

Supporting Information for:

Buckybowl and Its Chiral Hybrids Featuring Eight-Membered Rings and Helicene Units

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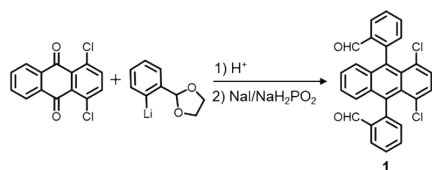
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1. Materials and Methods

All chemicals were used as received from commercial suppliers without further purification unless otherwise specified. THF and diethyl ether was refluxed with Na prior to use. ^1H NMR and ^{13}C NMR spectra were recorded in deuterated solvents on Bruker ADVANCE 400 NMR Spectrometer. Chemical shifts were reported in parts per million (ppm, δ) relative to the signal of tetramethylsilane ($\delta = 0.00$ ppm). ^1H NMR spectra were referenced to the signals of CDCl_3 ($\delta = 7.26$ ppm) and 1,1,2,2-tetrachloroethane- d_2 ($\delta = 6.00$ ppm). ^{13}C NMR spectra were referenced to the signal of CDCl_3 ($\delta = 77.2$ ppm) and 1,1,2,2-tetrachloroethane- d_2 ($\delta = 73.8$ ppm). Mass spectra (MALDI-TOF-MS) were determined on a Bruker BIFLEX III Mass Spectrometer. High resolution mass spectra (HRMS) were determined on Bruker Apex IV Fourier Transform Mass Spectrometer.

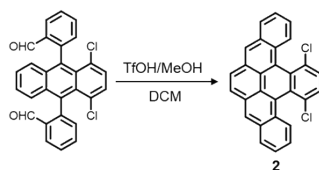
2. Synthesis and Characterization of Compounds



To a 250 mL two necked round-bottom flask was charged with 2-(2-bromophenyl)-1,3-dioxolane (9.9 g, 43.2 mmol) in dry ethyl ether (60 mL), the mixture was deoxygenated with nitrogen for 10 min at 0 °C, followed by adding n-BuLi (16.7 mL of 2.5 M solution; 41.8 mmol). The solution was stirred for 1 h and 1,4-dichloroanthraquinone (4 g, 14.4 mmol) in tetrahydrofuran (60 mL) was added, then warmed to room temperature and stirred for another 2 h. The reaction mixture was quenched with methanol and the solvent was removed under reduced pressure. The residue was dissolved in 60 mL glacial acetic acid followed by adding sodium iodide (15.1 g, 101 mmol) and sodium hypophosphite monohydrate (15.2 g, 144 mmol) and then heated to reflux for 30 min. The reaction mixture was cooled down to room temperature, poured into water, and filtered. The precipitate was washed with water, and dried over anhydrous sodium sulfate. The crude production was purified by silica gel chromatography using dichloromethane:petroleum ether (1:1) as eluent to afford a mixture of diastereomers **1** (*syn*-**1** and *anti*-**1**) (3.9 g, 60 %).

syn-**1**: ^1H NMR (400 MHz, CDCl_3): $\delta = 9.64$ (s, 2H), 8.17-8.15 (m, 2H), 7.76-7.68 (m, 4H), 7.42-7.39 (m, 4H), 7.37-7.31 (m, 4H). ^{13}C NMR (100 MHz, CDCl_3): $\delta = 191.5, 144.0, 136.2, 133.9, 133.4, 132.7, 132.1, 130.9, 128.9, 128.7, 128.4, 127.8, 127.4, 126.7$. HRMS (ESI) $[\text{M}+\text{Na}]^+$: Calcd (%) for $\text{C}_{28}\text{H}_{16}\text{Cl}_2\text{O}_2\text{Na}^+$: 477.0425, found: 477.0416;

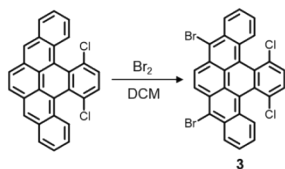
anti-**1**: ^1H NMR (400 MHz, CDCl_3) $\delta = 9.60$ (s, 2H), 8.17-8.15 (m, 2H), 7.75-7.68 (m, 4H), 7.43-7.41 (m, 4H), 7.36 (s, 4H). ^{13}C NMR (400 MHz, CDCl_3) $\delta = 191.2, 144.0, 136.2, 133.9, 133.2, 132.8, 132.1, 130.9, 129.0, 128.7, 128.5, 127.8, 127.4, 126.8$. HRMS (ESI) $[\text{M}+\text{Na}]^+$: Calcd (%) for $\text{C}_{28}\text{H}_{16}\text{Cl}_2\text{O}_2\text{Na}^+$: 477.0425, found: 477.0414.



To a mixture of **1** (100 mg, 0.2 mmol) and methanol (2 mL) in dichloromethane (200 mL) was added trifluoromethanesulfonic acid (triflic acid) (0.1 mL). The solution was stirred at room temperature for 48 h before the solvent was removed. The crude production was purified by silica

gel chromatography using dichloromethane:petroleum ether (1 : 9) as eluent to afford **2** (25 mg, 30%).

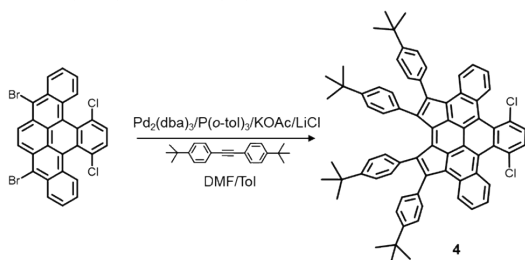
^1H NMR (400 MHz, CDCl_3): δ = 8.45 (s, 2H), 8.28-8.26 (m, 2H), 8.19-8.17 (m, 2H), 7.80 (d, J = 4.6 Hz, 4H), 7.67-7.60 (m, 4H). ^{13}C NMR (400 MHz, CDCl_3): δ = 132.5, 131.6, 130.9, 130.8, 130.2, 128.1, 128.0, 127.8, 127.8, 127.5, 127.4, 126.5, 125.9, 124.4. HRMS (EI): Calcd (%) for $\text{C}_{28}\text{H}_{14}\text{Cl}_2$:



420.0473, found: 420.0468.

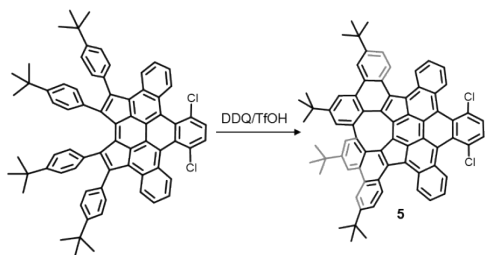
A solution of **2** (100 mg, 0.24 mmol) in dichloromethane (200 mL) was added elemental bromine (307 mg, 1.92 mmol) and the solution was stirred at room temperature for 10 min. The reaction was quenched by saturated aqueous sodium sulfite and the organic layer was extracted with dichloromethane. The combined organic layer was washed with brine and dried over anhydrous sodium sulfate. The filtrate was evaporated to give **3** as yellow solid (125 mg, 90%).

^1H NMR (400 MHz, CDCl_3): δ 8.72 (d, J = 8.9 Hz, 2H), 8.42 (s, 2H), 8.24 (d, J = 8.3 Hz, 2H), 7.79 (s, 2H), 7.79 – 7.71 (m, 2H), 7.67 (t, J = 7.6 Hz, 2H). ^{13}C NMR (400 MHz, $\text{CDCl}_3/\text{CS}_2$): δ = 132.6, 131.3, 130.9, 130.5, 129.8, 128.7, 127.5, 127.3, 126.3, 126.0, 125.4, 124.2, 122.7. .HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{28}\text{H}_{12}\text{Br}_2\text{Cl}_2$: 579.8632, found: 579.8628.



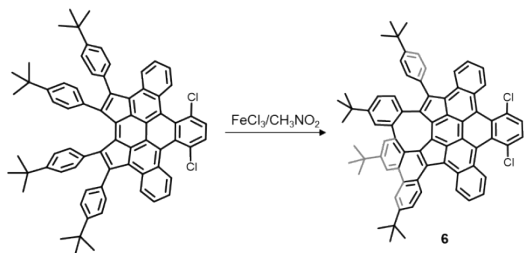
In a sealed tube, a solution of **3** (400 mg, 0.69 mmol), 1,2-bis(4-(tert-butyl)phenyl)ethyne (400 mg, 1.38 mmol), $\text{Pd}_2(\text{dba})_3$ (63 mg, 0.069 mmol), $\text{P}(\text{o-Tol})_3$ (32 mg, 0.1 mmol), KOAc (339 mg, 3.45 mmol), LiCl (58 mg, 1.38 mmol), and 1:1 DMF:Toluene (50 ml) was degassed with nitrogen for 15 min and then stirred at 130 °C for 12 h. The solvent was diluted with toluene and washed twice with water, and dried over anhydrous sodium sulfate. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 5) as eluent to afford **4** as green solid (410 mg, 60%).

^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$): δ 8.29 (d, J = 8.6 Hz, 2H), 7.75 (s, 2H), 7.70 – 7.61 (m, 4H), 7.53 – 7.45 (m, 2H), 7.36 (d, J = 8.2 Hz, 4H), 7.26 (d, J = 8.0 Hz, 4H), 6.94 (d, J = 8.3 Hz, 4H), 6.73 (d, J = 8.3 Hz, 4H), 1.37 (s, 18H), 1.13 (s, 18H). ^{13}C NMR (400 MHz, CDCl_3): δ = 150.7, 150.0, 148.2, 134.4, 132.8, 131.8, 131.6, 131.5, 130.3, 130.2, 129.9, 129.4, 128.6, 126.0, 124.9, 124.8, 123.7, 123.6, 34.8, 34.3, 31.6, 31.4. HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{72}\text{H}_{62}\text{Cl}_2$: 996.4228, found: 996.4229.



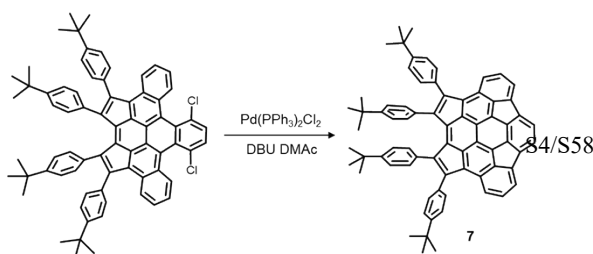
In a round bottom flask, **4** (100 mg, 0.10 mmol) was dissolved in CH_2Cl_2 (20 ml) and degassed with nitrogen for 15 min. The mixture was cooled to -10°C and DDQ (91 mg, 0.4 mmol) was added in one portion, then TfOH (0.5 mL) was added dropwise. After 15 min, the mixture was quenched with H_2O (10 mL) and was extracted with CH_2Cl_2 (30 mL). The organic layer was dried over anhydrous sodium sulfate and the solvent was removed in vacuo. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 8) as eluent to afford **5** as red solid (59 mg, 60%).

^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$): δ 9.09 (d, $J = 8.8$ Hz, 1H), 8.86 (d, $J = 12.8$ Hz, 2H), 8.76 (d, $J = 12.4$ Hz, 3H), 8.62 (s, 1H), 8.53 (s, 1H), 8.34 (d, $J = 8.0$ Hz, 2H), 7.94 – 7.83 (m, 2H), 7.80 (s, 2H), 7.70 (t, $J = 7.3$ Hz, 1H), 7.73 – 7.48 (m, 3H), 7.16 (d, $J = 17.8$ Hz, 2H), 1.65 (s, 9H), 1.60 (s, 9H), 1.48 (s, 9H), 1.45 (s, 9H). ^{13}C NMR (400 MHz, $\text{CDCl}_3/\text{CS}_2$): $\delta = 146.9, 146.8, 144.3, 141.1, 134.8, 134.1, 132.5, 132.3, 131.9, 131.6, 131.3, 131.1, 130.9, 129.9, 128.3, 128.0, 126.9, 126.5, 125.8, 125.6, 125.3, 124.3, 124.2, 124.2, 120.7, 119.8, 119.1, 118.8, 35.4, 35.3, 34.8, 34.6, 31.6, 31.4, 31.3, 31.2$. HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{72}\text{H}_{56}\text{Cl}_2$: 990.3759, found: 990.3760.



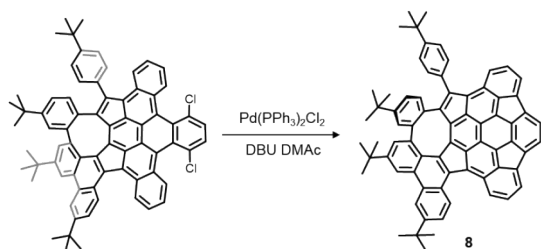
In a round bottom flask, **4** (300 mg, 0.30 mmol) was dissolved in CH_2Cl_2 (120 ml) and degassed with nitrogen for 15 min. Then the mixture was cooled to 0°C and FeCl_3 (293 mg, 1.8 mmol) in CH_3NO_2 (2 ml) was added dropwise. The reaction mixture was stirred at 0°C for 12 h and quenched with MeOH (10 mL), washed with water. The organic layer was dried over anhydrous sodium sulfate and the solvent was removed in vacuo. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 8) as eluent to afford **6** as red solid (90 mg, 30%).

^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$): δ 8.74 (t, $J = 9.3$ Hz, 2H), 8.60 (s, 1H), 8.53 (s, 1H), 8.34 (d, $J = 8.3$ Hz, 1H), 8.24 (d, $J = 8.3$ Hz, 1H), 8.01 (d, $J = 7.7$ Hz, 1H), 7.88 (d, $J = 6.1$ Hz, 2H), 7.77 (s, 2H), 7.67 (d, $J = 8.6$ Hz, 1H), 7.60 (s, 2H), 7.56–7.42 (m, 4H), 7.34 (t, $J = 8.0$ Hz, 1H), 7.08 (s, 2H), 6.68 (s, 1H), 1.64 (s, 9H), 1.55 (s, 9H), 1.47 (s, 9H), 1.20 (s, 9H). ^{13}C NMR (400 MHz, $\text{CDCl}_3/\text{CS}_2$): $\delta = 150.3, 148.6, 133.6, 133.0, 133.0, 132.6, 131.7, 131.5, 131.5, 131.4, 131.2, 131.2, 131.0, 130.4, 128.4, 126.7, 125.9, 125.8, 125.6, 125.3, 125.2, 124.3, 124.1, 123.9, 123.7, 120.5, 118.3, 35.3, 34.8, 34.8, 34.2, 31.6, 31.5, 31.4, 31.2$. HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{72}\text{H}_{58}\text{Cl}_2$: 992.3915, found: 992.3924.



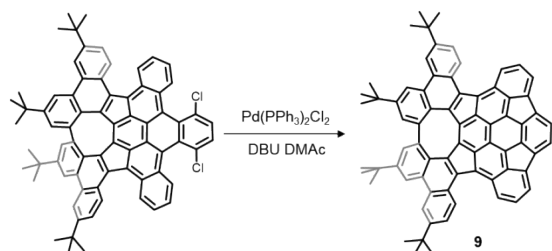
In a sealed tube, PdCl₂(PPh₃)₂ (42 mg, 0.06 mmol) was added to a solution of **4** (100 mg, 0.10 mmol) and DBU (91 mg, 0.60 mmol) in dried DMAc (6 mL) under nitrogen. The mixture was heated to 180 °C and stirred for 2 h. After cooling, the solvent was diluted with dichloromethane and washed with water, dried over anhydrous sodium sulfate. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 6) as eluent to afford **7** as brown solid (14 mg, 15%).

¹H NMR (400 MHz, CDCl₃): δ 7.46 (d, *J* = 6.8 Hz, 2H), 7.38 (s, 2H), 7.31 (d, *J* = 8.6 Hz, 4H), 7.17 (d, *J* = 6.3 Hz, 4H), 7.04 (dd, *J* = 8.6, 6.9 Hz, 2H), 6.90 (t, *J* = 8.6 Hz, 6H), 6.71 (d, *J* = 8.5 Hz, 4H), 1.34 (s, 18H), 1.11 (s, 18H). ¹³C NMR (400 MHz, C₂D₂Cl₄): δ = 150.8, 148.2, 147.8, 144.2, 142.8, 142.0, 140.9, 139.9, 139.2, 138.7, 138.7, 138.3, 133.1, 132.5, 131.1, 129.9, 129.3, 128.5, 125.3, 125.1, 124.6, 123.5, 121.7, 34.5, 34.0, 31.2, 31.1. HR-MALDI-TOF (*m/z*): Calcd (%) for C₇₂H₆₀: 924.4695, found: 924.4685.



In a sealed tube, a solution of **6** (100 mg, 0.10 mmol) and DBU (91 mg, 0.60 mmol) in super dry DMAc (6 mL) was added PdCl₂(PPh₃)₂ (42 mg, 0.06 mmol) under nitrogen. The mixture was heated to 180 °C in an oil bath and stirred for 2 h before cooling to room temperature. Then the solvent was diluted with dichloromethane and washed twice with water, dried over anhydrous sodium sulfate and the solvent removed in vacuo. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 6) as eluent to afford **8** as brown solid (18 mg, 20%).

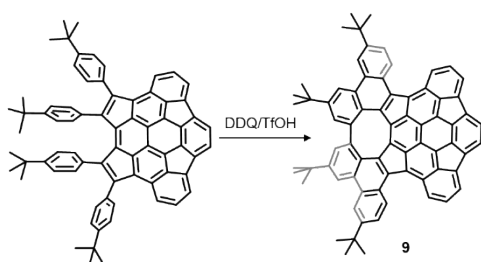
¹H NMR (400 MHz, C₂D₂Cl₄): δ 8.88 (d, *J* = 8.3 Hz, 1H), 8.51 (s, 1H), 8.41 (s, 1H), 8.31 (d, *J* = 8.3 Hz, 1H), 8.22 (d, *J* = 8.9 Hz, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.68 (d, *J* = 6.8 Hz, 1H), 7.52 (d, *J* = 6.8 Hz, 1H), 7.48 (d, *J* = 6.9 Hz, 1H), 7.43 – 7.31 (m, 6H), 7.29 – 7.19 (m, 2H), 7.14 (t, *J* = 9.3 Hz, 2H), 6.85 (s, 1H), 1.60 (s, 9H), 1.44 (s, 18H), 1.26 (s, 9H). ¹³C NMR (400 MHz, CDCl₃/CS₂): δ = 151.5, 150.4, 148.9, 148.7, 146.3, 145.9, 144.5, 143.8, 143.0, 142.8, 142.7, 141.3, 140.7, 140.4, 140.1, 139.9, 139.7, 139.5, 139.4, 139.4, 139.2, 139.0, 138.7, 136.1, 134.1, 132.6, 132.6, 132.2, 132.1, 131.7, 131.7, 130.7, 130.6, 130.6, 130.2, 130.1, 129.5, 128.8, 128.5, 128.1, 127.8, 126.7, 125.8, 125.6, 125.4, 125.0, 124.4, 121.7, 121.6, 120.3, 118.4, 35.3, 34.8, 34.6, 34.3, 31.6, 31.5, 31.3. HR-MALDI-TOF (*m/z*): Calcd (%) for C₇₂H₅₆: 920.4382, found: 920.4374.



In a sealed tube, PdCl₂(PPh₃)₂ (42 mg, 0.06 mmol) was added to a solution of **5** (100 mg, 0.10 mmol) and DBU (91 mg, 0.60 mmol) in super dry DMAc (6 mL) under nitrogen. The mixture was heated to 180 °C and stirred for 2 h. After cooling, the solvent was diluted with dichloromethane and washed with water, dried over anhydrous sodium sulfate. The crude product was further purified by

silica gel column chromatography using dichloromethane:petroleum ether (1 : 6) as eluent to afford **9** as red solid (37 mg, 40%).

^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$): δ 9.18 (d, $J = 8.7$ Hz, 1H), 8.94 (d, $J = 8.4$ Hz, 1H), 8.80 (s, 1H), 8.65 (s, 1H), 8.56 (s, 1H), 8.46 (s, 1H), 8.35 (d, $J = 8.7$ Hz, 1H), 8.23 (d, $J = 8.8$ Hz, 1H), 7.93 (d, $J = 8.6$ Hz, 2H), 7.64 (d, $J = 6.9$ Hz, 1H), 7.57 (d, $J = 6.9$ Hz, 1H), 7.53 – 7.38 (m, 3H), 7.33 (s, 1H), 7.32 – 7.24 (m, 1H), 6.81 (s, 1H), 1.61 (s, 18H), 1.51 (s, 9H), 1.31 (s, 9H). ^{13}C NMR (400 MHz, $\text{CDCl}_3/\text{CS}_2$): $\delta = 150.4, 150.2, 149.1, 146.7, 145.6, 144.6, 144.5, 143.8, 143.7, 142.5, 141.6, 141.0, 140.8, 140.8, 140.5, 139.8, 139.6, 139.2, 139.2, 139.0, 138.6, 138.2, 135.2, 134.6, 134.5, 133.8, 132.5, 132.2, 132.0, 131.1, 130.4, 130.2, 130.1, 129.1, 128.7, 127.7, 127.3, 126.9, 126.8, 126.5, 125.8, 125.6, 125.4, 125.0, 124.6, 121.9, 121.8, 120.4, 119.9, 118.9, 118.7, 35.3, 35.3, 34.7, 34.4, 31.6, 31.5, 31.2, 31.1$. HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{72}\text{H}_{54}$: 918.4225, found: 918.4219.



In a round bottom flask, **7** (20 mg, 0.02 mmol) was dissolved in CH_2Cl_2 (10 mL) and degassed with nitrogen for 15 min. The mixture was chilled to -15°C and DDQ (20 mg, 0.08 mmol) was added in one portion, then TFOH (0.5 mL) was added dropwise. After 15 min, the mixture was quenched with H_2O (10 mL) and was extracted with CH_2Cl_2 (30 mL). The organic layer was dried over anhydrous sodium sulfate and the solvent was removed in vacuo. The crude product was further purified by silica gel column chromatography using dichloromethane:petroleum ether (1 : 8) as eluent to afford **9** as red solid (5 mg, 30%).

^1H NMR (400 MHz, $\text{C}_2\text{D}_2\text{Cl}_4$): δ 9.18 (d, $J = 8.7$ Hz, 1H), 8.94 (d, $J = 8.4$ Hz, 1H), 8.80 (s, 1H), 8.65 (s, 1H), 8.56 (s, 1H), 8.46 (s, 1H), 8.35 (d, $J = 8.7$ Hz, 1H), 8.23 (d, $J = 8.8$ Hz, 1H), 7.93 (d, $J = 8.6$ Hz, 2H), 7.64 (d, $J = 6.9$ Hz, 1H), 7.57 (d, $J = 6.9$ Hz, 1H), 7.53 – 7.38 (m, 3H), 7.33 (s, 1H), 7.32 – 7.24 (m, 1H), 6.81 (s, 1H), 1.61 (s, 18H), 1.51 (s, 9H), 1.31 (s, 9H). ^{13}C NMR (400 MHz, $\text{CDCl}_3/\text{CS}_2$): $\delta = 150.4, 150.2, 149.1, 146.7, 145.6, 144.6, 144.5, 143.8, 143.7, 142.5, 141.6, 141.0, 140.8, 140.8, 140.5, 139.8, 139.6, 139.2, 139.2, 139.0, 138.6, 138.2, 135.2, 134.6, 134.5, 133.8, 132.5, 132.2, 132.0, 131.1, 130.4, 130.2, 130.1, 129.1, 128.7, 127.7, 127.3, 126.9, 126.8, 126.5, 125.8, 125.6, 125.4, 125.0, 124.6, 121.9, 121.8, 120.4, 119.9, 118.9, 118.7, 35.3, 35.3, 34.7, 34.4, 31.6, 31.5, 31.2, 31.1$. HR-MALDI-TOF (m/z): Calcd (%) for $\text{C}_{72}\text{H}_{54}$: 918.4225, found: 918.4219.

3. CV and UV Spectra of Compounds

Cyclic voltammograms (CVs) were recorded on a 1000B model electrochemical workstation using glassy carbon discs as the working electrode, Pt wire as the counter electrode, Ag/Ag^+ electrode as the reference electrode, ferrocene/ferrocenium as an internal potential marker, and tetrabutylammonium hexafluorophosphate (TBAPF₆, 0.1 M) as the supporting electrolyte. UV-vis absorption spectra were measured with Hitachi (model U-3010) UV-Vis spectrophotometer (chloroform solution, $\sim 10^{-5}$ M).

4. X-ray Crystallographic Data for **5**, **7**, **8**, **9**, and **9**· C_{60}

Single crystals **5** and **7** suitable for X-ray diffraction analysis could be obtained by slow diffusion of methanol into a chloroform solution at room temperature. Single crystals **9** suitable for X-ray

diffraction analysis could be obtained by slow diffusion of methanol into toluene solution at room temperature. Single crystals **8** suitable for X-ray diffraction analysis could be obtained by slow diffusion of isopropyl alcohol into a CS₂ solution at room temperature. Single crystals of **9.C₆₀** suitable for X-ray diffraction analysis could be obtained by slow diffusion of toluene solution at room temperature. The X-ray diffraction data were collected on a MM007HF Saturn724+ diffractometer with graphite monochromated Cu K α radiation (1.54184 Å). Using Olex2, these structures were solved with the ShelXS and refined with the ShelXL-2014 refinement package using Least Squares minimization. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC 2205342 (**5**), 2205221 (**7**), 2208030 (**8**), 2208032 (**9**), and 2234896(**9.C₆₀**). The single crystal X-ray crystallographic data were summarized in Table S1.

Table S1. Crystal data and structure refinement for **5**, **7**, **8**, **9**, and **9.C₆₀**.

Identification code	5	7	8	9	9.C₆₀
Empirical formula	C ₇₂ H ₅₆ Cl ₂ , CHCl ₃	2C ₇₂ H ₆₀ ,3CHCl ₃	C ₇₂ H ₅₆	C ₇₂ H ₅₄ , 2C ₇ H ₈	C ₇₂ H ₅₄ , C ₆₀
Formula weight	1111.43	2208.50	921.16	1086.34	1639.75
Crystal system	Trigonal	Triclinic	Triclinic	Monoclinic	Monoclinic
Space group	<i>R</i> -3	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ /c	<i>P</i> 2 ₁ /c
Radiation type	Cu K α	Cu K α	Cu K α	Cu K α	Cu K α
Radiation wavelength(Å)	1.54184	1.54184	1.54184	1.54184	1.54184
T(K)	169.99(12)	169.99(11)	169.99(10)	170.00(10)	172.99(10)
a(Å)	31.90908(14)	11.5164(5)	12.6634(6)	11.53234(11)	172.99(10)
b(Å)	31.90908(14)	17.9050(5)	19.4621(6)	17.84770(19)	18.02860(10)
c(Å)	37.27060(18)	31.0340(10)	22.1410(6)	30.0310(3)	26.3919(3)
α (deg)	90	77.629(2)	101.227(2)	90	90
β (deg)	90	80.917(3)	95.079(3)	91.5252(9)	100.3460(10)
γ (deg)	120	84.108(3)	100.078(3)	90	90
V(Å ³)	32864.4(3)	6156.5(4)	5227.1(3)	6178.96(11)	9113.61(15)
Z	18	2	4	4	4
ρ_{calc} (g cm ⁻³)	1.011	1.191	1.171	1.168	1.195
θ , range(°)	2.77 – 75.28	2.533 -75.449	3.444 – 67.002	3.848-63.023	2.307-77.844
R(int)	3.26%	15.34%	10.73%	12.57%	5.86%
μ (mm ⁻¹)	2.070	2.256	0.498	0.496	0.522
F(000)	10440.0	2316.0	1952.0	2307.0	3384.0
Crystal size (mm ³)	0.42 × 0.21 × 0.19	0.3 × 0.13 × 0.11	0.25 × 0.14 × 0.021	0.35 × 0.07 × 0.04	0.21 × 0.11 × 0.01
Index ranges	-33 ≤ h ≤ 39, -40 ≤ k ≤ 39, -46 ≤ l ≤ 46	-14 ≤ h ≤ 14, -22 ≤ k ≤ 22, -9 ≤ l ≤ 38	-14 ≤ h ≤ 14, -23 ≤ k ≤ 22, -24 ≤ l ≤ 26	-13 ≤ h ≤ 13, -16 ≤ k ≤ 20, -34 ≤ l ≤ 31	-24 ≤ h ≤ 24, -20 ≤ k ≤ 22, -33 ≤ l ≤ 33
Absorption correction	spherical harmonics	spherical harmonics	spherical harmonics	spherical harmonics	spherical harmonics

Max. transmission	1.0000	1.0000	1.0000	1.0000	1.0000
Min. transmission	0.33936	0.82986	0.17338	0.15635	0.41165
Goodness-of-fit on F^2	1.049	1.536	1.043	1.069	1.078
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0643$, $wR_2 = 0.1845$	$R_1 = 0.1631$, $wR_2 = 0.4168$	$R_1 = 0.0953$, $wR_2 = 0.2567$	$R_1 = 0.0601$, $wR_2 = 0.1527$	$R_1 = 0.0769$, $wR_2 = 0.2206$
R indices (all data)	$R_1 = 0.0671$, $wR_2 = 0.1871$	$R_1 = 0.2019$, $wR_2 = 0.4440$	$R_1 = 0.1265$, $wR_2 = 0.2838$	$R_1 = 0.0647$, $wR_2 = 0.1590$	$R_1 = 0.0914$, $wR_2 = 0.2338$
Largest diff. peak and hole ($e \cdot \text{\AA}^{-3}$)	1.57 and -1.09	1.10 and -1.05	0.55 and -0.42	0.35 and -0.39	1.19 and -0.41

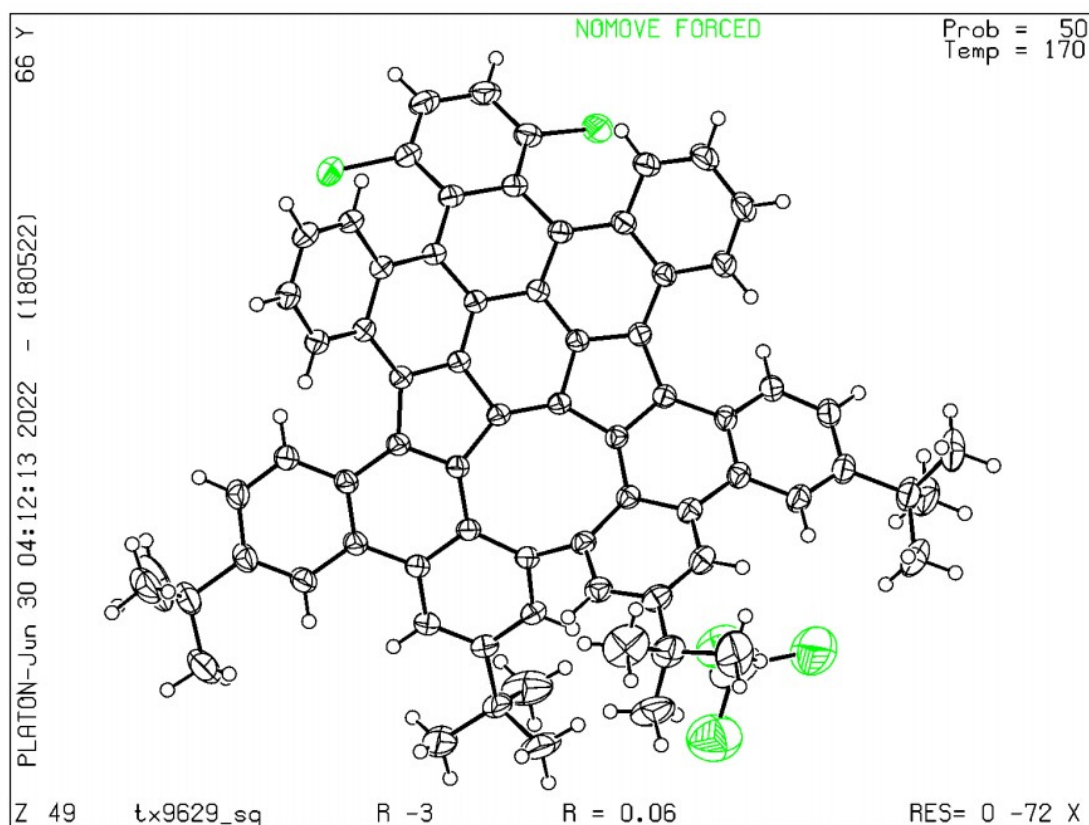


Fig. S1 Ellipsoid plots of **5** with 50% probability ellipsoids. Chlorine atoms are depicted by green ellipsoids; Hydrogens are depicted by white circles.

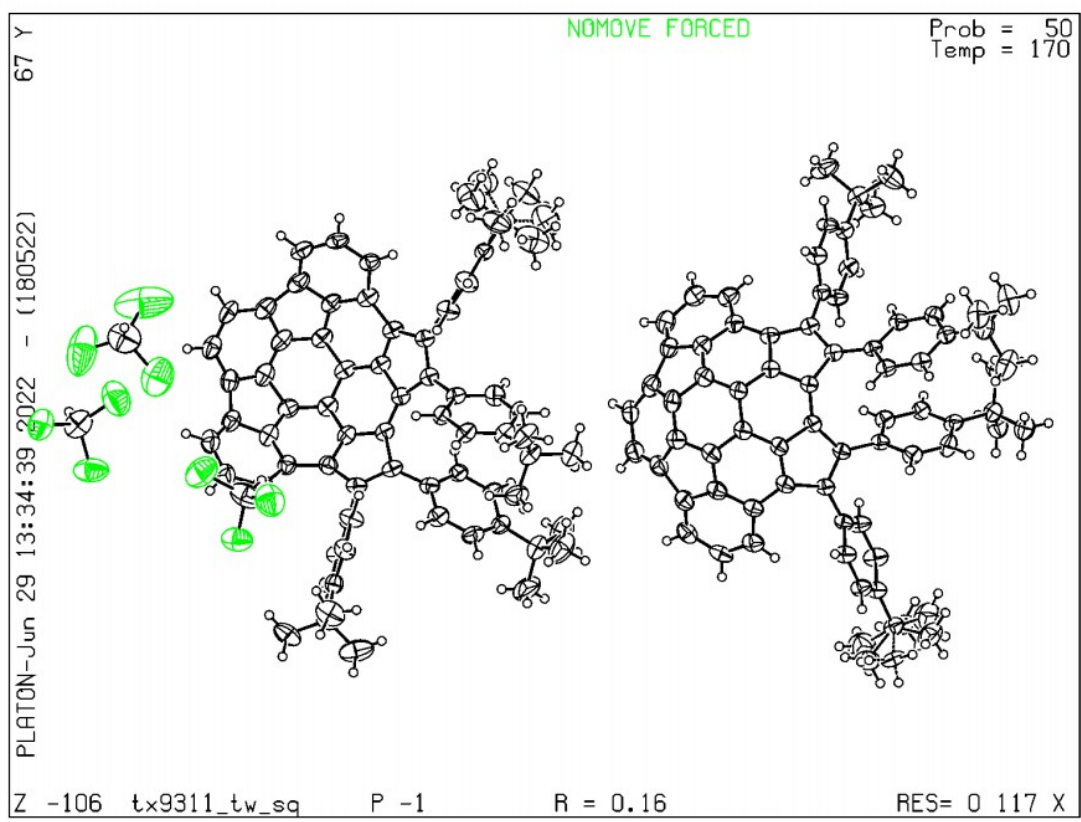


Fig. S2 Ellipsoid plots of 7 with 50% probability ellipsoids. Chlorine atoms are depicted by green ellipsoids; Hydrogens are depicted by white circles.

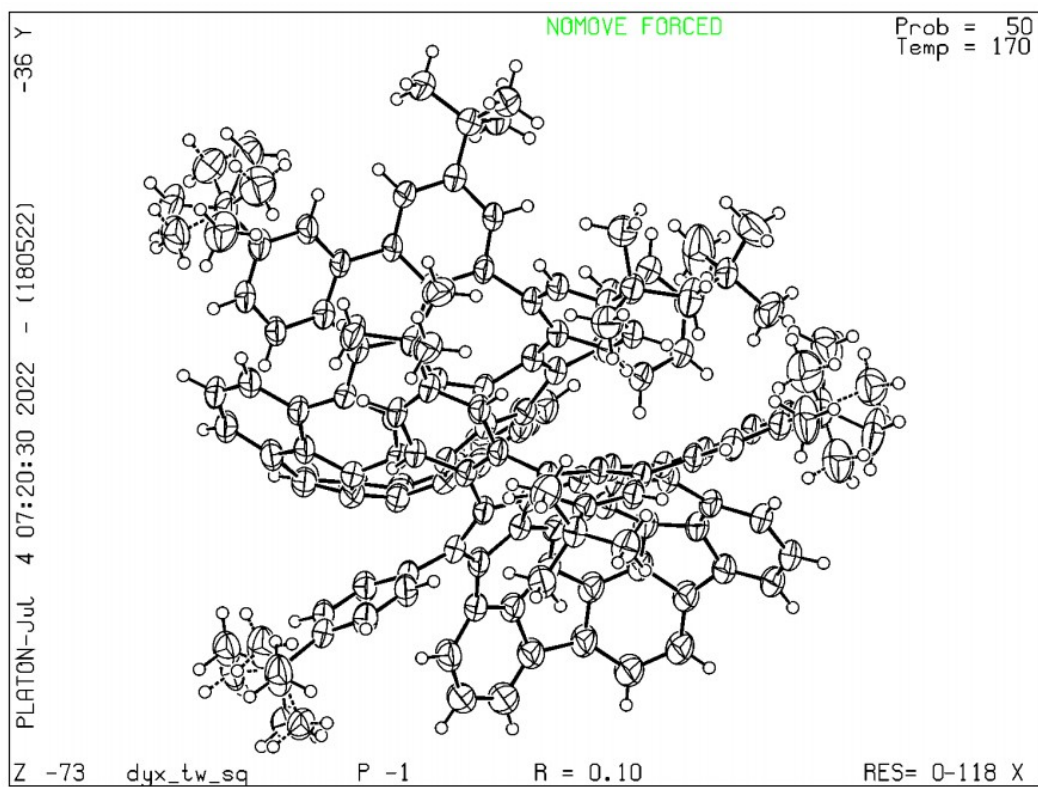


Fig. S3 Ellipsoid plots of **8** with 50% probability ellipsoids. Hydrogens are depicted by white circles.

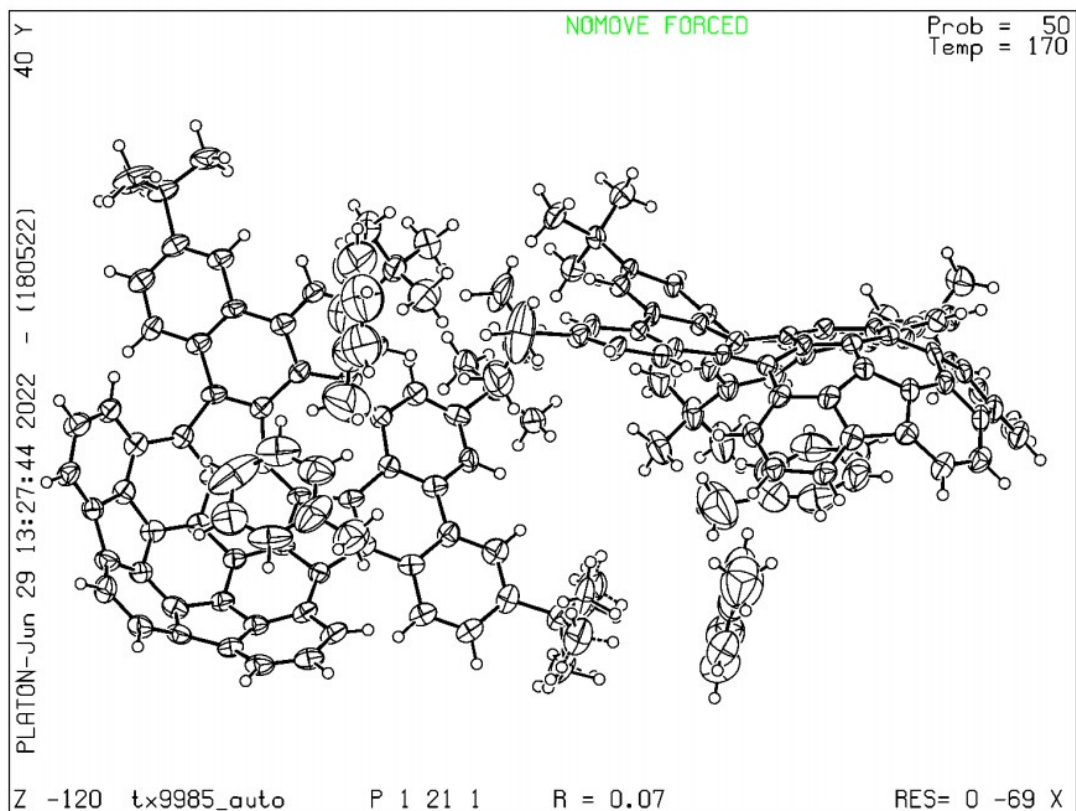


Fig. S4 Ellipsoid plots of **9** with 50% probability ellipsoids. Hydrogens are depicted by white circles.

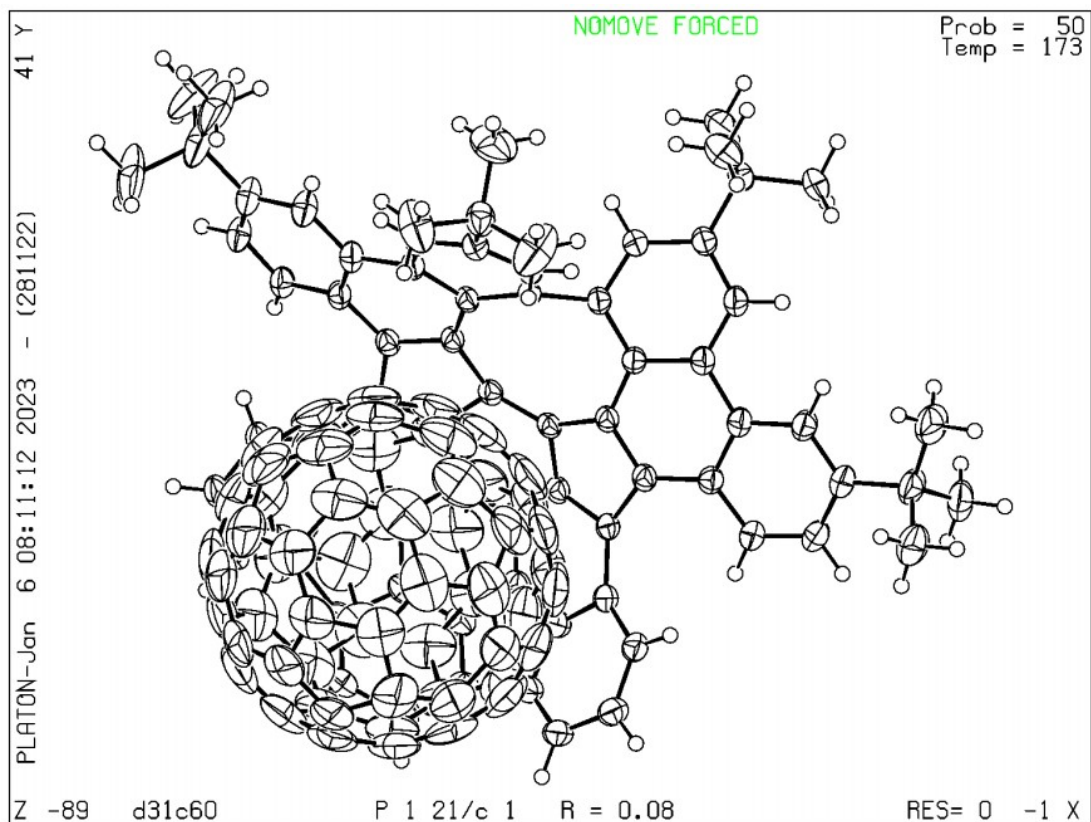


Fig. S5 Ellipsoid plots of **9**·C₆₀ with 50% probability ellipsoids. Hydrogens are depicted by white circles.

5. Density Functional Theory Results

All density functional theory (DFT) calculations were performed using Gaussian 09, Revision D.01 program^[1]. The geometry of **7**, **8** and **9** was optimized at the B3LYP level with the 6-311G(d,p) basis set at gas phase. Time-dependent density functional theory (TD-DFT) UV-vis were calculated at the CAM-B3LYP/6-311G(d,p) level in CHCl₃ with the IEFPCM solvent model and at least the 100 excited states were considered. For better comparison with experimental data, Lorentz broadening with a half width at half height of 0.4 eV was applied to the line spectra obtained. Major orbital transition contributions in excited states were generated using Multiwfn 3.8 software^[2]. NICS values were calculated (B3LYP/6-31G(d,p)) using the standard GIAO procedure (NMR pop=NCSall);^[3] ACID plot (B3LYP/6-31G(d,p)) was calculated by using the method developed by Herges based on the optimized ground-state geometries.^[4] The iso-chemical shielding surface (ICSS)^[5] calculations were carried out and the VMD programme^[6] was used to plot ICSS cube files; Charge transfer integrals were calculated by fragment orbital method with the GGA:PW91/TZP level of theory using Amsterdam Density Functional (ADF) program^[7].

The optimization and freq calculations of the TS were conducted at the B3LYP/6-311G(d,p) level in vacuo and only one imaginary frequency exists. The connection between the transition states and the ground state was confirmed by IRC calculation.

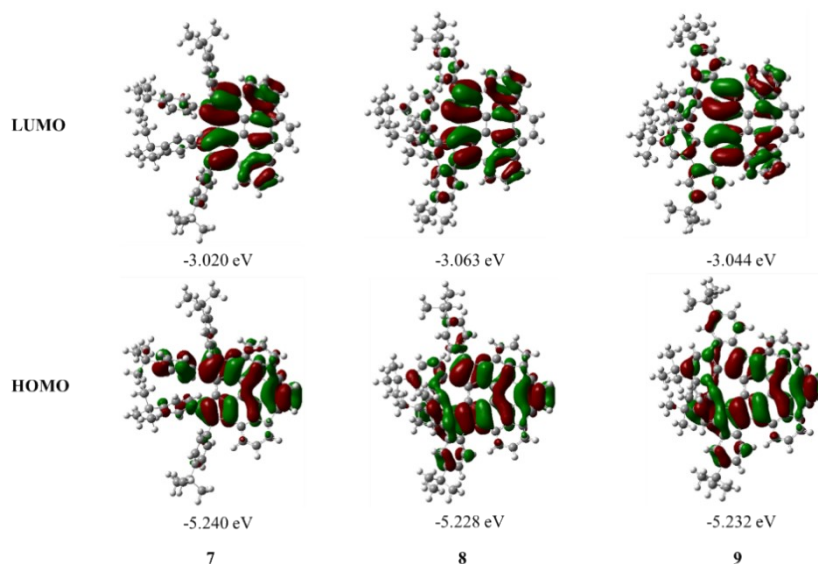


Fig. S6 Frontier orbitals and frontier orbital energies of **7**, **8**, and **9** at the optimized S₀ geometry at B3LYP/6-311G(d,p) level.

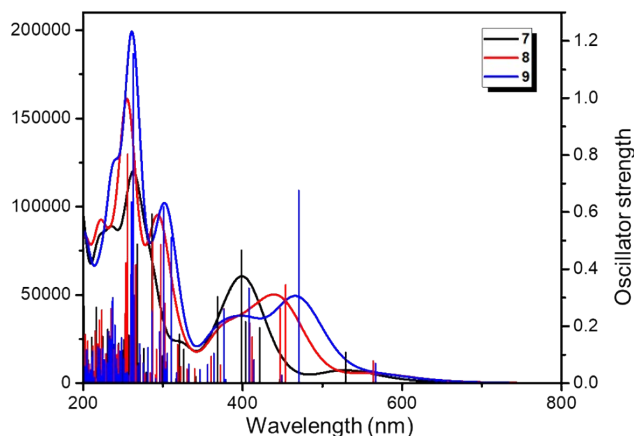


Fig. S7 Calculated UV-vis spectra of **7**, **8**, and **9** at the CAM-B3LYP/6-311G(d,p) level in CHCl₃ solution.

Table S2. TD-DFT singlet excitation energies *E*, excitation wavelengths λ , oscillator strengths *f* > 0.1, and orbital contributions for **7** at the optimized S₀ ground state geometry at the CAM-B3LYP/6-311G(d,p) level in CHCl₃ solution.

Excited state	Energy (eV)	Wavelength (nm)	Osc. Strength	Contributions
S ₁	1.9448	637.52	0.0079	HOMO→LUMO: 94.8%
S ₂	2.3422	529.35	0.1072	HOMO-1→LUMO:79.0% HOMO-2→LUMO:10.2%
S ₄	2.9424	421.37	0.1937	HOMO-3→LUMO:36.8% HOMO-2→LUMO+1:24.4% HOMO-1→LUMO+1:20.5% HOMO-2→LUMO:7.1%
S ₅	3.0732	403.44	0.2151	HOMO-2→LUMO:47.1% HOMO→LUMO+1:31.9% HOMO-2→LUMO+1:6.3%
S ₆	3.1122	398.38	0.4667	HOMO-3→LUMO:49.3% HOMO-2→LUMO+1:18.4% HOMO-1→LUMO+1:17.4%
S ₇	3.3651	368.44	0.3029	HOMO-4→LUMO:73.0% HOMO→LUMO+1:7.4% HOMO-2→LUMO:6.8%
S ₁₁	3.8608	321.14	0.1713	HOMO-4→LUMO+1:51.1% HOMO-3→LUMO+1:16.0%
S ₁₇	4.3327	286.16	0.5928	HOMO→LUMO+2:47.1% HOMO-12→LUMO+1:6.6%
S ₂₄	4.7201	262.67	0.4964	HOMO→LUMO+4:13.2% HOMO-1→LUMO+2:8.0% HOMO→LUMO+5:7.9% HOMO-2→LUMO+3:7.6%

Table S3. TD-DFT singlet excitation energies *E*, excitation wavelengths λ , oscillator strengths *f* > 0.1, and orbital contributions for **9** at the optimized S₀ ground state geometry at the CAM-B3LYP/6-311G(d,p) level in CHCl₃ solution.

Excited state	Energy (eV)	Wavelength (nm)	Osc. Strength	Contributions
S ₁	1.8856	657.53	0.0054	HOMO→LUMO:92.9%
S ₃	2.7311	453.97	0.3449	HOMO-2→LUMO:70.1% HOMO→LUMO+1:12.8%
S ₄	2.7734	447.05	0.2628	HOMO-3→LUMO:31.3% HOMO→LUMO+1:25.8% HOMO-2→LUMO:14.3%
S ₇	3.2899	376.86	0.2602	HOMO-4→LUMO:70.7%

				HOMO-5→LUMO:8.4% HOMO-1→LUMO+1:5.9%
S ₁₃	3.8939	318.41	0.1350	HOMO-6→LUMO:60.2% HOMO-5→LUMO+1:10.9% HOMO-4→LUMO+1:7.3%
S ₁₆	4.1687	297.42	0.4863	HOMO→LUMO+2:54.6%
S ₁₉	4.3168	287.21	0.4942	HOMO-1→LUMO+2:30.4% HOMO→LUMO+4:23.4% HOMO-10→LUMO:6.3% HOMO-1→LUMO+4:5.1%

Table S4. TD-DFT singlet excitation energies E , excitation wavelengths λ , oscillator strengths $f > 0.1$, and orbital contributions for **8** at the optimized S_0 ground state geometry at the CAM-B3LYP/6-311G(d,p) level in CHCl_3 solution.

Excited state	Energy (eV)	Wavelength (nm)	Osc. Strength	Contributions
S ₁	1.9277	643.17	0.0054	HOMO→LUMO:94.9%
S ₃	2.6369	470.19	0.6755	HOMO-2→LUMO: 90.2%
S ₆	3.0398	407.87	0.3317	HOMO-3→LUMO:58.4% HOMO→LUMO+1:31.4%
S ₈	3.2942	376.37	0.2587	HOMO-4→LUMO:76.2%
S ₉	3.4086	363.74	0.1044	HOMO-5→LUMO:79.6%
S ₁₄	3.9888	310.83	0.5117	HOMO→LUMO+2:22.1% HOMO→LUMO+3:15.3% HOMO-8→LUMO:12.9% HOMO-1→LUMO+2:8.3% HOMO-1→LUMO+4:6.2%
S ₁₅	4.0579	305.54	0.1045	HOMO-8→LUMO:29.8% HOMO→LUMO+5:12.2% HOMO→LUMO+2:6.8%
S ₁₇	4.1151	301.29	0.6180	HOMO→LUMO+2:26.4% HOMO→LUMO+3:17.0% HOMO-1→LUMO+4:12.1% HOMO-1→LUMO+5:6.1%
S ₂₀	4.3319	286.21	0.2517	HOMO-10→LUMO:27.5% HOMO-8→LUMO+1:11.4% HOMO→LUMO+6:9.7% HOMO-2→LUMO+2:8.8% HOMO→LUMO+4:5.1%

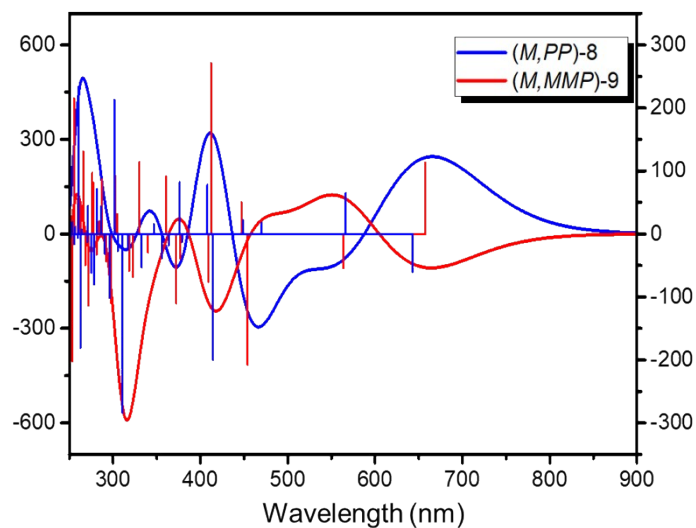


Fig. S8 Calculated CD spectra of *(M,PP)*-**8**, and *(M,MMP)*-**9** at the CAM-B3LYP/6-311G(d,p) level in CHCl_3 solution.

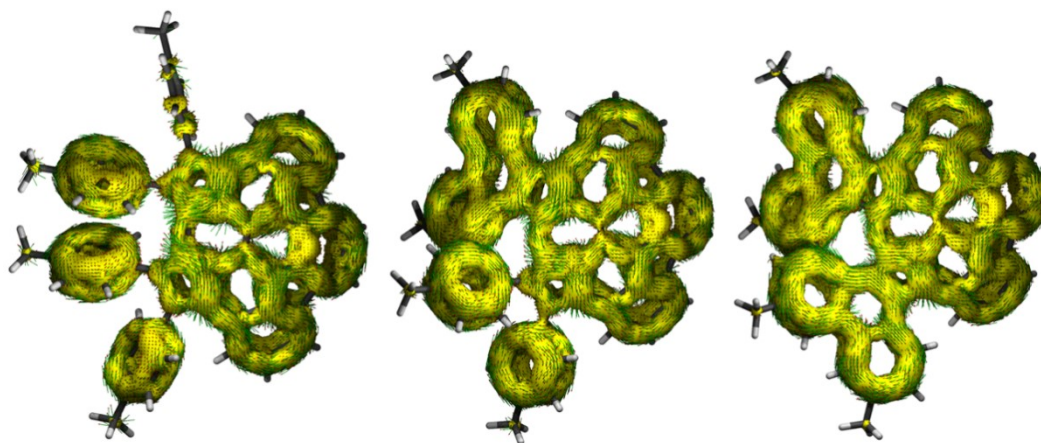


Fig. S9 ACID plots of **7**, **8**, **9**.

Table S5. Cartesian coordinates of optimized structures calculated by B3LYP/6-311G(d,p) level of theory.

7							
C	14.16500000	16.61600000	15.03100000	C	14.65200000	18.38600000	11.70600000
C	14.11500000	17.48500000	16.09000000	H	14.46300000	19.21200000	11.32400000
C	14.36200000	16.79600000	17.36700000	C	15.38300000	17.46600000	10.97700000
C	14.12400000	17.13300000	18.74800000	C	15.59000000	16.23400000	11.60100000
C	13.56800000	18.31900000	19.27600000	H	16.03700000	15.56600000	11.13200000
H	13.52200000	19.08400000	18.74700000	C	15.15900000	15.96900000	12.86800000
C	13.09100000	18.35100000	20.56100000	H	15.35200000	15.14100000	13.24400000
H	12.79200000	19.16200000	20.90200000	C	15.97700000	17.73900000	9.58700000
C	13.03200000	17.21600000	21.39200000	C	17.46900000	17.61200000	9.60200000
H	12.61200000	17.25200000	22.22100000	H	17.83900000	18.24400000	10.22300000
C	13.61200000	16.05200000	20.94500000	H	17.81400000	17.78800000	8.72300000
C	13.45000000	14.58800000	21.30800000	H	17.71200000	16.72200000	9.86900000
C	12.51000000	13.84300000	22.01600000	C	15.54000000	19.08200000	9.05000000
H	12.11700000	14.21500000	22.77500000	H	14.59000000	19.07500000	8.90800000

C	12.13900000	12.54300000	21.61700000	H	15.98700000	19.25600000	8.22000000
H	11.48700000	12.09000000	22.10100000	H	15.76300000	19.76800000	9.68400000
C	12.71800000	11.92500000	20.53700000	C	15.46400000	16.65900000	8.59600000
C	12.21700000	10.97500000	19.45900000	H	15.89200000	15.82200000	8.78700000
C	11.06700000	10.22000000	19.33900000	H	15.66700000	16.92700000	7.69800000
H	10.55800000	10.00300000	20.08700000	H	14.51400000	16.56200000	8.69500000
C	10.68900000	9.78600000	18.05100000	C	12.40800000	14.22800000	13.02600000
H	9.95500000	9.21800000	17.98600000	C	11.65800000	15.38200000	13.18900000
C	11.32900000	10.14400000	16.89300000	H	11.45500000	15.68100000	14.04700000
H	11.02500000	9.82100000	16.07500000	C	11.20600000	16.10600000	12.08100000
C	12.45600000	11.00500000	16.94100000	H	10.69700000	16.87200000	12.21700000
C	12.99400000	11.87200000	15.90200000	C	11.49500000	15.71500000	10.78800000
C	12.42600000	12.22200000	14.58900000	C	12.24200000	14.55400000	10.64100000
C	12.89700000	13.47300000	14.20600000	H	12.45500000	14.25300000	9.78600000
C	13.79400000	13.98200000	15.27300000	C	12.68000000	13.82900000	11.74500000
C	14.28300000	15.25400000	15.61700000	H	13.17100000	13.05100000	11.61100000
C	14.62100000	15.45700000	17.01500000	C	11.01100000	16.54200000	9.58700000
C	14.72500000	14.43300000	17.95800000	C	11.61100000	17.95100000	9.68300000
C	14.61700000	14.77700000	19.28500000	H	11.36700000	18.34800000	10.52300000
C	14.24700000	16.07600000	19.68400000	H	11.27500000	18.49200000	8.96400000
C	14.14200000	13.86700000	20.30600000	H	12.56800000	17.89700000	9.62200000
C	13.81100000	12.59600000	19.92100000	C	11.41800000	15.96200000	8.26600000
C	13.94000000	12.21800000	18.55900000	H	12.37200000	16.01300000	8.17400000
C	14.36800000	13.10400000	17.55100000	H	11.00200000	16.45900000	7.55700000
C	13.85900000	12.91200000	16.25500000	H	11.14000000	15.04500000	8.22000000
C	12.95000000	11.26300000	18.26100000	C	9.47700000	16.65400000	9.62000000
C	13.77700000	18.94600000	16.01200000	H	9.09000000	15.77900000	9.54200000
C	14.69300000	19.93600000	16.30400000	H	9.18000000	17.20300000	8.89100000
H	15.55700000	19.70100000	16.55900000	H	9.20400000	17.05100000	10.45100000
C	14.34500000	21.28100000	16.22600000	C	11.44200000	11.40200000	13.85200000
H	14.97800000	21.92900000	16.43400000	C	10.18900000	11.89600000	13.53400000
C	13.05900000	21.67400000	15.83800000	H	9.97600000	12.77200000	13.76200000
C	12.13500000	20.66400000	15.58400000	C	9.24300000	11.11800000	12.88600000
H	11.26200000	20.88500000	15.34800000	H	8.41700000	11.48800000	12.67600000
C	12.50500000	19.33000000	15.68000000	C	9.50000000	9.79900000	12.54400000
H	11.86600000	18.67500000	15.51300000	C	10.75500000	9.30400000	12.85000000
C	12.72400000	23.16700000	15.71000000	H	10.96700000	8.42800000	12.61800000
C	13.54900000	23.76700000	14.57300000	C	11.70800000	10.09100000	13.49800000
H	14.48200000	23.60300000	14.73300000	H	12.54000000	9.72600000	13.69400000
H	13.39300000	24.71200000	14.52600000	C	8.43700000	8.94400000	11.85300000
H	13.29300000	23.35800000	13.74200000	C	8.78500000	8.70000000	10.44200000
C	11.24100000	23.41500000	15.40100000	H	9.06500000	9.52300000	10.03600000
H	11.05100000	23.13500000	14.50200000	H	8.01700000	8.35800000	9.97900000
H	11.04600000	24.35000000	15.49300000	H	9.49900000	8.06000000	10.39600000

H	10.69900000	22.91300000	16.01300000	C	7.07100000	9.58900000	11.83800000
C	13.00100000	23.89000000	17.05200000	H	6.68400000	9.54400000	12.71400000
H	12.45900000	23.50400000	17.74200000	H	6.50500000	9.12600000	11.21400000
H	12.78900000	24.82300000	16.96300000	H	7.15400000	10.50800000	11.57100000
H	13.92800000	23.79500000	17.28200000	C	8.29500000	7.58300000	12.53400000
C	14.44100000	16.90500000	13.62600000	H	9.15400000	7.15700000	12.58000000
C	14.19200000	18.12500000	12.99100000	H	7.69200000	7.03400000	12.02800000
H	13.70600000	18.77700000	13.43800000	H	7.95000000	7.70400000	13.42200000

TS-7

C	0.71729900	0.71772600	0.04074400	C	-0.94200100	-6.42721300	1.98048500
C	-0.71730300	0.71772700	-0.04067800	C	-3.21950500	-5.75276500	2.81304900
C	-1.38320400	2.01522200	-0.17249700	C	-8.61229900	-1.38859300	-0.15274700
C	-0.68092200	3.17612900	-0.10855800	C	-8.97120800	-2.20825600	1.10004600
C	0.68092400	3.17612700	0.10864200	C	-9.56647600	-0.17343900	-0.22186100
C	1.38320300	2.01521800	0.17257100	C	-8.83364000	-2.28407200	-1.39429400
C	-1.31113200	4.36675300	-0.19084200	H	-1.17999100	8.85823300	-0.11268900
C	-0.67163600	5.59756900	-0.08873100	H	1.18002000	8.85823000	0.11262700
C	0.67164700	5.59756700	0.08876800	H	4.70806400	7.20041600	0.34396000
C	1.31113900	4.36675100	0.19090400	H	6.25857100	5.32000300	0.43717700
C	-1.52468000	6.68273500	-0.16393000	H	5.65333900	2.99472200	0.42088700
C	-0.73117000	7.87120400	-0.07290100	H	-5.65333100	2.99473800	-0.42091900
C	0.73119300	7.87120200	0.07287000	H	-6.25855400	5.32002200	-0.43725500
C	1.52469700	6.68273100	0.16392300	H	-4.70804100	7.20043100	-0.34403700
C	2.65726600	4.51107500	0.31187200	H	4.29119900	-0.98389500	-1.71800100
C	-2.65725600	4.51107900	-0.31184000	H	6.59245000	-1.77492200	-1.75605600
C	2.94128100	5.93994800	0.29869400	H	7.30495400	0.12932800	2.02622200
C	4.29239900	6.19863600	0.35160200	H	5.00483300	0.93973700	2.04444400
C	5.20094900	5.07996400	0.40281700	H	3.06115000	-2.24670000	1.43930300
C	4.85896700	3.73048900	0.39791400	H	3.23469100	-4.58091600	0.77131000
C	3.48148100	3.33866000	0.34619800	H	0.88354800	-3.74570600	-2.72333200
C	-3.48147300	3.33867000	-0.34617300	H	0.69672400	-1.41865900	-2.03556200
C	-4.85895700	3.73050300	-0.39793100	H	-3.06112500	-2.24670700	-1.43928400
C	-5.20093400	5.07997900	-0.40286300	H	-3.23464200	-4.58092700	-0.77130200
C	-4.29238000	6.19864800	-0.35164500	H	-0.88358100	-3.74569100	2.72338900
C	-2.94126500	5.93995500	-0.29869800	H	-0.69677400	-1.41864500	2.03562800
C	2.77589300	2.02515900	0.28661300	H	-4.29126200	-0.98383200	1.71803600
C	-2.77589200	2.02516700	-0.28656600	H	-6.59252000	-1.77485800	1.75603600
C	3.08012500	0.56198600	0.18673200	H	-7.30489900	0.12929900	-2.02631200
C	1.90241900	-0.18949000	0.03748300	H	-5.00478100	0.93969900	-2.04448200
C	-1.90242700	-0.18948600	-0.03744100	H	9.86767500	-2.64118600	1.42580300
C	-3.08012800	0.56199300	-0.18670200	H	8.63861400	-1.74428500	2.32372500
C	4.46190300	0.03865600	0.16480000	H	8.17330100	-3.15512200	1.36874000
C	1.88648100	-1.63890800	-0.25454500	H	10.01346200	-2.53273400	-1.03957700
C	-4.46190800	0.03866300	-0.16480000	H	8.86098200	-1.62091300	-2.01562600

C	-1.88649200	-1.63890400	0.25458700	H	8.35170000	-3.10454700	-1.19118700
C	4.94786600	-0.73679000	-0.89287600	H	9.39605300	0.42683300	1.11832000
C	6.26563900	-1.18728600	-0.90833100	H	10.60798200	-0.50912000	0.23841600
C	7.15474600	-0.89713800	0.13225500	H	9.43267600	0.47679700	-0.64704200
C	6.65980300	-0.12059800	1.19141100	H	3.03901300	-7.73517800	-0.92624900
C	5.35126500	0.34481800	1.20630500	H	3.95229100	-6.38727900	-0.25330600
C	2.57712800	-2.57116400	0.52558400	H	2.35063900	-6.78123300	0.39157500
C	2.67749300	-3.90496400	0.13587200	H	1.09216300	-7.44974600	-2.34004000
C	2.09911600	-4.36897100	-1.05098300	H	0.45486100	-5.86566100	-2.77976900
C	1.36505200	-3.43891500	-1.80215200	H	0.25462900	-6.46236500	-1.13193000
C	1.25207400	-2.11113200	-1.41309800	H	2.78513600	-5.14112300	-3.60802500
C	-2.57711600	-2.57116600	-0.52555500	H	4.19240800	-5.32556300	-2.55640100
C	-2.67746800	-3.90496800	-0.13585000	H	3.38214100	-6.75939900	-3.21162500
C	-2.09910600	-4.36897300	1.05101600	H	-3.03866000	-7.73526600	0.92607800
C	-1.36507600	-3.43890800	1.80220400	H	-3.95195400	-6.38746600	0.25296700
C	-1.25210500	-2.11112200	1.41315300	H	-2.35012500	-6.78122100	-0.39159400
C	-4.94790300	-0.73675100	0.89288400	H	-1.09220500	-7.44971000	2.34021000
C	-6.26567700	-1.18724600	0.90830600	H	-0.45521300	-5.86561500	2.78032400
C	-7.15474900	-0.89713700	-0.13232000	H	-0.25441400	-6.46209100	1.13246900
C	-6.65977600	-0.12061800	-1.19147800	H	-2.78567000	-5.14111300	3.60789300
C	-5.35123800	0.34479900	-1.20634000	H	-4.19268300	-5.32574600	2.55595500
C	8.61229200	-1.38860200	0.15269000	H	-3.38241000	-6.75946900	3.21141800
C	8.83363900	-2.28405000	1.39425700	H	-10.01349600	-2.53269600	1.03950600
C	8.97116800	-2.20830600	-1.10008700	H	-8.35173600	-3.10448800	1.19120000
C	9.56647900	-0.17345200	0.22174500	H	-8.86106400	-1.62083100	2.01557000
C	2.29547000	-5.80390500	-1.57230800	H	-10.60797900	-0.50910300	-0.23859100
C	2.94762300	-6.72308900	-0.52262000	H	-9.39599200	0.42684200	-1.11842900
C	0.94195400	-6.42730700	-1.98015000	H	-9.43272400	0.47681400	0.64693100
C	3.21921700	-5.75269800	-2.81325700	H	-8.17335900	-3.15518500	-1.36871000
C	-2.29546500	-5.80391600	1.57231600	H	-9.86769700	-2.64114300	-1.42588400
C	-2.94730200	-6.72316200	0.52248100	H	-8.63852800	-1.74435300	-2.32377100
(M,PP)-8							
C	2.75988100	1.87693400	1.12567200	H	-7.31949000	-2.37275600	-3.42384100
C	3.49142800	3.08094800	0.76305900	H	-8.83839000	-3.02958600	-2.81321900
C	4.68678800	3.20216400	-0.01361500	H	-7.31433300	-3.51938600	-2.07243200
H	5.30473200	2.33956200	-0.21233300	C	-2.79422500	-1.90673900	2.05510300
C	5.03488800	4.40585700	-0.59707500	H	-3.61860400	-1.22632000	2.22707000
H	5.93940800	4.44431900	-1.19430700	C	-2.77623700	-3.12479400	2.72004100
C	4.21590400	5.56754600	-0.54150000	H	-3.60280200	-3.36544700	3.37555200
H	4.47507100	6.43088700	-1.14468300	C	-1.70076900	-4.00430000	2.57171600
C	3.06705800	5.52460200	0.21296600	C	-0.68662300	-3.61016100	1.69333000
C	1.79101800	6.32591500	0.22557800	H	0.15449300	-4.27180300	1.52469500
C	1.19474600	7.22269100	-0.67249500	C	-1.60029000	-5.34901500	3.31229300
H	1.80158100	7.79238800	-1.36861600	C	-0.31872500	-5.36592000	4.17744300

C	-0.22033600	7.27487600	-0.84682200	H	0.58148700	-5.23993400	3.57192000
H	-0.59782000	7.88014700	-1.66447400	H	-0.23312400	-6.31798000	4.71052700
C	-1.07720400	6.43316100	-0.12419600	H	-0.33795000	-4.56164700	4.91771900
C	-2.37381800	5.72283800	-0.43706500	C	-1.53949500	-6.50317300	2.28472200
C	-3.32640700	5.83153500	-1.42472200	H	-2.43763700	-6.51706300	1.66099200
H	-3.38515600	6.69903600	-2.07316500	H	-1.46792100	-7.46654400	2.79918500
C	-4.20914400	4.73534100	-1.64954300	H	-0.67395000	-6.41297200	1.62456200
H	-4.96227500	4.83801800	-2.42324000	C	-2.80681000	-5.59393600	4.23690200
C	-4.09631100	3.51947400	-1.00025600	H	-2.89104200	-4.82283100	5.00737200
H	-4.73408100	2.69901900	-1.30110900	H	-2.69120000	-6.55581200	4.74364300
C	-3.09968100	3.32799300	0.00558300	H	-3.74701600	-5.62581400	3.67959000
C	-2.57196000	2.08846900	0.53932800	C	0.30963000	-3.22535900	-1.04735500
C	-2.86875900	0.64583000	0.32814500	H	-0.61408700	-3.78759300	-1.11293300
C	-1.77463300	-0.10635400	0.72789700	C	1.35659500	-3.51670100	-1.94297800
C	-1.75947300	-1.50362900	1.19595900	C	2.56681500	-2.90391100	-1.68597900
C	-0.69122200	-2.39477100	0.99215000	H	3.42609200	-3.14581300	-2.29296300
C	0.39851800	-2.27604500	-0.03761300	C	2.72127200	-1.93025300	-0.67732300
C	1.58163000	-1.47528600	0.06297700	C	1.13493600	-4.51554200	-3.08916000
C	1.71185300	-0.21418600	0.75880900	C	2.38964400	-4.68605700	-3.96446800
C	2.94832400	0.45207000	0.77985600	H	2.70257600	-3.73927500	-4.41293200
C	2.80258800	4.31055200	0.94295200	H	2.17716600	-5.38405700	-4.77860900
C	1.50595900	4.37427100	1.47734200	H	3.23098300	-5.09226200	-3.39625100
C	0.90539600	5.60335100	1.05331700	C	0.75839800	-5.89962700	-2.51031800
C	-0.46320700	5.66013700	0.88636200	H	1.55764800	-6.28503800	-1.87127900
C	-1.22934300	4.48585900	1.14629900	H	0.59485500	-6.61729500	-3.32017500
C	-2.37040100	4.50448800	0.32936700	H	-0.15625400	-5.85734200	-1.91481000
C	-1.33466900	2.11673900	1.19870400	C	-0.01574600	-4.00745100	-3.98893200
C	-0.69945100	0.81033000	1.13975300	H	-0.94911900	-3.90262700	-3.43124900
C	0.68143000	0.74115400	1.22501900	H	-0.19341500	-4.70847800	-4.81033100
C	1.41191700	1.98269900	1.50238000	H	0.22763000	-3.03244100	-4.41948500
C	0.77029800	3.21859500	1.69647200	C	4.04304300	-1.40776700	-0.35691100
C	-0.64560900	3.28701200	1.51907000	C	4.15350800	-0.23087000	0.42338300
C	-4.15037100	0.11051200	-0.15536900	C	5.43503800	0.17800600	0.85489000
C	-5.37484500	0.64130200	0.28373400	H	5.51942600	1.02547600	1.52335000
H	-5.37748500	1.46407700	0.98987200	C	6.56590800	-0.51139700	0.48326700
C	-6.58165300	0.11422000	-0.15500500	H	7.52695300	-0.17546700	0.85460500
H	-7.50029200	0.54992800	0.22128900	C	6.48931800	-1.65492300	-0.34646700
C	-6.63567000	-0.95746100	-1.06041100	C	5.22903200	-2.07769700	-0.73711500
C	-5.41257700	-1.47530700	-1.50118400	H	5.14040100	-2.98549000	-1.31418200
H	-5.39133000	-2.29564100	-2.20647800	C	7.77951900	-2.39248200	-0.74189500
C	-4.19828200	-0.95749100	-1.05941100	C	8.50108900	-2.88989100	0.53276100
H	-3.27051400	-1.37632100	-1.43078000	H	8.76672900	-2.06604500	1.19891000
C	-7.99569000	-1.50631400	-1.52372000	H	9.42450100	-3.41280400	0.26559800
C	-8.79557600	-0.38074300	-2.22039100	H	7.86770400	-3.58233400	1.09367400

H	-8.97586800	0.46356700	-1.55121600	C	8.70644900	-1.42003100	-1.50883200
H	-9.76811400	-0.75633000	-2.55315100	H	8.22322100	-1.05853800	-2.42060000
H	-8.25850100	-0.00538800	-3.09572000	H	9.63439700	-1.92577900	-1.79267900
C	-8.78906400	-2.01376500	-0.29668000	H	8.97324600	-0.55022700	-0.90440300
H	-8.24717100	-2.81455600	0.21371300	C	7.51056800	-3.60909100	-1.64572100
H	-9.76153600	-2.40619000	-0.60961500	H	6.89262700	-4.35982100	-1.14572300
H	-8.96907700	-1.21706900	0.42861900	H	8.45839100	-4.08635000	-1.90830200
C	-7.84820500	-2.67442900	-2.51560400	H	7.01677500	-3.32158100	-2.57799500

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C	-0.76917400	0.65243800	0.13168100	C	-0.79723600	-5.18686800	3.33238800
C	0.62532100	0.77873500	0.33561500	C	-0.52899600	-6.42518000	2.44572600
C	1.19872000	2.11568500	0.44371900	C	-1.96226400	-5.52085200	4.28204200
C	0.40427600	3.20214200	0.23421600	C	0.45490900	-4.89076800	4.19015500
C	-0.93752100	3.07181400	-0.07170900	C	-8.15178700	-2.63096200	-0.75237100
C	-1.54535200	1.85787200	-0.08672000	C	-8.06095800	-3.85522400	-1.68145300
C	0.92505200	4.44383100	0.26127200	C	-8.62071000	-3.11626900	0.63940300
C	0.18520800	5.60455500	0.06412300	C	-9.20402300	-1.65986300	-1.33708200
C	-1.14154500	5.47717100	-0.18363300	H	0.36560500	8.89815000	0.17152000
C	-1.66363200	4.19224900	-0.25803600	H	-1.96494400	8.67286400	-0.20085000
C	0.91931300	6.76637600	0.20957600	H	-5.28720600	6.69797100	-0.68429500
C	0.02049800	7.87322700	0.08400200	H	-6.65168900	4.68320800	-0.86468100
C	-1.42417400	7.73351600	-0.15082700	H	-5.84720100	2.42674900	-0.74063300
C	-2.09128900	6.47571600	-0.29705500	H	5.35847600	3.53461000	0.84503500
C	-3.01411700	4.20331400	-0.43083000	H	5.71946200	5.88323500	0.86211400
C	2.23789700	4.71216200	0.49550000	H	3.99977500	7.60226500	0.62937800
C	-3.42523100	5.60028700	-0.47931400	H	5.38393700	1.70415300	1.38813700
C	-4.78695200	5.73705200	-0.63238800	H	7.57338300	0.72007600	1.00889300
C	-5.58473300	4.54187400	-0.72695200	H	5.74374800	-2.59158900	-0.98449600
C	-5.12555200	3.22899000	-0.65169100	H	4.17282300	-3.14410700	-2.05012500
C	-3.73097200	2.96014700	-0.46408800	H	0.05713700	-3.97916400	-1.32425300
C	3.16406100	3.62239300	0.63531600	H	0.77804200	-4.04738700	1.43132600
C	4.48562800	4.16656900	0.76292800	H	-3.09176100	-3.54646200	3.18795300
C	4.69423600	5.54290100	0.76079000	H	-3.43489800	-1.60206500	1.80216900
C	3.68926600	6.56319300	0.62383600	H	-3.54890900	-1.99604200	-1.62732700
C	2.38167300	6.16415000	0.47161400	H	-5.65370800	-3.19663200	-1.89771300
C	-2.92128200	1.71335900	-0.27241200	H	-7.57735600	-0.39320200	0.72485300
C	2.58755000	2.23294500	0.59272100	H	-5.47028500	0.80052400	0.98860200
C	2.98352500	0.77437900	0.48861200	H	8.65975900	-0.41227700	-2.06743500
C	-3.06391000	0.21888800	-0.15056700	H	9.20753100	0.34281500	-0.56798200
C	1.83554000	-0.05017500	0.33481000	H	10.10245500	-1.02285700	-1.24042600
C	-1.81368100	-0.38182900	0.12624000	H	7.75117900	-2.81604500	-2.05452900
C	4.27717200	0.18102800	0.34956500	H	9.20757300	-3.31557000	-1.19386500
C	1.92070100	-1.38977600	-0.17202000	H	7.62348800	-3.70593500	-0.52590800
C	-1.56067800	-1.68926400	0.76462700	H	8.99307000	-0.95737800	1.67449000

C	-4.33841300	-0.50119100	-0.30344900	H	8.29550500	-2.57979700	1.67647900
C	5.46227300	0.79222200	0.81438600	H	9.88869900	-2.29832300	0.95498700
C	6.69625800	0.22131000	0.61360500	H	1.03153600	-5.25088400	-4.79695300
C	6.83167500	-1.00672000	-0.07562800	H	0.04737100	-4.35876900	-3.63164100
C	5.67029500	-1.62641300	-0.50697200	H	1.28694700	-3.51341000	-4.56218000
C	4.38112200	-1.08248000	-0.30308000	H	2.47630200	-6.34648000	-1.49615400
C	3.17803400	-1.80495500	-0.69794300	H	0.75873900	-6.06885100	-1.80462400
C	3.22789000	-2.90084800	-1.58831700	H	1.74069000	-6.91303000	-3.00426400
C	2.10128600	-3.62676900	-1.92231800	H	4.25438800	-5.19827100	-2.93134400
C	0.91617600	-3.32819600	-1.21228600	H	3.41555000	-5.72253300	-4.39003500
C	0.80302900	-2.27896200	-0.31445100	H	3.77880700	-4.01083400	-4.15927600
C	-0.34686300	-2.41456600	0.66676300	H	0.31966500	-6.26808900	1.77631500
C	-0.16373600	-3.51945700	1.51664400	H	-0.30641800	-7.29735900	3.06842100
C	-1.10782600	-3.97224900	2.44151700	H	-1.40221000	-6.66048700	1.83090600
C	-2.30906200	-3.26331100	2.49639600	H	-2.87546300	-5.76830100	3.73389200
C	-2.51306600	-2.15529000	1.68918500	H	-1.69967200	-6.38767800	4.89448200
C	-4.43155100	-1.64492100	-1.10593000	H	-2.18360600	-4.69234000	4.96019900
C	-5.63681000	-2.32445700	-1.25751600	H	1.33154500	-4.68683800	3.57141900
C	-6.80447800	-1.90262700	-0.61164600	H	0.29035000	-4.02126600	4.83213800
C	-6.70478000	-0.75748700	0.19430700	H	0.68836700	-5.74770400	4.82986500
C	-5.50854800	-0.06816300	0.34139900	H	-7.76063700	-3.57546500	-2.69482700
C	8.23040900	-1.60968600	-0.28514600	H	-7.35251200	-4.59882800	-1.30658900
C	9.09979900	-0.61234200	-1.08678500	H	-9.03988100	-4.33726900	-1.74889100
C	8.19006500	-2.93875600	-1.06060000	H	-9.58065800	-3.63520300	0.55673300
C	8.88903600	-1.87387000	1.08939000	H	-7.89570100	-3.80911100	1.07502100
C	2.10274500	-4.76139100	-2.95941400	H	-8.74998100	-2.28562200	1.33692300
C	1.05187400	-4.45062600	-4.05072400	H	-8.89838000	-1.30206400	-2.32398800
C	1.74561900	-6.10014000	-2.27154000	H	-10.16937600	-2.16460500	-1.44179400
C	3.47155600	-4.92506200	-3.64431000	H	-9.35217400	-0.78763800	-0.69636600

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C	-2.95105400	0.04575000	-0.63801900	C	-2.38929600	7.01193700	0.53577100
C	-1.65189200	-0.40196200	-0.39537400	C	-2.72109000	6.01909000	-0.39850600
C	-1.28925300	-1.54938400	0.46386800	C	-3.87578000	5.05635800	-0.57609800
C	-0.10967800	-2.32124200	0.39376700	C	-5.17123100	4.97740200	-0.12060100
C	1.07811400	-2.23165800	-0.53183000	C	-5.85853500	3.73408500	-0.24350300
C	2.08102600	-1.21683600	-0.39288200	C	-5.24974900	2.56220600	-0.65579000
C	1.80962400	0.16210700	-0.11898100	C	-3.87353400	2.55607200	-1.04718100
C	2.82864900	1.08292200	0.16498100	C	-2.92001600	1.45713400	-1.10028900
C	-4.18130900	-0.77651200	-0.51028900	H	-5.08103000	0.31041100	1.11442200
C	-5.19076700	-0.51682100	0.42246900	H	-7.06854500	-1.08189600	1.25371100
C	-6.32507900	-1.32245500	0.50496700	H	-5.58136800	-3.51504500	-1.95516200
C	-6.50849500	-2.42004100	-0.34327500	H	-3.58931800	-2.10977700	-2.08722700
C	-5.49168200	-2.67615800	-1.27425100	H	-8.80271200	-2.27331800	-1.88919600
C	-4.35566700	-1.88083000	-1.35572900	H	-7.83501500	-3.63457500	-2.46238500

C	-7.74913500	-3.32791800	-0.28559100	H	-9.36195400	-3.93337700	-1.62589100
C	-8.47749300	-3.28927000	-1.64933700	H	-8.29987600	-2.92333300	1.80057300
C	-8.74561000	-2.88887600	0.80272100	H	-9.60731100	-3.56167200	0.80356400
C	-7.31096500	-4.77927900	0.01987400	H	-9.11872500	-1.87602000	0.62824400
C	-2.17479200	-1.84570700	1.52393900	H	-6.79419200	-4.83624000	0.98169300
C	-1.96589400	-2.86344900	2.43216000	H	-8.18363000	-5.43834800	0.06208100
C	-0.82142100	-3.66521900	2.35689900	H	-6.63564300	-5.16897600	-0.74505000
C	0.07626400	-3.35519700	1.34102500	H	-3.05168800	-1.23088400	1.64792700
C	-0.58769600	-4.79385700	3.37380200	H	-2.69819200	-3.01505800	3.21703900
C	-0.52869400	-4.19538900	4.79879200	H	0.99634500	-3.91595100	1.26603500
C	0.72498600	-5.55606900	3.11819800	H	-1.45438000	-3.67751500	5.05981100
C	-1.75652100	-5.80326000	3.29147100	H	0.29175400	-3.47812300	4.88608500
C	1.40136100	-3.37941800	-1.23346100	H	-0.36934500	-4.98754700	5.53701800
C	2.70287200	-3.64999400	-1.71708100	H	0.73881000	-6.02166400	2.12907300
C	3.70536900	-2.78264300	-1.32926800	H	0.83664500	-6.35177100	3.85975900
C	3.43498500	-1.57564500	-0.64027400	H	1.59779800	-4.90307800	3.20122800
C	2.95366800	-4.90533100	-2.56791200	H	-1.81746400	-6.24867600	2.29474300
C	4.42158900	-5.02525500	-3.01540800	H	-1.61358900	-6.61008300	4.01705800
C	2.59361900	-6.17188600	-1.75591800	H	-2.71730500	-5.32907300	3.50427700
C	2.06676900	-4.83983600	-3.83315700	H	0.62752600	-4.12952500	-1.34735800
C	4.50088200	-0.67035500	-0.23006700	H	4.72644600	-3.00001100	-1.60245900
C	4.19513500	0.65853700	0.19275700	H	4.73730300	-4.16026600	-3.60488200
C	5.27479400	1.52657600	0.48100800	H	4.54306500	-5.91414600	-3.64013000
C	6.57914600	1.09739200	0.43552600	H	5.10051600	-5.12846500	-2.16437800
C	6.90330100	-0.23575300	0.09128800	H	3.20661300	-6.24340800	-0.85320800
C	5.85604300	-1.07600500	-0.24515800	H	1.54472600	-6.17751500	-1.45130700
C	8.37297300	-0.68645200	0.09613700	H	2.76861100	-7.06923500	-2.35733700
C	8.95895600	-0.50288600	1.51592900	H	2.31058500	-3.96009700	-4.43466700
C	9.17674400	0.17603300	-0.90549200	H	2.22092100	-5.72949700	-4.45154200
C	8.53885300	-2.16361700	-0.30340700	H	1.00525900	-4.78727100	-3.58096200
C	0.28412900	3.32256200	-1.14374600	H	5.07313100	2.55969800	0.72034000
C	-1.06851400	3.04226400	-1.49503200	H	7.36716500	1.80359300	0.66919700
C	-1.55893100	1.74886100	-1.27879800	H	6.07618800	-2.09853100	-0.51083100
C	-0.71857500	0.65723800	-0.80423500	H	8.91239100	0.53801800	1.84378500
C	0.62402200	0.90509400	-0.57621700	H	10.00848200	-0.81206800	1.53559200
C	1.08444400	2.28192100	-0.67161500	H	8.41216000	-1.10773000	2.24434100
C	1.65924400	4.82624100	0.15217300	H	9.13956600	1.23767000	-0.65158500
C	0.64319200	4.60992300	-0.78905800	H	8.78590700	0.06111700	-1.92004500
C	-0.31507600	5.66157100	-0.68548200	H	10.22770900	-0.12875600	-0.90853100
C	-1.62328600	5.40175600	-1.03568600	H	8.01470300	-2.83276500	0.38437900
C	-1.97590500	4.08754900	-1.47022100	H	8.17343600	-2.35485200	-1.31607100
C	-3.32119000	3.86076500	-1.15983500	H	9.59832100	-2.43205700	-0.28041600
C	2.28120300	2.46911700	0.03467200	H	4.02221500	3.44370700	2.15418400
C	2.53282200	3.78840500	0.58764000	H	3.76490800	5.59749000	3.20980500

C	3.33117900	4.15195400	1.71595800	H	1.99507500	7.19109400	2.58418100
C	3.15812700	5.37522000	2.33881300	H	-0.87269400	7.94110000	1.74781100
C	2.15747500	6.31696900	1.96305500	H	-3.16315900	7.51497000	1.10634300
C	1.37031900	6.04322000	0.86753400	H	-5.66880500	5.81550000	0.35509800
C	0.03301300	6.54166600	0.36125900	H	-6.89856100	3.69305200	0.06177900
C	-1.03411100	7.26571300	0.91402900	H	-5.82164100	1.64591000	-0.65114800
TS2-8							
C	1.62541200	-2.30045100	-1.02436400	C	-7.34737200	-2.44770200	2.65404800
C	2.50355800	-3.29620300	-1.48111200	C	-8.62061100	-1.74820800	2.12373100
C	3.88558600	-3.34960500	-1.26758700	C	-7.29287300	-2.25132300	4.18002300
C	4.42651200	-2.37589300	-0.45040500	C	-7.43978000	-3.96452900	2.36657000
C	3.65643000	-1.28210700	-0.03957500	C	-1.42882700	-6.25043800	-1.41969100
C	4.27762500	-0.23577400	0.76401800	C	-1.21643200	-7.27430100	-0.28027500
C	5.36031400	-0.51311000	1.61870100	C	-0.51221900	-6.63739600	-2.59383900
C	5.93240400	0.44155100	2.45193000	C	-2.89439500	-6.32920300	-1.90956000
C	5.36513600	1.72982000	2.43371200	H	2.09818300	-4.14807000	-1.99428400
C	4.31334100	2.03989600	1.59333700	H	5.47188600	-2.40155100	-0.18304500
C	3.76499300	1.08739500	0.71321000	H	5.72416500	-1.53134400	1.66562000
C	2.65280600	1.31605200	-0.16700500	H	5.72991400	2.49666100	3.10404400
C	2.13719800	2.54892700	-0.81257800	H	3.86172600	3.01741400	1.66346700
C	2.44620900	3.97251100	-0.75428100	H	4.42617700	4.16131300	0.15638600
C	3.52101100	4.67833400	-0.12455900	H	4.26064000	6.52783200	0.61344600
C	3.42521300	6.03444700	0.12884700	H	2.18893300	7.82191100	0.21244500
C	2.25830900	6.80305600	-0.15247100	H	-0.89999300	8.16458200	0.07634300
C	1.24289200	6.20715200	-0.86206300	H	-3.22151800	7.48730900	0.14286000
C	1.44922400	4.84023000	-1.27020500	H	-5.53809000	5.55130700	0.55374200
C	0.30066400	4.38092300	-1.92686700	H	-6.49941700	3.36576900	1.17832500
C	-0.69486300	5.39713700	-1.85911100	H	-5.42951100	1.26446100	0.61823400
C	-0.20834900	6.51737100	-1.14726000	H	-3.16298700	-0.24542100	2.51690100
C	-1.18279200	7.30725800	-0.52565700	H	-5.09856200	-1.13869100	3.70597500
C	-2.55543600	6.90751200	-0.48771500	H	-6.78079300	-2.42819700	-0.02879700
C	-2.98904100	5.71209900	-1.07390800	H	-4.84328600	-1.52351900	-1.20859100
C	-2.02047200	5.01541800	-1.83363200	H	-2.49077000	-2.54708600	1.16484300
C	-2.33504400	3.62655000	-1.89852200	H	-2.62137400	-4.90676400	0.71413700
C	-3.52629500	3.41292300	-1.18257100	H	0.49643300	-4.46065000	-2.11968200
C	-4.02944700	4.67935200	-0.71709200	H	4.34434600	-5.87738000	-0.21787700
C	-5.10997400	4.64686600	0.13509200	H	4.81740600	-6.67164800	-1.72933300
C	-5.63095200	3.38216300	0.52892300	H	3.17961000	-6.04199000	-1.53417400
C	-5.03295300	2.17855000	0.20033500	H	4.87830400	-3.55146000	-3.84396300
C	-3.87669600	2.15003200	-0.63829800	H	5.11362600	-5.30727700	-3.86239000
C	-2.89305700	1.09318500	-0.81193900	H	3.48970600	-4.63201400	-3.70438700
C	-2.70684300	-0.21616700	-0.16732200	H	6.61706200	-3.41317400	-1.95149800
C	-3.84611900	-0.82772300	0.56553300	H	6.41571500	-4.40564300	-0.49636800
C	-3.95434800	-0.73008700	1.95548200	H	6.76306700	-5.16986800	-2.04568300

C	-5.06300200	-1.24129700	2.62932400	H	5.80680100	-0.68949400	4.97922500
C	-6.11045600	-1.86826600	1.94538900	H	7.46103100	-1.32139600	5.03225800
C	-5.99553600	-1.95408400	0.54916200	H	6.31155500	-1.94332100	3.84338800
C	-4.89564500	-1.44223400	-0.12877000	H	8.62620300	0.28265700	1.82478800
C	-1.81119200	-2.96113700	0.44104700	H	9.11711000	-0.75225400	3.17610600
C	-1.90915000	-4.30314200	0.16452300	H	7.99532300	-1.36155600	1.95572400
C	-1.15423600	-4.83399900	-0.89351100	H	7.96273600	2.06792700	3.55936800
C	-0.14030800	-4.02254100	-1.37388700	H	6.83921300	1.65258300	4.86587600
C	0.16098800	-2.69948100	-0.93750600	H	8.45091100	0.93955100	4.82507800
C	-0.93170800	-2.07127100	-0.23058000	H	-8.74287100	-1.88733500	1.04729700
C	-1.40267500	-0.68972200	-0.38478500	H	-9.50959800	-2.15453400	2.61575000
C	-0.69077600	0.38127200	-1.12045400	H	-8.58542700	-0.67313000	2.32003200
C	-1.68808600	1.37362500	-1.46931900	H	-6.42784800	-2.75101900	4.62438800
C	-1.36756000	2.63471100	-1.98693400	H	-8.19000300	-2.67780300	4.63651700
C	0.00764000	3.03014700	-1.99086600	H	-7.25551700	-1.19328200	4.45320300
C	0.95544300	2.14242800	-1.46202800	H	-6.55285100	-4.48596300	2.73676500
C	0.63047800	0.76054200	-1.14276700	H	-8.31700400	-4.39210300	2.86171400
C	1.82912100	0.22078800	-0.49954700	H	-7.52710800	-4.17057900	1.29741300
C	2.29059800	-1.13535100	-0.45976700	H	-0.18657300	-7.24251600	0.08538100
C	4.71029200	-4.49654400	-1.87697200	H	-1.42082400	-8.28840200	-0.63765800
C	4.23047900	-5.85116000	-1.30493300	H	-1.87799500	-7.08137800	0.56727100
C	4.53367400	-4.49524900	-3.41312700	H	0.54007000	-6.66932700	-2.29779300
C	6.21246800	-4.35425800	-1.56951200	H	-0.77885300	-7.63459700	-2.95408500
C	7.10036500	0.05737200	3.37885500	H	-0.61415800	-5.94501800	-3.43413400
C	6.63990200	-1.04145500	4.36493200	H	-3.60009400	-6.09765800	-1.10869700
C	8.27773200	-0.47651300	2.53026000	H	-3.07051700	-5.62190700	-2.72454000
C	7.61078700	1.25541500	4.20090500	H	-3.12002000	-7.33545100	-2.27629900
(P,MM)-8							
C	2.77772000	1.85509100	-1.12268600	H	-7.23896900	-3.54863000	1.56636200
C	3.52177100	3.05063000	-0.75745300	H	-8.99842200	-3.40618700	1.49691300
C	4.71714600	3.15788900	0.02123800	H	-8.02277300	-3.08235900	0.05422700
H	5.32531000	2.28836000	0.21994300	C	-2.81482900	-1.86643700	-2.06829100
C	5.07746400	4.35703000	0.60665600	H	-3.63129000	-1.17674100	-2.24110700
H	5.98140800	4.38490800	1.20534900	C	-2.80877400	-3.08376600	-2.73482300
C	4.27130800	5.52765200	0.55116500	H	-3.63650700	-3.31450500	-3.39241400
H	4.53893000	6.38741900	1.15576200	C	-1.74346900	-3.97529300	-2.58521100
C	3.12323900	5.49811000	-0.20512600	C	-0.72683900	-3.59341900	-1.70422800
C	1.85602900	6.31328900	-0.21867300	H	0.10659700	-4.26449000	-1.53473900
C	1.26824200	7.21539300	0.67965300	C	-1.65627900	-5.32021200	-3.32709000
H	1.88022800	7.77759800	1.37735700	C	-0.37322200	-5.35028700	-4.18964000
C	-0.14642500	7.28268800	0.85204500	H	0.52707900	-5.23467600	-3.58218000
H	-0.51849700	7.89096700	1.66994700	H	-0.29691900	-6.30273400	-4.72344200
C	-1.01132100	6.45118600	0.12715600	H	-0.38215600	-4.54518000	-4.92920900
C	-2.31591900	5.75449500	0.43739300	C	-1.61028800	-6.47608000	-2.30064600

C	-3.26838800	5.87226900	1.42410200	H	-2.50977800	-6.48069600	-1.67873100
H	-3.31843800	6.73950500	2.07362800	H	-1.54837100	-7.43962700	-2.81603200
C	-4.16309100	4.78536800	1.64650900	H	-0.74509500	-6.39620700	-1.63868900
H	-4.91579300	4.89507000	2.41966700	C	-2.86355000	-5.55087900	-4.25435700
C	-4.06279100	3.56926800	0.99561700	H	-2.93760600	-4.77823000	-5.02432600
H	-4.70959200	2.75532400	1.29474000	H	-2.75760400	-6.51354700	-4.76170300
C	-3.06732500	3.36822500	-0.00955100	H	-3.80517900	-5.57277400	-3.69897400
C	-2.55270000	2.12370000	-0.54472500	C	0.26813700	-3.22320000	1.03893600
C	-2.86580800	0.68381900	-0.33723300	H	-0.66161700	-3.77573300	1.10177200
C	-1.77876800	-0.07936500	-0.73587800	C	1.31002100	-3.52685200	1.93639800
C	-1.77762600	-1.47594000	-1.20626900	C	2.52730100	-2.92681700	1.68265800
C	-0.71957300	-2.37901400	-1.00144800	H	3.38266700	-3.17871700	2.29110600
C	0.36927700	-2.27352900	0.03068600	C	2.69431800	-1.95366200	0.67550800
C	1.56114300	-1.48544200	-0.06644400	C	1.07511100	-4.52461200	3.08088400
C	1.70633000	-0.22494600	-0.76040000	C	2.32595000	-4.70966300	3.95877400
C	2.95002400	0.42783400	-0.77835600	H	2.64812900	-3.76681800	4.40898000
C	2.84666200	4.28788500	-0.93695500	H	2.10411700	-5.40622300	4.77164800
C	1.55160300	4.36637800	-1.47321500	H	3.16409300	-5.12433900	3.39195800
C	0.96382200	5.60140700	-1.04858600	C	0.68497500	-5.90386400	2.49955500
C	-0.40433400	5.67285000	-0.88353600	H	1.48146700	-6.29711300	1.86185200
C	-1.18282000	4.50728700	-1.14603500	H	0.51186600	-6.62068800	3.30817100
C	-2.32476500	4.53717600	-0.33066100	H	-0.22779000	-5.85099400	1.90200300
C	-1.31394900	2.13955500	-1.20180700	C	-0.07202500	-4.00519700	3.97870800
C	-0.69303000	0.82625500	-1.14392100	H	-1.00294900	-3.88967300	3.41903700
C	0.68717900	0.74216500	-1.22701300	H	-0.25909600	-4.70521200	4.79888600
C	1.43158300	1.97602100	-1.50141200	H	0.18084900	-3.03335500	4.41094200
C	0.80373100	3.21906600	-1.69486700	C	4.02229900	-1.44516400	0.35825900
C	-0.61161600	3.30266100	-1.51946800	C	4.14702400	-0.26865700	-0.42048700
C	-4.15426500	0.16070700	0.14122300	C	5.43373100	0.12670200	-0.84916700
C	-5.36974600	0.70821500	-0.28959200	H	5.52857500	0.97392000	-1.51654000
H	-5.36401100	1.53768300	-0.98785200	C	6.55633000	-0.57539300	-0.47623900
C	-6.58874500	0.19236300	0.14483300	H	7.52167200	-0.24953600	-0.84539100
H	-7.49719500	0.64646500	-0.22851100	C	6.46575100	-1.71894400	0.35204700
C	-6.65321200	-0.88404700	1.03637400	C	5.20021500	-2.12839300	0.73990900
C	-5.43105300	-1.42201300	1.47108700	H	5.10066000	-3.03580700	1.31580500
H	-5.42522800	-2.25128100	2.16936900	C	7.74711400	-2.47095600	0.74898200
C	-4.21362300	-0.91901900	1.03699300	C	8.46581700	-2.97436500	-0.52493500
H	-3.29036400	-1.35233900	1.40275400	H	8.74160700	-2.15251700	-1.18942200
C	-7.97929900	-1.47671400	1.54195000	H	9.38302400	-3.50753000	-0.25666800
C	-8.04253700	-1.35699200	3.08268900	H	7.82613400	-3.65920000	-1.08803600
H	-7.99084000	-0.31042300	3.39498100	C	8.68296700	-1.50961500	1.51908800
H	-8.98045300	-1.77808100	3.45766400	H	8.20181300	-1.14407400	2.43034000
H	-7.22097300	-1.89062100	3.56574200	H	9.60478700	-2.02576700	1.80416800
C	-9.20536200	-0.75451900	0.95425200	H	8.96043800	-0.64197100	0.91635400

H	-9.23665500	-0.82741600	-0.13621000	C	7.46325700	-3.68583100	1.65057700
H	-10.12006200	-1.21127500	1.34138200	H	6.83809300	-4.42907400	1.14837800
H	-9.22435200	0.30387700	1.22792100	H	8.40533100	-4.17376300	1.91421100
C	-8.06075500	-2.96831800	1.14093900	H	6.97089300	-3.39424000	2.58233900
<i>(M,MMP)-9</i>							
C	0.33682100	-2.27280400	0.27991300	C	-0.95977600	-2.26733200	-0.49786700
C	0.32399600	-3.24406000	1.27713300	C	-2.00981200	-1.30514900	-0.38627400
H	-0.62894500	-3.70765300	1.49836800	C	-1.80932200	0.09975100	-0.20597400
C	1.46621400	-3.67047000	1.97958400	C	-0.66605200	0.90163600	-0.68294900
C	2.67455200	-3.16707200	1.54201700	C	-1.19809000	2.26000800	-0.74284200
H	3.59211100	-3.51128300	1.99454900	C	-0.45891800	3.36012600	-1.18161700
C	2.75690100	-2.16926400	0.55052800	C	0.91524000	3.17247800	-1.50762500
C	4.05673500	-1.73862400	0.05244700	C	1.46994100	1.89512400	-1.34657600
C	5.22435500	-2.51736800	0.22497200	C	0.68484700	0.72021900	-0.94846800
H	5.14327900	-3.44648500	0.76826400	C	1.69546400	-0.31422500	-0.64866700
C	6.44769100	-2.16980100	-0.32505800	C	1.56177600	-1.58536400	0.01472500
C	6.50130600	-0.98950100	-1.10339200	C	1.32996200	-4.68181400	3.12840900
H	7.42554400	-0.70515800	-1.59261100	C	0.41010800	-4.08627000	4.21980400
C	5.38978300	-0.19814500	-1.27796000	H	0.83083800	-3.16033800	4.62089800
H	5.44968000	0.67625300	-1.91329800	H	-0.58511500	-3.85915400	3.83120200
C	4.15175200	-0.53401400	-0.68578000	H	0.29381800	-4.79429200	5.04620700
C	2.96732800	0.25186600	-0.84055700	C	0.71097300	-5.99654600	2.59886400
C	2.84429700	1.68683300	-1.15502600	H	0.60747000	-6.72104300	3.41250900
C	3.70701300	2.83394400	-0.91367700	H	-0.28037900	-5.83657200	2.16931900
C	4.98982300	2.87068100	-0.28261200	H	1.34405600	-6.44182500	1.82635200
H	5.55615400	1.96340400	-0.13203200	C	2.68722300	-5.01602800	3.77308500
C	5.49537400	4.05327000	0.22563900	H	2.53886700	-5.71908700	4.59702400
H	6.46240300	4.02909500	0.71615500	H	3.37214100	-5.48518400	3.06128400
C	4.76984200	5.27692400	0.23142600	H	3.17233000	-4.12529900	4.18136200
H	5.16518000	6.12684800	0.77706300	C	7.71478600	-3.02461400	-0.15528300
C	3.54156200	5.31484600	-0.38701000	C	7.47612100	-4.26542100	0.72384300
C	3.10160400	4.11179700	-1.04587000	H	8.40841600	-4.82741000	0.82436200
C	1.76054300	4.26851600	-1.42884200	H	7.14515000	-3.99319800	1.72982100
C	1.31107400	5.55182100	-0.98595400	H	6.73305500	-4.93796400	0.28682400
C	2.33801400	6.21808600	-0.28314200	C	8.20327300	-3.50423100	-1.54239800
C	1.91514200	7.18337900	0.64200400	H	9.10829100	-4.11030200	-1.43670100
H	2.63641300	7.71785600	1.25151400	H	7.44066800	-4.11393900	-2.03431500
C	0.53516500	7.35871500	0.96111800	H	8.43915900	-2.66724200	-2.20331000
H	0.29785100	8.01407400	1.79274400	C	8.81972400	-2.17037700	0.50987800
C	-0.46034500	6.57554400	0.36002000	H	9.73287900	-2.76080400	0.63237700
C	-0.02300400	5.72755900	-0.68087200	H	9.06992600	-1.29121300	-0.08806300
C	-0.90863000	4.61801500	-0.82068600	H	8.50321100	-1.82431300	1.49759300
C	-1.95948500	4.76109100	0.09723500	C	-8.31791500	-1.10049500	0.23406700
C	-1.77211000	5.98842500	0.82604700	C	-9.18426800	-0.36729100	-0.81719200

C	-2.59467700	6.19976400	1.90921800	H	-10.21606200	-0.72942000	-0.77580100
H	-2.50417400	7.07949200	2.53705300	H	-9.20413600	0.71170800	-0.64896900
C	-3.52746900	5.18510500	2.26567800	H	-8.80253000	-0.54126200	-1.82678500
H	-4.16031600	5.35469500	3.12995200	C	-8.89174700	-0.83501600	1.64584700
C	-3.59882900	3.95688100	1.63307100	H	-9.92172400	-1.19890900	1.71084900
H	-4.23880100	3.19557400	2.05869500	H	-8.30070500	-1.34777800	2.40950100
C	-2.76269000	3.66332600	0.51138800	H	-8.89895100	0.23005000	1.88812400
C	-2.41207600	2.37100100	-0.05005600	C	-8.40644100	-2.61203600	-0.04268600
C	-2.87758100	0.96416900	0.07940400	H	-9.44846900	-2.93577400	0.02379500
C	-4.21921300	0.47066000	0.15107500	H	-8.04751700	-2.86415500	-1.04428100
C	-5.34191400	1.30016000	0.38673300	H	-7.83391300	-3.19338600	0.68520600
H	-5.19645000	2.35909500	0.53354900	C	-2.75160500	-5.19843100	-2.24197800
C	-6.62145500	0.80011600	0.39569400	C	-4.22677700	-5.43591800	-2.61208600
H	-7.44374700	1.48065900	0.58275600	H	-4.32034600	-6.37710400	-3.16030400
C	-6.87625700	-0.57172600	0.16464600	H	-4.86332900	-5.50901800	-1.72587600
C	-5.78904300	-1.37611400	-0.12900200	H	-4.61714200	-4.63976700	-3.25175400
H	-5.95726400	-2.42572400	-0.31363300	C	-2.28341500	-6.37383600	-1.35214100
C	-4.45871000	-0.89588800	-0.17383700	H	-2.42500200	-7.32449600	-1.87537300
C	-3.35015700	-1.76153900	-0.55197800	H	-1.22563800	-6.29338600	-1.09230600
C	-3.57705400	-3.02901800	-1.13715300	H	-2.85660400	-6.41018800	-0.42152200
H	-4.59345800	-3.32192700	-1.34923200	C	-1.92251800	-5.18313500	-3.54742800
C	-2.54346500	-3.86788200	-1.50138600	H	-2.04920700	-6.12579700	-4.08870800
C	-1.24550100	-3.48363700	-1.09942400	H	-2.24236800	-4.36833900	-4.20241100
H	-0.43020300	-4.18877400	-1.20606800	H	-0.85641100	-5.05212400	-3.34901800

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C	-1.02361600	2.39935000	-1.23273700	C	-7.27311000	0.13340700	4.38363100
C	-1.74920600	3.49604200	-1.72335800	C	6.23594400	2.42151600	3.50727500
C	-3.08663500	3.80533200	-1.44731100	C	7.70503900	2.00388700	3.26208700
C	-3.73710700	2.98995800	-0.54282300	C	5.83004100	2.04287700	4.95101400
C	-3.15127700	1.78984000	-0.12327300	C	6.14458700	3.95187100	3.36928600
C	-3.91323600	0.89579800	0.74054300	C	2.69614200	5.67804700	-2.07369100
C	-4.87600700	1.39105300	1.63911600	C	2.93694900	6.71500300	-0.95210000
C	-5.57142900	0.57918700	2.52788300	C	1.67129000	6.26779500	-3.05972500
C	-5.26014100	-0.79379300	2.51849200	C	4.01683600	5.44149400	-2.84398900
C	-4.33442300	-1.31486900	1.63548700	H	-1.24645400	4.21858200	-2.33845600
C	-3.66440100	-0.50140200	0.70140000	H	-4.74336300	3.21397400	-0.22336400
C	-2.66512800	-0.95430300	-0.22584500	H	-5.03688500	2.46079900	1.67426200
C	-2.40214100	-2.29020200	-0.82061000	H	-5.72619400	-1.46416800	3.22828500
C	-2.95472800	-3.63253500	-0.67697700	H	-4.07456300	-2.35933700	1.71079400
C	-4.12615300	-4.10172700	-0.00147000	H	-4.92080000	-3.41752900	0.25656000
C	-4.26646900	-5.43774000	0.32848400	H	-5.16754300	-5.74824900	0.84599100
C	-3.25810900	-6.41446400	0.08410500	H	-3.36317000	-7.40790500	0.50603100
C	-2.16519000	-6.04737500	-0.66516900	H	-0.37928300	-8.30798900	0.35700000
C	-2.13450300	-4.68983700	-1.14964300	H	2.02673600	-8.06312400	0.35125100

C	-0.93257400	-4.47612900	-1.83752000	H	4.76936600	-6.58018100	0.48583800
C	-0.13204000	-5.64747200	-1.71585400	H	6.20404400	-4.59083800	0.81744200
C	-0.79598500	-6.62598600	-0.94145800	H	5.48973400	-2.35786500	0.23075100
C	0.03729500	-7.54511400	-0.29247700	H	4.44894700	-1.49757900	1.69342900
C	1.46194600	-7.40011400	-0.29587000	H	5.89091100	-0.28608500	3.20986700
C	2.08986900	-6.33229500	-0.94839000	H	4.42459000	3.42050100	1.65729500
C	1.23870000	-5.50800000	-1.71913800	H	3.97773700	4.10189800	-0.23529200
C	1.78610100	-4.19938700	-1.84380300	H	0.34266000	4.38105400	-2.33731800
C	3.00965600	-4.16618000	-1.16173000	H	-3.02395300	6.43698900	-0.57102800
C	3.31570300	-5.48949100	-0.67829500	H	-3.45924000	7.20336000	-2.10797200
C	4.46401800	-5.62846500	0.06514800	H	-1.94449300	6.30918600	-1.96242600
C	5.25612800	-4.46844800	0.30495000	H	-4.19924900	4.01084800	-3.97347400
C	4.84774800	-3.18823200	-0.02341900	H	-4.12530000	5.77536400	-4.11393200
C	3.60231800	-2.96509400	-0.69258900	H	-2.63730100	4.83269300	-3.99305900
C	2.78969900	-1.76183800	-0.83272000	H	-5.33638000	5.33997200	-0.62182000
C	2.78065700	-0.40027800	-0.23822900	H	-5.64830300	6.05576200	-2.20169300
C	3.67158000	0.24420100	0.68657700	H	-5.80494700	4.31068900	-1.98702900
C	4.49481600	-0.42213300	1.61970000	H	-5.09327900	1.71435900	5.01083900
C	5.29635100	0.27376400	2.49720000	H	-6.59298200	2.64996500	5.12996100
C	5.32772700	1.68559400	2.50845000	H	-5.41510200	3.01910400	3.86587800
C	4.48439100	2.34242900	1.62574800	H	-7.28107600	2.73278700	2.08561000
C	3.63652400	1.65930000	0.72765200	H	-8.21659500	1.23580800	2.03410000
C	2.71006000	2.38382500	-0.13483100	H	-8.42830900	2.36995700	3.37827600
C	3.03666300	3.67417300	-0.55235900	H	-6.55451700	-0.39081900	5.01926800
C	2.23109700	4.34739100	-1.45570100	H	-8.00181500	0.61547700	5.04071500
C	0.98498500	3.78035800	-1.72522300	H	-7.80800900	-0.60920400	3.78525800
C	0.49830900	2.55399800	-1.23294000	H	8.02150500	2.26781300	2.24931400
C	1.51906300	1.72707400	-0.60995600	H	8.36707200	2.51281300	3.96940300
C	1.62183200	0.29571900	-0.64470700	H	7.84844500	0.92824400	3.38698800
C	0.74536100	-0.67739400	-1.29094500	H	4.79458900	2.33020000	5.15229400
C	1.56303100	-1.85601000	-1.51545700	H	6.47286800	2.55619400	5.67279500
C	1.01657900	-3.05796600	-1.98750500	H	5.91961000	0.96917900	5.13056700
C	-0.40964500	-3.20309500	-1.98421900	H	6.43749500	4.28753300	2.37064100
C	-1.18496400	-2.13557700	-1.50922400	H	6.81938100	4.42527900	4.08741700
C	-0.62048600	-0.81630000	-1.28779200	H	5.13594400	4.32049700	3.57437500
C	-1.67211500	-0.03917600	-0.63695500	H	3.69978700	6.37939800	-0.24592500
C	-1.85851900	1.38402700	-0.60124800	H	2.01852900	6.90126700	-0.38887800
C	-3.73778500	5.03842000	-2.09693800	H	3.27414000	7.66480600	-1.37860000
C	-2.99346700	6.32126100	-1.65777300	H	1.45664500	5.58136800	-3.88349200
C	-3.66723400	4.90411800	-3.63573800	H	0.72907400	6.52369600	-2.56696500
C	-5.21774300	5.18632900	-1.69790800	H	2.07063900	7.18797900	-3.49420800
C	-6.59209100	1.19636300	3.50161400	H	3.87399800	4.71503500	-3.64842000
C	-5.87804100	2.20630500	4.42999300	H	4.80501300	5.06265200	-2.18958600
C	-7.69287300	1.92810400	2.69886900	H	4.37085500	6.37706000	-3.28801000

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C	-0.33689800	-2.27289100	0.27981000	C	0.95973600	-2.26740800	-0.49792400
C	-0.32408200	-3.24406100	1.27713000	C	2.00977800	-1.30520900	-0.38629100
H	0.62885900	-3.70761500	1.49842700	C	1.80928700	0.09968900	-0.20603700
C	-1.46629400	-3.67040400	1.97961900	C	0.66602900	0.90159000	-0.68300200
C	-2.67463500	-3.16703600	1.54200300	C	1.19809100	2.25995300	-0.74292400
H	-3.59219400	-3.51119700	1.99456000	C	0.45893800	3.36008700	-1.18169700
C	-2.75696100	-2.16927200	0.55047700	C	-0.91524300	3.17246900	-1.50763700
C	-4.05679000	-1.73859900	0.05242200	C	-1.46996100	1.89512400	-1.34656000
C	-5.22441500	-2.51732800	0.22496400	C	-0.68487700	0.72019300	-0.94850400
H	-5.14331700	-3.44646900	0.76819800	C	-1.69550600	-0.31423900	-0.64869800
C	-6.44777200	-2.16970500	-0.32500100	C	-1.56183000	-1.58540900	0.01464000
C	-6.50137700	-0.98937900	-1.10329200	C	-1.33003600	-4.68172400	3.12847700
H	-7.42562000	-0.70501400	-1.59247900	C	-0.41005200	-4.08623100	4.21978900
C	-5.38984500	-0.19804100	-1.27787300	H	-0.83072700	-3.16029600	4.62093600
H	-5.44974900	0.67636700	-1.91318700	H	0.58514200	-3.85913200	3.83109900
C	-4.15180000	-0.53396600	-0.68575400	H	-0.29370300	-4.79427000	5.04616800
C	-2.96736400	0.25189200	-0.84052600	C	-0.71113700	-5.99647100	2.59888100
C	-2.84430800	1.68686300	-1.15494500	H	-0.60760100	-6.72098100	3.41251000
C	-3.70697300	2.83399400	-0.91349200	H	0.28019100	-5.83652500	2.16926500
C	-4.98971300	2.87073700	-0.28229300	H	-1.34429500	-6.44171800	1.82641400
H	-5.55602500	1.96346600	-0.13164500	C	-2.68726700	-5.01587800	3.77326200
C	-5.49520100	4.05333000	0.22601300	H	-2.53887400	-5.71889900	4.59722700
H	-6.46218200	4.02916600	0.71661400	H	-3.37224900	-5.48505600	3.06153600
C	-4.76965700	5.27697500	0.23171700	H	-3.17232200	-4.12511500	4.18152400
H	-5.16492800	6.12689900	0.77739100	C	-7.71490800	-3.02448700	-0.15529000
C	-3.54143600	5.31488600	-0.38684400	C	-7.47635600	-4.26546900	0.72363600
C	-3.10155600	4.11183400	-1.04574600	H	-8.40872000	-4.82735000	0.82411900
C	-1.76051800	4.26852600	-1.42882400	H	-7.14529400	-3.99344300	1.72963700
C	-1.31099600	5.55182700	-0.98596900	H	-6.73341500	-4.93805700	0.28647500
C	-2.33787200	6.21811300	-0.28309200	C	-8.20345300	-3.50380200	-1.54248800
C	-1.91492500	7.18340400	0.64203000	H	-9.10857000	-4.10974400	-1.43690300
H	-2.63615900	7.71789300	1.25156500	H	-7.44093400	-4.11354700	-2.03448600
C	-0.53492800	7.35872500	0.96104300	H	-8.43918300	-2.66666000	-2.20326600
H	-0.29753000	8.01408600	1.79264000	C	-8.81977100	-2.17026600	0.50999800
C	0.46052800	6.57553000	0.35987700	H	-9.73298600	-2.76062900	0.63235100
C	0.02310800	5.72754300	-0.68097300	H	-9.06987300	-1.29095200	-0.08776400
C	0.90870100	4.61797300	-0.82082000	H	-8.50325400	-1.82443400	1.49779300
C	1.95960500	4.76104300	0.09705500	C	8.31782800	-1.10065200	0.23433000
C	1.77230900	5.98840200	0.82583300	C	9.18439800	-0.36704900	-0.81645600
C	2.59493700	6.19973800	1.90896400	H	10.21620100	-0.72912400	-0.77490200
H	2.50448600	7.07947900	2.53678000	H	9.20414500	0.71190100	-0.64790800
C	3.52770700	5.18506000	2.26541400	H	8.80293800	-0.54072800	-1.82620200
H	4.16060700	5.35465400	3.12964300	C	8.89129100	-0.83561400	1.64635400

C	3.59899700	3.95681300	1.63283500	H	9.92124200	-1.19955400	1.71152300
H	4.23897000	3.19549800	2.05843100	H	8.30002700	-1.34859700	2.40968700
C	2.76277900	3.66326600	0.51121600	H	8.89844900	0.22937800	1.88896700
C	2.41209300	2.37093100	-0.05017100	C	8.40645600	-2.61210200	-0.04293200
C	2.87757500	0.96410800	0.07931500	H	9.44846400	-2.93585100	0.02378500
C	4.21918200	0.47058800	0.15103500	H	8.04787700	-2.86386200	-1.04473900
C	5.34190600	1.30009300	0.38662800	H	7.83369600	-3.19373300	0.68455700
H	5.19645800	2.35904600	0.53330900	C	2.75161300	-5.19840600	-2.24216100
C	6.62142500	0.80001400	0.39566300	C	4.22673700	-5.43569400	-2.61262900
H	7.44374700	1.48054700	0.58260700	H	4.32028800	-6.37682400	-3.16094400
C	6.87618600	-0.57187300	0.16476600	H	4.86350900	-5.50879500	-1.72657700
C	5.78897000	-1.37625000	-0.12888300	H	4.61685800	-4.63944100	-3.25232000
H	5.95715500	-2.42587500	-0.31344900	C	2.28376100	-6.37387000	-1.35220700
C	4.45865400	-0.89598100	-0.17379300	H	2.42541300	-7.32452000	-1.87544000
C	3.35012200	-1.76160400	-0.55194300	H	1.22601500	-6.29357700	-1.09219200
C	3.57704900	-3.02907700	-1.13713800	H	2.85712500	-6.41009800	-0.42169300
H	4.59346300	-3.32195800	-1.34918800	C	1.92220900	-5.18319900	-3.54739600
C	2.54347500	-3.86790600	-1.50147500	H	2.04880100	-6.12588000	-4.08865800
C	1.24547900	-3.48366800	-1.09955500	H	2.24187200	-4.36842500	-4.20249700
H	0.43020300	-4.18881000	-1.20629500	H	0.85614400	-5.05221000	-3.34874800
TS_{rot}-8							
C	2.88637700	1.68292400	0.94312300	H	-7.64270600	-3.18728600	-0.75110100
C	3.70451100	2.81792300	0.54213900	H	-9.14922500	-2.91099900	-1.63199900
C	4.86024300	2.83925700	-0.30012300	H	-8.64290800	-1.78493900	-0.36155300
H	5.37842800	1.92506900	-0.54767100	C	-2.76148700	-1.36222600	2.54074200
C	5.29037400	4.01512400	-0.88652700	H	-3.49246300	-0.57989500	2.70783900
H	6.15887800	3.97698600	-1.53504000	C	-2.75292100	-2.47458000	3.36136900
C	4.59510000	5.25016900	-0.76718100	H	-3.49118200	-2.54066500	4.15240300
H	4.90587200	6.09611500	-1.37059800	C	-1.79629500	-3.48791100	3.19651200
C	3.48965700	5.30495000	0.04928300	C	-0.88453300	-3.32308800	2.15602400
C	2.30247900	6.23023600	0.14701000	H	-0.13238400	-4.07888600	1.97596600
C	1.74604200	7.21281000	-0.68558200	C	-1.78400400	-4.70282400	4.13945900
H	2.36414000	7.74559800	-1.40075600	C	-0.66347700	-5.70128200	3.79741500
C	0.33428200	7.41764100	-0.76656600	H	-0.77248300	-6.10587500	2.78751700
H	-0.02504100	8.09389700	-1.53523500	H	-0.69725400	-6.54244400	4.49502600
C	-0.56083000	6.63892100	-0.01934200	H	0.32659000	-5.24490700	3.87831100
C	-1.95246900	6.09018100	-0.24025100	C	-3.13780700	-5.44375000	4.04016700
C	-3.02496900	6.42636300	-1.02619900	H	-3.97538500	-4.79844600	4.31452600
H	-3.07109200	7.35239900	-1.58813200	H	-3.14812100	-6.30753300	4.71206700
C	-4.10560200	5.50319100	-1.08699000	H	-3.31176100	-5.80309700	3.02212400
H	-5.00534400	5.79705600	-1.61646000	C	-1.57103500	-4.21900800	5.59302900
C	-4.06344600	4.23303800	-0.54351800	H	-0.61805900	-3.69263800	5.69248600
H	-4.95987600	3.64764700	-0.64306200	H	-1.56313800	-5.07140500	6.27937400
C	-2.91022600	3.74068900	0.16114900	H	-2.36314000	-3.53915900	5.91480200

C	-2.44847600	2.39169700	0.53789000	C	-0.15557100	-3.30569400	-0.74432300
C	-2.84624400	0.91607500	0.35011100	H	-1.11917500	-3.79690800	-0.68059700
C	-1.80154700	0.12811700	0.84077700	C	0.77920700	-3.74253200	-1.70400600
C	-1.83088200	-1.19762700	1.49544800	C	2.04930300	-3.20816700	-1.61027100
C	-0.87954900	-2.20452600	1.29949300	H	2.82436200	-3.56308200	-2.27244300
C	0.10000400	-2.29077800	0.16528400	C	2.37396100	-2.18216300	-0.69740100
C	1.34482800	-1.58973500	0.10187800	C	0.37645700	-4.80056300	-2.74279100
C	1.63071100	-0.31233700	0.71170100	C	1.52977900	-5.14555300	-3.70207100
C	2.92098300	0.23870600	0.62293300	H	1.87625900	-4.26640100	-4.25199500
C	3.14595700	4.10535700	0.77249200	H	1.18931300	-5.88141200	-4.43540900
C	1.88853400	4.28196400	1.37128700	H	2.38327700	-5.57983500	-3.17404100
C	1.39477900	5.57219000	1.00290200	C	-0.05807800	-6.09989700	-2.02487800
C	0.03455300	5.76356400	0.91046700	H	0.75978500	-6.50465300	-1.42240200
C	-0.82224000	4.65283800	1.15542000	H	-0.34810200	-6.85857200	-2.75827200
C	-2.00407700	4.81056700	0.43114000	H	-0.91183300	-5.93497700	-1.36385200
C	-1.17454000	2.31517800	1.14060300	C	-0.80471300	-4.25960400	-3.58204400
C	-0.65319100	0.96319900	1.14025500	H	-1.67027200	-4.02394100	-2.95892000
C	0.71870200	0.75186100	1.18629300	H	-1.11614000	-5.00280000	-4.32262400
C	1.57457900	1.91648800	1.38495000	H	-0.51952800	-3.34769800	-4.11329100
C	1.05449200	3.19891700	1.60420400	C	3.75519000	-1.75279600	-0.52157100
C	-0.35554100	3.39707600	1.47070600	C	4.02821900	-0.56284700	0.19970100
C	-4.03841600	0.31567000	-0.29014300	C	5.37174200	-0.25478200	0.51003900
C	-5.03028100	1.06372200	-0.93329500	H	5.58263500	0.59899000	1.14104300
H	-4.92165700	2.12486800	-1.00360300	C	6.40640500	-1.04796100	0.07173100
C	-6.13777600	0.48917900	-1.55372700	H	7.41972100	-0.78488000	0.35165700
H	-6.85243500	1.15143000	-2.02520300	C	6.16596300	-2.20297200	-0.70926000
C	-6.32620500	-0.89127400	-1.58420800	C	4.84637400	-2.52960400	-0.97588100
C	-5.31258300	-1.65948000	-0.98740600	H	4.63551900	-3.44292200	-1.51072700
H	-5.37557000	-2.74189600	-1.00412300	C	7.35283700	-3.05667100	-1.18624600
C	-4.21004600	-1.08784800	-0.37816000	C	8.13462600	-3.58372700	0.04004300
H	-3.46875100	-1.75349100	0.03099000	H	8.52138300	-2.76986100	0.65735500
C	-7.53733500	-1.57052700	-2.23927400	H	8.98652800	-4.18883000	-0.28502600
C	-7.05527000	-2.49425200	-3.38241700	H	7.49521700	-4.20698100	0.67091300
H	-6.52373800	-1.92241600	-4.14777600	C	8.28984800	-2.18506000	-2.05532400
H	-7.90927800	-2.98748000	-3.85691600	H	7.76341900	-1.80444500	-2.93481500
H	-6.38094000	-3.27253400	-3.01816500	H	9.14503400	-2.77492100	-2.39906700
C	-8.52878800	-0.55131200	-2.82919100	H	8.67857100	-1.32774000	-1.50123200
H	-8.92362200	0.12090700	-2.06255600	C	6.90896500	-4.26650400	-2.02806200
H	-9.37654900	-1.07876500	-3.27456200	H	6.27702900	-4.95145600	-1.45624700
H	-8.06923200	0.05560100	-3.61399500	H	7.78859100	-4.82739600	-2.35478200
C	-8.28465400	-2.41475000	-1.18033200	H	6.36209200	-3.95954900	-2.92380100

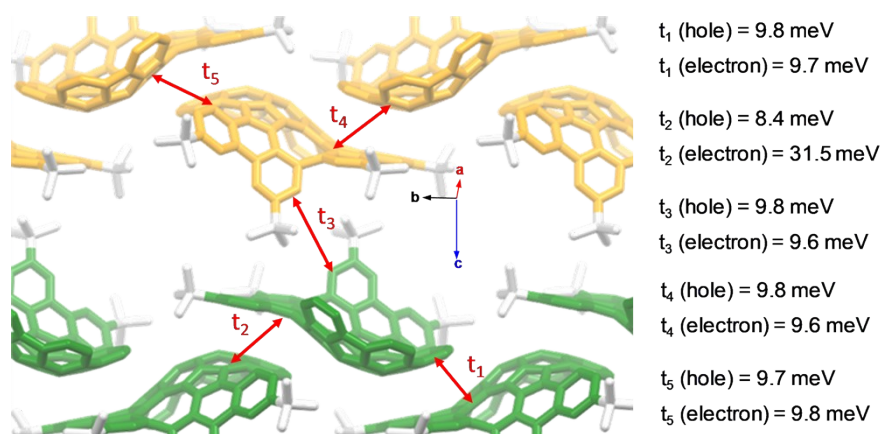


Fig. S10 The calculated transfer integrals of **9**.

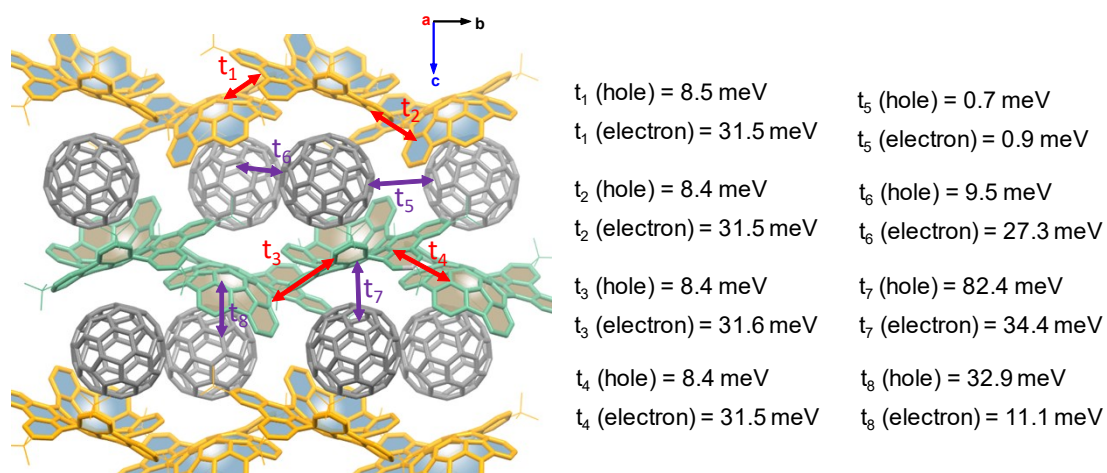


Fig. S11 The calculated transfer integrals of **9·C₆₀**.

6. VT-NMR spectra of 7, 8, and 9

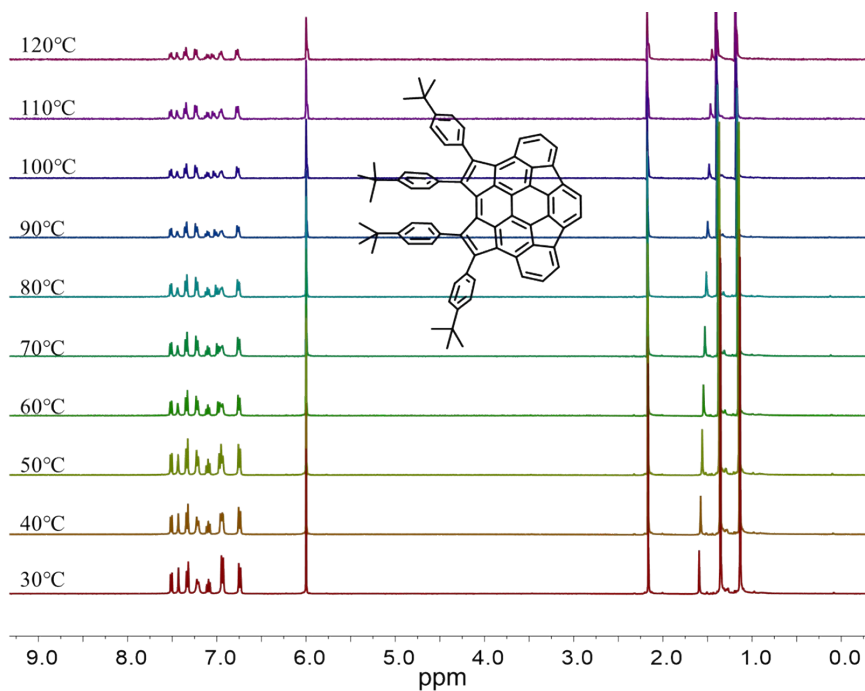


Fig. S12 Variable-temperature ^1H NMR spectra of **7** in 1,1,2,2-tetrachloroethane- d_2 .

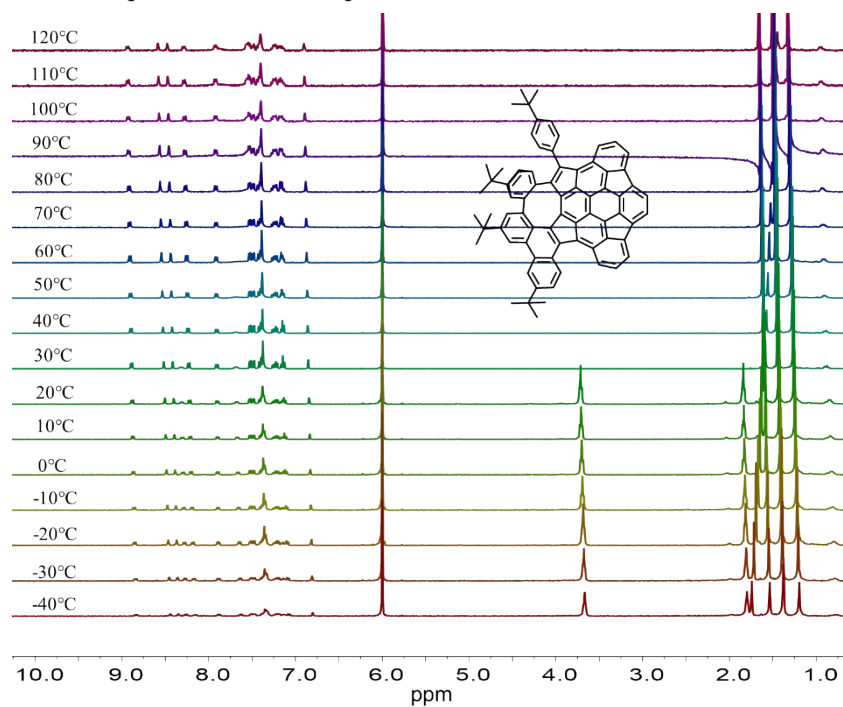


Fig. S13 Variable-temperature ^1H NMR spectra of **8** in 1,1,2,2-tetrachloroethane- d_2 .

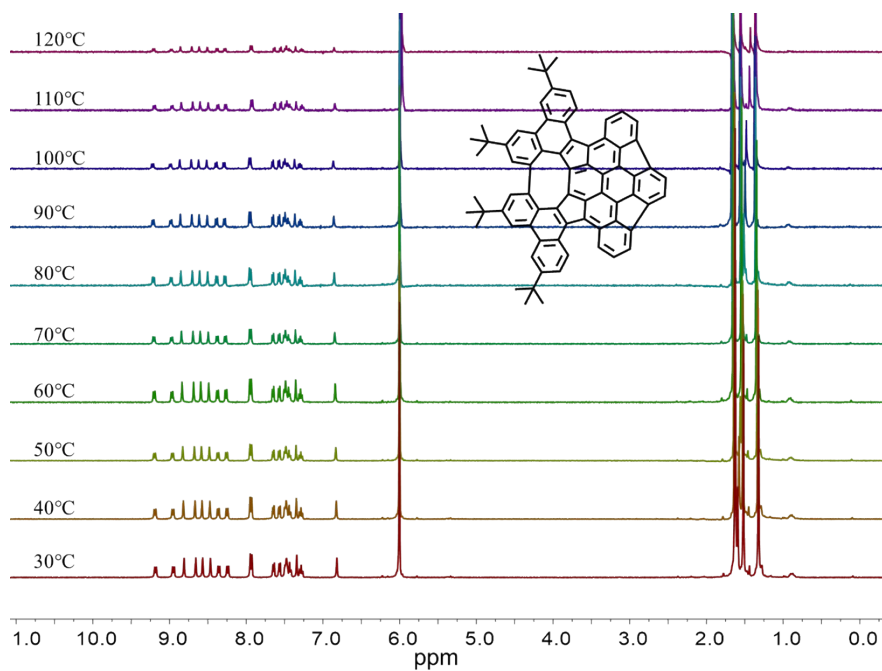


Fig. S14 Variable-temperature ^1H NMR spectra of **9** in 1,1,2,2-tetrachloroethane- d_2 .

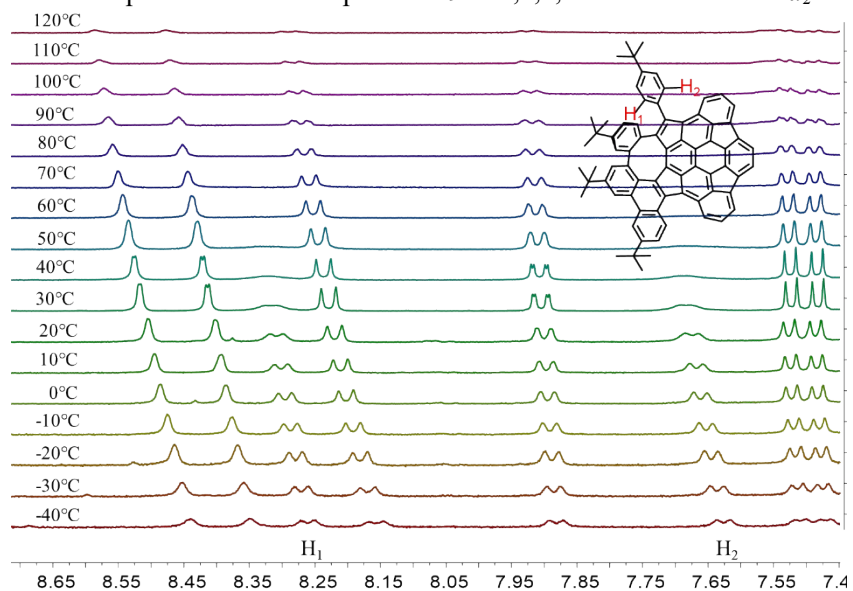


Fig. S15 Variable-temperature ^1H NMR spectra of **8** in 1,1,2,2-tetrachloroethane- d_2 .

For the coalescence temperature k_{exch} for **8** can be calculated using^[8]:

$$k_{\text{exch}} = \frac{\pi\Delta V_0}{\sqrt{2}} \quad (1)$$

$$k_{\text{exch}} = \frac{k_b T_c}{h} e^{-\Delta G^\ddagger / RT_c} \quad (2)$$

$h = 6.626 \cdot 10^{-34} \text{ J} \cdot \text{sec}$, $T_c = \text{coalescence temperature in K}$; $k_b = 1.381 \cdot 10^{-23} \text{ J/K}$, $R = 3.814 \text{ J/mol} \cdot \text{K}$,

In this particular case, $\Delta\nu = 252 \text{ Hz}$. $\Delta G^\ddagger = 15.4 \text{ kcal} \cdot \text{mol}^{-1}$ ($T_c = 333 \text{ K}$).

7. Chiral HPLC analysis and kinetic study of racemization barrier of **8** and **9**

HPLC analysis was conducted on a Shimadzu LC-20A instrument equipped with equipped with a CHIRALPAK® IC column.

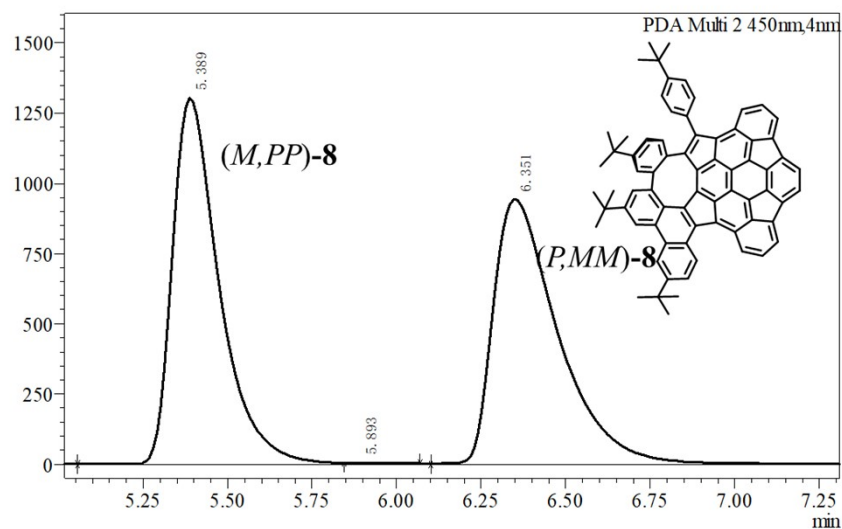


Fig. S16 The HPLC analysis spectra of **8** (eluent: n-hexane/dichloromethane = 50:50, 0.8 mL·min⁻¹, 25 °C, Detector: PDA Ch2 450nm 4nm).

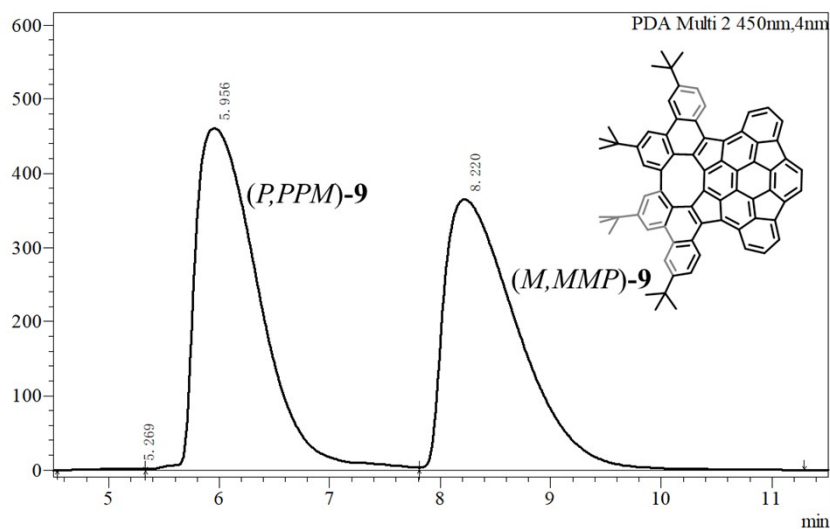


Fig. S17 The HPLC analysis spectra of **9** (eluent: n-hexane/dichloromethane = 50:50, 0.8 mL·min⁻¹, 25 °C, Detector: PDA Ch2 450nm 4nm).

Table S6 Thermal stability tests of (*P,PPM*)-**9** heated at different temperature in toluene.

T/°C	Time/min	Time/s	Major ent.(%)	Minor ent.(%)	ee	ln([ee] _t /[ee] ₀)
65	0	0	99.2	0.8	98.4	0
	70	4200	94.9	5.1	89.8	-0.09145
	180	10800	88.9	11.1	77.8	-0.2349
T/°C	Time/min	Time/s	Major ent.(%)	Minor ent.(%)	ee	ln([ee] _t /[ee] ₀)
80	0	0	99.2	0.8	98.4	0
	45	2700	87.2	12.8	74.4	-0.2796

	90	5400	78.7	21.3	57.4	-0.5390
	120	7200	74.2	25.8	48.4	-0.7095
	180	10800	65.9	34.1	31.8	-1.1296
T/°C	Time/min	Time/s	Major ent.(%)	Minor ent.(%)	ee	ln([ee] _t /[ee] ₀)
85	0	0	99.2	0.8	98.4	0
	30	1800	87.8	12.2	75.6	-0.2636
	70	4200	75.7	24.3	51.4	-0.6494
	120	7200	65.8	34.2	31.6	-1.1359
	180	10800	59.2	40.8	18.4	-1.6767
T/°C	Time/min	Time/s	Major ent.(%)	Minor ent.(%)	ee	ln([ee] _t /[ee] ₀)
90	0	0	99.2	0.8	98.4	0
	30	1800	77.3	22.7	54.6	-0.5890
	50	3000	70.7	29.3	41.4	-0.8658
	80	4800	62.0	38.0	24	-1.4110
	112	6720	55.7	44.3	11.4	-2.1554

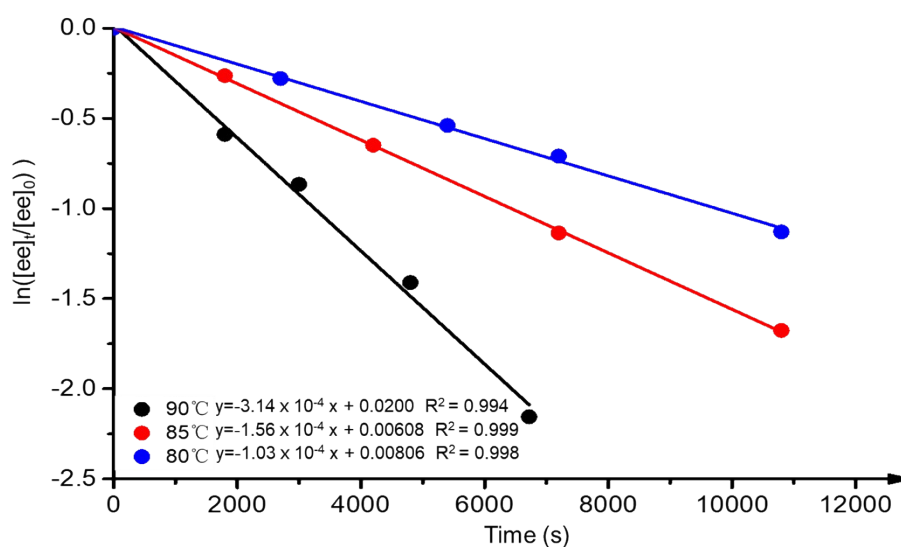


Fig. S18 Temperature-dependent plots of the decreasing *ee* ratio of enantioenriched (*P,PPM*)-**9** in toluene.

The exchange rate constant (*k*) was determined, then fitting with Eyring equation:

$$\ln \frac{k}{T} = -\frac{\Delta H^\ddagger}{RT} + \frac{\Delta S^\ddagger}{R} + \ln \frac{k_B}{h}, \text{ and } \Delta G^\ddagger = \Delta H^\ddagger - T\Delta S^\ddagger,$$

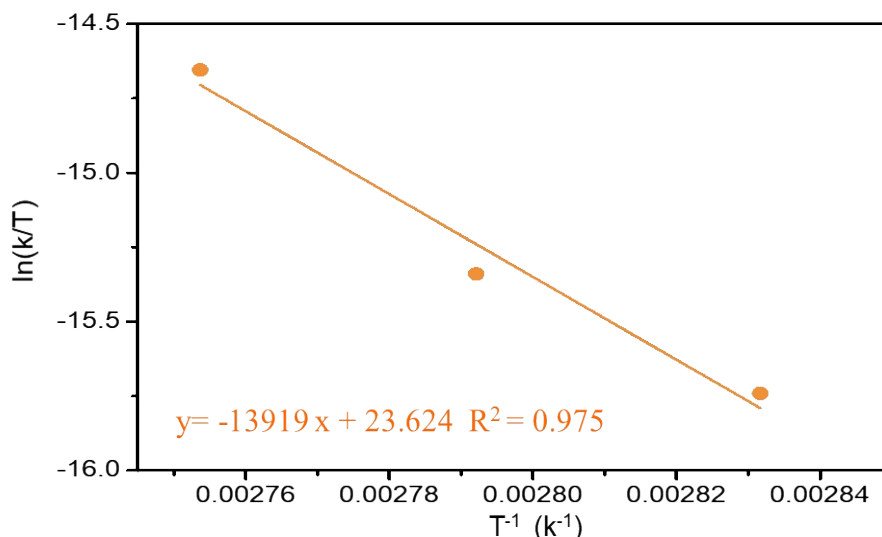


Fig. S19 Fitting of the exchange rate constants with temperature by Eyring equation for (*P,PPM*)-**9** in toluene giving thermodynamic parameters: $\Delta H^\ddagger = 27.6 \text{ kcal}\cdot\text{mol}^{-1}$; $\Delta S^\ddagger = -1.05 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$; $\Delta G^\ddagger = 27.7 \text{ kcal}\cdot\text{mol}^{-1}$ (298 K).

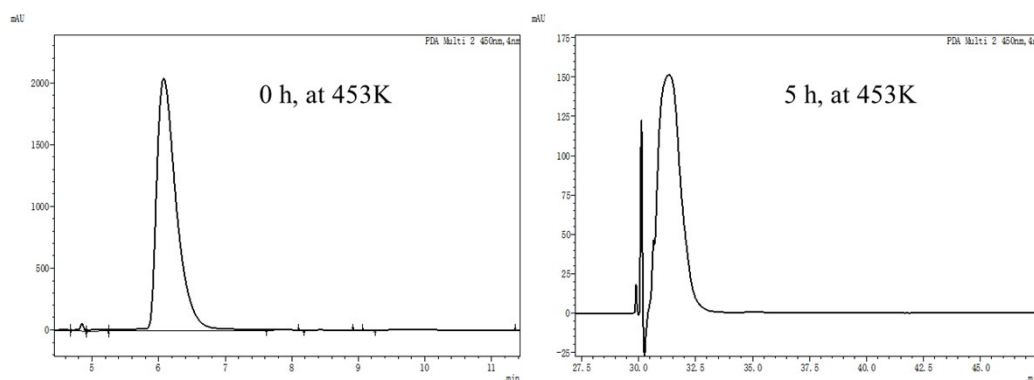


Fig. S20 HPLC chromatogram of (*M,PP*)-**8** after heating at 453K for different times: 0 h (left) and 5 h (right).

The half-life time ($t_{1/2}$) of racemization was calculated from the equation:

$$t_{\frac{1}{2}} = \frac{\ln 2}{k_r}$$

The estimated values of the Gibbs activation energy ($\Delta G^\ddagger(T)$) for enantiomerization of (*M,PP*)-**8** were obtained by using Eyring equation. The rate constant of racemization was calculated from the maximum time to which compounds (*M,PP*)-**8** remain unchanged at a specific temperature (453 K).

8. Binding behaviors with C_{60}

The association behaviors of **7/8/9** and C_{60} were analyzed by NMR titrations. A solution of **7/8/9** ($6.0 \times 10^{-4} \text{ M}$ in toluene- d_8) and a solution of C_{60} ($6.0 \times 10^{-4} \text{ M}$ in toluene- d_8) were prepared. The solutions were mixed with different ratios.

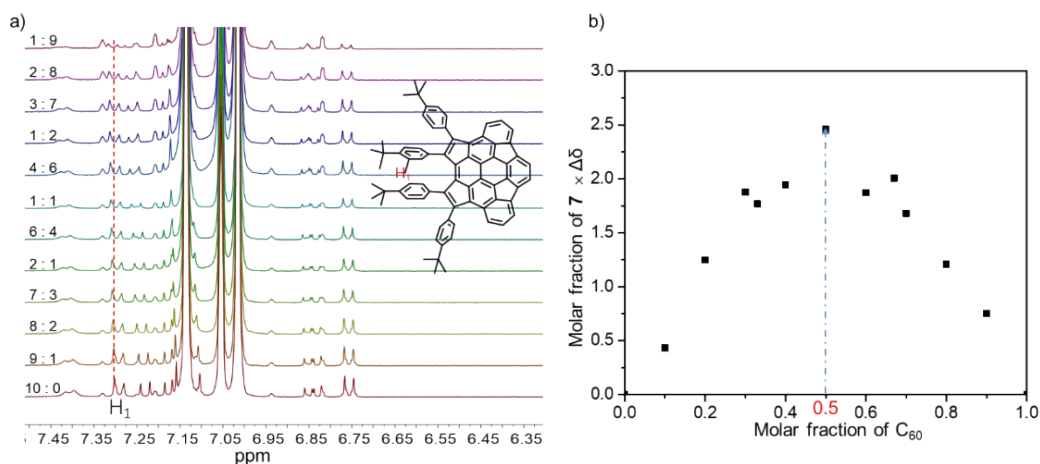


Fig. S21 a) NMR spectra of **7** and C_{60} mixed in different ratio in toluene- d_8 at 298 K (total concentration of 6.0×10^{-4} M), b) Job plot showing complexation between **7** and C_{60} .

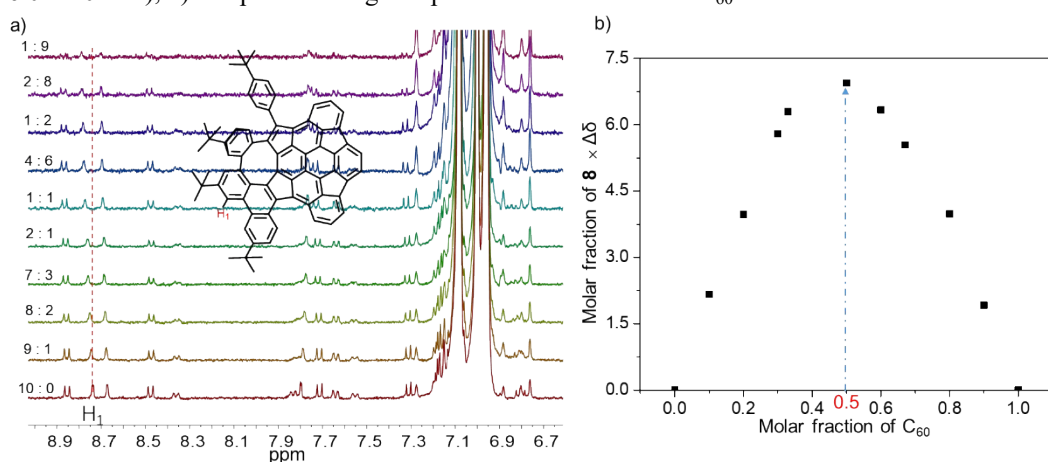


Fig. S22 a) NMR spectra of **8** and C_{60} mixed in different ratio in toluene- d_8 at 298 K (total concentration of 6.0×10^{-4} M), b) Job plot showing complexation between **8** and C_{60} .

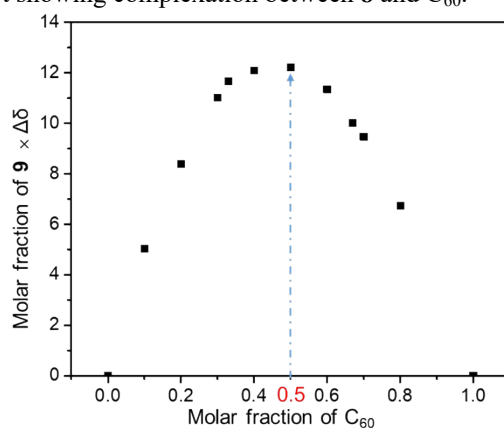


Fig. S23 Job plot showing complexation between **9** and C_{60} .

A solutions of **7/8/9** at a concentration of approximately 4×10^{-4} M. Those solutions were utilized as solvents in the C_{60} solution (1.2×10^{-3} M), to ensure working at constant concentration of host. The K_a were determined by the equation:^[9]

$$\Delta\delta = \delta_{\Delta HG} * \frac{1}{2H_0} \left[\left(G_0 + H_0 + \frac{1}{K_a} \right) - \sqrt{\left(G_0 + H_0 + \frac{1}{K_a} \right)^2 + 4[H_0][G_0]} \right]$$

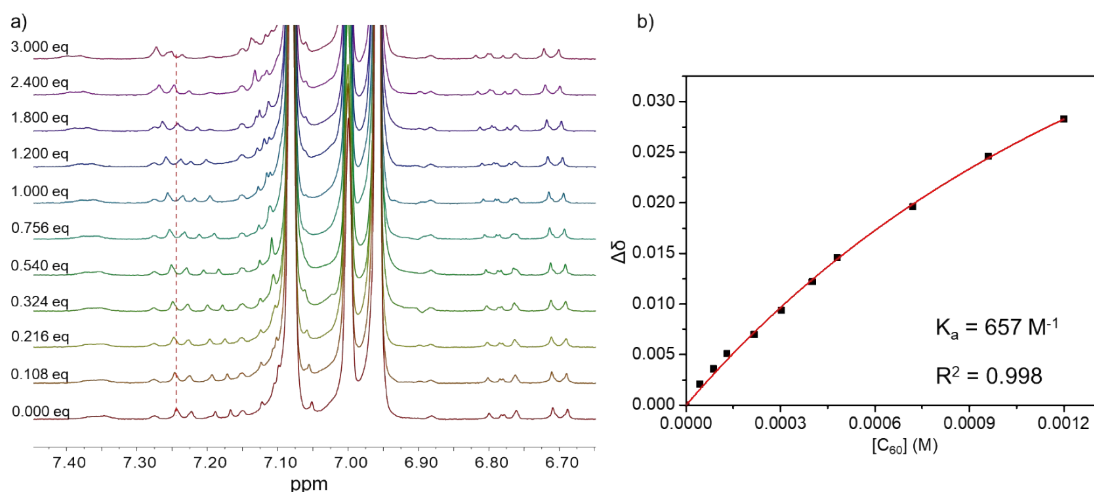


Fig. S24 (a) Proton NMR spectra from a mixture of different ratios of C_{60} and **7** in toluene- d_8 at 298 K, (b) Binding isotherms fitted to a 1:1 binding model.

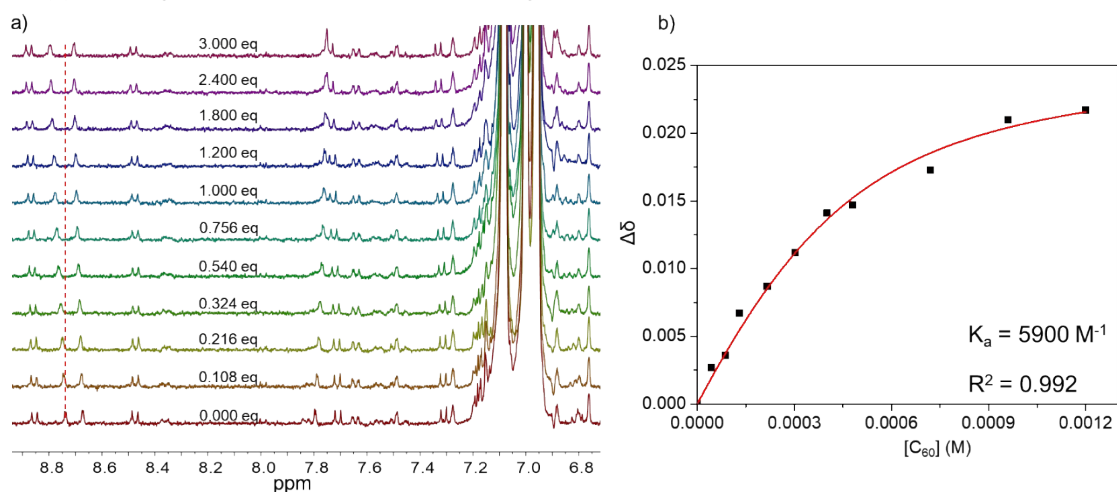


Fig. S25 (a) Proton NMR spectra from a mixture of different ratios of C_{60} and **8** in toluene- d_8 at 298 K, (b) Binding isotherms fitted to a 1:1 binding model.

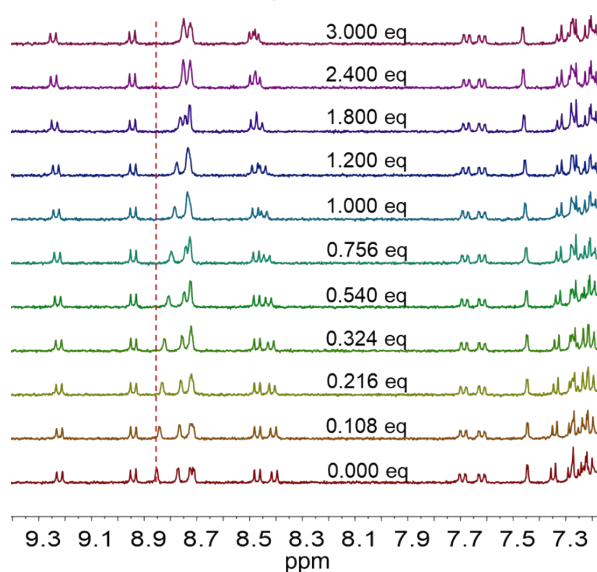


Fig. S26 Proton NMR spectra from a mixture of different ratios of C_{60} and **9** in toluene- d_8 at 298 K.

9. OFET Fabrication and Characterization

Thin-film devices fabrication: OTFT devices were fabricated in bottom-gate/bottom-contact (BGBC) type, where heavily doped silicon substrates were employed as substrate and gate electrodes, Au as source and drain electrodes. The source and drain gold electrodes were prepared by photolithography. The thin films of compound **7**, **8** and **9** were fabricated by spin-coating 5 mg/mL chlorobenzene solution at 1500 rpm for 40 s, respectively, which were subsequently annealed at 120 °C under vacuum.

The micro/nanometer-sized single-crystals devices fabrication: The heavily n-doping Si wafers with 300 nm SiO₂ layer were used as substrates in this work. The SiO₂/Si wafers were cleaned with deionized water, piranha solution (H₂SO₄/H₂O₂=2:1), deionized water, isopropyl alcohol, and finally were blown dry with high-purity nitrogen gas. Treatment of wafers with octadecyltrichlorosilane (OTS) was conducted by the vaper-desposition method. Clean wafers were dried under vacuum at 90 °C for 90 minutes to remove the moisture. When the temperature was reduced to room temperature, a small drop of OTS was dropped around the wafers and kept 120 °C for 2 hours under the vacuum. After that the OTS treated SiO₂/Si substrates were cleaned with n-hexane, chloroform, isopropyl alcohol, respectively. Micro/nanometer-sized single-crystals were prepared by drop casting method in a sealed container with toluene as the solvent. The single crystals of compound **9** were fabricated by slow solution evaporation on OTS modified SiO₂/Si substrates. The micro/nanometer-sized co-crystals of **9**·C₆₀ were prepared by slow solution evaporation of toluene on OTS modified SiO₂/Si substrates. The bottom-gate top-contact (BGTC) devices based on single crystals were fabricated in “gold strips” method^[10].

Devices characterization: All electrical characteristics of the devices were measured at room temperature using a semiconductor parameter analyser (Keithley 4200 SCS) in nitrogen atmosphere. The mobilities of the devices were calculated in the saturation regime. The equation is listed as follows:

$$I_{DS} = (W/2L) C_i \mu (V_{GS} - V_t)^2$$

where W/L is the channel width/length, C_i is the insulator capacitance per unit area (10 nF /cm²), and V_{GS} and V_t are the gate voltage and threshold voltage, respectively. This equation defines the important characteristics of electron mobility (μ), on/off ratio (I_{on}/I_{off}), and threshold voltage (V_t), which could be deduced by the equation from the plot of current–voltage. The microscope images of microcrystal were acquired by SOPTOP RX50M microscope. Atomic force microscopy (AFM) measurements were carried out with a Nanoscope IIIa instrument (Digital Instruments). X-ray diffraction (XRD) was measured on a D/max 2500 with a Cu Kα source (κ = 1.541 Å). TEM observation was carried out with a JEOL 1011 JEM-2100F microscope operated at 200 kV.

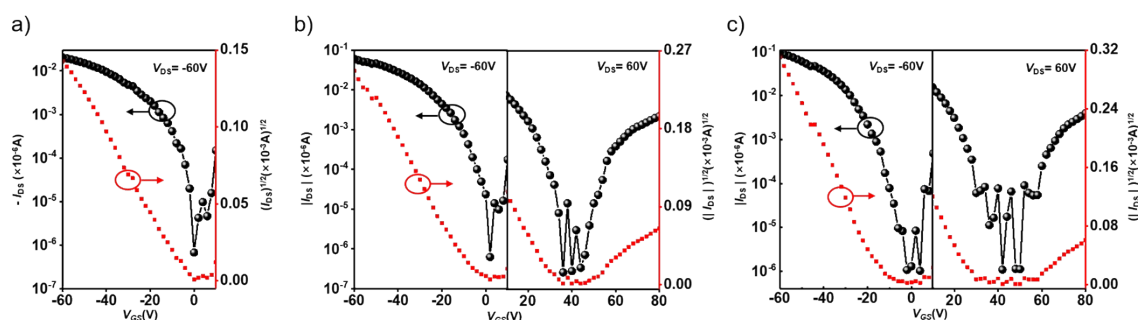


Fig. S27 The transfer characteristics of the thin films of **7** (a), **8** (b), **9** (c).

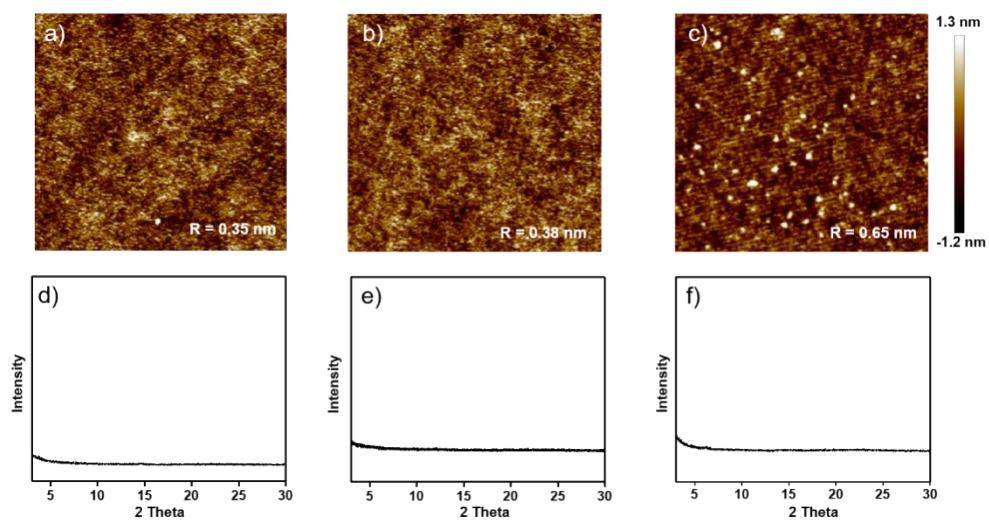


Fig. S28 AFM images and XRD patterns of thin films of **7** (a, d), **8** (b, e), **9** (c, f).

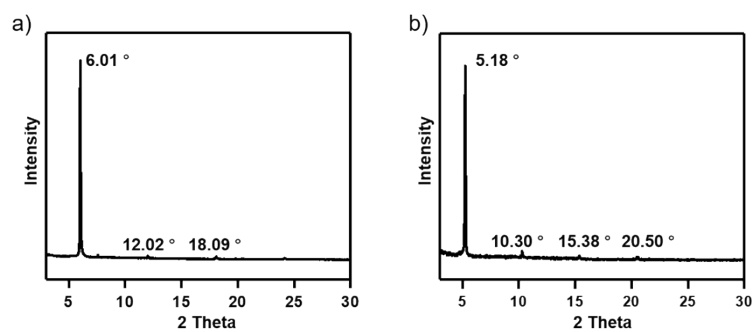


Fig. S29 XRD pattern of microbelts of **9** (a) and **9·C₆₀** (b).

10. ^1H NMR, ^{13}C NMR and HRMS spectra of compounds

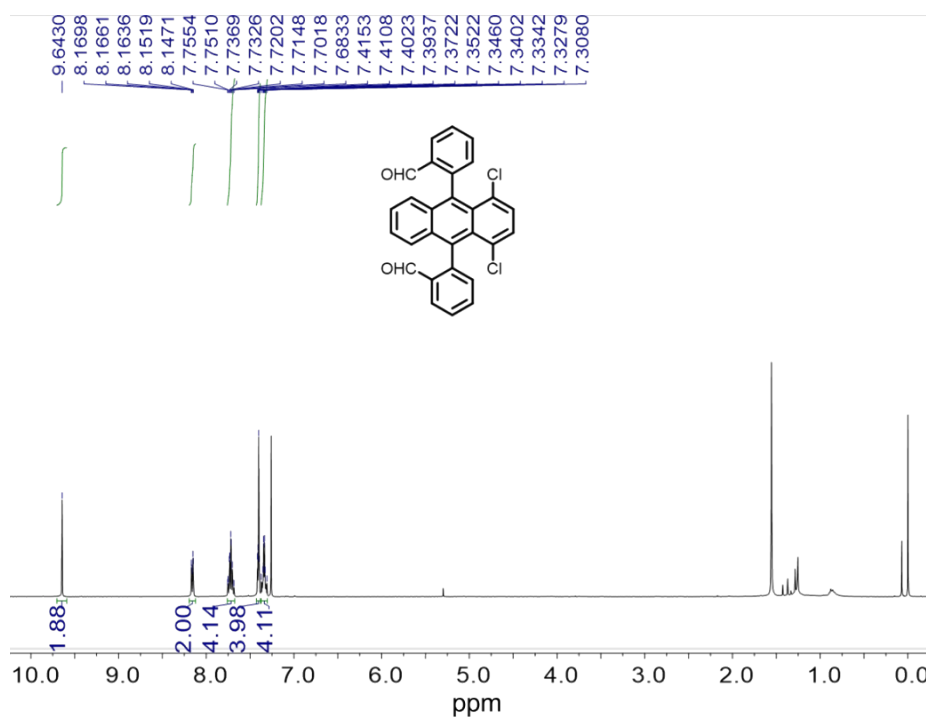


Fig. S30 ^1H NMR spectrum of *syn-1* in CDCl_3 (400 MHz, 298 K).

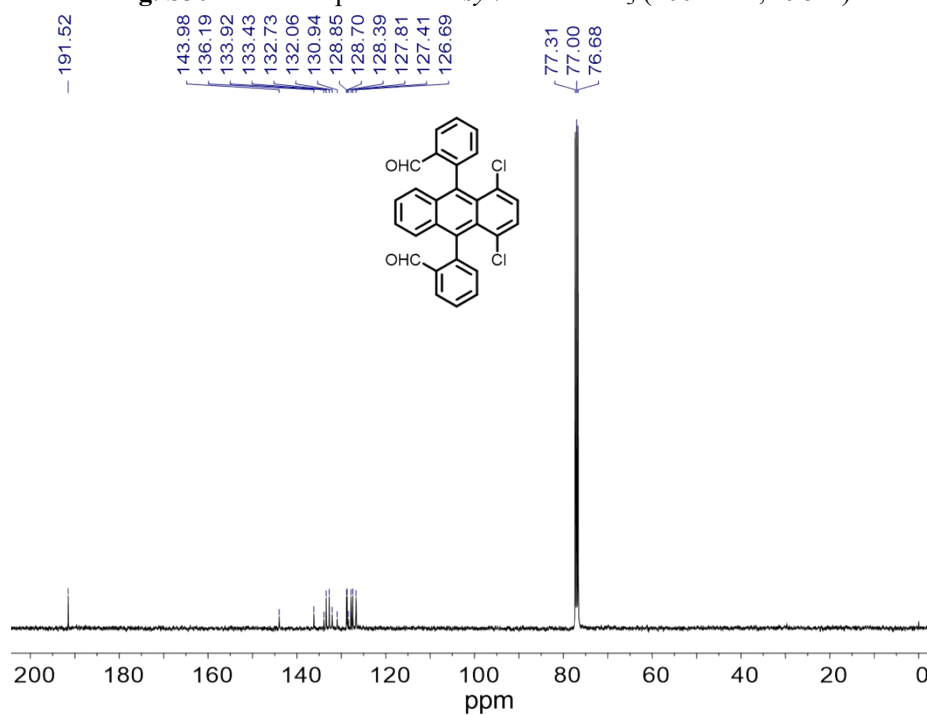


Fig. S31 ^{13}C NMR spectrum of *syn-1* in CDCl_3 (400 MHz, 298 K).

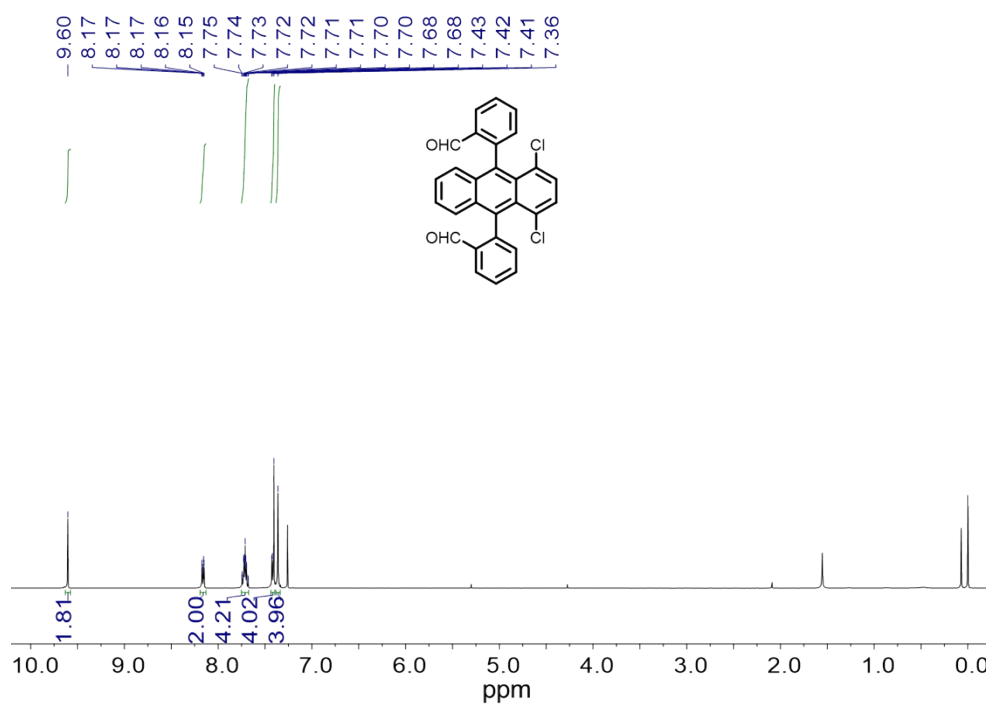


Fig. S32 ^1H NMR spectrum of *anti-1* in CDCl_3 (400 MHz, 298 K).

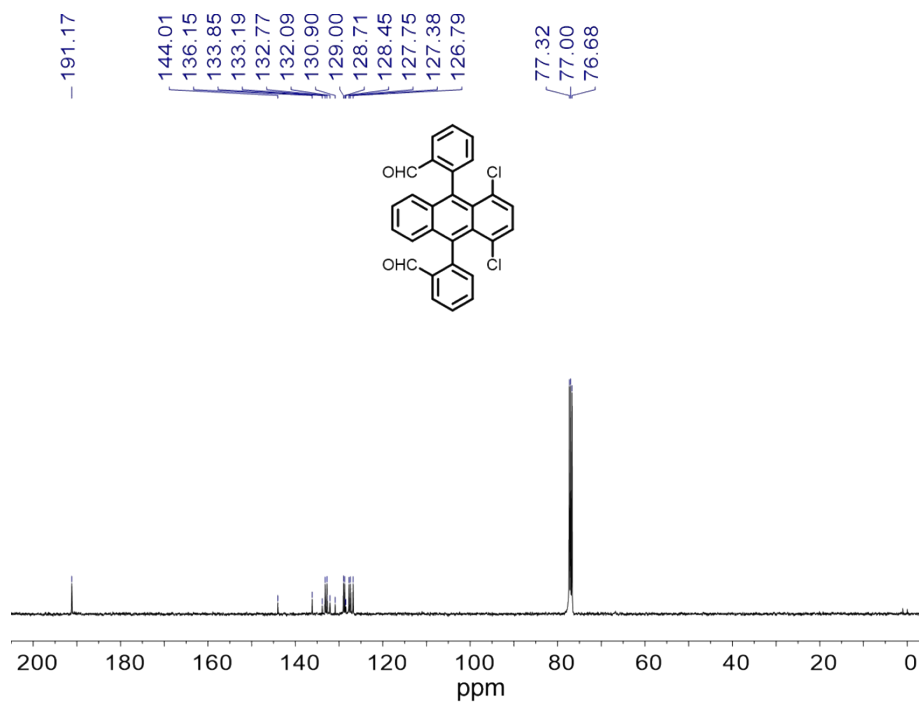


Fig. S33 ^{13}C NMR spectrum of *anti-1* in CDCl_3 (400 MHz, 298 K).

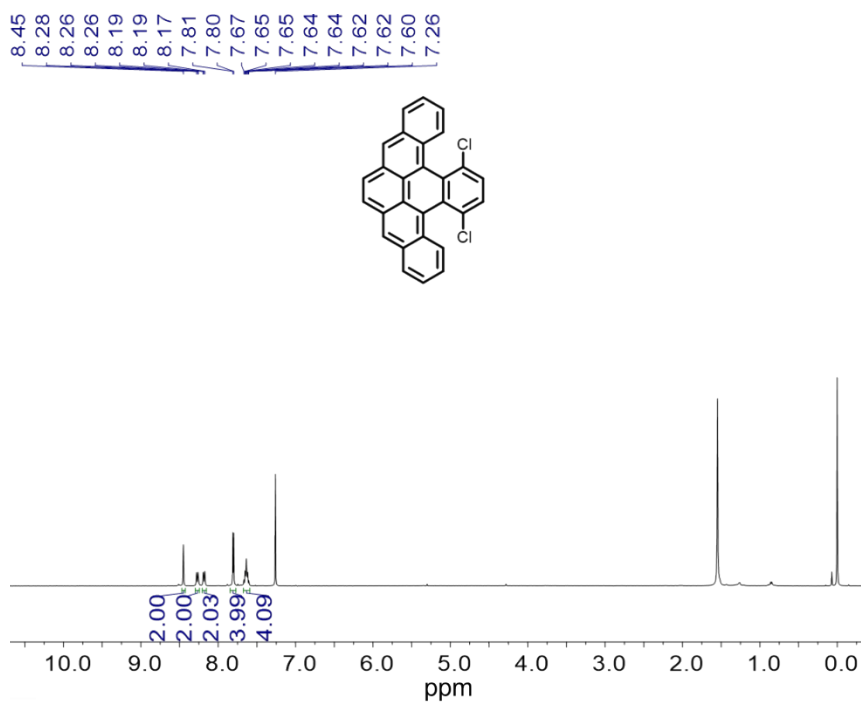


Fig. S34 ^1H NMR spectrum of **2** in CDCl_3 (400 MHz, 298 K).

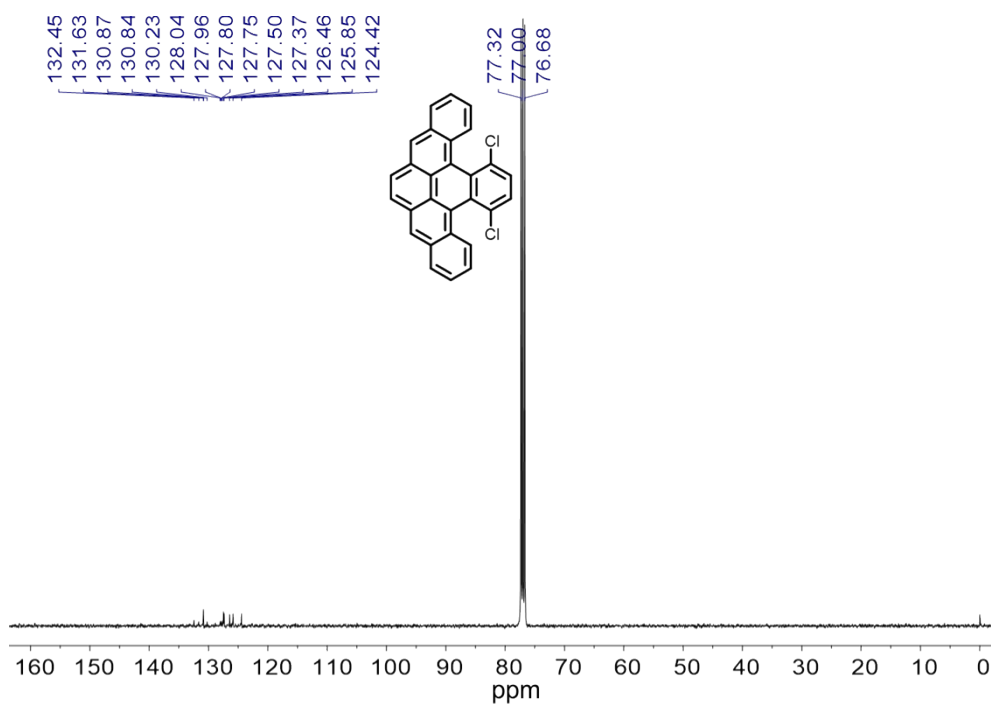


Fig. S35 ^{13}C NMR spectrum of **2** in CDCl_3 (400 MHz, 298 K).

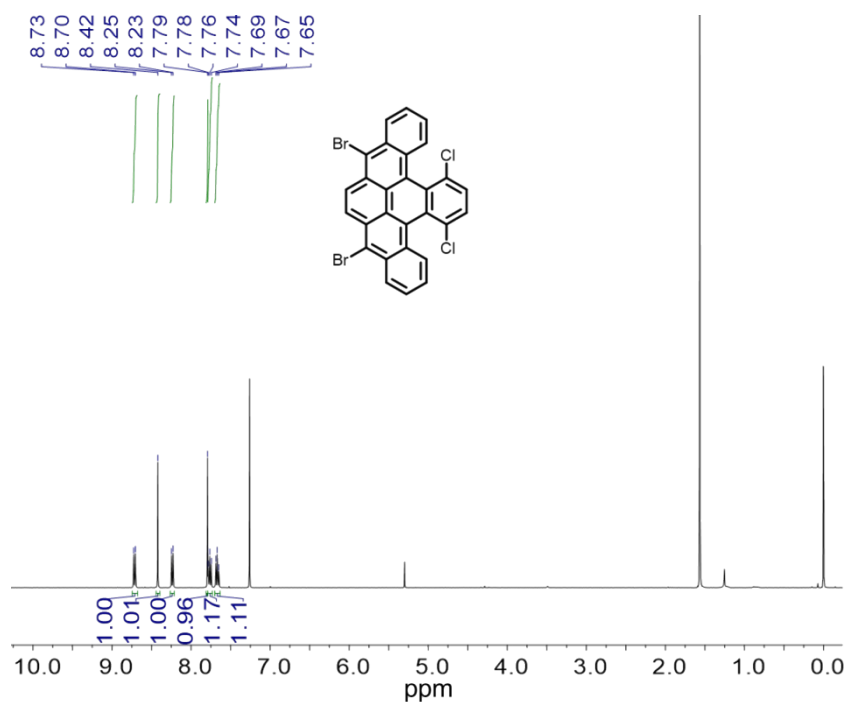


Fig. S36 ^1H NMR spectrum of **3** in CDCl_3 (400 MHz, 298 K).

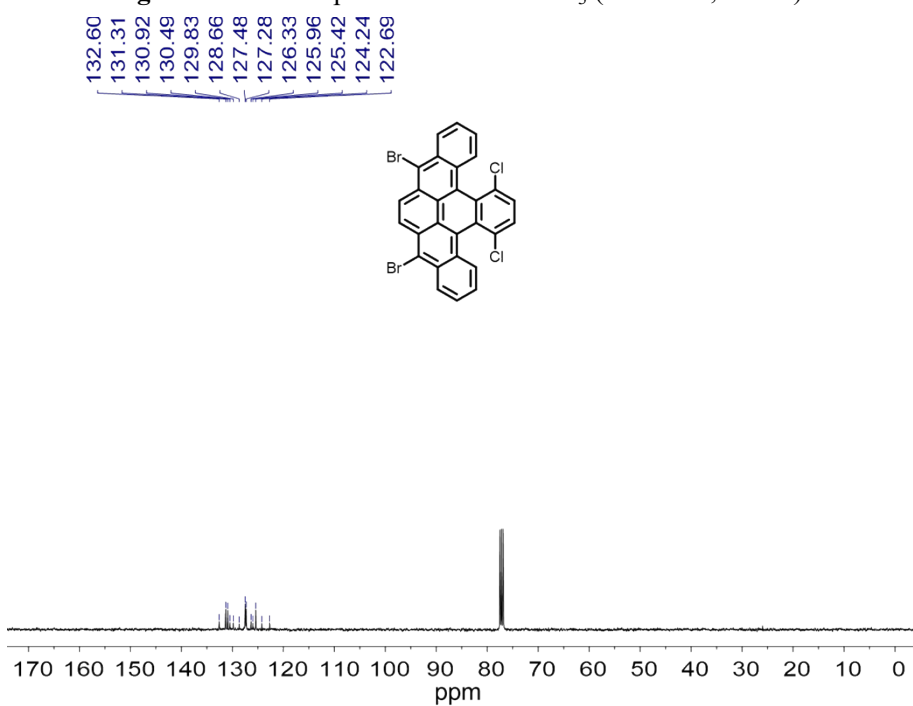


Fig. S37 ^{13}C NMR spectrum of **3** in $\text{CDCl}_3/\text{CS}_2$ ($v=1:1$) (400 MHz, 298 K).

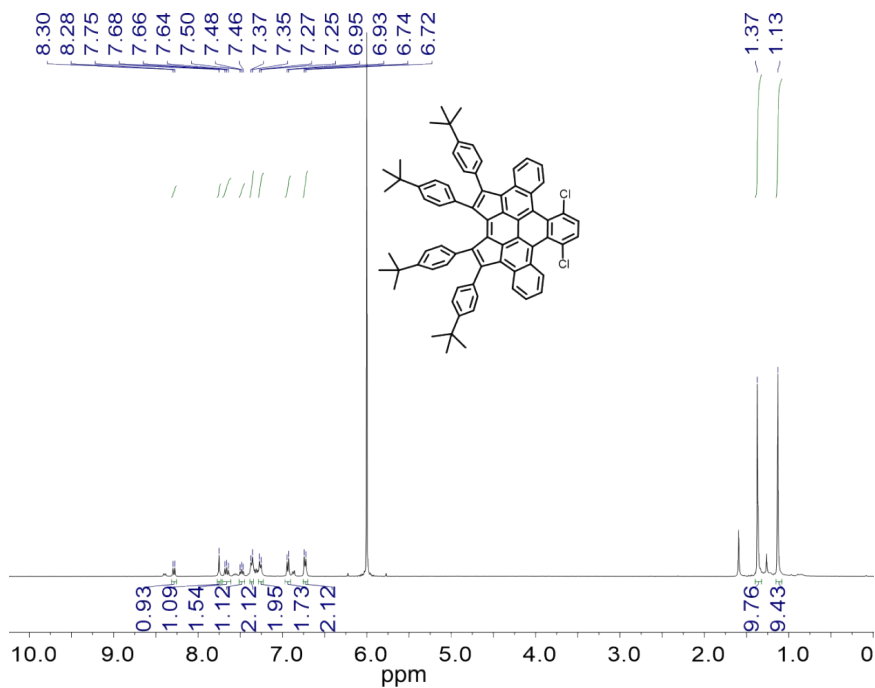


Fig. S38 ^1H NMR spectrum of **4** in $\text{C}_2\text{D}_2\text{Cl}_4$ (400 MHz, 298 K).

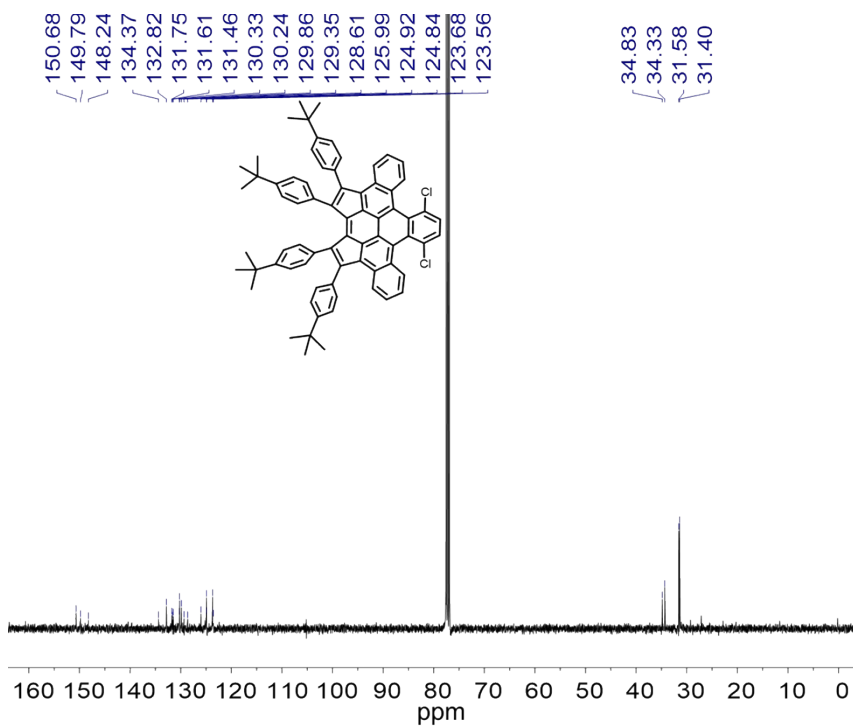


Fig. S39 ^{13}C NMR spectrum of **4** in CDCl_3 (400 MHz, 298 K).

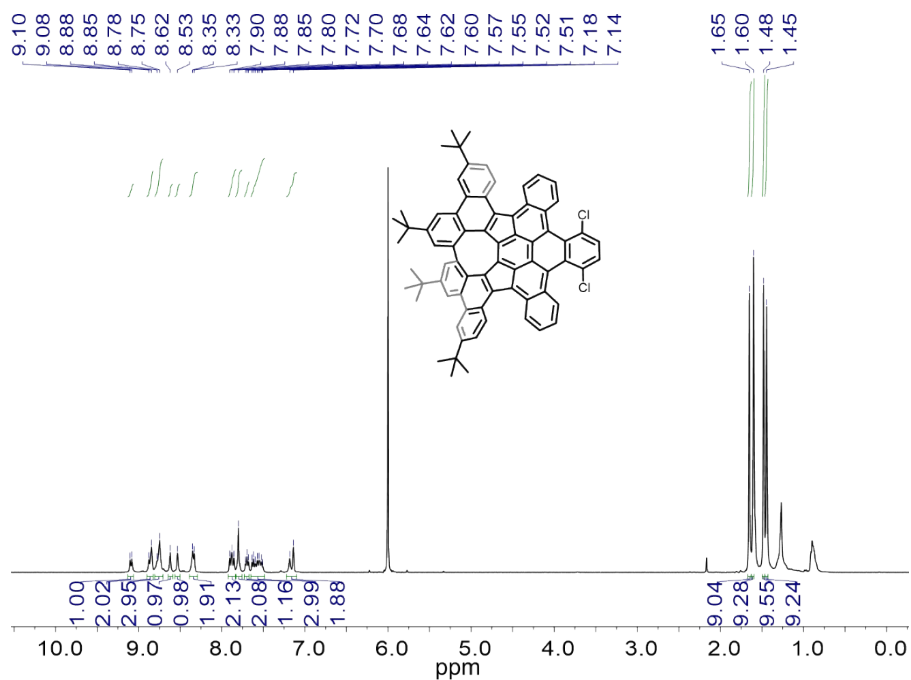


Fig. S40 ^1H NMR spectrum of **5** in $\text{C}_2\text{D}_2\text{Cl}_4$ (400 MHz, 298 K).

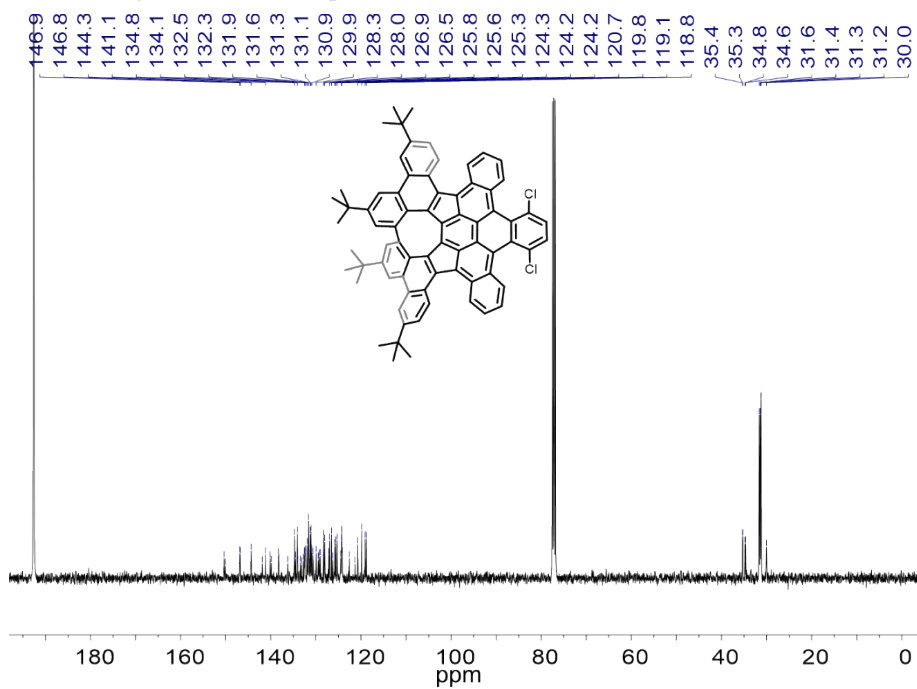


Fig. S41 ^{13}C NMR spectrum of **5** in $\text{CDCl}_3/\text{CS}_2$ ($v=1:1$)(400 MHz, 298 K).

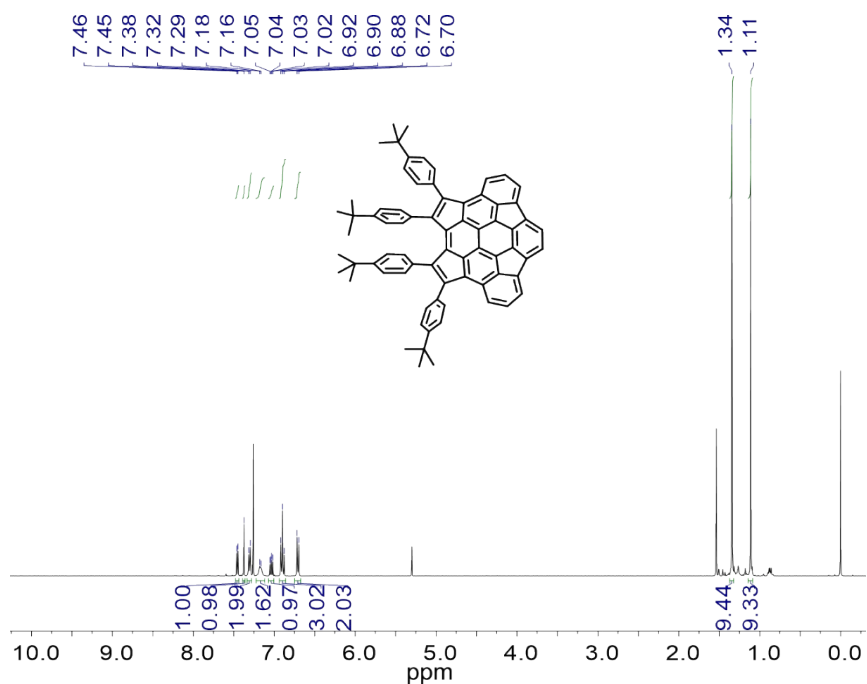


Fig. S44 ^1H NMR spectrum of **7** in CDCl_3 (400 MHz, 298 K).

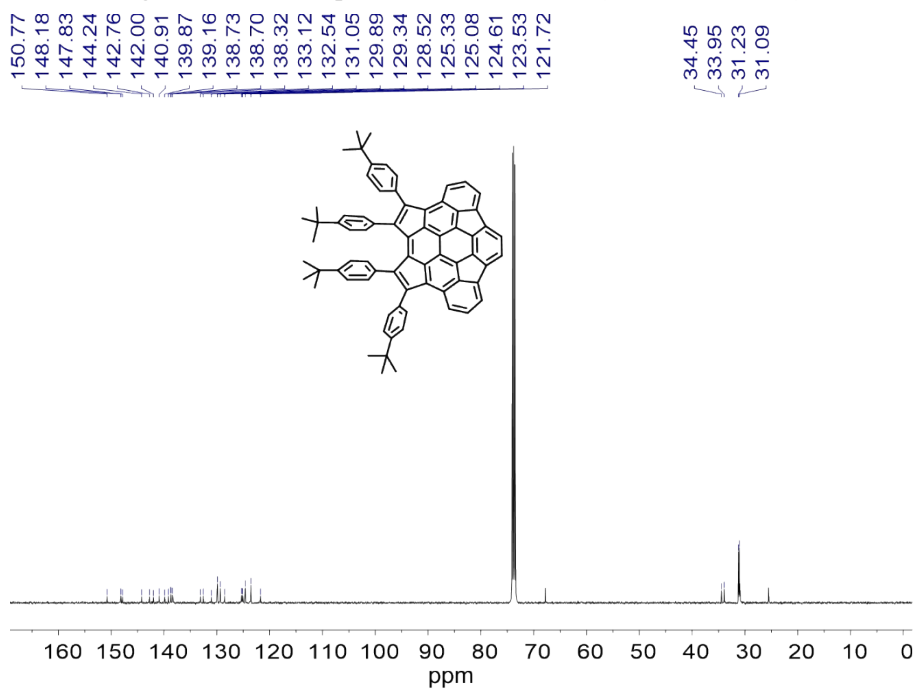


Fig. S45 ^{13}C NMR spectrum of **7** in $\text{CDCl}_3/\text{CS}_2$ ($\nu=1:1$)(400 MHz, 298 K).

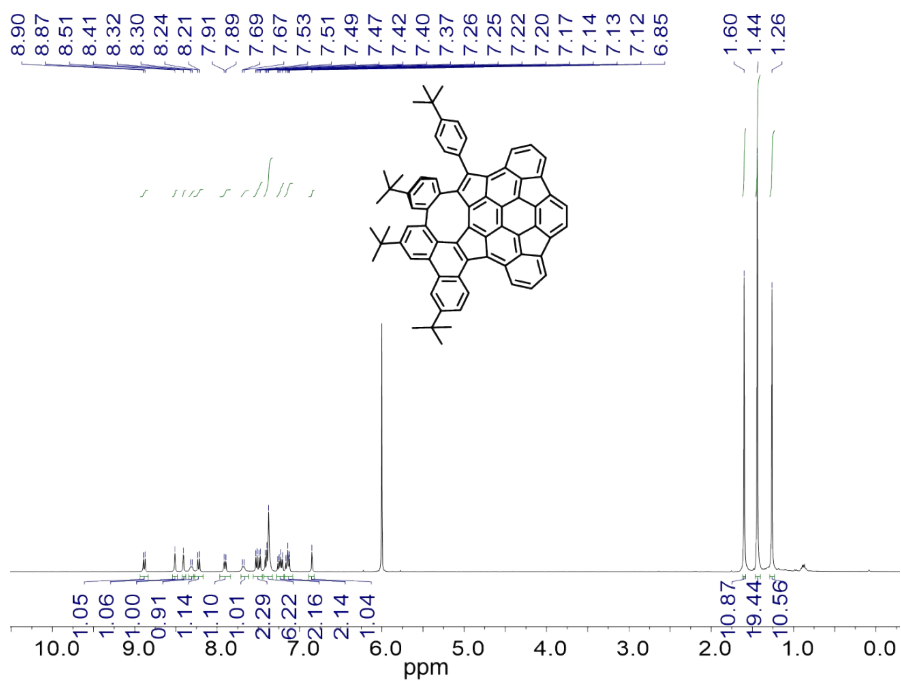


Fig. S46 ^1H NMR spectrum of **8** in $\text{C}_2\text{D}_2\text{Cl}_4$ (400 MHz, 298 K).

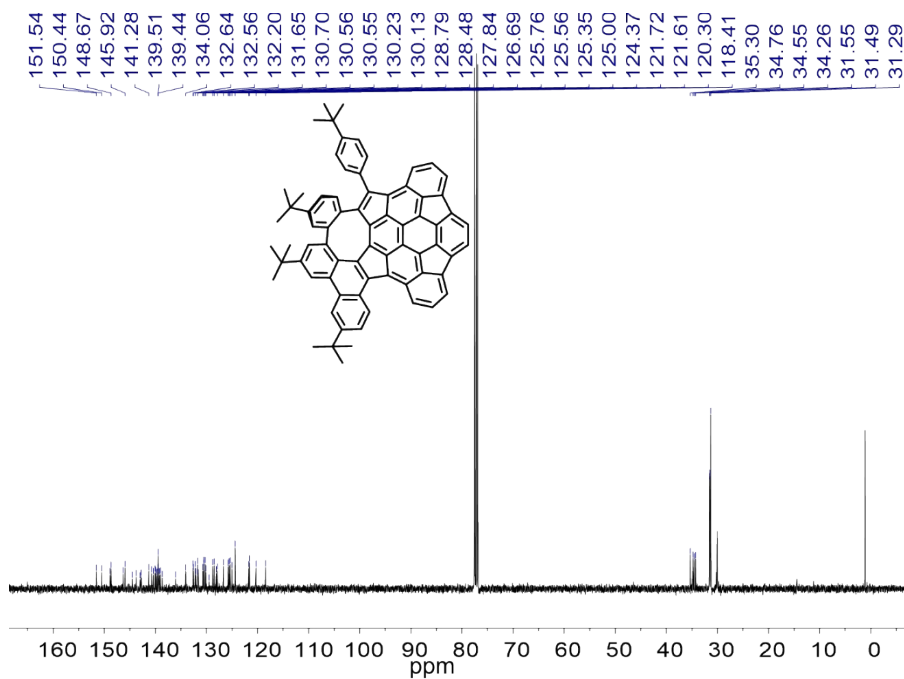


Fig. S47 ^{13}C NMR spectrum of **8** in $\text{CDCl}_3/\text{CS}_2$ ($\nu=1:1$)(400 MHz, 298 K).

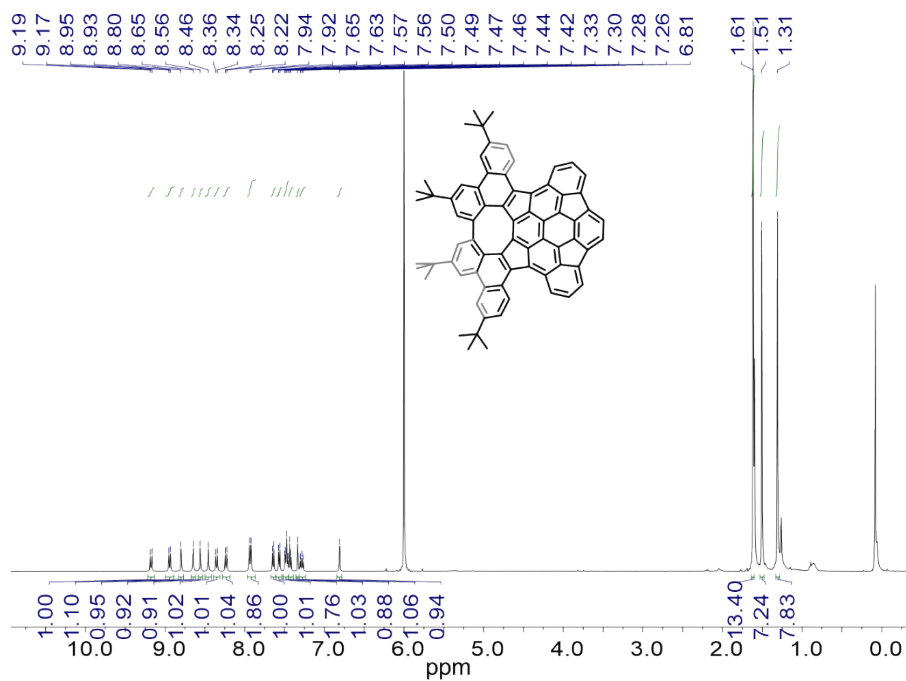


Fig. S48 ^1H NMR spectrum of **9** in $\text{C}_2\text{D}_2\text{Cl}_4$ (400 MHz, 298 K).

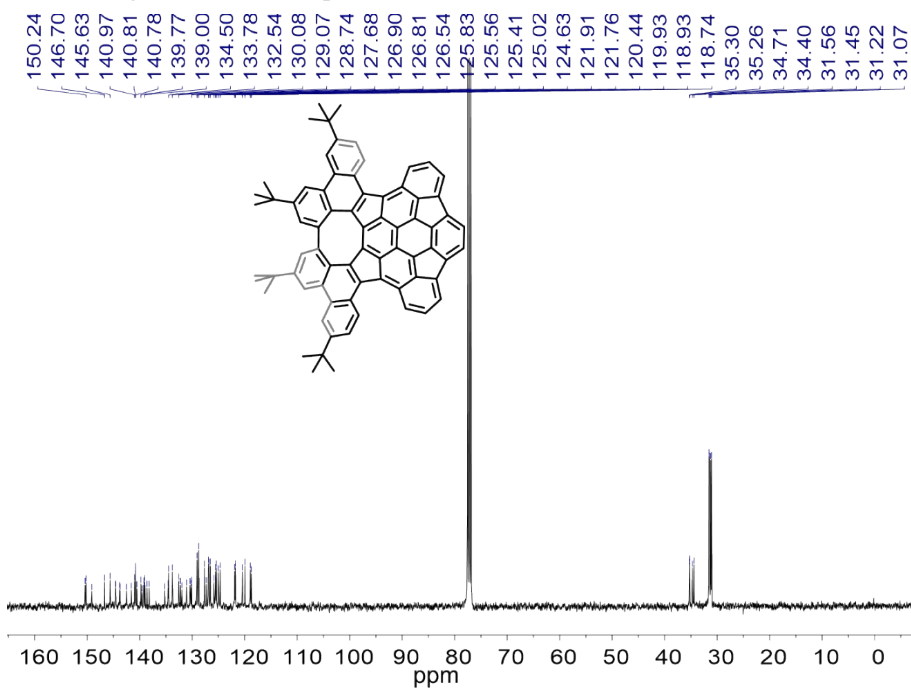


Fig. S49 ^{13}C NMR spectrum of **9** in $\text{CDCl}_3/\text{CS}_2$ ($v=1:1$) (400 MHz, 298 K).

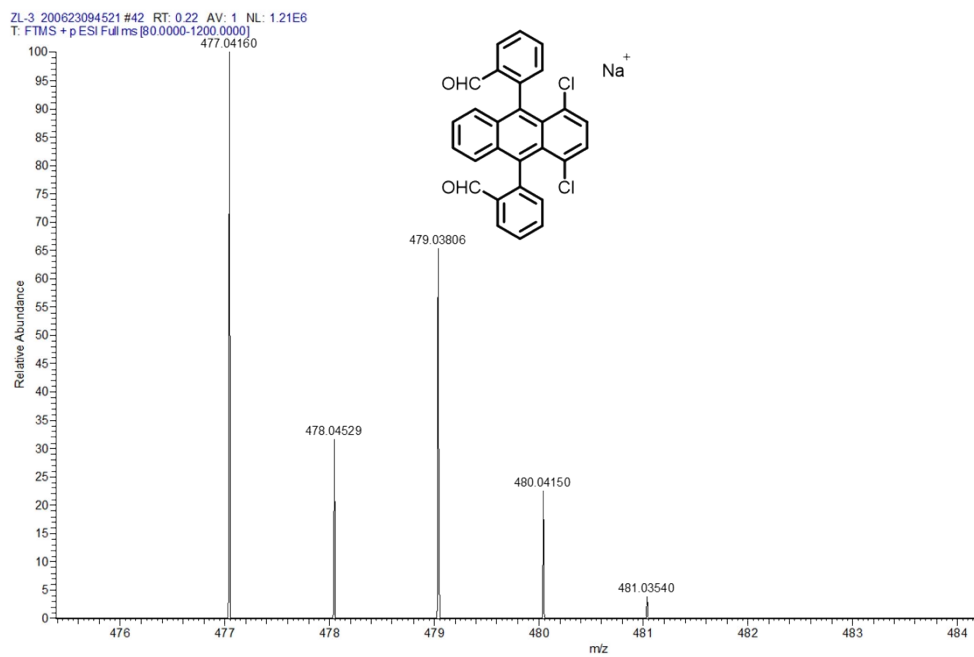


Fig. S50 HR-ESI spectra of *syn-1*.

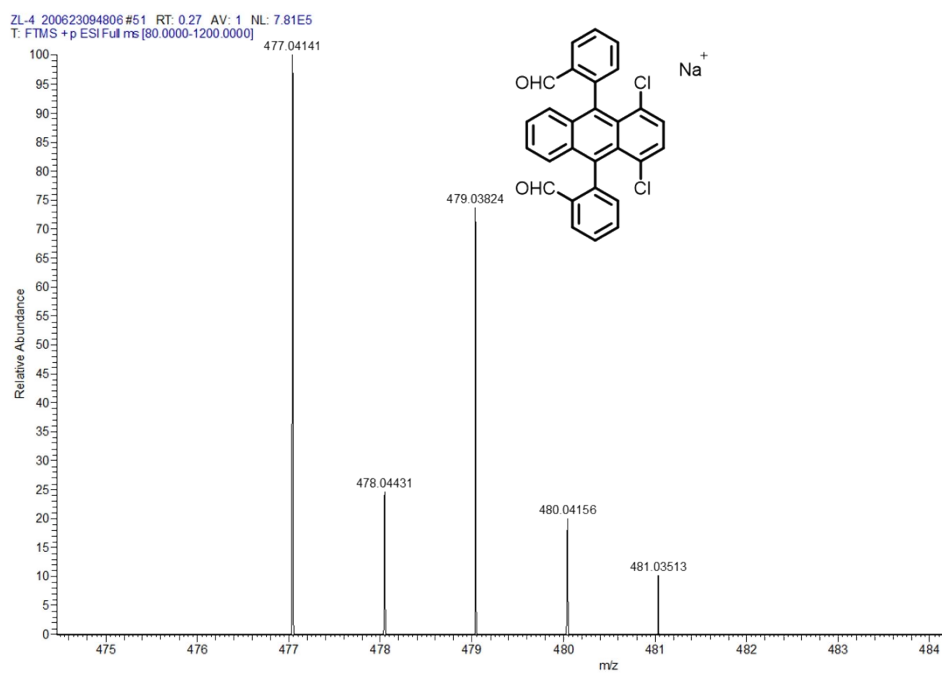


Fig. S51 HR-ESI spectra of *anti-1*.

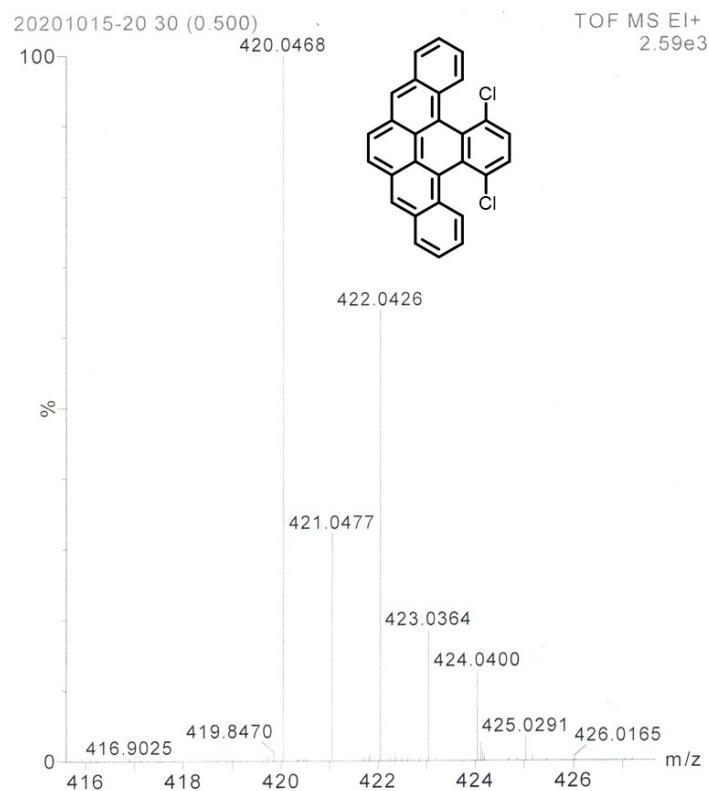


Fig. S52 HR-EI spectra of 2.

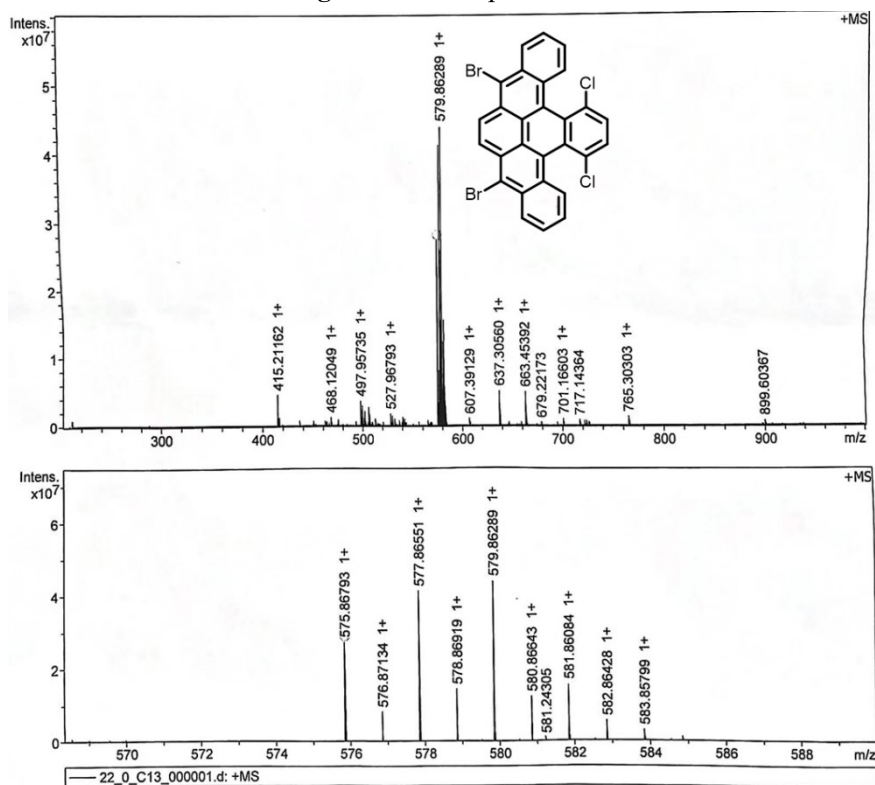


Fig. S53 HR-EI spectra of 3.

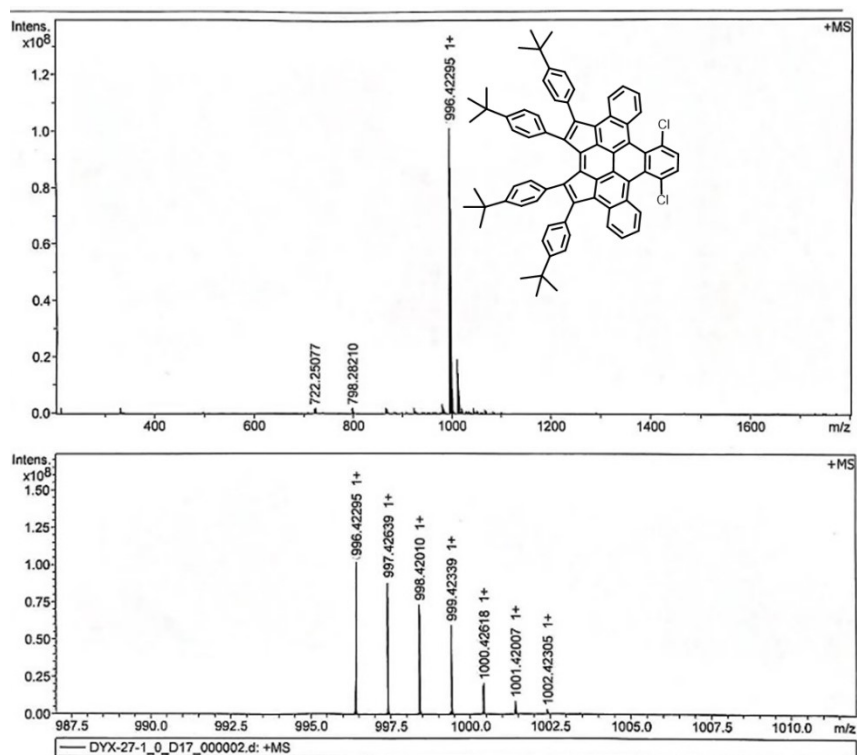


Fig. S54 HR-EI spectra of 4.

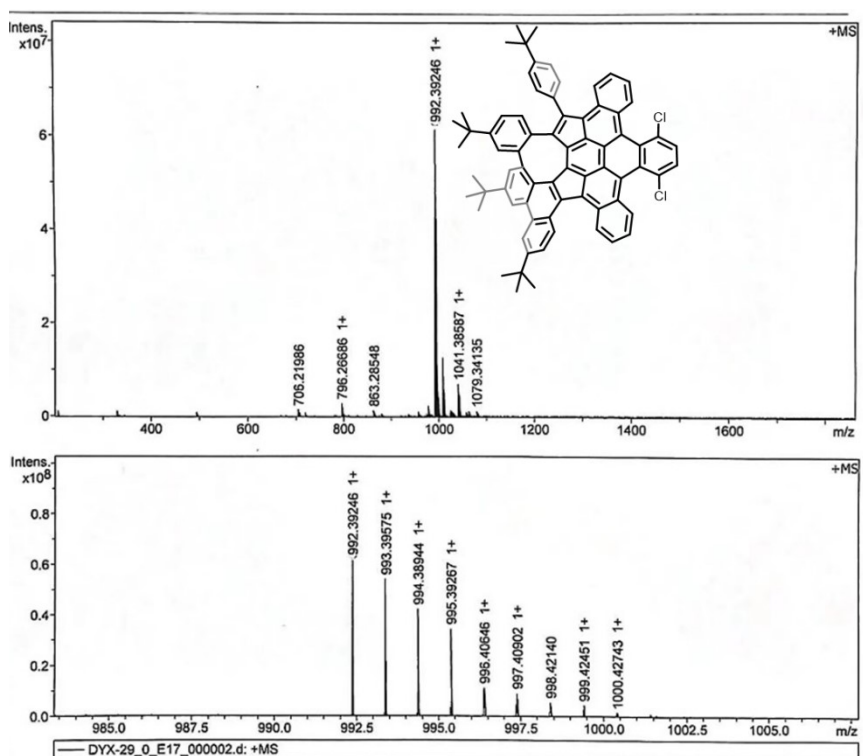


Fig. S55 HR-MALDI-TOF spectra of 5.

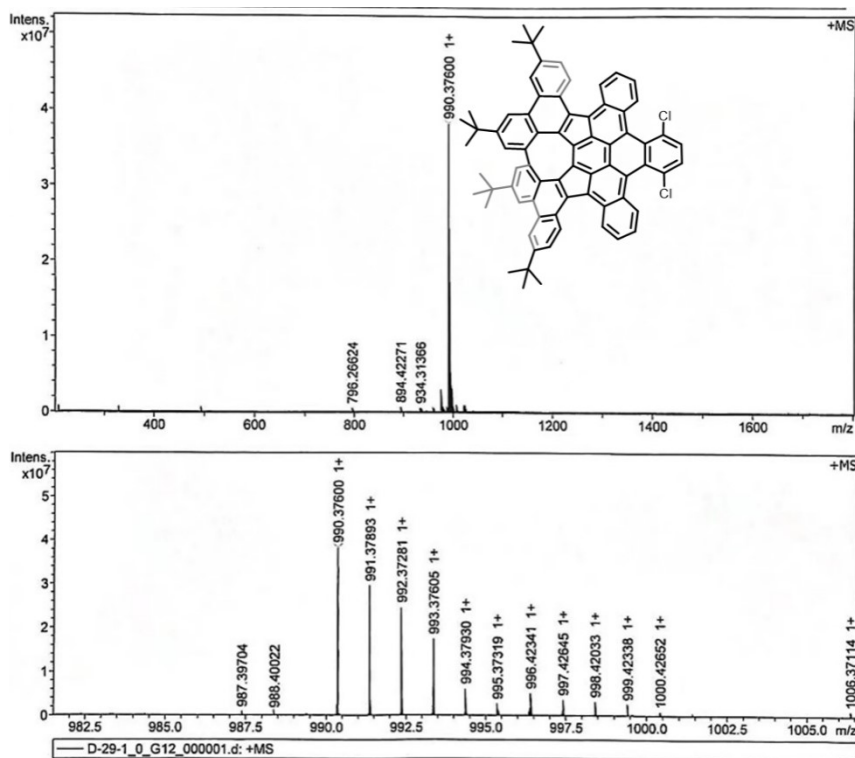


Fig. S56 HR-MALDI-TOF spectra of 6.

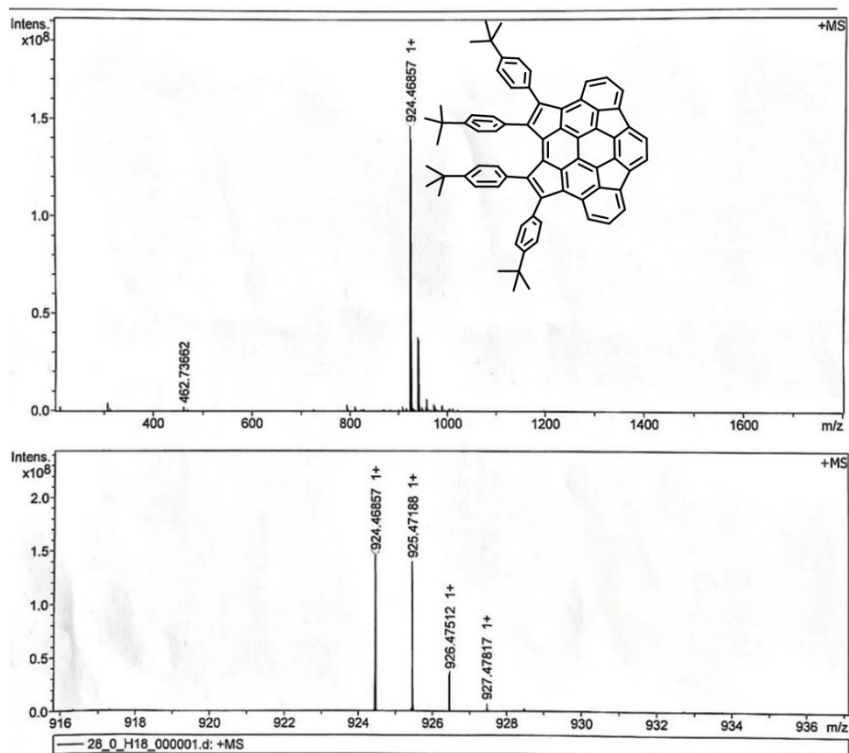


Fig. S57 HR-MALDI-TOF spectra of 7.

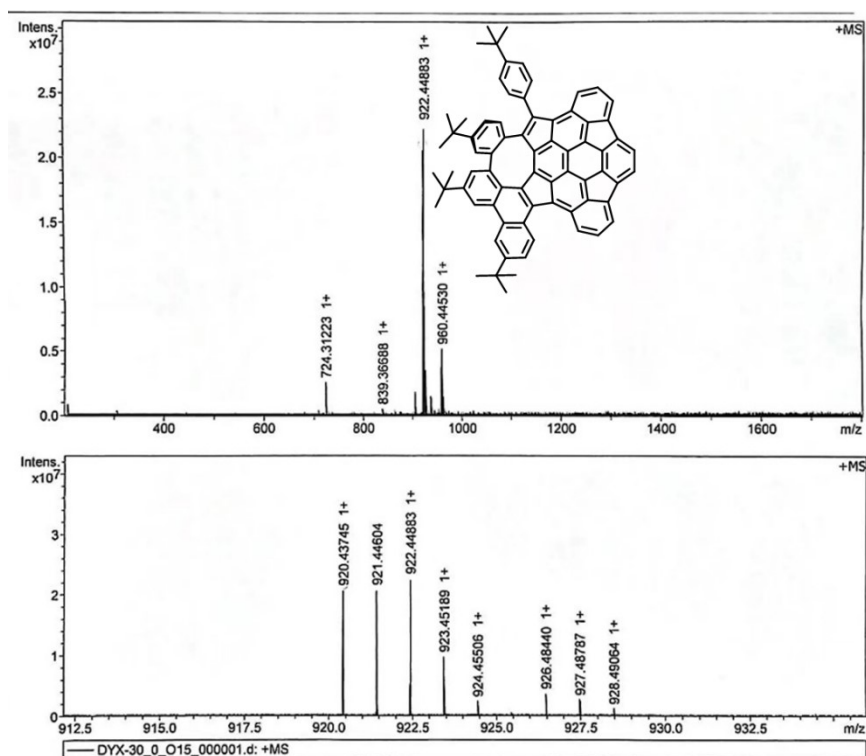


Fig. S58 HR-MALDI-TOF spectra of 8.

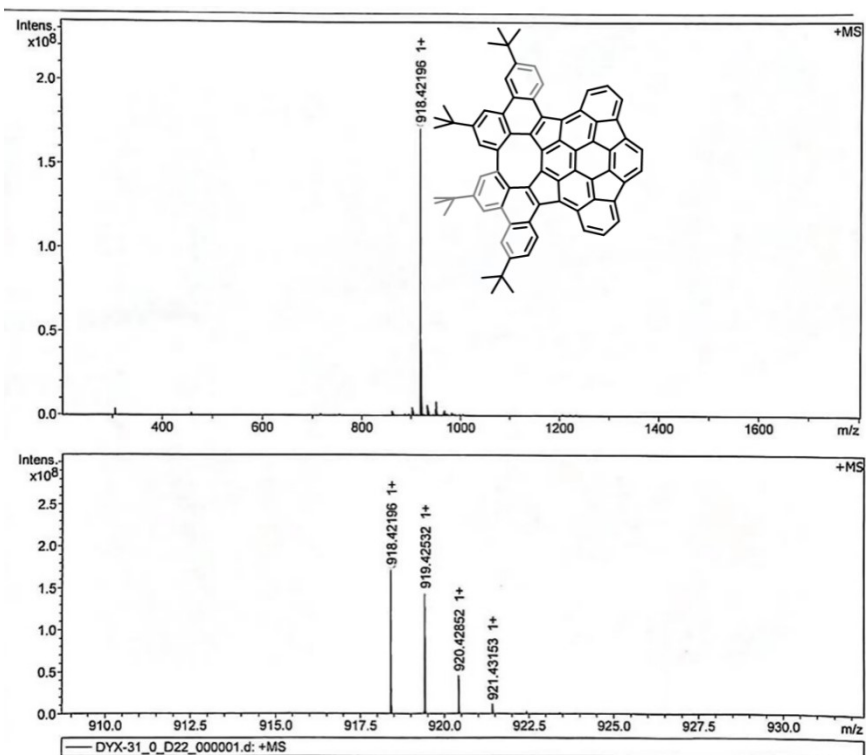


Fig. S59 HR-MALDI-TOF spectra of 9.

11. References

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