68149300				
C	-0.37079700	-7.05780800	0.43295300				
C	-0.18690200	-7.39754400	1.75707100				
H	-2.08398800	-6.67427200	-1.72945100				
C	-2.78843900	-4.94035500	-2.74906500				
H	-3.39970500	-2.96981900	-3.40992300				
C	-0.11827200	-8.07438300	-0.57730200				
C	-0.05772300	-8.75573900	2.21246600				
C	-3.63481800	-5.68297500	-3.78798900				
C	0.00016600	-9.42426200	-0.17837200				
C	0.14629500	-7.72923000	-1.91919000				
C	-0.00215700	-9.08325600	3.57703500				
C	-0.04523400	-9.77970900	1.23752200				
C	-3.16892300	-5.29034500	-5.20263900				
C	-3.51971100	-7.20615000	-3.64142600				
C	-5.11488400	-5.29204700	-3.61308700				
C	0.25185200	-10.38146800	-1.18175100				
H	0.16120200	-6.67926700	-2.17315400				
C	0.42148200	-8.66960400	-2.89288300				
C	0.04523400	-10.39329600	4.02450800				
H	-0.01495400	-8.27256900	4.30065800				
C	-0.01558800	-11.10550100	1.70099900				
H	-3.24262300	-4.21163000	-5.36883200				
H	-2.12902400	-5.58568500	-5.37164600				
H	-3.78938800	-5.78763100	-5.95586900				

AR-11(PPMM)
-3966.797829 Hartree

C	-4.37188900	0.25806800	10.15873200
C	-3.81837700	0.06336500	8.90870100
C	-2.42795800	-0.06680500	8.71775200
C	-1.55202500	-0.02726200	9.82314900
C	-3.48342500	0.33221300	11.25248300
C	-0.13250700	-0.29511600	9.61948800
C	0.38767200	-0.40539000	8.31068700
C	1.67965900	-0.94414300	8.13209800
H	2.00104400	-1.14538900	7.12048200
C	2.50465300	-1.27539000	9.18910700
C	2.01942600	-1.02530500	10.48878100
H	-4.45816700	0.02780500	8.03375200
H	-3.87248700	0.50369300	12.25151500
H	2.64057900	-1.24415700	11.35215000
C	-1.84772400	-0.17047100	7.40634800
C	-0.48752400	-0.14275500	7.17765300
S	-2.76951400	-0.31291300	5.93558700
C	-1.31109700	-0.22272500	4.98356900
C	-1.28802100	-0.27882200	3.55443800
C	-0.18664500	-0.02261700	5.75790000
C	-2.44356000	-0.65751600	2.82297700
C	-0.08980400	0.00838200	2.87894500

C	1.03770500	0.34920500	5.08128400	C	-2.44356000	-0.65751600	-2.82297700
H	-3.34651100	-0.92792400	3.36164100	C	-1.31109700	-0.22272500	-4.98356900
C	1.11485200	0.23977100	3.66883900	C	1.03770500	0.34920500	-5.08128400
C	2.12916700	0.90996300	5.78373700	C	2.41251400	0.34934800	-3.10861400
H	1.97775200	1.14692700	6.82706800	H	-3.34651100	-0.92792400	-3.36164100
C	3.34068800	1.18807100	5.18707100	C	-0.18664500	-0.02261700	-5.75790000
C	3.48646400	0.79778100	3.83839100	S	-2.76951400	-0.31291300	-5.93558700
H	4.45234100	0.87684900	3.34869600	C	2.12916700	0.90996300	-5.78373700
C	3.86883100	-1.94636100	8.99334500	C	3.48646400	0.79778100	-3.83839100
C	4.17551800	-2.19975500	7.51145800	H	2.57488200	0.05488300	-2.08066700
C	4.98029200	-1.05911300	9.58376800	C	-0.48752400	-0.14275500	-7.17765300
C	3.86811700	-3.30532100	9.72062500	C	-1.84772400	-0.17047100	-7.40634800
H	3.46355600	-2.90307900	7.06810500	H	1.97775200	1.14692700	-6.82706800
H	4.14644200	-1.27773000	6.92343700	C	3.34068800	1.18807100	-5.18707100
H	5.17620400	-2.63135300	7.40998200	H	4.45234100	0.87684900	-3.34869600
H	4.81167700	-0.84965200	10.64423100	C	0.38767200	-0.40539000	-8.31068700
H	5.95031700	-1.55967300	9.49283100	C	-2.42795800	-0.06680500	-8.71775200
H	5.04406900	-0.10182300	9.05869900	C	4.47822000	1.91322000	-5.91241500
H	4.82383600	-3.81738300	9.56533100	C	-0.13250700	-0.29511600	-9.61948800
H	3.72329600	-3.19036200	10.79868400	C	1.67965900	-0.94414300	-8.13209800
H	3.06866800	-3.94828100	9.34021600	C	-3.81837700	0.06336500	-8.90870100
C	4.47822000	1.91322000	5.91241500	C	-1.55202500	-0.02726200	-9.82314900
C	4.12228800	2.21818700	7.37334200	C	5.76631400	1.07007700	-5.88644600
C	5.76631400	1.07007700	5.88644600	C	4.12228800	2.21818700	-7.37334200
C	4.73841400	3.24795500	5.18616200	C	4.73841400	3.24795500	-5.18616200
H	3.27098700	2.90225400	7.44622400	C	0.73762000	-0.57069000	-10.69409100
H	3.87259200	1.30979700	7.93033500	H	2.00104400	-1.14538900	-7.12048200
H	4.97359500	2.69438000	7.86963300	C	2.50465300	-1.27539000	-9.18910700
H	6.07876900	0.82949100	4.86628600	C	-4.37188900	0.25806800	-10.15873200
H	6.58395900	1.62390900	6.35988400	H	-4.45816700	0.02780500	-8.03375200
H	5.63850400	0.13000700	6.42973800	C	-2.12412700	0.19252000	-11.09110500
H	5.53229700	3.80777100	5.69236100	H	6.07876900	0.82949100	-4.86628600
H	5.04849700	3.08669900	4.14932600	H	5.63850400	0.13000700	-6.42973800
H	3.83553900	3.86603600	5.17516300	H	6.58395900	1.62390900	-6.35988400
C	-5.87860600	0.40825500	10.39171500	H	3.27098700	2.90225400	-7.44622400
C	-6.35607100	-0.70204600	11.34706000	H	4.97359500	2.69438000	-7.86963300
C	-6.16112800	1.78577600	11.02089500	H	3.87259200	1.30979700	-7.93033500
C	-6.68197100	0.30015100	9.08891700	H	5.53229700	3.80777100	-5.69236100
H	-6.16217500	-1.69101100	10.92072400	H	3.83553900	3.86603600	-5.17516300
H	-5.85218200	-0.64934200	12.31642100	H	5.04849700	3.08669900	-4.14932600
H	-7.43274100	-0.61041800	11.52574400	C	2.01942600	-1.02530500	-10.48878100
H	-5.82424700	2.59056500	10.36043400	H	0.38281100	-0.47360300	-11.71385300
H	-7.23558200	1.91007000	11.19301500	C	3.86883100	-1.94636100	-8.99334500
H	-5.65412300	1.90575500	11.98260400	C	-3.48342500	0.33221300	-11.25248300
H	-7.74901000	0.40666700	9.30665000	C	-5.87860600	0.40825500	-10.39171500
H	-6.40976800	1.08666000	8.37788900	H	-1.48909000	0.26231700	-11.96705900
H	-6.53830500	-0.67056900	8.60379100	H	2.64057900	-1.24415700	-11.35215000
C	0.73762000	-0.57069000	10.69409100	C	4.98029200	-1.05911300	-9.58376800
H	0.38281100	-0.47360300	11.71385300	C	4.17551800	-2.19975500	-7.51145800
C	-2.12412700	0.19252000	11.09110500	C	3.86811700	-3.30532100	-9.72062500
H	-1.48909000	0.26231700	11.96705900	H	-3.87248700	0.50369300	-12.25151500
C	2.41251400	0.34934800	3.10861400	C	-6.35607100	-0.70204600	-11.34706000
H	2.57488200	0.05488300	2.08066700	C	-6.68197100	0.30015100	-9.08891700
C	-2.41927100	-0.75050100	1.46639400	C	-6.16112800	1.78577600	-11.02089500
H	-3.30606600	-1.10790800	0.95971800	H	4.81167700	-0.84965200	-10.64423100
C	-0.14941200	0.12821000	1.43895200	H	5.04406900	-0.10182300	-9.05869900
C	0.81652900	0.85980500	0.67881600	H	5.95031700	-1.55967300	-9.49283100
C	-1.27740400	-0.33952200	0.72531300	H	3.46355600	-2.90307900	-7.06810500
C	0.81652900	0.85980500	-0.67881600	H	5.17620400	-2.63135300	-7.40998200
H	1.51210900	1.50755700	1.19499900	H	4.14644200	-1.27773000	-6.92343700
H	1.51210900	1.50755700	-1.19499900	H	4.82383600	-3.81738300	-9.56533100
C	-0.14941200	0.12821000	-1.43895200	H	3.06866800	-3.94828100	-9.34021600
C	-0.08980400	0.00838200	-2.87894500	H	3.72329600	-3.19036200	-10.79868400
C	-1.27740400	-0.33952200	-0.72531300	H	-5.85218200	-0.64934200	-12.31642100
C	-1.28802100	-0.27882200	-3.55443800	H	-6.16217500	-1.69101100	-10.92072400
C	1.11485200	0.23977100	-3.66883900	H	-7.43274100	-0.61041800	-11.52574400

H	-6.40976800	1.08666000	-8.37788900	H	-4.82761600	-3.96115500	4.97304000
H	-7.74901000	0.40666700	-9.30665000	H	-3.70024600	-4.21938500	6.31431100
H	-6.53830500	-0.67056900	-8.60379100	C	5.67606600	0.03123600	10.56508200
H	-7.23558200	1.91007000	-11.19301500	C	6.03550300	-1.41882500	10.18839100
H	-5.82424700	2.59056500	-10.36043400	C	6.52494500	1.00533900	9.72598100
H	-5.65412300	1.90575500	-11.98260400	C	6.02119900	0.24404200	12.04535800
C	-2.41927100	-0.75050100	-1.46639400	H	5.43814100	-2.13032600	10.76702200
H	-3.30606600	-1.10790800	-0.95971800	H	5.86328800	-1.61748000	9.12662100

AR-11(PMPM)

-3966.8117663 Hartree

C	4.18971600	0.27780600	10.27597200	H	7.08931100	0.06383000	12.19944500
C	3.70217700	0.13506400	8.98654200	H	5.80760300	1.26779200	12.36877200
C	2.35036500	0.34544700	8.66648600	H	5.47225800	-0.44609000	12.69393900
C	1.43622900	0.73835300	9.67178300	C	-0.82843800	1.68203000	10.20743200
C	3.26605100	0.63826900	11.27381300	H	-0.52006600	1.86694800	11.22993300
C	0.05771100	1.05643700	9.30642300	C	1.93528000	0.86199600	10.97984600
C	-0.40128300	0.82666200	7.98985300	H	1.27073000	1.13401000	11.79189400
C	-1.65582100	1.34130100	7.60003900	C	-2.16124300	-1.60110400	3.12636700
H	-1.93439200	1.25137100	6.56008700	H	-2.17969900	-1.89017100	2.08339400
C	-2.50776900	1.98151100	8.47972000	C	2.64638400	-0.90036800	1.47205000
C	-2.07529200	2.11316300	9.81497500	H	3.59889200	-1.00488900	0.96911700
H	4.37892800	-0.16662000	8.19155300	C	0.22065900	-0.69072600	1.43263100
H	3.58930300	0.74768800	12.30217900	C	-0.94596000	-0.34693200	0.67856800
H	-2.71170400	2.60059500	10.54722300	C	1.43866200	-0.81867100	0.72552900
C	1.83344300	0.11789600	7.34297300	C	-0.94596000	-0.34693200	-0.67856800
C	0.49175200	0.19253500	7.03052000	H	-1.83159100	-0.00867000	1.20168600
S	2.81888700	-0.30876500	5.96980500	H	-1.83159100	-0.00867000	-1.20168600
C	1.40108000	-0.46799500	4.96962100	C	0.22065900	-0.69072600	-1.43263100
C	1.42598600	-0.69948600	3.55399000	C	0.20192100	-0.76880100	-2.86940600
C	0.23240100	-0.27171800	5.67805600	C	1.43866200	-0.81867100	-0.72552900
C	2.64231600	-0.79131400	2.83062300	C	1.42598600	-0.69948600	-3.55399000
C	0.20192100	-0.76880100	2.86940600	C	-1.00868100	-0.97946400	-3.65974200
C	-0.99560000	-0.73365800	5.05529400	C	2.64231600	-0.79131400	-2.83062300
H	3.58577100	-0.78410700	3.36800100	C	1.40108000	-0.46799500	-4.96962100
C	-1.00868100	-0.97946400	3.65974200	C	-0.99560000	-0.73365800	-5.05529400
C	-2.10039800	-1.12710400	5.83984500	C	-2.16124300	-1.60110400	-3.12636700
H	-2.02036300	-1.00866900	6.91063600	H	3.58577100	-0.78410700	-3.36800100
C	-3.23272700	-1.70750900	5.30317300	C	0.23240100	-0.27171800	-5.67805600
C	-3.24093400	-1.93235100	3.91213200	S	2.81888700	-0.30876500	-5.96980500
H	-4.08904100	-2.42410800	3.44566200	C	-2.10039800	-1.12710400	-5.83984500
C	-3.84959600	2.57949000	8.04309400	C	-3.24093400	-1.93235100	-3.91213200
C	-4.14798000	2.30519800	6.56290000	H	-2.17969900	-1.89017100	-2.08339400
C	-4.98912300	1.98159900	8.88956000	C	0.49175200	0.19253500	-7.03052000
C	-3.80847700	4.10533700	8.25576400	C	1.83344300	0.11789600	-7.34297300
H	-3.41769300	2.78794800	5.90574000	H	-2.02036300	-1.00866900	-6.91063600
H	-4.14767400	1.23332800	6.33996900	C	-3.23272700	-1.70750900	-5.30317300
H	-5.13577300	2.70090100	6.30804400	H	-4.08904100	-2.42410800	-3.44566200
H	-4.84537200	2.16864900	9.95749700	C	-0.40128300	0.82666200	-7.98985300
H	-5.94486200	2.43023100	8.59916000	C	2.35036500	0.34544700	-8.66648600
H	-5.06517700	0.89999400	8.74344400	C	-4.41597000	-2.16187300	-6.16378900
H	-4.75363100	4.55666300	7.93576600	C	0.05771100	1.05643700	-9.30642300
H	-3.65354400	4.36232000	9.30783600	C	-1.65582100	1.34130100	-7.60003900
H	-2.99876600	4.55644200	7.67377700	C	3.70217700	0.13506400	-8.98654200
C	-4.41597000	-2.16187300	6.16378900	C	1.43622900	0.73835300	-9.67178300
C	-4.19730000	-1.85445900	7.65115100	C	-5.69509600	-1.44175900	-5.69671100
C	-5.69509600	-1.44175900	5.69671100	C	-4.19730000	-1.85445900	-7.65115100
C	-4.60355100	-3.68332400	6.00699100	C	-4.60355100	-3.68332400	-6.00699100
H	-3.34797700	-2.41160800	8.05926600	C	-0.82843800	1.68203000	-10.20743200
H	-4.01721700	-0.78880700	7.82407000	H	-1.93439200	1.25137100	-6.56008700
H	-5.08692000	-2.14104200	8.22008900	C	-2.50776900	1.98151100	-8.47972000
H	-5.91070800	-1.64073600	4.64289000	C	4.18971600	0.27780600	-10.27597200
H	-6.55358600	-1.78391600	6.28410700	H	4.37892800	-0.16662000	-8.19155300
H	-5.60733800	-0.35856200	5.82484400	C	1.93528000	0.86199600	-10.97984600
H	-5.43481200	-4.02579600	6.63222700	H	-5.91070800	-1.64073600	-4.64289000

H	-5.60733800	-0.35856200	-5.82484400	C	2.81567400	2.54306700	0.20833900
H	-6.55358600	-1.78391600	-6.28410700	C	2.90991600	0.11223700	0.34962900
H	-3.34797700	-2.41160800	-8.05926600	C	5.09915900	-1.02421800	0.69588900
H	-5.08692000	-2.14104200	-8.22008900	H	3.33039800	3.49914800	0.20212900
H	-4.01721700	-0.78880700	-7.82407000	C	3.68352200	-1.06320100	0.73705600
H	-5.43481200	-4.02579600	-6.63222700	C	5.83823600	-2.08538900	1.25990100
H	-3.70024600	-4.21938500	-6.31431100	H	6.91293500	-1.98165200	1.29583200
H	-4.82761600	-3.96115500	-4.97304000	C	5.24390100	-3.20023600	1.81613100
C	-2.07529200	2.11316300	-9.81497500	C	3.83576700	-3.23576800	1.83472100
H	-0.52006600	1.86694800	-11.22993300	H	3.31964300	-4.07042200	2.29961000
C	-3.84959600	2.57949000	-8.04309400	C	8.60025900	-3.96329100	-1.97286600
C	3.26605100	0.63826900	-11.27381300	C	9.36249700	-5.04830600	-1.18933900
C	5.67606600	0.03123600	-10.56508200	C	7.10054100	-4.28318000	-1.91071500
H	1.27073000	1.13401000	-11.79189400	C	9.04290800	-3.99896200	-3.44846500
H	-2.71170400	2.60059500	-10.54722300	H	10.44388200	-4.88639300	-1.21472400
C	-4.98912300	1.98159900	-8.88956000	H	9.05120400	-5.07172900	-0.14094400
C	-4.14798000	2.30519800	-6.56290000	H	9.16427200	-6.03409900	-1.62342500
C	-3.80847700	4.10533700	-8.25576400	H	6.51400600	-3.59687400	-2.52953300
H	3.58930300	0.74768800	-12.30217900	H	6.92433900	-5.29709100	-2.28320300
C	6.52494500	1.00533900	-9.72598100	H	6.71418600	-4.22839500	-0.88796500
C	6.03550300	-1.41882500	-10.18839100	H	8.80970900	-4.97320500	-3.89155000
C	6.02119900	0.24404200	-12.04535800	H	8.52689700	-3.22644500	-4.02657000
H	-4.84537200	2.16864900	-9.95749700	H	10.11936500	-3.83341500	-3.55169600
H	-5.06517700	0.89999400	-8.74344400	C	6.05148500	-4.33299200	2.45796300
H	-5.94486200	2.43023100	-8.59916000	C	5.72829400	-5.66019500	1.74630900
H	-3.41769300	2.78794800	-5.90574000	C	7.56313800	-4.08545900	2.36640400
H	-5.13577300	2.70090100	-6.30804400	C	5.67092700	-4.44843900	3.94659200
H	-4.14767400	1.23332800	-6.33996900	H	4.66069900	-5.89457100	1.79080400
H	-4.75363100	4.55666300	-7.93576600	H	6.02050100	-5.62421600	0.69253200
H	-2.99876600	4.55644200	-7.67377700	H	6.27135900	-6.48456200	2.22076600
H	-3.65354400	4.36232000	-9.30783600	H	7.86303600	-3.19852300	2.93335200
H	6.28408000	2.04383100	-9.97380000	H	8.10274600	-4.94234500	2.78159600
H	6.36056100	0.86686300	-8.65350100	H	7.89241400	-3.95008600	1.33155800
H	7.58969300	0.84383800	-9.92451700	H	6.25659200	-5.23995600	4.42632600
H	5.43814100	-2.13032600	-10.76702200	H	5.86922700	-3.50897800	4.47127700
H	7.09337100	-1.61048700	-10.39677700	H	4.61257100	-4.69088200	4.07886000
H	5.86328800	-1.61748000	-9.12662100	C	10.52220600	5.74907100	0.37378400
H	7.08931100	0.06383000	-12.19944500	C	9.81784300	6.52198700	-0.75737200
H	5.47225800	-0.44609000	-12.69393900	C	9.93007800	6.17147800	1.73177200
H	5.80760300	1.26779200	-12.36877200	C	12.00965700	6.12716500	0.35958800
C	2.64638400	-0.90036800	-1.47205000	H	10.21834400	6.23302400	-1.73386900
H	3.59889200	-1.00488900	-0.96911700	H	8.74055100	6.33383100	-0.76796100

AR-11(TS-1)

-3966.7989549 Hartree

C	10.30469400	4.24407100	0.17083000	H	10.41062400	5.62836900	2.55126600
C	9.01942300	3.72787200	0.14876400	H	10.08258800	7.24379700	1.89466000
C	8.76119100	2.35894100	-0.02892100	H	8.85540100	5.97545400	1.78450800
C	9.83193800	1.45473100	-0.21565900	H	12.11400100	7.20736100	0.49968100
C	11.36337900	3.33206600	0.01529100	H	12.56159300	5.63502700	1.16673900
C	9.54602900	0.05177900	-0.50398200	H	12.48466300	5.86956800	-0.59245900
C	8.21966700	-0.43059800	-0.44520100	C	10.54656100	-0.84129800	-0.93711700
C	7.93580600	-1.72071700	-0.93974600	H	11.57848400	-0.51305200	-0.98630300
H	6.89927400	-2.02132600	-0.98971400	C	11.13236300	1.98405700	-0.17264800
C	8.91737100	-2.58071100	-1.39263100	H	11.98845500	1.32809100	-0.28227900
C	10.24811700	-2.11952800	-1.34916100	C	3.08660300	-2.19618800	1.33539900
H	8.17378100	4.39545700	0.29089400	H	2.01308700	-2.22376800	1.47240000
H	12.38985100	3.67817800	0.04106000	C	1.45601700	2.51458300	0.12991400
H	11.05673300	-2.76121400	-1.68602100	H	0.93214400	3.45956300	0.07962200
C	7.42946000	1.81860400	0.02987000	C	1.49951300	0.09050800	0.06768500
C	7.15893800	0.46681300	-0.01197400	C	0.81749100	-1.09560600	-0.32596400
S	5.98939700	2.78516900	0.19192100	C	0.74906800	1.28253800	0.03050400
C	5.00575800	1.35131500	0.28371900	C	-0.51852000	-1.12262700	-0.56502700
C	3.57222100	1.34766700	0.30474100	H	1.39165000	-1.99314400	-0.52022100
C	5.75858200	0.19412600	0.26187400	H	-0.89313100	-2.05078300	-0.94344300
				C	-1.37807500	0.01231600	-0.39667900
				C	-2.83806900	-0.02026700	-0.48826100
				C	-0.69342000	1.23479700	-0.14385600

C	-3.50246600	1.21979400	-0.34264100	H	-8.46358500	6.41893800	0.79717400
C	-3.70084200	-1.19738100	-0.75560400	H	-9.63694700	7.73465400	0.66255700
C	-2.78543400	2.42653500	-0.15658000	H	-10.14585800	5.80367800	-2.53369800
C	-4.93185400	1.28599200	-0.29028400	H	-9.75561200	7.40028600	-1.86514900
C	-5.12010100	-1.06139100	-0.72829300	H	-8.58138200	6.08253800	-1.75801900
C	-3.26025100	-2.49511900	-1.12501000	H	-11.79271900	7.43779400	-0.47849900
H	-3.33442200	3.35695000	-0.05461200	H	-12.30112200	5.88980800	-1.15859300
C	-5.73392900	0.17312300	-0.29688600	H	-12.22283600	6.10889800	0.60258700
S	-5.85323700	2.76422200	-0.17145800	C	-1.43596200	2.43746900	-0.05037600
C	-5.95292100	-2.07078400	-1.26001900	H	-0.94211300	3.38035400	0.13886500
C	-4.10007600	-3.49044500	-1.56726400				
H	-2.22659600	-2.77043300	-1.07810700				
C	-7.12264000	0.49682400	-0.01052700				
C	-7.33439000	1.85865000	-0.03303200				
H	-7.00573100	-1.84306200	-1.34157400	C	-10.26068200	3.96309300	-0.44856900
C	-5.48261700	-3.28356700	-1.70825200	C	-8.97233800	3.46081700	-0.53022500
H	-3.65838300	-4.44238800	-1.84708900	C	-8.62492000	2.19531800	-0.03011600
C	-8.21628400	-0.35545400	0.43252500	C	-9.60088400	1.39191300	0.60323400
C	-8.64275600	2.45350100	0.03023100	C	-11.23025700	3.14340800	0.15533400
C	-6.37548100	-4.33987200	-2.36286400	C	-9.20433300	0.12472300	1.21166600
C	-9.52213400	0.17876300	0.49238600	C	-7.89161400	-0.36759000	1.03870500
C	-7.97947500	-1.64798000	0.94514900	C	-7.46403200	-1.46836200	1.81016400
C	-8.84394200	3.83310600	-0.13785000	H	-6.42387200	-1.75250400	1.74402600
C	-9.75061300	1.59245300	0.20588600	C	-8.30570500	-2.15630300	2.66251900
C	-6.27113700	-5.67136400	-1.59648200	C	-9.64064100	-1.71314900	2.74588200
C	-7.84704700	-3.90602500	-2.39134600	H	-8.19880800	4.05243100	-1.01256700
C	-5.90076100	-4.55415200	-3.81321400	H	-12.25760900	3.47948200	0.23107200
C	-10.55614200	-0.67320000	0.93042900	H	-10.34362800	-2.22612500	3.39533900
H	-6.95463600	-1.98577500	0.99622600	C	-7.30471600	1.64694400	-0.18893300
C	-8.99078200	-2.46260200	1.41526800	C	-6.97077900	0.36001900	0.17794200
C	-10.10728000	4.40105500	-0.16236100	S	-5.96476200	2.51334000	-0.88769000
H	-7.97131800	4.46679200	-0.27192100	C	-4.94519300	1.10267400	-0.75996500
C	-11.02820600	2.17419900	0.16033800	C	-3.54793900	1.08008500	-1.05143500
H	-5.24127900	-6.03721000	-1.55132400	C	-5.63477400	0.00746700	-0.27026000
H	-6.63677400	-5.56843200	-0.57087800	C	-2.84691400	2.24512900	-1.45234400
H	-6.87397100	-6.43834700	-2.09429900	C	-2.84821800	-0.12258600	-0.86566600
H	-7.99251400	-3.01282300	-3.00706100	C	-5.01264400	-1.29005900	-0.46243200
H	-8.45974900	-4.70598500	-2.81849500	H	-3.39927500	3.16169000	-1.63644900
H	-8.22748400	-3.68895100	-1.38816700	C	-3.62824200	-1.35258500	-0.75630400
H	-6.53468400	-5.29314700	-4.31504800	C	-5.79559600	-2.45964100	-0.55790300
H	-5.94918000	-3.61905900	-4.37932800	H	-		

-3966.7797937 Hartree

H	-7.73978100	-4.24740400	0.28995700	C	9.66264000	3.00077400	2.29514800
H	-6.65423200	-6.37572100	-2.57599200	H	6.71999000	-4.42028800	-3.76590500
H	-6.36073000	-4.73146200	-3.17482500	H	7.79145200	-3.74867200	-2.54106300
H	-5.00074200	-5.76644900	-2.71714200	H	7.84141800	-5.47839800	-2.88802900
C	-10.57889600	5.35177700	-1.01742100	H	5.90334600	-5.63431800	0.29742400
C	-9.71090900	6.40513800	-0.30325300	H	7.42556400	-6.09395200	-0.49387300
C	-10.26991800	5.36800800	-2.52654100	H	7.17697400	-4.44007500	0.09638200
C	-12.05291500	5.73342500	-0.82447300	H	5.92390400	-6.95215600	-2.39214700
H	-9.90942000	6.40789200	0.77285700	H	4.48532600	-6.38913000	-1.54064700
H	-8.64328600	6.21607400	-0.44659500	H	4.78710200	-5.87772500	-3.21513600
H	-9.92868600	7.40447400	-0.69510200	C	10.18905700	-1.24343400	2.21563900
H	-10.86975500	4.62025300	-3.05428600	H	10.34329100	0.64994700	3.13660200
H	-10.49827500	6.35216000	-2.94961300	C	10.24052200	-3.38142300	0.86144600
H	-9.21616600	5.15488400	-2.72735000	C	9.64798800	-4.37264700	2.14653500
H	-12.22971100	6.73106800	-1.23772100	C	8.81381400	6.51716700	0.96974000
H	-12.72328200	5.03890300	-1.34078700	H	10.33153300	2.57973700	3.03574300
H	-12.32983300	5.75996900	0.23428600	H	10.92693600	-1.67329400	2.88327700
C	-10.06668600	-0.60016700	2.05854800	C	9.62673300	-4.40071700	1.83909400
H	-11.08533500	-0.26178900	2.20951500	C	9.97431600	-3.81219600	-0.58539300
C	-10.90869400	1.90106100	0.66416900	C	11.77130200	-3.37641400	1.04911300
H	-11.69929000	1.31193500	1.11482900	H	10.29286500	4.96480500	2.78499900
C	-3.10288500	-2.61459500	-1.11591500	C	9.23493900	6.83429300	-0.47763400
H	-2.07195500	-2.69064800	-1.43736700	C	7.38776800	7.04457000	1.21800000
C	-1.49503100	2.22973700	-1.62046000	C	9.76965800	7.25109300	1.92016700
H	-1.00854800	3.13477100	-1.96090600	H	9.86943700	-4.13896400	2.87393800
C	-1.41033300	-0.07931800	-0.85756500	H	8.53782800	-4.43170400	1.75210700
C	-0.62501100	-1.12949700	-0.28479200	H	10.01584300	-5.40592100	1.64250400
C	-0.72754000	1.07758800	-1.29774300	H	10.38568200	-3.08701100	-1.29495200
C	0.73059100	-1.12422800	-0.34641800	H	10.44238200	-4.78245600	-0.77913100
H	-1.12279100	-1.91084700	0.27595200	H	8.91300500	-3.92682900	-0.79228900
H	1.28512300	-1.90338600	0.16241400	H	12.18062600	-4.34511000	0.74466800
C	1.45041200	-0.06688200	-0.98716200	H	12.24051700	-2.60003700	0.43720100
C	2.88184400	-0.08779900	-1.12170900	H	12.06842300	-3.21660800	2.08862900
C	0.72112600	1.08303100	-1.36522300	H	10.24389200	6.46187800	-0.67960700
C	3.54812900	1.11109100	-1.34857700	H	8.55763500	6.37956200	-1.20610100
C	3.70038400	-1.29328400	-1.11732700	H	9.22841700	7.91656800	-0.64588200
C	2.80958500	2.26728700	-1.70668400	H	7.06389200	6.82351500	2.23957600
C	4.96167900	1.15028700	-1.08095900	H	7.35471900	8.12993200	1.07448300
C	5.12257400	-1.23861200	-0.95567000	H	6.66367600	6.59493600	0.53265500
C	3.11060500	-2.51024300	-1.49611900	H	9.71946900	8.32757400	1.73033700
H	3.33341600	3.18478900	-1.95629600	H	9.50334100	7.08819300	2.96938400
C	5.75963600	0.07385300	-0.71377100	H	10.80818800	6.93765500	1.77332500
S	5.70973900	2.68731100	-0.86575600	C	1.44849600	2.23596900	-1.76858600
C	5.82343200	-2.43380000	-1.18372000	H	0.92788300	3.12874900	-2.09027700
C	3.84035600	-3.66211100	-1.67970400				
H	2.05338500	-2.53175000	-1.72569900				
C	7.04344100	0.55263100	-0.12206000				
C	7.08070700	1.94098500	-0.13449400				
H	6.89748800	-2.39941600	-1.16195000				
C	5.22690400	-3.64393200	-1.52798300				
H	3.32434300	-4.56176900	-1.99181000				
C	8.17036900	-0.08949800	0.60452700				
C	8.01789600	2.78235900	0.56460000				
C	6.08174400	-4.89758300	-1.74213000				
C	8.92111800	0.70810600	1.51812600				
C	8.62896800	-1.41436800	0.42098500				
C	8.03278500	4.17841100	0.41061500				
C	8.85672500	2.16494200	1.50194700				
C	7.17526400	-4.61466200	-2.78990500				
C	6.68922000	-5.29047500	-0.38254500				
C	5.26179500	-6.09195200	-2.25228300				
C	9.84423000	0.07528200	2.36640500				
H	8.21172900	-1.98863300	-0.38469000				
C	9.65892000	-1.99087500	1.15566400				
C	8.83736400	4.99845900	1.18348200				
H	7.38952700	4.62389800	-0.34316700				

ARO-11

C	3.93345300	0.25385100	10.41472600
C	3.47699000	0.10379100	9.11737100
C	2.13143600	0.33077600	8.77442100
C	1.19429200	0.73476600	9.75618400
C	2.99026100	0.63342100	11.39090100
C	-0.16909200	1.05067700	9.35337500
C	-0.59626800	0.83511500	8.01917900
C	-1.85036800	1.33395000	7.60049700
H	-2.10232600	1.25133200	6.55344300
C	-2.73046300	1.94908500	8.46605700
C	-2.32979300	2.06905300	9.81492500
H	4.16228100	-0.21896500	8.34012800
H	3.29654700	0.75025600	12.42356500
H	-2.99297100	2.53604200	10.53636900
C	1.63265000	0.10824800	7.45718100
C	0.32596300	0.22143600	7.09017900
C	1.23664700	-0.29403100	4.95025600
C	1.28562000	-0.51139500	3.54698600
C	0.08766200	-0.20839200	5.68030700

C	2.50944700	-0.53713800	2.82550100	C	1.28562000	-0.51139500	-3.54698600
C	0.06014500	-0.64240000	2.86771400	C	-1.12616900	-0.92309300	-3.66259000
C	-1.11853400	-0.70276400	5.06742300	C	2.50944700	-0.53713800	-2.82550100
H	3.45095100	-0.47777300	3.36026400	C	1.23664700	-0.29403100	-4.95025600
C	-1.12616900	-0.92309300	3.66259000	C	-1.11853400	-0.70276400	-5.06742300
C	-2.20881300	-1.13898100	5.85439300	C	-2.26403700	-1.57352900	-3.12698800
H	-2.12876000	-1.03206200	6.92610500	H	3.45095100	-0.47777300	-3.36026400
C	-3.32097100	-1.74569100	5.31261300	C	0.08766200	-0.20839200	-5.68030700
C	-3.32354900	-1.95121300	3.91572300	C	-2.20881300	-1.13898100	-5.85439300
H	-4.15683800	-2.46525200	3.44690800	C	-3.32354900	-1.95121300	-3.91572300
C	-4.07363800	2.52584700	8.00811900	H	-2.28119800	-1.84847000	-2.08075900
C	-4.33412600	2.26124300	6.51909100	C	0.32596300	0.22143600	-7.09017900
C	-5.21769300	1.89420500	8.82357100	C	1.63265000	0.10824800	-7.45718100
C	-4.06608800	4.04944900	8.23925700	H	-2.12876000	-1.03206200	-6.92610500
H	-3.59870600	2.76361200	5.88265900	C	-3.32097100	-1.74569100	-5.31261300
H	-4.31142500	1.19146000	6.28632500	H	-4.15683800	-2.46525200	-3.44690800
H	-5.32272600	2.64233400	6.24669500	C	-0.59626800	0.83511500	-8.01917900
H	-5.10144500	2.07076700	9.89658700	C	2.13143600	0.33077600	-8.77442100
H	-6.17540500	2.32759400	8.51776700	C	-4.48963100	-2.24517800	-6.16655200
H	-5.26913500	0.81324200	8.66242300	C	-0.16909200	1.05067700	-9.35337500
H	-5.01348600	4.48510300	7.90522500	C	-1.85036800	1.33395000	-7.60049700
H	-3.93821100	4.29732900	9.29712100	C	3.47699000	0.10379100	-9.11737100
H	-3.25419300	4.52330100	7.67897600	C	1.19429200	0.73476600	-9.75618400
C	-4.48963100	-2.24517800	6.16655200	C	-5.78890600	-1.55910100	-5.70367400
C	-4.28137100	-1.94361100	7.65651500	C	-4.28137100	-1.94361100	-7.65651500
C	-5.78890600	-1.55910100	5.70367400	C	-4.62791900	-3.77010100	-5.99385400
C	-4.62791900	-3.77010100	5.99385400	C	-1.09051900	1.65105500	-10.23821700
H	-3.41515500	-2.47674600	8.06115000	H	-2.10232600	1.25133200	-6.55344300
H	-4.13750900	-0.87374800	7.83866800	C	-2.73046300	1.94908500	-8.46605700
H	-5.16154100	-2.26380700	8.22175500	C	3.93345300	0.25385100	-10.41472600
H	-5.99865200	-1.75459100	4.64805500	H	4.16228100	-0.21896500	-8.34012800
H	-6.63654300	-1.93286400	6.28711700	C	1.66753300	0.86529500	-11.07463900
H	-5.73405900	-0.47501500	5.84258300	H	-5.99865200	-1.75459100	-4.64805500
H	-5.44993400	-4.14387900	6.61294800	H	-5.73405900	-0.47501500	-5.84258300
H	-4.84033100	-4.04503800	4.95666600	H	-6.63654300	-1.93286400	-6.28711700
H	-3.70934400	-4.28039800	6.29935500	H	-3.41515500	-2.47674600	-8.06115000
C	5.41010100	-0.00514300	10.73820800	H	-5.16154100	-2.26380700	-8.22175500
C	5.75923200	-1.46350200	10.38409500	H	-4.13750900	-0.87374800	-7.83866800
C	6.28479200	0.95936000	9.90401200	H	-5.44993400	-4.14387900	-6.61294800
C	5.72696300	0.22125200	12.22262200	H	-3.70934400	-4.28039800	-6.29935500
H	5.14315900	-2.16180700	10.95916000	H	-4.84033100	-4.04503800	-4.95666600
H	5.60547600	-1.67212500	9.32150200	C	-2.32979300	2.06905300	-9.81492500
H	6.81061600	-1.66385500	10.61517400	H	-0.81574400	1.82169200	-11.27220300
H	6.05151600	1.99414300	10.13627000	C	-4.07363800	2.52584700	-8.00811900
H	7.34342900	0.77853700	10.12459000	C	2.99026100	0.63342100	-11.39090100
H	6.13863900	0.80214000	8.83030800	C	5.41010100	-0.00514300	-10.73820800
H	6.78983800	0.03206000	12.39966000	H	0.99166600	1.15059300	-11.87220400
H	5.51817100	1.25089000	12.53022500	H	-2.99297100	2.53604200	-10.53636900
H	5.15882600	-0.45620300	12.86809400	C	-5.21769300	1.89420500	-8.82357100
C	-1.09051900	1.65105500	10.23821700	C	-4.33412600	2.26124300	-6.51909100
H	-0.81574400	1.82169200	11.27220300	C	-4.06608800	4.04944900	-8.23925700
C	1.66753300	0.86529500	11.07463900	H	3.29654700	0.75025600	-12.42356500
H	0.99166600	1.15059300	11.87220400	C	6.28479200	0.95036000	-9.90401200
C	-2.26403700	-1.57352900	3.12698800	C	5.75923200	-1.46350200	-10.38409500
H	-2.28119800	-1.84847000	2.08075900	C	5.72696300	0.22125200	-12.22262200
C	2.51004800	-0.64743200	1.46942400	H	-5.10144500	2.07076700	-9.89658700
H	3.46425800	-0.70319700	0.96292100	H	-5.26913500	0.81324200	-8.66242300
C	0.07181900	-0.55721700	1.42942200	H	-6.17540500	2.32759400	-8.51776700
C	-1.10844000	-0.26442800	0.67897900	H	-3.59870600	2.76361200	-5.88265900
C	1.29531300	-0.62686400	0.72458800	H	-5.32272600	2.64233400	-6.24669500
C	-1.10844000	-0.26442800	-0.67897900	H	-4.31142500	1.19146000	-6.28632500
H	-2.00775300	0.03554800	1.20183000	H	-5.001348600	4.48510300	-7.90522500
H	-2.00775300	0.03554800	-1.20183000	H	-3.25419300	4.52330100	-7.67897600
C	0.07181900	-0.55721700	-1.42942200	H	-3.93821100	4.29732900	-9.29712100
C	0.06014500	-0.64240000	-2.86771400	H	6.05151600	1.99414300	-10.13627000
C	1.29531300	-0.62686400	-0.72458800	H	6.13863900	0.80214000	-8.83030800

H	7.34342900	0.77853700	-10.12459000	C	-1.20284200	0.42448400	-0.30733300
H	5.14315900	-2.16180700	-10.95916000	C	-0.68645900	-0.85394000	-0.23535900
H	6.81061600	-1.66385500	-10.61517400	C	-1.49035500	-1.92544800	-0.79345500
H	5.60547600	-1.67212500	-9.32150200	C	-2.86670300	-1.69489300	-1.03965500
H	6.78983800	0.03206000	-12.39966000	C	-3.56854600	-2.69552900	-1.75093200
H	5.15882600	-0.45620300	-12.86809400	C	-2.96448400	-3.86453000	-2.15239100
H	5.51817100	1.25089000	-12.53022500	C	-1.59670600	-4.10456400	-1.91235000
C	2.51004800	-0.64743200	-1.46942400	C	-0.93808300	-5.38918000	-2.42473500
H	3.46425800	-0.70319700	-0.96292100	C	-1.07016800	-5.45116600	-3.95863100
S	2.64955900	-0.18852800	-6.02687300	C	-1.64617400	-6.60790400	-1.80300800
S	2.64955900	-0.18852800	6.02687300	C	0.55239400	-5.45669200	-2.06509800
O	3.32612300	-1.48722000	-6.06885700	C	-0.89051800	-3.11536700	-1.25723100
O	3.47277600	0.99399800	-5.76429400	C	-3.45900800	-0.39712400	-0.72438600
O	3.32612300	-1.48722000	6.06885700	C	-2.59313800	0.69249300	-0.53629900
O	3.47277600	0.99399800	5.76429400	C	-3.11517400	2.01109800	-0.51596400

AR-17

C	15.95806100	-3.87972500	-1.40689800	C	-4.87673300	-0.15833400	-0.65122900
C	14.96499700	-2.94514700	-2.12317400	C	-5.81190600	-1.21590700	-0.41682700
C	13.54085600	-3.44750000	-1.84985600	C	-7.15193100	-1.00121800	-0.42770400
C	15.21845000	-3.00622900	-3.64209800	C	-7.70592700	0.29481500	-0.67460000
C	15.16804500	-1.50368600	-1.64397500	C	-6.81396500	1.39211500	-0.68551000
C	14.14743500	-0.74971800	-1.09680200	C	-7.35986600	2.70520800	-0.66642500
C	14.32036200	0.59112500	-0.69308200	C	-8.70465400	2.90640900	-0.57406800
C	15.55442100	1.23183700	-0.94498600	C	-9.61158500	1.81646400	-0.60073300
C	15.68940500	2.67344600	-0.74846400	C	-9.12551300	0.51005200	-0.77062800
C	16.90523600	3.36190700	-0.90069700	C	-10.08972400	-0.53746900	-1.09874700
C	16.98021800	4.73671500	-0.79239000	C	-11.47227900	-0.32434300	-0.87219900
C	15.84059500	5.51741400	-0.52683700	C	-12.40906600	-1.25231000	-1.37432200
C	15.88634600	7.04611600	-0.40607200	C	-12.04068900	-2.40118400	-2.04613200
C	17.29870300	7.60318400	-0.63085600	C	-13.06352600	-3.38818800	-2.61766600
C	15.42208300	7.45961600	1.00363200	C	-12.82676900	-4.78221600	-2.00659300
C	14.94865300	7.66763500	-1.45865200	C	-12.89280100	-3.46800000	-4.14705600
C	14.64045400	4.84510200	-0.35830900	C	-14.50609700	-2.96091800	-2.31598100
C	14.54264800	3.44661500	-0.45205800	C	-10.66235400	-2.61137000	-2.25019700
C	13.31092600	2.74764400	-0.19737600	C	-9.72653000	-1.70272200	-1.81263900
C	13.21511000	1.37201300	-0.15585500	C	-11.90755000	0.94234400	-0.31072000
C	11.90755000	0.94234500	0.31072800	C	-11.01940400	1.99631700	-0.39139900
C	11.01940100	1.99631900	0.39135600	S	-11.78886100	3.53577200	-0.11978300
C	9.61157500	1.81647100	0.60065400	C	-13.31091100	2.74765300	0.19738900
C	8.70464600	2.90641700	0.57393800	C	-13.21509500	1.37202200	0.15589500
C	7.35985600	2.70521900	0.66626700	C	-14.32032900	0.59114500	0.69317800
C	6.81395400	1.39212700	0.68537300	C	-15.55437800	1.23186300	0.94511300
C	7.70591500	0.29482600	0.67451000	C	-16.60112500	0.44865000	1.47368300
C	7.15192300	-1.00121200	0.42763100	C	-16.42202500	-0.87767800	1.79505100
C	5.81189800	-1.21590000	0.41673300	C	-15.16797700	-1.50364600	1.64414500
C	4.87672100	-0.15832100	0.65109400	C	-14.96491300	-2.94509800	2.12336300
C	5.38124000	1.16259800	0.67195700	C	-15.21831800	-3.00615500	3.64229600
C	4.45331400	2.23980000	0.63415500	C	-13.54078000	-3.44745400	1.85000800
C	3.11516500	2.01110800	0.51574800	C	-15.95799800	-3.87968900	1.40713200
C	2.59312800	0.69250400	0.53611200	C	-14.14738700	-0.74969000	1.09691900
C	3.45899500	-0.39710900	0.72423800	C	-15.68936900	2.67346700	0.74856500
C	2.86668600	-1.69487000	1.03953500	C	-14.54262400	3.44663000	0.45209900
C	1.49034000	-1.92542900	0.79332900	C	-14.64043500	4.84511500	0.35832100
C	0.89049800	-3.11533600	1.25713100	C	-15.84057000	5.51743000	0.52687900
C	1.59667900	-4.10451600	1.91228300	C	-15.88632700	7.04612900	0.40608000
C	0.93805000	-5.38911800	2.42469500	C	-17.29867600	7.60320100	0.63090300
C	-0.55242300	-5.45663800	2.06504400	C	-15.42211600	7.45959700	-1.00365100
C	1.07011700	-5.45106200	3.95859500	C	-14.94859500	7.66767300	1.45861100
C	1.64614700	-6.60785900	1.80301000	C	-16.98018200	4.73673600	0.79249300
C	2.96445500	-3.86447600	2.15233100	C	-16.90519500	3.36193100	0.90082800
C	3.56852200	-2.69548600	1.75084600	C	9.12549900	0.51006400	0.77056700
C	0.68644900	-0.85393500	0.23520000	C	10.08969900	-0.53745000	1.09873700
C	1.20283400	0.42449000	0.30714300	C	11.47226200	-0.32433000	0.87222300
S	-0.00000300	1.64880100	-0.00011200	C	12.40903300	-1.25228800	1.37439200
				C	12.04063700	-2.40114700	2.04621600

C	13.06345700	-3.38814000	2.61779900	H	-9.08768000	3.91876800	-0.48865900
C	12.89269000	-3.46792100	4.14718500	H	-13.45700900	-1.01405700	-1.26421000
C	14.50603600	-2.96087800	2.31614400	H	-13.53160700	-5.50324600	-2.43368500
C	12.82671500	-4.78218000	2.00674600	H	-12.97303800	-4.76761400	-0.92223800
C	10.66229600	-2.61132700	2.25024800	H	-11.81458200	-5.14593200	-2.20604000
C	9.72648500	-1.70268700	1.81264500	H	-13.63105600	-4.15609900	-4.57211400
S	11.78886600	3.53576800	0.11973000	H	-13.03717600	-2.48469600	-4.60535000
C	16.60118700	0.44861300	-1.47350000	H	-11.89945600	-3.83022600	-4.42723100
C	16.42209900	-0.87772200	-1.79484700	H	-14.75769200	-2.01292500	-2.80212500
H	16.99631100	-3.58524900	-1.58444600	H	-14.68028100	-2.84670500	-1.24144800
H	15.83598600	-4.90469700	-1.77238000	H	-15.19971800	-3.72029100	-2.68949400
H	15.78842400	-3.88404400	-0.32607700	H	-10.32107700	-3.47771700	-2.80853900
H	12.79463100	-2.87539200	-2.41028500	H	-8.69160000	-1.86199500	-2.08695100
H	13.45550700	-4.49420100	-2.15707900	H	-17.56783200	0.89781900	1.66971900
H	13.28547000	-3.38732800	-0.78694400	H	-17.25888100	-1.42991900	2.21156800
H	16.24144900	-2.71060100	-3.89294000	H	-15.06406700	-4.02615000	4.01001600
H	14.53271700	-2.34164100	-4.17682100	H	-16.24130900	-2.71052500	3.89316500
H	15.06421200	-4.02623000	-4.00980600	H	-14.53256900	-2.34155700	4.17698600
H	13.16211600	-1.18155700	-0.99672300	H	-13.45542000	-4.49415000	2.15724800
H	17.81858500	2.81456700	-1.10360500	H	-13.28542800	-3.38730200	0.78708700
H	17.94752700	5.20844500	-0.91779000	H	-12.79453700	-2.87533500	2.41040300
H	17.27812100	8.69341300	-0.54101900	H	-15.78839400	-3.88402500	0.32630700
H	17.67701100	7.35960700	-1.62878100	H	-16.99624200	-3.58521000	1.58470800
H	18.00827600	7.22334300	0.11108600	H	-15.83591100	-4.90465500	1.77262800
H	15.45436200	8.54943600	1.10596300	H	-13.16207200	-1.18153200	0.99681200
H	14.39697700	7.13538600	1.20490000	H	-13.74115600	5.41001100	0.12755500
H	16.07113000	7.02436500	1.76993100	H	-17.27809800	8.69342700	0.54103900
H	13.91194300	7.34848000	-1.31807700	H	-17.67694600	7.35964700	1.62884800
H	15.25610400	7.38311800	-2.46979800	H	-18.00827600	7.22334100	-0.111100400
H	14.97453500	8.76008700	-1.38741300	H	-15.45440100	8.54941400	-1.10600600
H	13.74116600	5.41000200	-0.12759000	H	-14.39701700	7.13536400	-1.20494900
H	9.08767500	3.91877300	0.48851200	H	-16.07119000	7.02432700	-1.76991600
H	6.71170100	3.57169600	0.67954100	H	-15.25601000	7.38317900	2.46977500
H	7.81463200	-1.81865900	0.17260600	H	-13.91189000	7.34851600	1.31800600
H	5.44229200	-2.19863600	0.15236000	H	-14.97448100	8.76012300	1.38734800
H	4.79874900	3.26522400	0.65216600	H	-17.94748700	5.20846900	0.91791800
H	2.43712300	2.85327000	0.41624500	H	-17.81853600	2.81459500	1.10378200
H	-0.17645600	-3.22309500	1.12654800	H	13.45698000	-1.01403900	1.26430300
H	-0.96737100	-6.41189200	2.40041800	H	13.63093200	-4.15601300	4.57227700
H	-0.71424200	-5.38159000	0.98484500	H	11.89933700	-3.83013800	4.42734100
H	-1.12361300	-4.65852100	2.54975300	H	13.03705700	-2.48460800	4.60546400
H	0.59299600	-6.35954900	4.34095600	H	15.19964700	-3.72024500	2.68968900
H	2.11687400	-5.46493300	4.27583100	H	14.68024900	-2.84668600	1.24161300
H	0.58577600	-4.58747500	4.42484800	H	14.75762000	-2.01287600	2.80227500
H	2.71158400	-6.62812200	2.04971200	H	12.97300900	-4.76759900	0.92239500
H	1.55212400	-6.60458700	0.71265700	H	11.81452200	-5.14589100	2.20617600
H	1.19846500	-7.53354600	2.17939200	H	13.53154100	-5.50320200	2.43387000
H	3.55459500	-4.58773900	2.70672200	H	10.32100200	-3.47766000	2.80860000
H	4.59480500	-2.52147900	2.04769600	H	8.69154800	-1.86195300	2.08693200
H	-4.59483200	-2.52152800	-2.04777600	H	17.56790200	0.89777800	-1.66950800
H	-3.55462900	-4.58780700	-2.70675800	H	17.25897000	-1.42997100	-2.21132000
H	-0.59304900	-6.35966300	-4.34097300				
H	-0.58583400	-4.58759100	-4.42491400				
H	-2.11692900	-5.46504800	-4.27585400				
H	-1.19849800	-7.53360200	-2.17937300				
H	-1.55213600	-6.60460400	-0.71265700				
H	-2.71161400	-6.62817100	-2.04969500				
H	0.71422600	-5.38161500	-0.98490300				
H	1.12357900	-4.65858800	-2.54983500				
H	0.96733800	-6.41195500	-2.40045100				
H	0.17643700	-3.22312400	-1.12665500				
H	-2.43713000	2.85326300	-0.41649400				
H	-4.79875900	3.26521100	-0.65239100				
H	-5.44229700	-2.19863800	-0.15243900				
H	-7.81463600	-1.81865900	-0.17264900				
H	-6.71171100	3.57168300	-0.67973700				
				ARO-17			
C	15.87906400	-4.15995200	1.47921700	C	15.87906400	-4.15995200	1.47921700
C	14.91616300	-3.18850300	2.18774300	C	14.91616300	-3.18850300	2.18774300
C	13.47708600	-3.64973300	1.92080800	C	13.47708600	-3.64973300	1.92080800
C	15.17133600	-3.23771200	3.70671800	C	15.17133600	-3.23771200	3.70671800
C	15.16141000	-1.76041600	1.69093900	C	15.16141000	-1.76041600	1.69093900
C	14.16512700	-0.98240800	1.13924500	C	14.16512700	-0.98240800	1.13924500
C	14.38640400	0.34739000	0.71526300	C	14.38640400	0.34739000	0.71526300
C	15.64748800	0.95263600	0.94428400	C	15.64748800	0.95263600	0.94428400
C	15.84078100	2.37679700	0.70919300	C	15.84078100	2.37679700	0.70919300
C	17.07830600	3.02980900	0.85542700	C	17.07830600	3.02980900	0.85542700
C	17.19370600	4.39599100	0.70207200	C	17.19370600	4.39599100	0.70207200
C	16.08335200	5.20652900	0.39119100	C	16.08335200	5.20652900	0.39119100

C	16.18353200	6.72726200	0.21957700	C	-12.80884200	-4.97668100	1.97247700
C	17.61024800	7.24404000	0.44880000	C	-12.88864800	-3.65570400	4.11008700
C	15.75382900	7.10570500	-1.21087700	C	-14.51372400	-3.17873100	2.27911100
C	15.24997400	7.41268200	1.23574500	C	-10.67387500	-2.78088900	2.19642900
C	14.86371200	4.57446500	0.22668100	C	-9.74618400	-1.87289100	1.74681200
C	14.72524100	3.18201000	0.37369600	C	-11.95345700	0.74141200	0.26093800
C	13.49112800	2.50907900	0.13371700	C	-11.06197500	1.77373600	0.26781100
C	13.32128100	1.15817100	0.16911400	C	-13.49112500	2.50908000	-0.13374500
C	11.95345800	0.74141100	-0.26095200	C	-13.32127800	1.15817200	-0.16913700
C	11.06197600	1.77373400	-0.26782100	C	-14.38639700	0.34738900	-0.71529100
C	9.66285400	1.62933300	-0.46913600	C	-15.64748000	0.95263500	-0.94432200
C	8.77014700	2.73341300	-0.41227700	C	-16.66848400	0.13755800	-1.47876200
C	7.42682800	2.54205000	-0.51216800	C	-16.43885900	-1.17317400	-1.82352800
C	6.86765500	1.23219800	-0.56284500	C	-15.16139700	-1.76041900	-1.69096700
C	7.74457800	0.12342300	-0.57440700	C	-14.91614700	-3.18850700	-2.18776700
C	7.17909700	-1.16944100	-0.34983700	C	-15.17131100	-3.23771900	-3.70674300
C	5.83590700	-1.36890600	-0.34350700	C	-13.47707200	-3.64973700	-1.92082300
C	4.91701100	-0.29637600	-0.56084200	C	-15.87905300	-4.15995500	-1.47924500
C	5.43421700	1.01929400	-0.55485300	C	-14.16511700	-0.98241000	-1.13926900
C	4.51935700	2.11023600	-0.49236600	C	-15.84077400	2.37679600	-0.70923600
C	3.17974600	1.90321000	-0.37693100	C	-14.72523600	3.18201000	-0.37373300
C	2.64516000	0.58762200	-0.43133900	C	-14.86370800	4.57446500	-0.22672200
C	3.49487300	-0.51419400	-0.64419600	C	-16.08334700	5.20653000	-0.39124200
C	2.88157400	-1.78627400	-0.99550800	C	-16.18352800	6.72726200	-0.21963300
C	1.49324600	-2.00002500	-0.77517300	C	-17.61024200	7.24404000	-0.44886700
C	0.87632100	-3.17804800	-1.25455300	C	-15.75383400	7.10570900	1.21082300
C	1.57510100	-4.17001900	-1.90687700	C	-15.24996300	7.41268000	-1.23579600
C	0.90599500	-5.44117900	-2.43651100	C	-17.19369900	4.39599100	-0.70212800
C	-0.58903400	-5.48949500	-2.09339100	C	-17.07829800	3.02980800	-0.85547900
C	1.05635400	-5.49261100	-3.96907500	C	9.16755800	0.32775000	-0.67094200
C	1.59025700	-6.67290900	-1.81369100	C	10.12186500	-0.71011600	-1.03166300
C	2.95229600	-3.94693800	-2.12551600	C	11.51432700	-0.50981900	-0.82374200
C	3.57476900	-2.79666300	-1.70530600	C	12.44364900	-1.44497800	-1.33373300
C	0.71268400	-0.92699700	-0.21694400	C	12.05882200	-2.58608800	-2.00331600
C	1.26623400	0.31975700	-0.21887300	C	13.06522600	-3.58493400	-2.58101600
C	-1.26623500	0.31975800	0.21891700	C	12.88862400	-3.65571300	-4.11009600
C	-0.71268500	-0.92699600	0.21699300	C	14.51371100	-3.17873800	-2.27913100
C	-1.49324900	-2.00002300	0.77522300	C	12.80883000	-4.97668700	-1.97248400
C	-2.88157800	-1.78627000	0.99555400	C	10.67386300	-2.78089500	-2.19642600
C	-3.57477500	-2.79665700	1.70535100	C	9.74617500	-1.87289700	-1.74680500
C	-2.95230300	-3.94693100	2.12556700	C	16.66849600	0.13756000	1.47871900
C	-1.57510700	-4.17001300	1.90693300	C	16.43887200	-1.17317100	1.82349000
C	-0.90600300	-5.44117100	2.43657400	H	16.92652400	-3.89739900	1.65227100
C	-1.05636700	-5.49259800	3.96913800	H	15.72514500	-5.17636600	1.85574200
C	-1.59026300	-6.67290300	1.81375600	H	15.70717800	-4.17028000	0.39876900
C	0.58902700	-5.48948900	2.09345700	H	12.74861800	-3.04849400	2.47406200
C	-0.87632500	-3.17804300	1.25460900	H	13.36002300	-4.68910900	2.24137300
C	-3.49487500	-0.51419100	0.64423600	H	13.22448600	-3.59645500	0.85661600
C	-2.64516100	0.58762400	0.43137900	H	16.20319800	-2.96952600	3.95213600
C	-3.17974700	1.90321200	0.37696500	H	14.50636900	-2.54736700	4.23479000
C	-4.51935800	2.11023900	0.49239400	H	14.98847100	-4.24834900	4.08631100
C	-5.43421800	1.01929600	0.55488000	H	13.16493700	-1.38073500	1.05081500
C	-4.91701200	-0.29637300	0.56087500	H	17.97119600	2.46262100	1.09052600
C	-5.83590700	-1.36890400	0.34353900	H	18.17261600	4.84327600	0.82673000
C	-7.17909700	-1.16944000	0.34986200	H	17.62707400	8.33066300	0.32301600
C	-7.74458000	0.12342500	0.57442400	H	17.96516100	7.02208900	1.46031500
C	-6.86765600	1.23220000	0.56286300	H	18.31802100	6.81738900	-0.26909200
C	-7.42682900	2.54205200	0.51218000	H	15.82412500	8.18963500	-1.34895700
C	-8.77014700	2.73341500	0.41228000	H	14.72154200	6.80899400	-1.41735100
C	-9.66285500	1.62933500	0.46913600	H	16.39948100	6.62355700	-1.95153400
C	-9.16756000	0.32775200	0.67094800	H	14.20624800	7.12006200	1.09043800
C	-10.12186900	-0.71011300	1.03166600	H	15.53410600	7.15476500	2.26071200
C	-11.51433000	-0.50981600	0.82373400	H	15.31093200	8.50047100	1.12663900
C	-12.44365600	-1.44497400	1.33372100	H	13.98889400	5.15635700	-0.04544400
C	-12.05883300	-2.58608300	2.00330900	H	9.16305300	3.73769300	-0.29829300
C	-13.06524100	-3.58492700	2.58100500	H	6.78587000	3.41338100	-0.50469900

H	7.83190400	-1.99844300	-0.10747800	H	-14.20623800	7.12006000	-1.09048200
H	5.45464800	-2.35133900	-0.09559300	H	-15.31092200	8.50046900	-1.12669400
H	4.88006300	3.13002200	-0.48697700	H	-18.17260800	4.84327600	-0.82679400
H	2.51395500	2.75031900	-0.25444100	H	-17.97118600	2.46262000	-1.09058400
H	-0.19357800	-3.26906200	-1.13825800	H	13.49435600	-1.21657500	-1.23173300
H	-1.01338200	-6.43621400	-2.44023300	H	13.61477600	-4.35402700	-4.53873300
H	-0.76111000	-5.42105200	-1.01412200	H	11.88917100	-4.00159400	-4.38925200
H	-1.14389400	-4.68033500	-2.57880800	H	13.04775200	-2.67338200	-4.56530500
H	0.57114200	-6.39144700	-4.36324100	H	15.19579400	-3.94581100	-2.65743700
H	2.10643200	-5.51966100	-4.27417600	H	14.69088300	-3.07394900	-1.20390000
H	0.58978800	-4.61906200	-4.43462700	H	14.77856100	-2.23231000	-2.76121800
H	2.65897100	-6.70562100	-2.04419400	H	12.95683200	-4.96676700	-0.88828700
H	1.47857600	-6.67766900	-0.72498900	H	11.79201400	-5.32714300	-2.17191200
H	1.13656700	-7.58918000	-2.20497400	H	13.50348400	-5.70552200	-2.40239700
H	3.53646000	-4.67500800	-2.67963300	H	10.32221300	-3.64144700	-2.75695600
H	4.60786200	-2.64107800	-1.98647600	H	8.70887500	-2.02656700	-2.01301500
H	-4.60786900	-2.64107200	1.98651700	H	17.65397500	0.55100100	1.65644000
H	-3.53646900	-4.67500000	2.67968400	H	17.25767000	-1.74946600	2.24276000
H	-0.57115500	-6.39143200	4.36330800	S	0.00000000	1.55211800	0.00002100
H	-0.58980200	-4.61904600	4.43468700	S	-11.92186600	3.32048000	0.08255300
H	-2.10644500	-5.51964700	4.27423500	S	11.92186700	3.32047900	-0.08257200
H	-1.13657600	-7.58917300	2.20504500	O	0.15962300	2.31070000	2.14222400
H	-1.47857900	-6.67766800	0.72505500	O	-0.15962300	2.31069700	-1.24218400
H	-2.65897800	-6.70561400	2.04425600	O	-11.83841100	4.07578700	1.33505000
H	0.76110600	-5.42105000	1.01418900	O	-11.56467000	4.02003100	-1.15363100
H	1.14388500	-4.68032700	2.57887300	O	11.56468000	4.02003300	1.15361200
H	1.01337400	-6.43620700	2.44030500	O	11.83840500	4.07578200	-1.33507200
H	0.19357400	-3.26905800	1.13831700				
H	-2.51395500	2.75032100	0.25447600				
H	-4.88006500	3.13002400	0.48700100	AR-23			
H	-5.45464600	-2.35133800	0.09563200	C	-0.34109100	-0.50924400	-3.55376000
H	-7.83190300	-1.99844300	0.10750200	C	0.87553400	-0.42415200	-2.82981600
H	-6.78587100	3.41338300	0.50471200	C	0.89478400	-0.53074400	-1.47145900
H	-9.16305300	3.73769500	0.29829100	C	-0.31272500	-0.62160800	-0.72548300
H	-13.49436200	-1.21657100	1.23171300	C	-1.53636500	-0.66775000	-1.43288300
H	-13.50349900	-5.70551500	2.40238800	C	-1.54361900	-0.75186900	-2.87002200
H	-12.95683600	-4.96676300	0.88828000	C	-0.31272500	-0.62160800	0.72548300
H	-11.79202700	-5.32713800	2.17191200	C	-1.53636500	-0.66775000	1.43288300
H	-13.61480200	-4.35401600	4.53872000	C	-2.73893400	-0.48745200	0.67859800
H	-13.04777900	-2.67337200	4.56529300	C	-2.73893400	-0.48745200	-0.67859800
H	-11.88919600	-4.00158400	4.38924900	C	0.89478400	-0.53074400	1.47145900
H	-14.77857700	-2.23230200	2.76119500	C	0.87553400	-0.42415200	2.82981600
H	-14.69088900	-3.07394300	1.20387900	C	-0.34109100	-0.50924400	3.55376000
H	-15.19580900	-3.94580400	2.65741300	C	-1.54361900	-0.75186900	2.87002200
H	-10.32222900	-3.64144000	2.75696300	C	-2.71407300	-1.12992700	-3.65837000
H	-8.70888600	-2.01302900	2.01302900	C	-2.71407300	-1.12992700	3.65837000
H	-17.65396300	0.55099800	-1.65648900	C	-3.77736700	-1.89077100	-3.11968100
H	-17.25765400	-1.74947000	-2.24280100	C	-4.81477000	-2.34810200	-3.89900400
H	-14.98844400	-4.24835700	-4.08633300	C	-4.84650400	-2.11771300	-5.28895500
H	-16.20317100	-2.96953400	-3.95216800	C	-3.79093000	-1.41366900	-5.83343700
H	-14.50634100	-2.54737500	-4.23481300	C	-2.73531900	-0.89311900	-5.05537900
H	-13.36000700	-4.68911300	-2.24138400	C	-2.73531900	-0.89311900	5.05537900
H	-13.22447800	-3.59645700	-0.85662800	C	-3.79093000	-1.41366900	5.83343700
H	-12.74860100	-3.04849900	-2.47407300	C	-4.84650400	-2.11771300	5.28895500
H	-15.70717300	-4.17028100	-0.39879600	C	-4.81477000	-2.34810200	3.89900400
H	-16.92651100	-3.89740200	-1.65230600	C	-3.77736700	-1.89077100	3.11968100
H	-15.72513100	-5.17637000	-1.85576700	C	-5.98427200	-2.69101300	-6.13950700
H	-13.16492800	-1.38073700	-1.05083100	C	-5.99559700	-4.22594700	-6.00564400
H	-13.98889200	5.15635800	0.04540700	C	-7.32785200	-2.12654200	-5.64003700
H	-17.62706900	8.33066400	-0.32308600	C	-5.82925800	-2.33668500	-7.62472600
H	-17.96514800	7.02208700	-1.46038400	C	-5.98427200	-2.69101300	6.13950700
H	-18.31802100	6.81739000	0.26902100	C	-7.32785200	-2.12654200	5.64003700
H	-15.82413200	8.18964000	1.34890000	C	-5.99559700	-4.22594700	6.00564400
H	-14.72154900	6.80899900	1.41730500	C	-5.82925800	-2.33668500	7.62472600
H	-16.39949100	6.62356300	1.95147700	C	0.42875200	0.56768400	8.68140900
H	-15.53408900	7.15476000	-2.26076500	C	1.81287100	0.61267900	8.98763300

C	2.24485000	0.74238900	10.27344400	C	0.03246300	1.28701800	-18.69065200
C	1.32806700	0.72707600	11.36061500	C	0.82293400	0.83557200	-17.61262400
C	-0.05354100	0.64113600	11.07186800	C	-2.34017000	0.69444400	-8.00917300
C	-0.51760800	0.70205700	9.71042800	C	-3.63114200	1.09896200	-7.60861400
C	1.78167800	0.75072900	12.73865800	C	-4.52651600	1.70531700	-8.46709000
C	0.84231500	0.68246600	13.79357100	C	-4.08502900	1.95712900	-9.78156200
C	-0.51181700	0.37285200	13.44996300	C	-2.81705200	1.61352800	-10.19009500
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C	-5.92214900	2.15419100	8.02293600	C	6.77557500	-0.61263600	22.21403300
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C	0.38111100	1.05636700	-16.28427100	H	1.85230000	-0.49832800	-0.96832300
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