Electronic Supplementary Information

Synthesis, Structures and Fluorescence Properties of gem-Linked Cyclic Tetraphenylethylenes and Cyclic Hexaphenylethylenes

Huowang He,[‡a] Jian-An Li,[‡a] Yihuan Zhang,[a] Sumra Idrees,[a] Jin Cai,[a] Yongying Li,[a] Atsuhiro Osuka,*[b] Bingjia Xu,*[a] and Hua-Wei Jiang*[a]

a. School of Chemistry, South China Normal University, Guangzhou 510006, P. R. China; E-mail: bingjiaxu@m.scnu.edu.cn； hwjiang@m.scnu.edu.cn.
b. Key Laboratory of the Assembly and Application of Organic Functional Molecules of Hunan Province, College of Chemistry and Chemical Engineering, Hunan Normal University, Changsha 410081, P. R. China; Email: oosuka.atsuhiro.46c@st.kyoto-u.ac.jp.
‡ These authors contributed equally.
* Corresponding authors.

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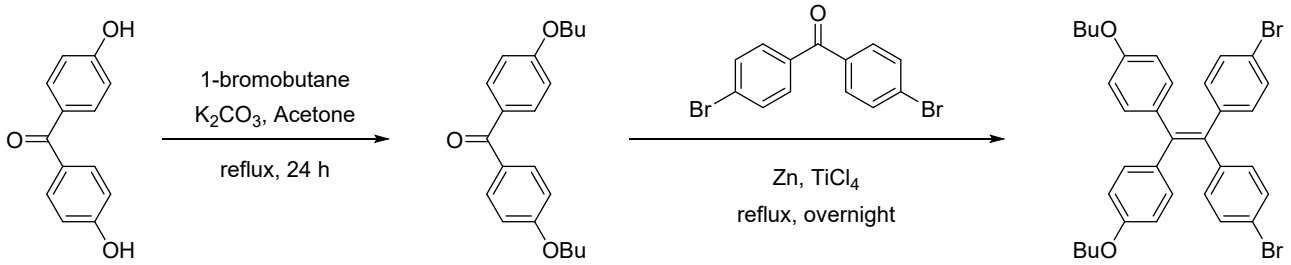
1. General Information

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE NEO 600 spectrometer (operating as 600 MHz for ^{1}H and 151 MHz for ^{13}C) at 298.0 K using the residual solvent signals as the internal reference for ^{1}H (δ = 7.26 ppm in $CDCl_3$) and ^{13}C (δ = 77.16 ppm in $CDCl_3$). Mass spectra (MS) were obtained from a Thermo Scientific Q Exactive HF Orbitrap-FTMS. Semipreparative GPC was carried out on a Shimadzu recycling GPC system equipped with a LC-20 AD pump, SPD20A UV detector and a set of JAIGEL 2.5H (20 × 600 mm) columns in Chloroform as the eluent at a flow rate of 5.0 mL/min. Absolute PL quantum yields and emission decay curves of the compounds were collected by using a spectrometer (FLS980) from Edinburgh Instruments equipped with an integrating sphere. Steady-state PL spectra were obtained by the spectrophotometers of QE65 Pro and FLS980. Measurement of UV-visible absorption spectra was conducted on a spectrometer from HITACHI Instruments (UV-3900H) and Shimadzu UV-2700 spectrometers.

TLC analyses were performed on silica gel plate and column chromatography over silica gel (mesh 200-300). Unless otherwise noted, commercially available solvents and reagents were used without further purification.

2. Synthetic Procedure and Characterization Data

2.1 Synthesis of compound **S2**



Compound **S1** was synthesized according to the previously reported method.[1]

A 250 mL two-necked flask equipped with a magnetic stirrer was charged with zinc powder (12.01 g, 184 mmol, 12.0 equiv.) and THF (140 mL) under nitrogen atmosphere. The mixture was cooled to -40 °C, and $TiCl_4$ (10.10 mL, 92 mmol, 6.0 equiv.) was added slowly by a syringe. The mixture was refluxed for 2 h and then cooled to room temperature. A THF solution (80 mL) of **S1** (5.00 g, 15 mmol, 1.0 equiv.) and 4,4'-dibromobenzophenone (5.21 g, 15 mmol, 1.0 equiv.) was added to the mixture, and the reaction mixture was stirred at reflux overnight. After cooling down to room temperature, saturated K_2CO_3 was added and the mixture was filtered. The filtrates were extracted with CH_2Cl_2 (200 mL x 3) and the combined organic phase was washed with brine (300 mL x 3). After solvent removal under reduced pressure, the crude product was purified by column chromatography on silica gel using PE / CH_2Cl_2 (6:1, v/v) as eluent to afford **S2** as light yellow solid (3.75 g, 39 % yield).

S2: Known compound. [2] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.6 Hz, 4H), 6.88 (broad, 8H), 6.64 (d, *J* = 8.6 Hz, 4H), 3.90 (t, *J* = 6.6 Hz, 4H), 1.76 - 1.70 (m, 4H), 1.51-1.44 (m, 4H), 0.97 (t, *J* = 7.4 Hz, 6H).

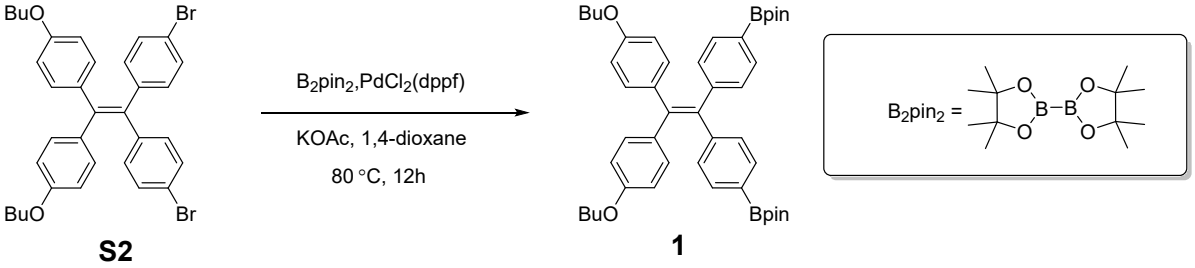
^{13}C NMR (151 MHz, $CDCl_3$) δ 158.16, 143.02, 141.80, 136.47, 135.53, 133.16, 132.63, 131.12, 120.35, 113.86,

67.68, 31.49, 19.39, 14.03.

UV/Vis (CH_2Cl_2): λ_{max} (log ε) = 257 (4.48), 302 (4.21) and 333 nm (4.27).

MS (MALDI-TOF) m/z: $[M]^+$ calcd. for $C_{34}H_{34}O_2Br_2^+$, 632.0920; found, 632.0925.

2.2 Synthesis of compound **1**



A mixture of compound **S2** (500 mg, 0.78 mmol, 1.0 equiv.), B_2pin_2 (500 mg, 1.97mmol, 2.5 equiv.), KOAc (232 mg, 1.97 mmol, 3.0 equiv.), and $PdCl_2(dppf)$ (35 mg, 0.05 mmol, 6 % equiv.) in anhydrous 1,4-dioxane (20 mL) were heated at 80 °C for 12 h under nitrogen, and then 1,4-dioxane was removed under vacuum, the residue was dissolved in CH_2Cl_2 washed with water, and dried over anhydrous $NaSO_4$. After removing CH_2Cl_2 under reduced pressure, the crude product was purified by column chromatography on silica gel using PE / CH_2Cl_2 (1:2, v/v) as eluent to afford **1** as light yellow solid (489 mg, 85 % yield).

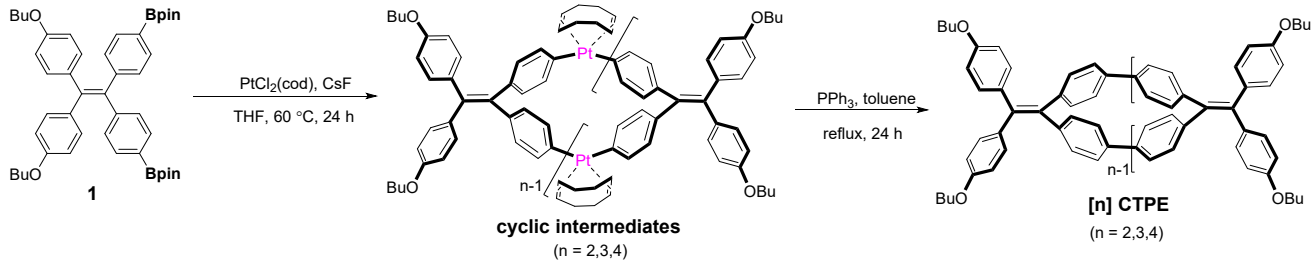
1: Known compound.[2] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 4H), 7.00 (d, *J* = 7.8 Hz, 4H), 6.90 (d, *J* = 8.7 Hz, 4H), 6.60 (d, *J* = 8.7 Hz, 4H), 3.88 (t, *J* = 6.5 Hz, 4H), 1.77-1.67 (m, 4H), 1.52-1.43 (m, 4H), 1.32 (s, 24H), 0.96 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 157.93, 147.47, 141.47, 138.90, 136.09, 134.24, 132.74, 130.97, 113.69, 83.79, 67.57, 31.52, 25.03, 19.40, 14.04.

UV/Vis (CH_2Cl_2): λ_{max} (log ε) = 257 (4.42), 303 (4.21) and 335 nm (4.23).

MS (MALDI-TOF) m/z: $[M]^+$ calcd. for $C_{46}H_{58}B_2O_6^+$, 728.4414; found,728.4415.

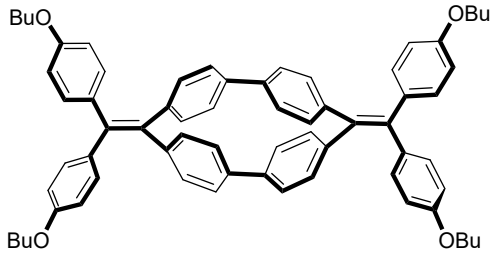
2.3 Synthesis of **[n]CTPE**s



A mixture of **1** (200.0 mg, 0.27 mmol), $PtCl_2(cod)$ (102.7 mg, 0.27 mmol) and CsF (250.2 mg, 1.64 mmol) in THF (25 ml) was stirred at ambient temperature for 30 min and then heated at 60 °C for 24 h under nitrogen atmosphere. After THF was removed rotary evaporation, the residue was dissolved in CH_2Cl_2 and was washed with brine, dried over Na_2SO_4, and concentrated in vacuo to afford crude product containing the cyclic intermediates. A mixture of crude cyclic intermediates and PPh_3 (1440.0 mg, 4.17 mmol) in toluene (25 ml) was refluxed for 24 h under nitrogen atmosphere. After cooling down to room temperature, toluene was removed under vacuum. The residue was dissolved in CH_2Cl_2 (30 mL) and washed with brine (30 mL x 3). After dried

over anhydrous Na_2SO_4, the organic layer was concentrated and then passed through a short silica gel column to afford a crude mixture, which was subjected to recycling preparative GPC-HPLC. **[2]CTPE**, **[3]CTPE** and **[4]CTPE** were collected separately as yellow solutions. Further purification by silica gel column chromatography and recrystallization from CH_2Cl_2/*n*-hexane gave pure **[2]CTPE**, **[3]CTPE** and **[4]CTPE**.

[2]CTPE, White solid, 20.7 mg, yield 15.9 %;



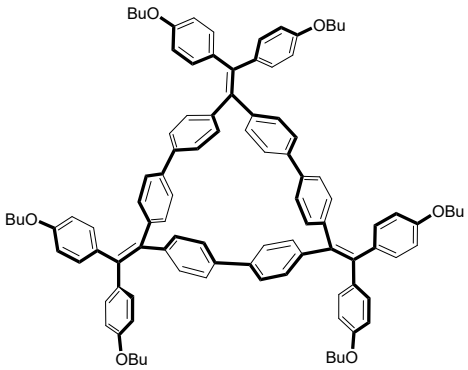
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.38 (d, *J* = 8.9 Hz, 8H), 6.96 (d, *J* = 8.5 Hz, 8H), 6.90 (d, *J* = 8.5 Hz, 8H), 6.76 (d, *J* = 8.9 Hz, 8H), 3.91 (t, *J* = 6.5 Hz, 8H), 1.76-1.69 (m, 8H), 1.50-1.42 (m, 8H), 0.95 (t, *J* = 7.4 Hz, 12H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.16, 148.90, 139.59, 138.80, 134.72, 133.96, 131.78, 130.06, 126.86, 113.73, 67.64, 31.49, 19.39, 13.99.

UV/Vis (THF): λ_{max} (log ε) = 252 (4.48), 288 (4.86) and 324 nm (4.66).

MS (MALDI-TOF): $[M]^+$ calcd. for $C_{68}H_{68}O_4^+$, 948.5112; found, 948.5111.

[3]CTPE, White solid, 12.9 mg, yield 9.9 %;



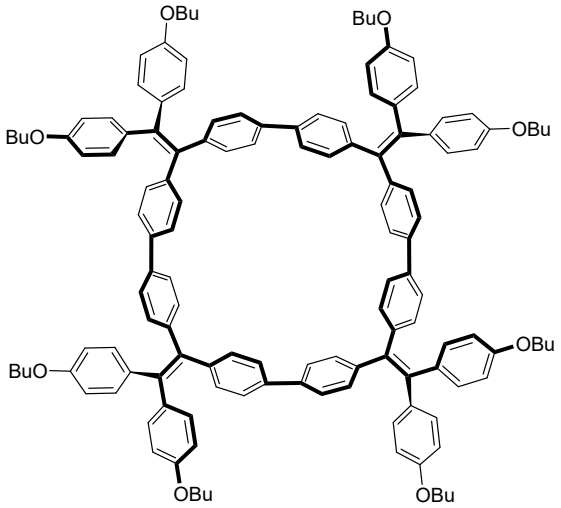
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.17 (d, *J* = 8.9 Hz, 12H), 7.13 (d, *J* = 8.4 Hz, 12H), 6.88 (d, *J* = 8.4 Hz, 12H), 6.69 (d, *J* = 8.9 Hz, 12H), 3.87 (t, *J* = 6.5 Hz, 12H), 1.74-1.67 (m, 12H), 1.48-1.40 (m, 12H), 0.93 (t, *J* = 7.4 Hz, 18H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 157.87, 144.13, 139.35, 137.97, 137.56, 134.62, 132.10, 129.66, 127.14, 113.64, 67.59, 31.51, 19.39, 14.00.

UV/Vis (THF): λ_{max} (log ε) = 255 (4.89) and 317 nm (4.88).

MS (MALDI-TOF): $[M]^+$ calcd. for $C_{102}H_{102}O_6^+$, 1422.7671; found, 1422.7663.

[4]CTPE-2OBu, yellow solid, 5.8 mg, yield 4.5 %;



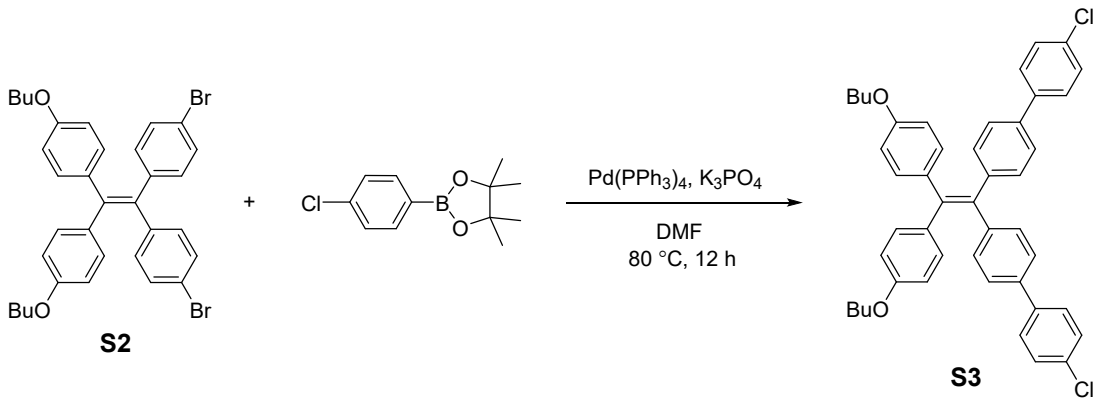
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.4 Hz, 16H), 7.06 (d, *J* = 8.8 Hz, 16H), 6.87 (d, *J* = 8.4 Hz, 16H), 6.65 (d, *J* = 8.8 Hz, 16H), 3.88 (t, *J* = 6.5 Hz, 16H), 1.77-1.68 (m, 16H), 1.50-1.42 (m, 16H), 0.95 (t, *J* = 7.4 Hz, 24H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.04, 144.61, 138.99, 138.25, 136.94, 135.51, 132.70, 131.73, 125.77, 113.69, 67.61, 31.52, 19.40, 14.01.

UV/Vis (THF): λ_{max} (log ε) = 262 (5.03) and 356 nm (5.10).

MS (MALDI-TOF) : $[M]^+$ calcd. for $C_{136}H_{137}O_8^+$, 1898.0308; found,1898.0313.

2.4 Synthesis of compound **S3**



To a 50 mL Schlenk flask charged with a magnetic stir bar, **S2** (400 mg, 0.63 mmol, 1.0 equiv), 4-chlorophenylboronic acid pinacol ester (301 mg, 1.26 mmol, 2.0 equiv), $Pd(PPh_3)_4$ (73 mg, 0.06 mmol, 0.1 equiv), and K_3PO_4 (803 mg, 3.78 mmol, 6.0 equiv) were added. The vessel was sealed with a rubber septum and evacuated/backfilled with N_2 (3 times) before adding DMF (15 mL) under N_2 atmosphere. The bright yellow reaction mixture was heated to 80 °C and stirred at this temperature for 12 h. The reaction mixture was then cooled down to room temperature and diluted with DCM (50 mL). The organic layer was washed with water (40 mL×5), dried over anhydrous Na_2SO_4, and concentrated. Further purification by silica gel column chromatography (PE / DCM, v/v = 3:1) afforded compound **S3** as light-yellow solid (367 mg, 83 % yield).

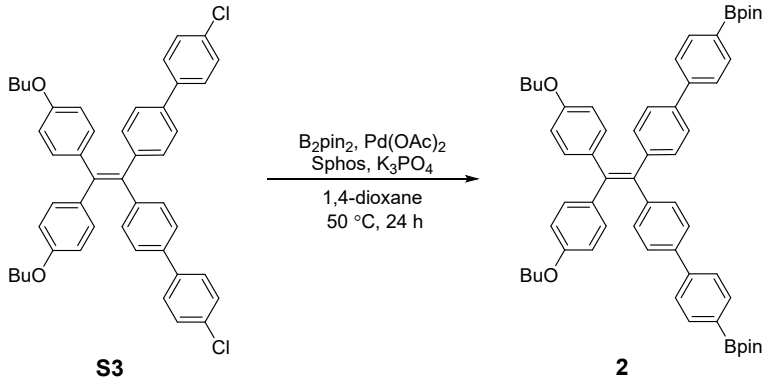
S3: ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49 (d, *J* = 8.6 Hz, 4H), 7.37 (d, *J* = 8.6 Hz, 4H), 7.33 (d, *J* = 8.0 Hz, 4H), 7.11 (broad, 4H), 6.97 (d, *J* = 8.0 Hz, 4H), 6.65 (d, J = 8.8 Hz, 4H), 3.89 (t, *J* = 6.5 Hz, 4H), 1.77 -1.69 (m, 4H), 1.51-1.42 (m, 4H), 0.96 (t, *J* = 7.4 Hz, 6H).

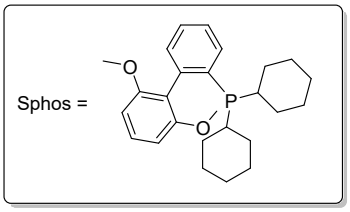
^{13}C NMR (151 MHz, $CDCl_3$) δ 157.99, 143.91, 141.20, 139.31, 137.41, 136.18, 133.27, 132.77, 132.15, 128.97, 128.21, 126.26, 113.77, 67.67, 31.51, 19.40, 14.03.

UV/Vis (CH_2Cl_2): λ_{max} (log ε) = 265 (4.64) and 335 nm (4.45).

MS (MALDI-TOF): $[M]^+$ calcd. for $C_{46}H_{42}O_2Cl_2^+$, 696.2556; found, 696.2562.

2.5 Synthesis of compound **2**





To a 50 mL schlenk flask were added **S3** (300 mg, 0.43 mmol, 1 equiv), B_2pin_2 (655 mg, 2.58 mmol, 6 equiv), $Pd(OAc)_2$ (6 mg, 0.026 mmol, 6% equiv), K_3PO_4 (548 mg, 2.58 mmol, 6 equiv) and Sphos (21 mg, 0.052 mmol, 12% equiv). The flask was degassed and purged with N_2 for three cycles. Then anhydrous 1,4-dioxane (10 mL) was added through a syringe under N_2 atmosphere. The mixture was stirred at 50 °C for 24 h. The solvent was removed and the residue was dissolved in 30 mL CH_2Cl_2. The solution was washed with brine (30 mL x 3) and then dried over anhydrous Na_2SO_4. After removing the organic solvent under reduced pressure, the crude product was purified by silica gel column chromatography using dichloromethane as eluent to afford compound **2** as Light yellow solid (310 mg, 82 % yield).

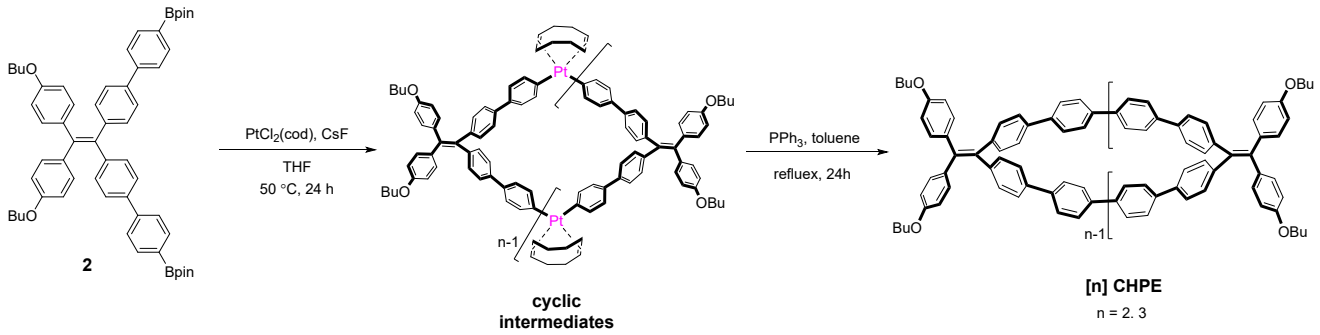
2: ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 4H), 7.58 (d, *J* = 8.4 Hz, 4H), 7.40 (d, *J* = 8.4 Hz, 4H), 7.12 (d, *J* = 8.0 Hz, 4H), 6.98 (d, *J* = 8.8 Hz, 4H), 6.65 (d, *J* = 8.8 Hz, 4H), 3.89 (t, *J* = 6.5 Hz, 4H), 1.78 – 1.69 (m, 4H), 1.52 – 1.43 (m, 4H), 1.36 (s, 24H), 0.96 (t, *J* = 7.4 Hz, 6H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 157.93, 143.92, 143.57, 140.98, 138.40, 136.29, 135.32, 132.78, 132.07, 126.50, 126.25, 113.76, 83.92, 67.64, 31.51, 25.03, 19.39, 14.03.

UV/Vis (CH_2Cl_2): λ_{max} (log ε) = 265 (4.66) and 327 nm (4.55).

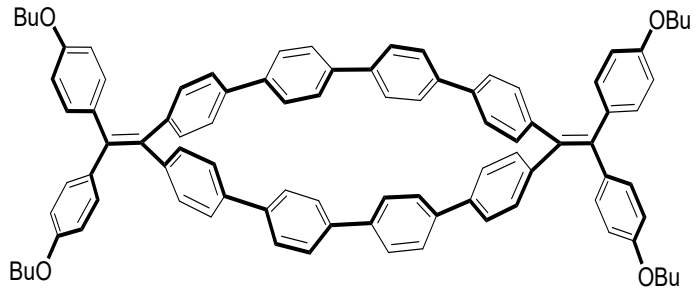
MS (MALDI-TOF): $[M]^+$ calcd. for $C_{58}H_{66}B_2O_6^+$, 880.5040; found, 880.5049.

2.6 Synthesis of **[n]CHPE**s



A mixture of **2** (200.0 mg, 0.23 mmol), $PtCl_2$(cod) (85.0 mg, 0.23 mmol) and CsF (207.0 mg, 1.36 mmol) in THF (25 ml) was heated at 60 °C for 24 h under N_2 atmosphere. After completion of reaction THF was removed under vacuum, the residue was dissolved in CH_2Cl_2 and was washed with brine, dried over anhydrous Na_2SO_4, and concentrated in vacuo to afford the cyclic intermediates. The crude cyclic intermediates and PPh_3 (1191.0 mg, 4.5 mmol) in toluene (25 ml) and the mixture was stirred at ambient temperature for 30 min and then at reflux for 24 h. After the mixture cooled down to room temperature, toluene was removed under vacuum. The residue was dissolved in CH_2Cl_2 (30 mL) and washed with brine (30 mL x 3). After dried over anhydrous sodium sulfate, the organic layer was concentrated and then passed through a short silica gel column to afford a crude mixture, which was subjected to recycling preparative GPC-HPLC. **[2]CHPE** and **[3]CHPE** were separately collected as a yellow solutions. Further purification by silica gel column chromatography and recrystallization from CH_2Cl_2/*n*-hexane gave pure **[2]CHPE** and **[3]CHPE**.

[2]CHPE, white solid, 21.6 mg, yield 15.2 %;



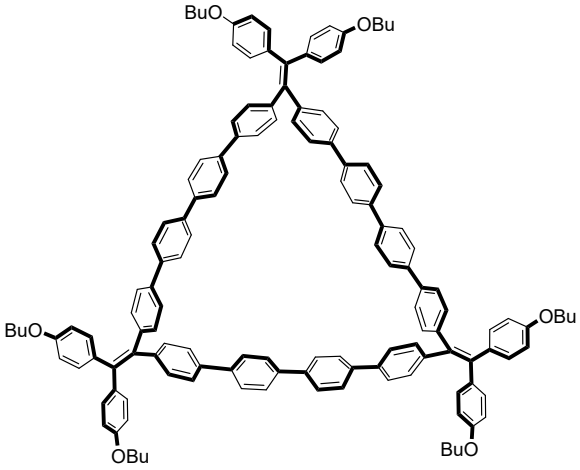
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.51 (d, *J* = 8.5 Hz, 8H), 7.38 (d, *J* = 8.5 Hz, 8H), 7.22 (d, *J* = 8.8 Hz, 8H), 7.17 (d, *J* = 8.4 Hz, 8H), 6.88 (d, *J* = 8.4 Hz, 8H), 6.73 (d, *J* = 8.8 Hz, 8H), 3.90 (t, *J* = 6.5 Hz, 8H), 1.76 -1.68 (m, 8H), 1.49-1.43 (m, 8H), 0.95 (t, *J* = 7.4 Hz, 12H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.02, 144.74, 139.83, 139.02, 137.90, 137.68, 137.29, 134.55, 132.29, 130.12, 127.68, 127.29, 126.72, 113.70, 68.73, 32.35, 20.83, 13.45.

UV/Vis (THF): λ_{max} (log ε) = 258 (4.73) and 337 nm (5.00).

MS (MALDI-TOF): $[M]^+$ calcd. for $C_{92}H_{84}O_4^+$, 1252.6364; found, 1252.6357.

[3] CHPE, yellow solid, 7.4 mg, yield 5.2 %



^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.6 Hz, 12H), 7.58 (d, *J* = 8.6 Hz, 12H), 7.34 (d, *J* = 8.4 Hz, 12H), 7.12 (d, *J* = 8.9 Hz, 12H), 6.96 (d, *J* = 8.4 Hz, 12H), 6.71 (d, *J* = 8.9 Hz, 12H), 3.90 (t, *J* = 6.5 Hz, 12H), 1.76-1.70 (m, 12H), 1.50-1.43 (m, 12H), 0.95 (t, *J* = 7.4 Hz, 18H).

^{13}C NMR (151 MHz, $CDCl_3$) δ 158.04, 144.71, 139.65, 139.12, 139.09, 138.35, 137.58, 135.53, 132.69, 131.62, 127.26, 127.21, 126.44, 113.77, 67.65, 31.53, 19.41, 14.02.

UV/Vis (THF): λ_{max} (log ε) = 263 (4.91) and 352 nm (5.19).

MS (MALDI-TOF): $[M]^+$ calcd. for $C_{138}H_{126}O_4^+$, 1878.9549; found, 1878.9546.

3. NMR spectra

3.1 ^{1}H and ^{13}C NMR spectra

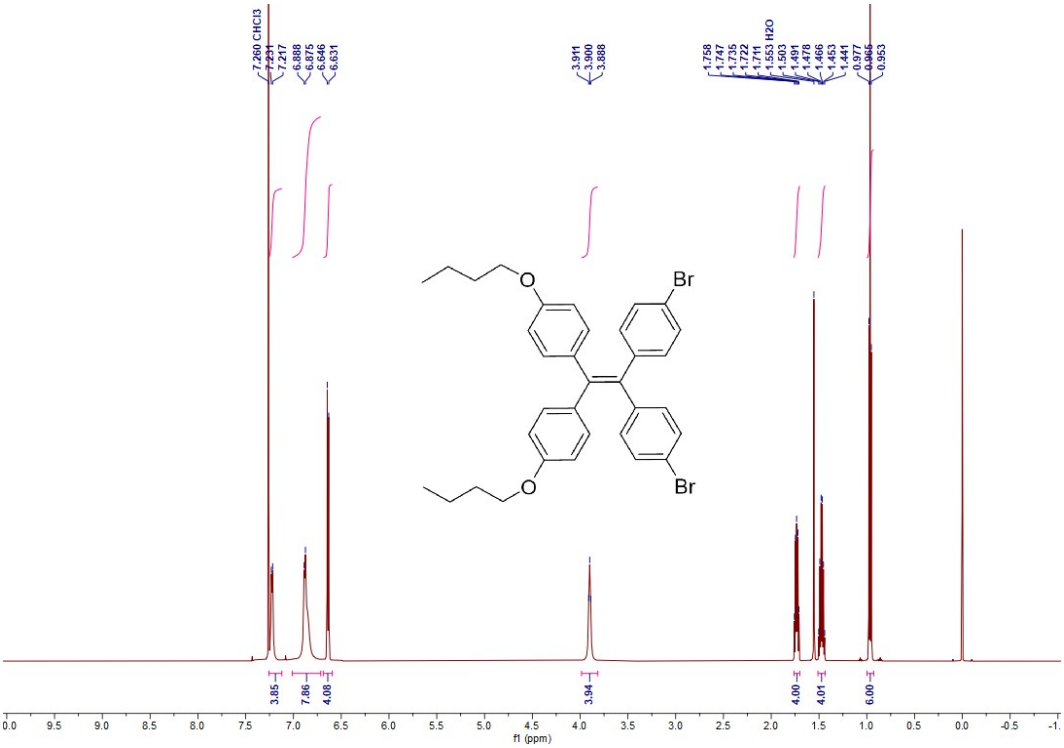


Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **S2**.

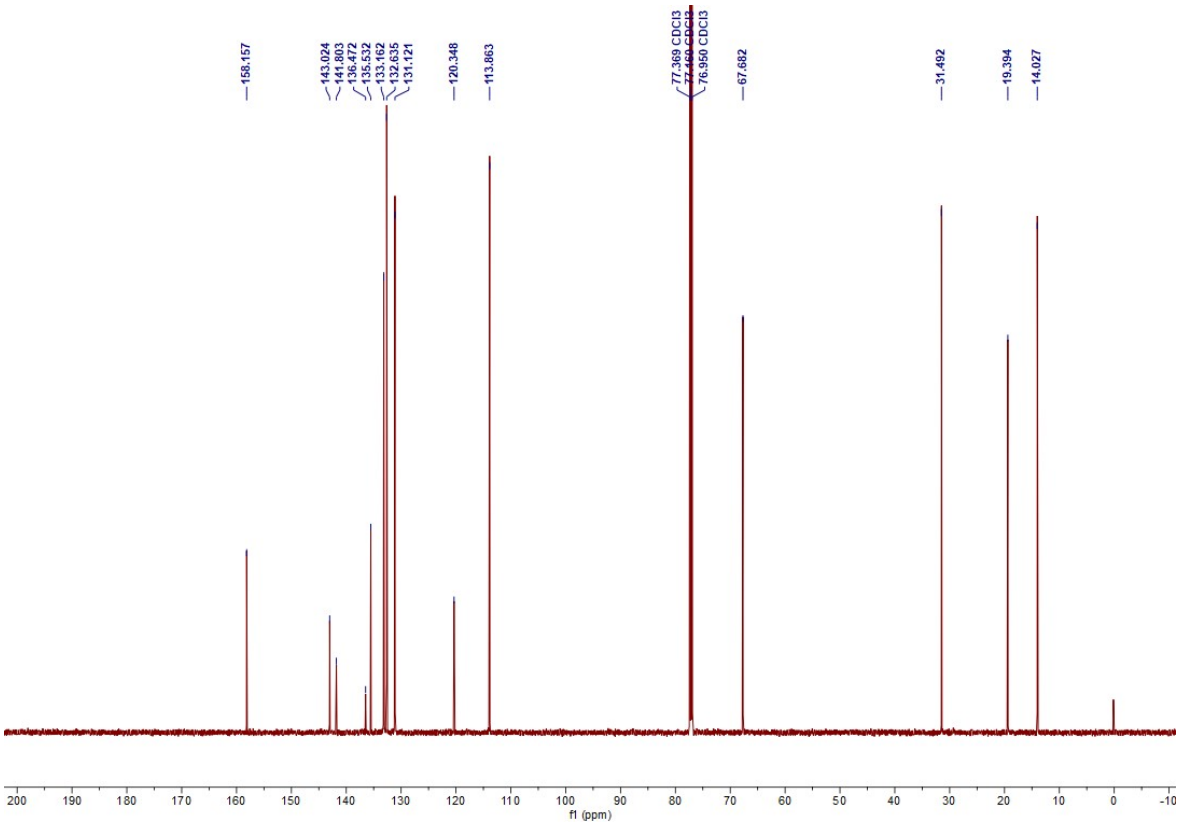


Figure S2. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **S2**.

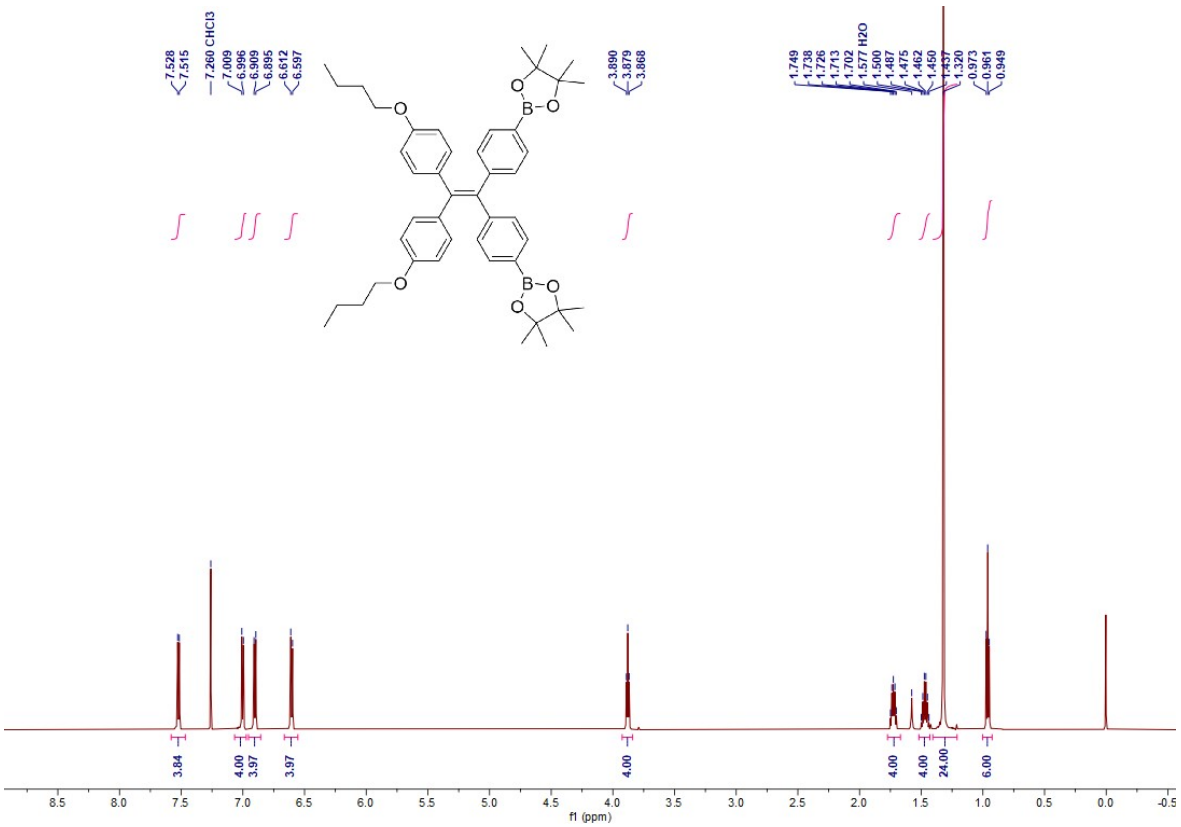


Figure S3. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **1**.

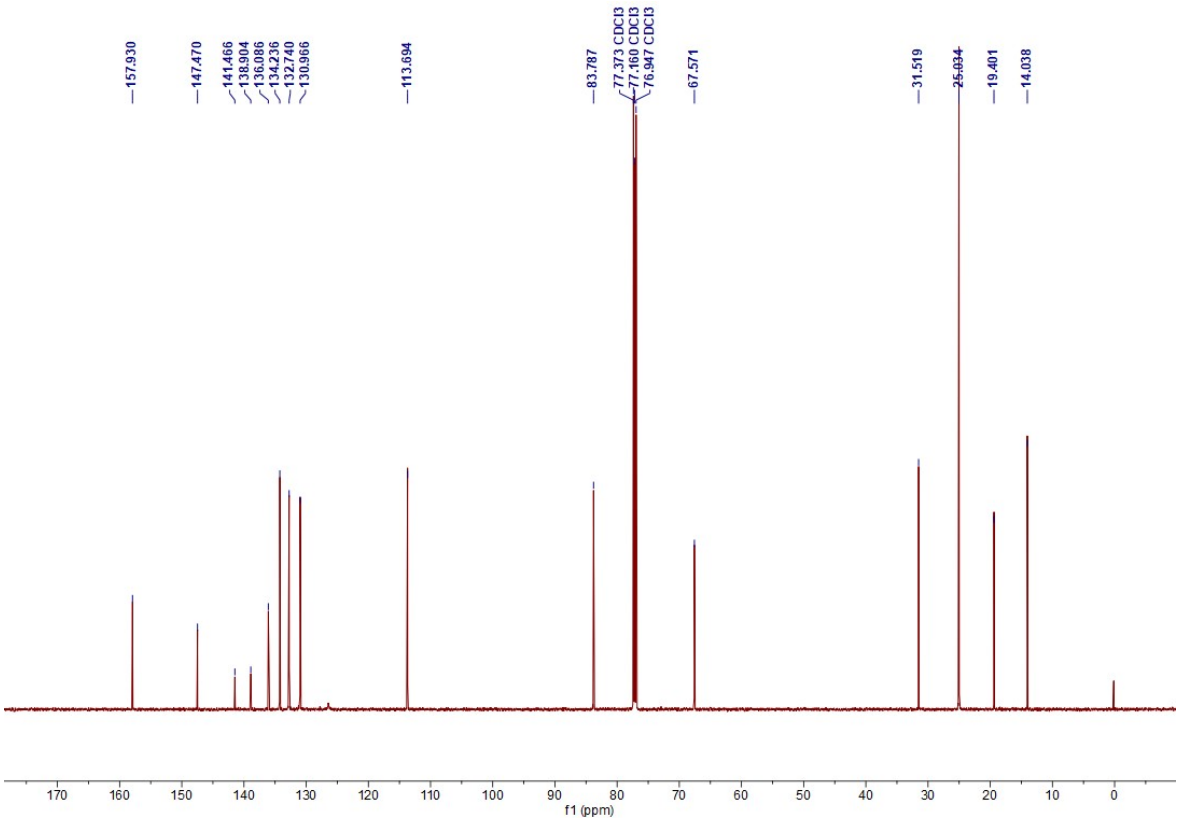


Figure S4. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **1**.

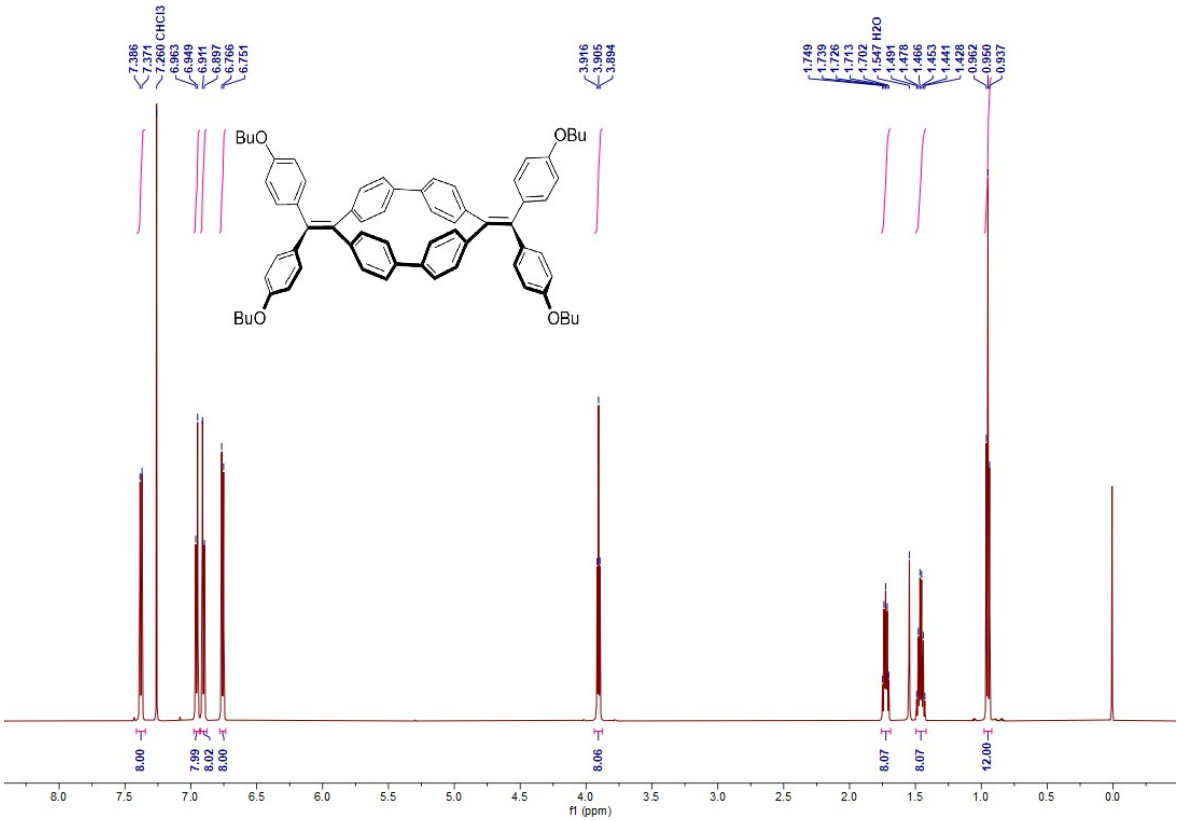


Figure S5. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **[2]CTPE**.

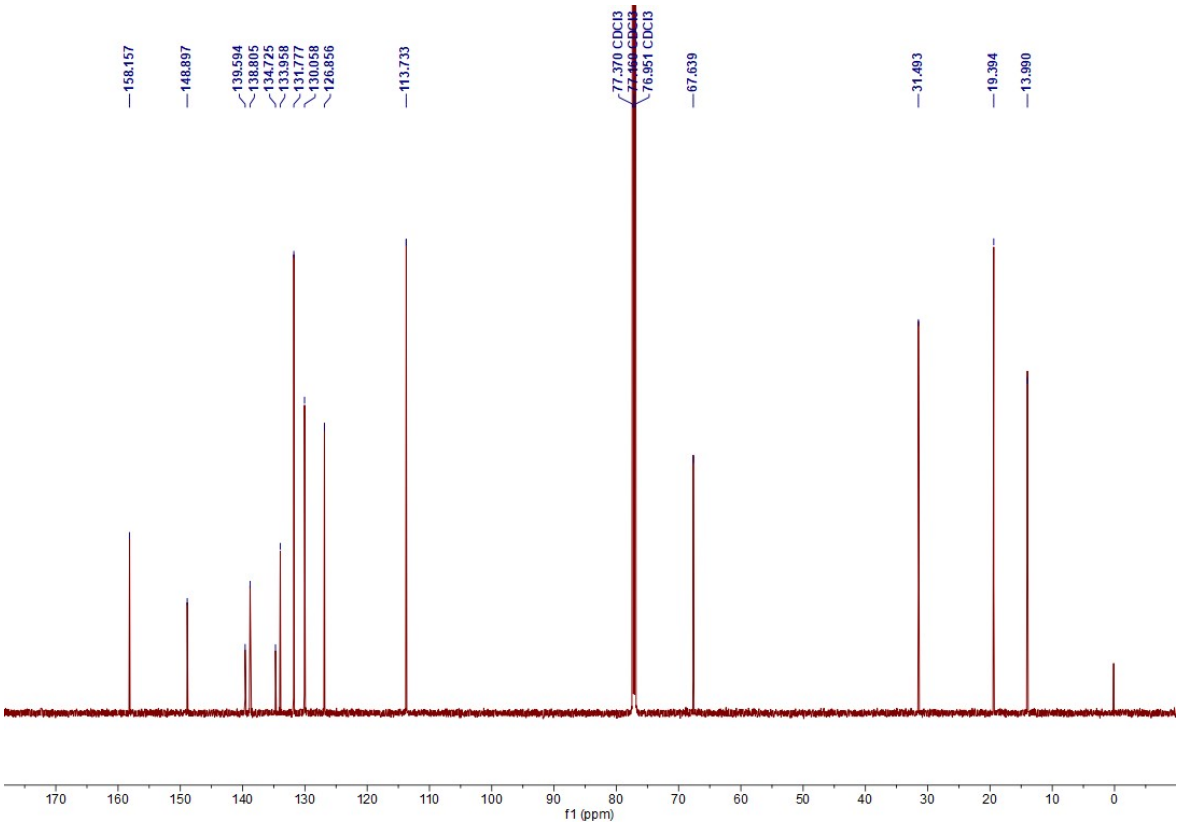


Figure S6. ^{13}C NMR (151 MHz, $CDCl_3$) of spectrum compound **[2]CTPE**.

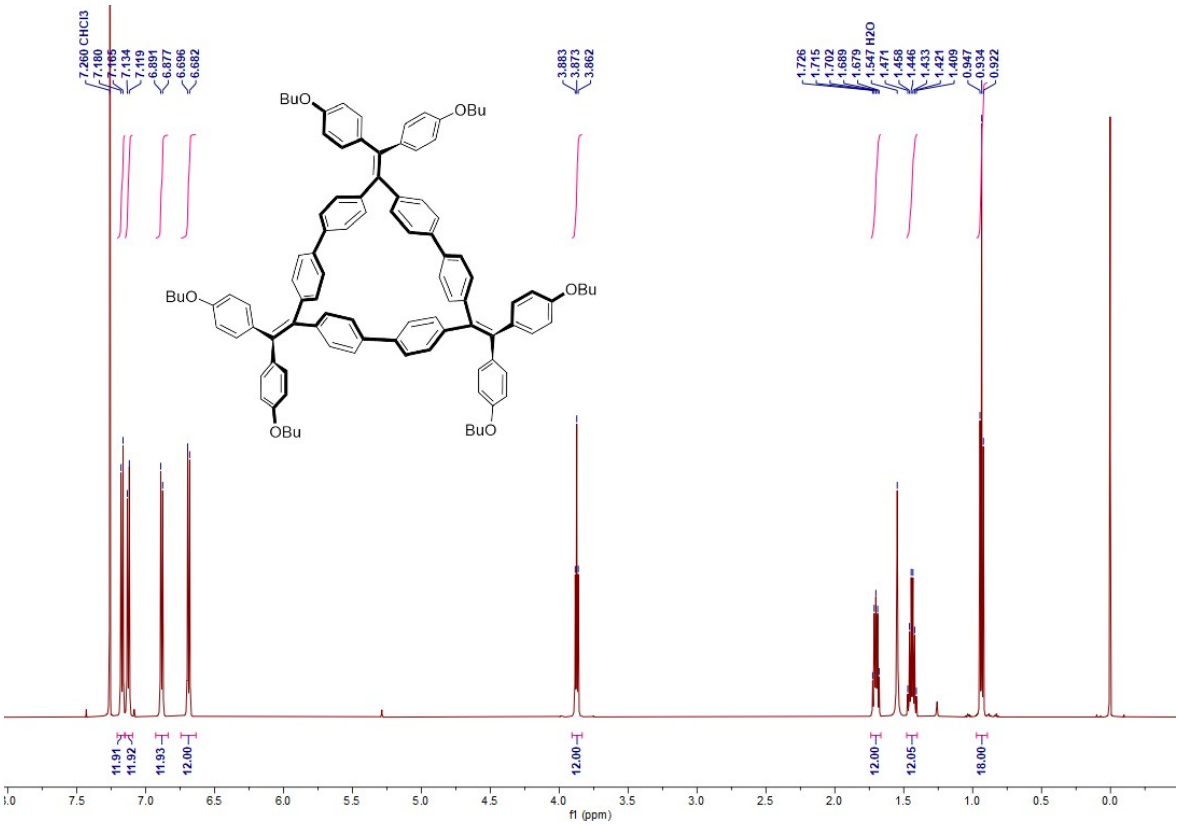


Figure S7. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **[3]CTPE**.

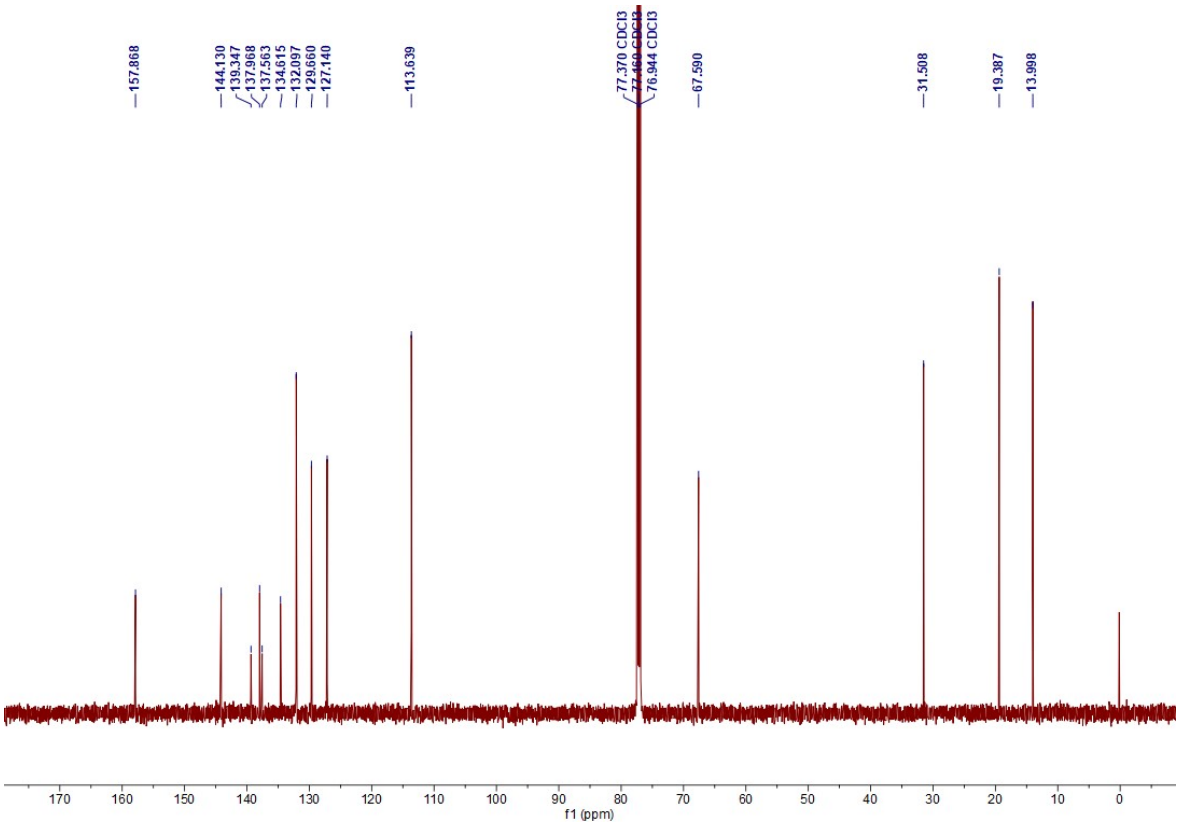


Figure S8. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **[3]CTPE**.

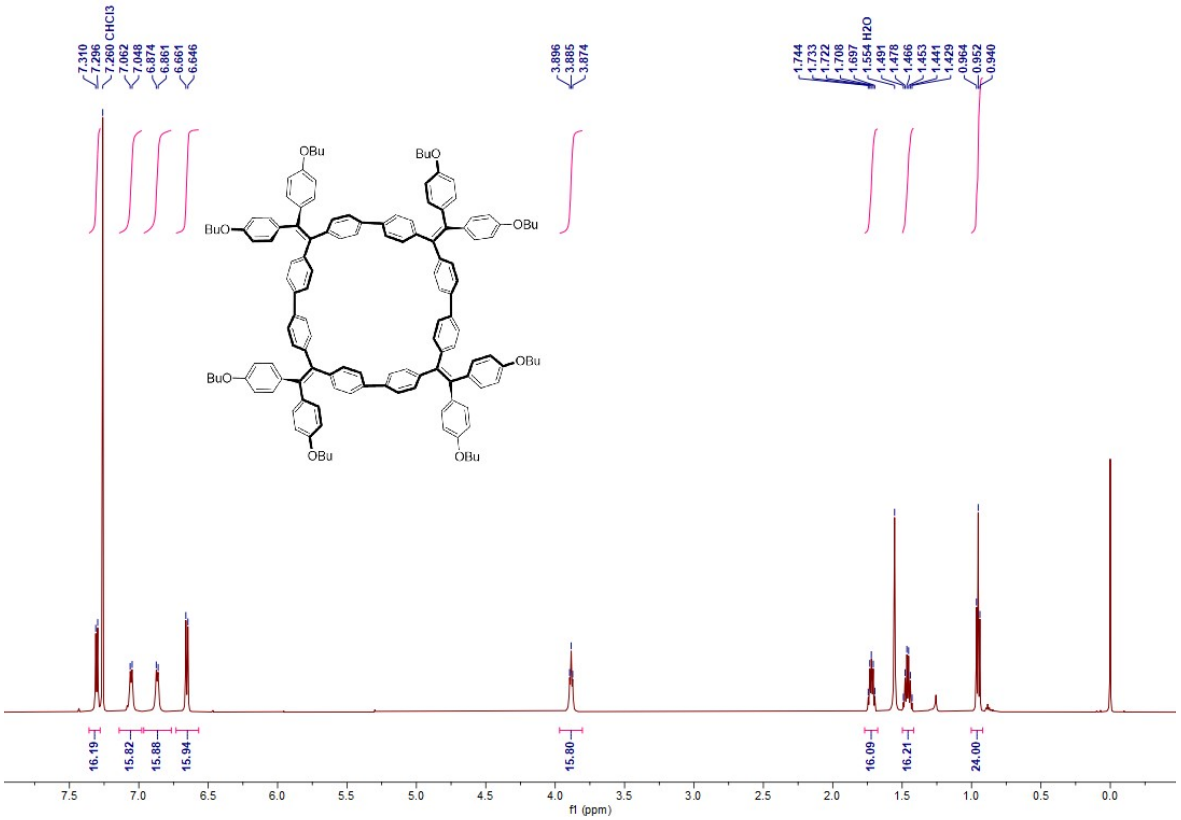


Figure S9. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **[4]CTPE**.

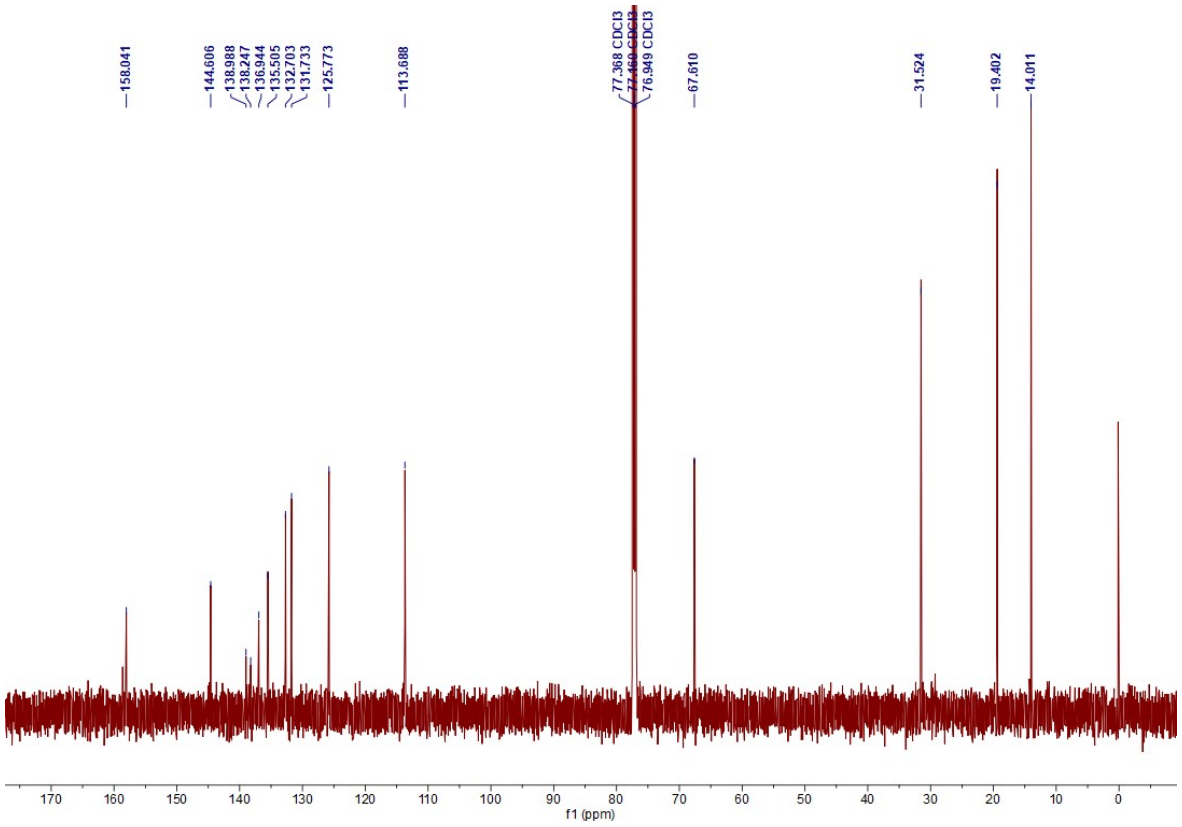


Figure S10. ^{13}C NMR (151 MHz, $CDCl_3$) spectrum of compound **[4]CTPE**.

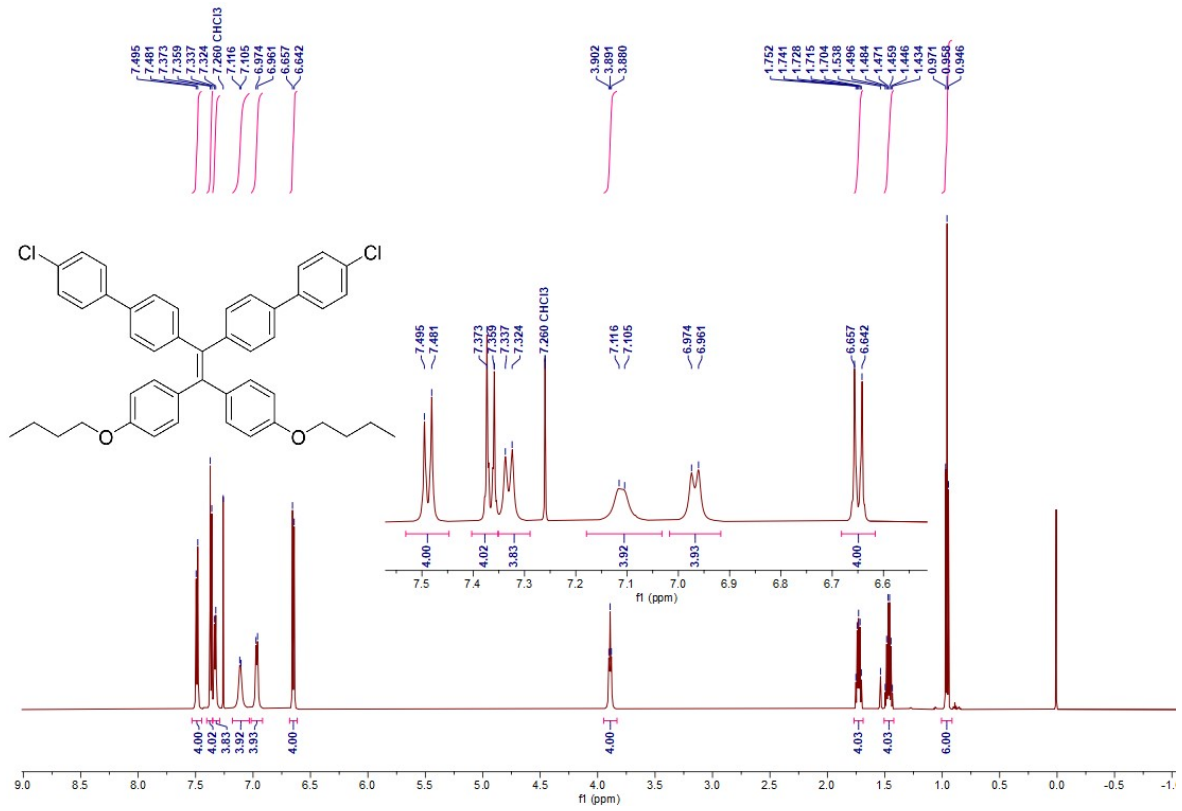


Figure S11. ^{1}H NMR spectrum of compound **S3** (600 MHz, $CDCl_3$).

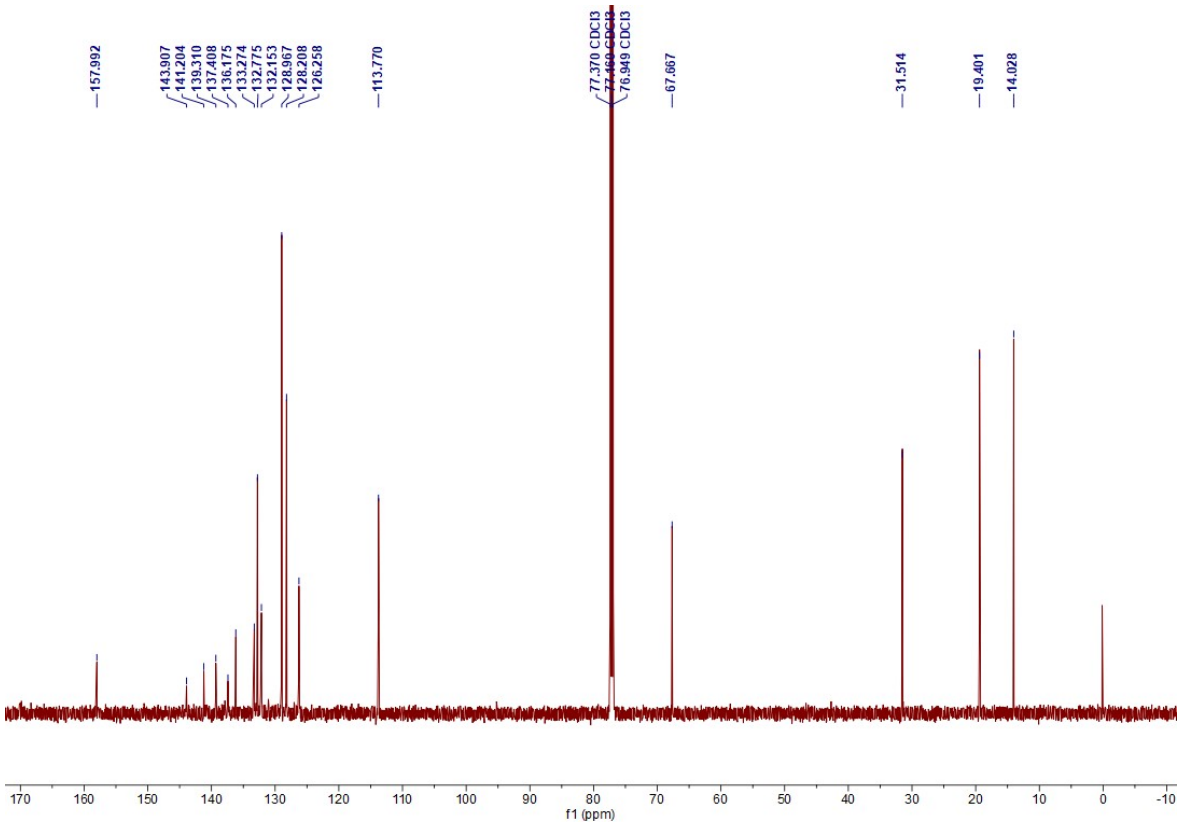


Figure S12. ^{13}C NMR spectrum of compound **S3** (151 MHz, $CDCl_3$).

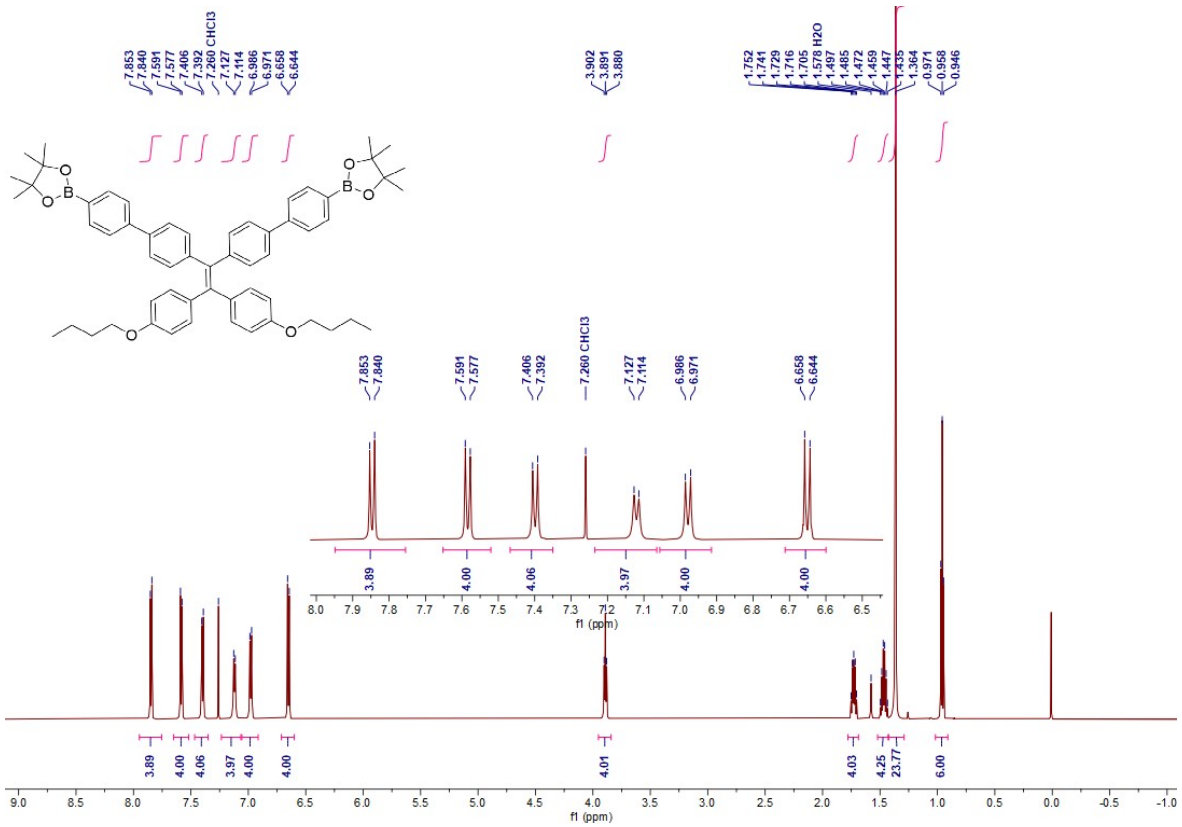


Figure S13. ^{1}H NMR spectrum of compound **2** (600 MHz, $CDCl_3$).

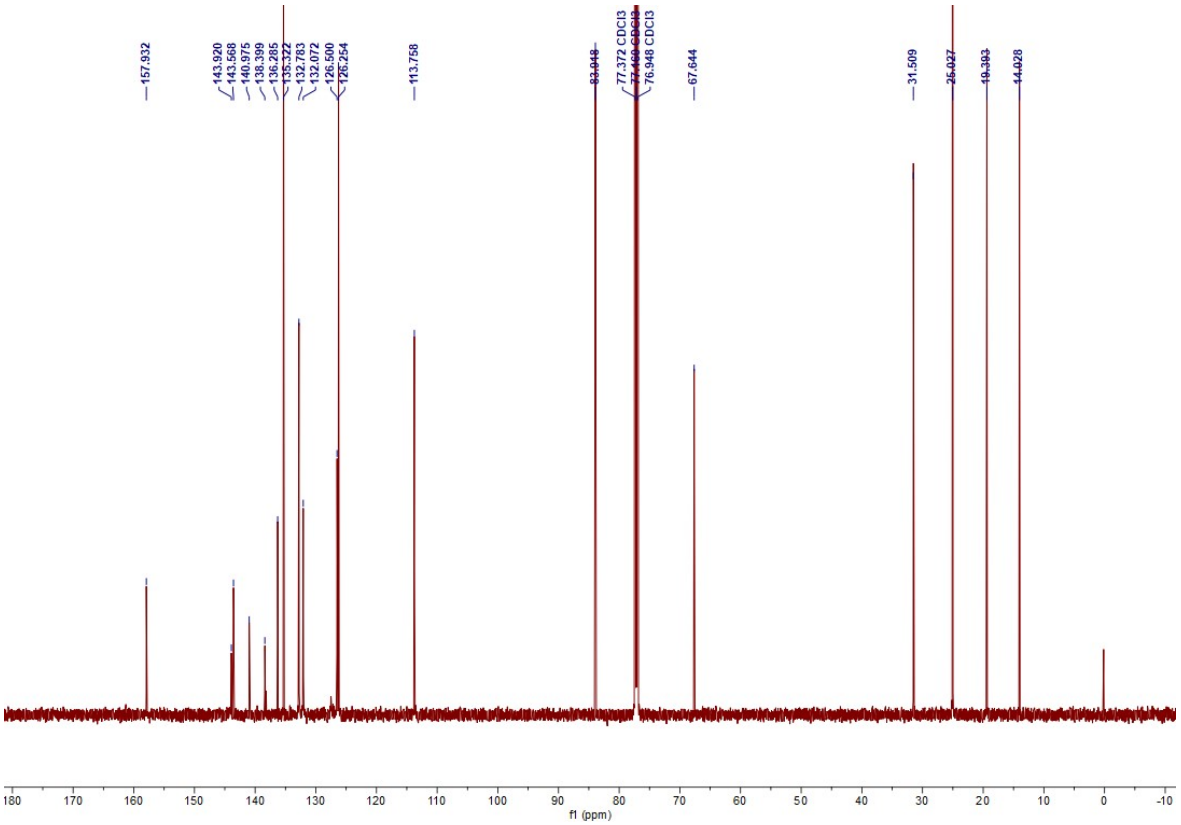


Figure S14. ^{13}C NMR spectrum of compound **2** (151 MHz, $CDCl_3$).

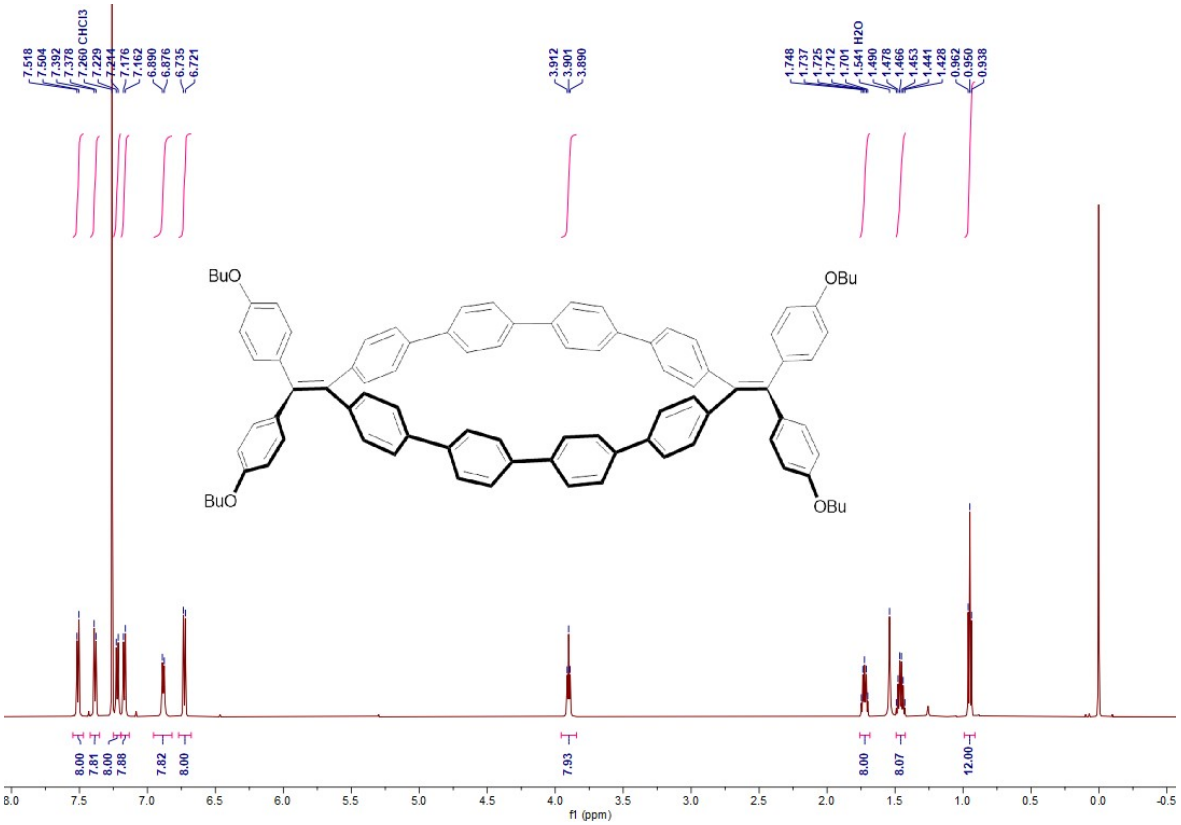


Figure S15. ^{1}H NMR spectrum of compound **[2]CHPE** (600 MHz, $CDCl_3$).

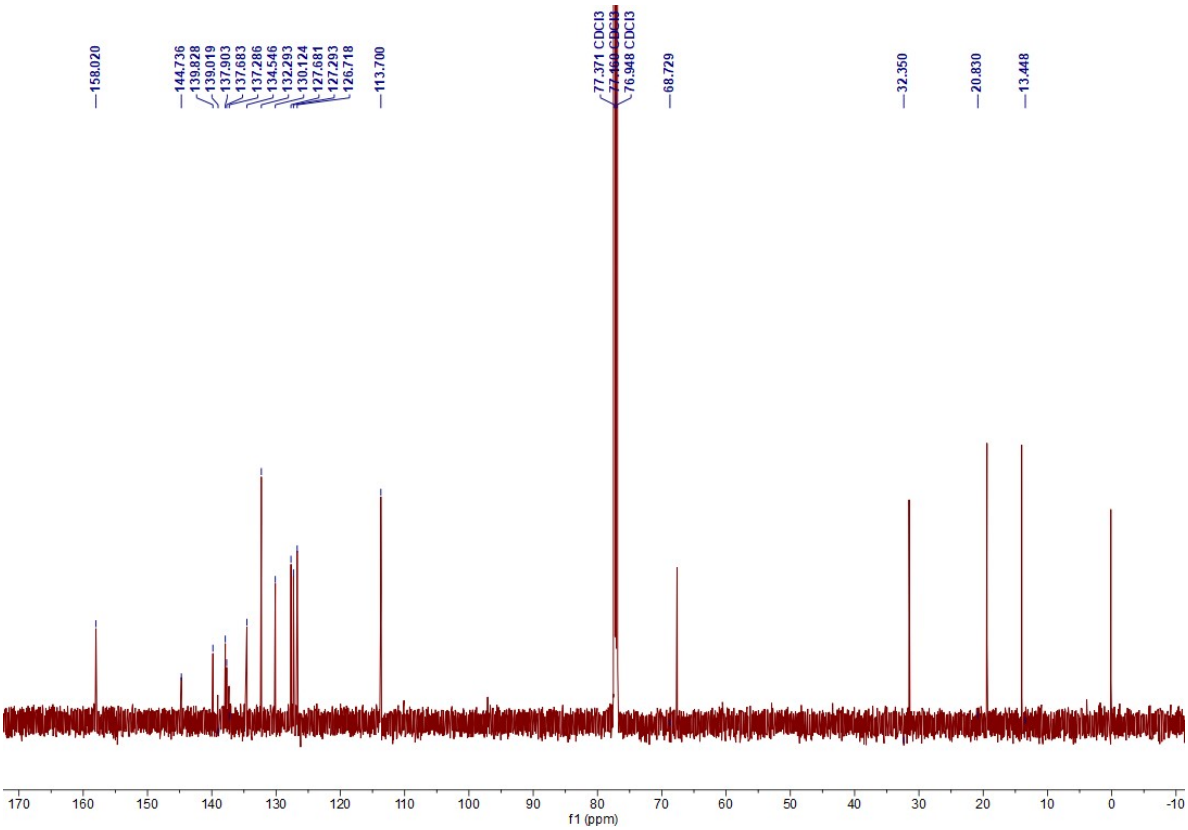


Figure S16. ^{13}C NMR spectrum of compound **[2]CHPE** (151 MHz, $CDCl_3$).

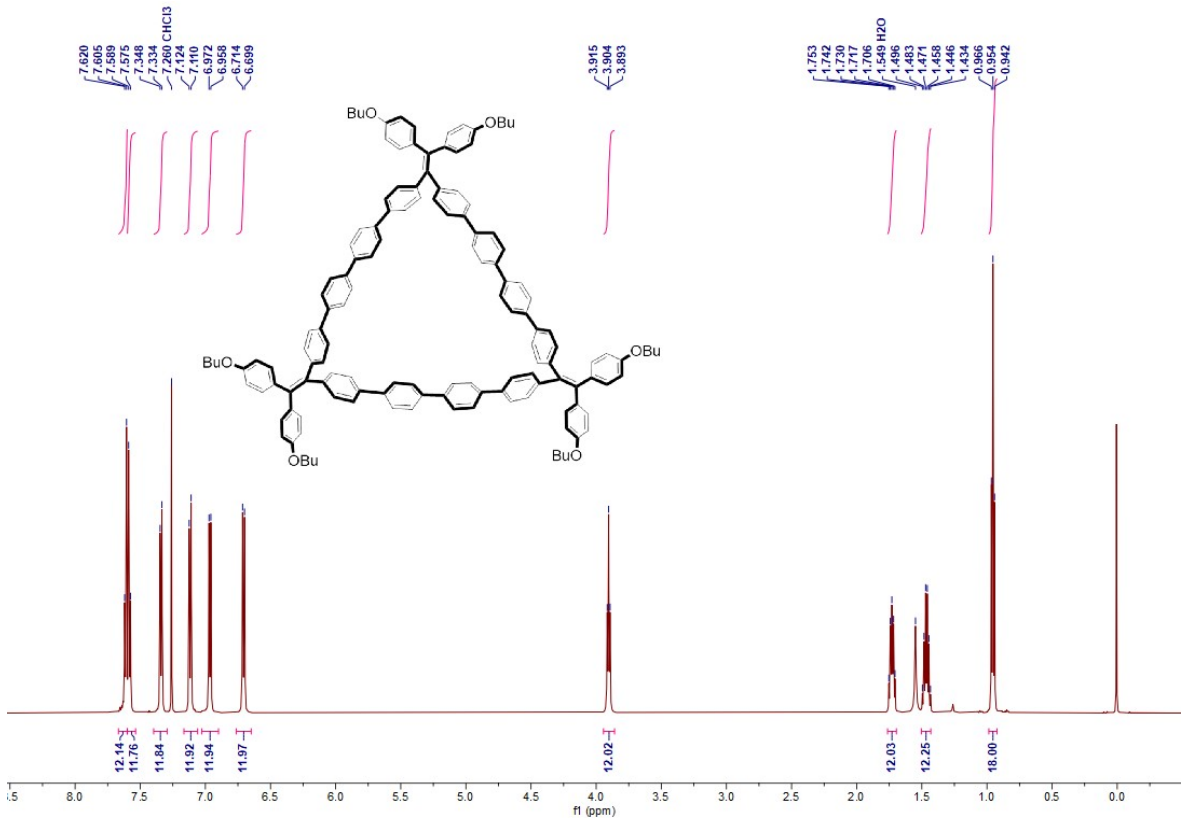


Figure S17. ^{1}H NMR spectrum of compound **[3]CHPE** (600 MHz, $CDCl_3$).

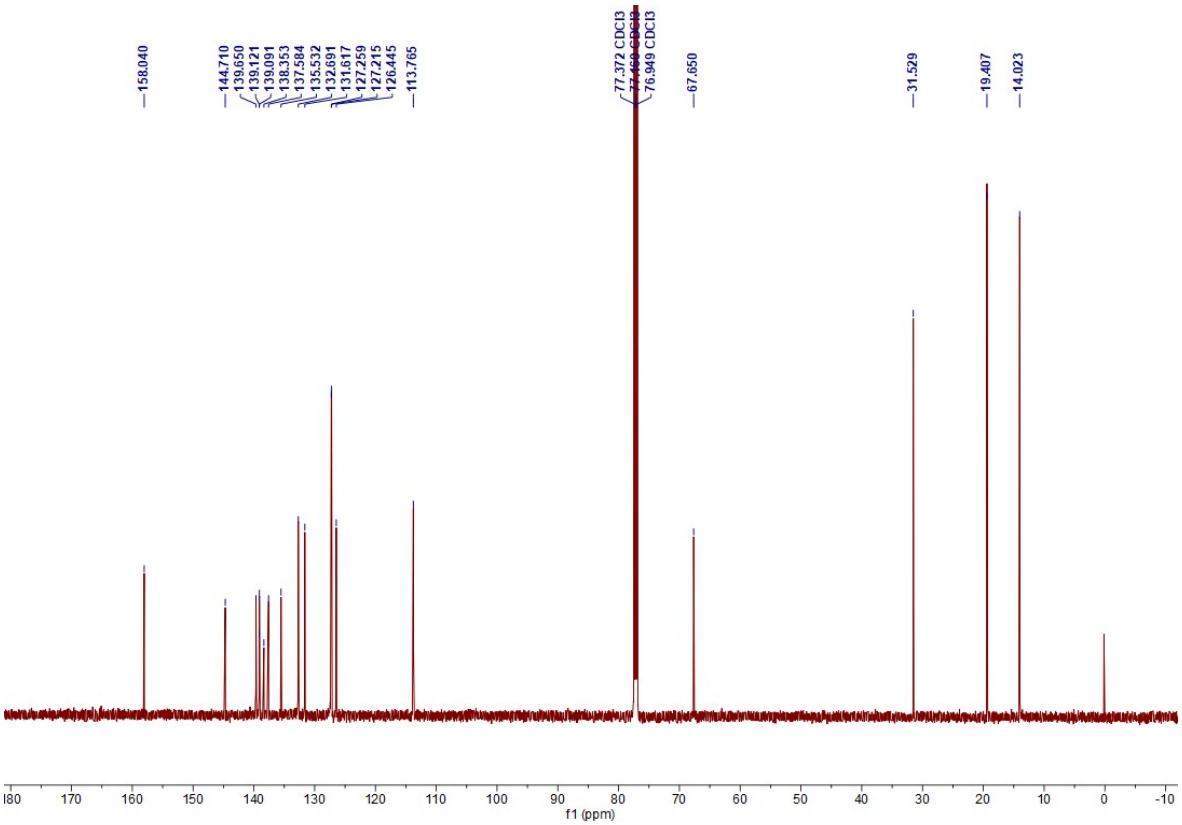
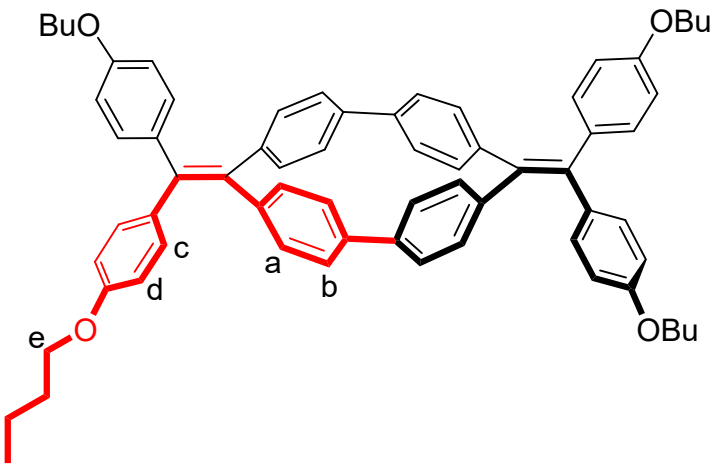


Figure S18. ^{13}**C NMR** spectrum of compound **[3]CHPE** (151 MHz, $CDCl_3$).

3.2. 2D spectra of **[2]CTPE**



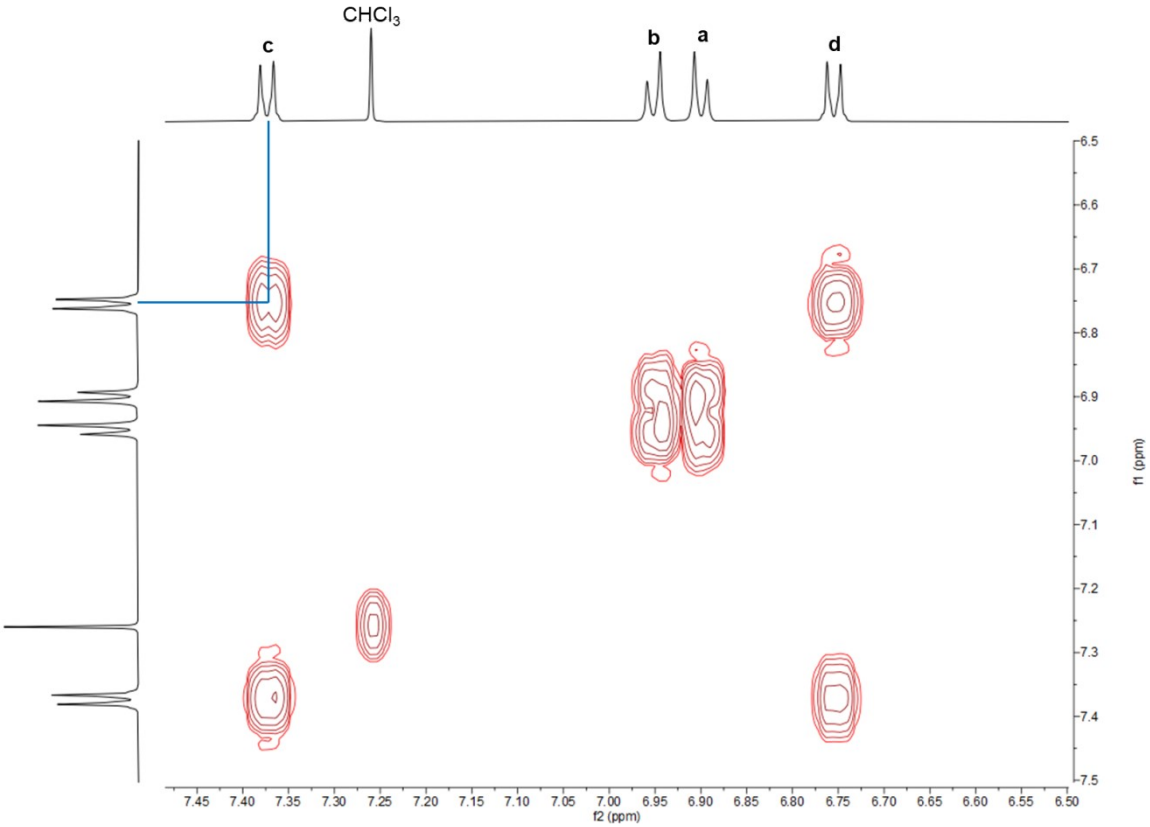


Figure S19. The COSY correlation spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CTPE**, indicating the COSY correlation between proton **a** and proton **b** , and proton **c** and proton **d**.

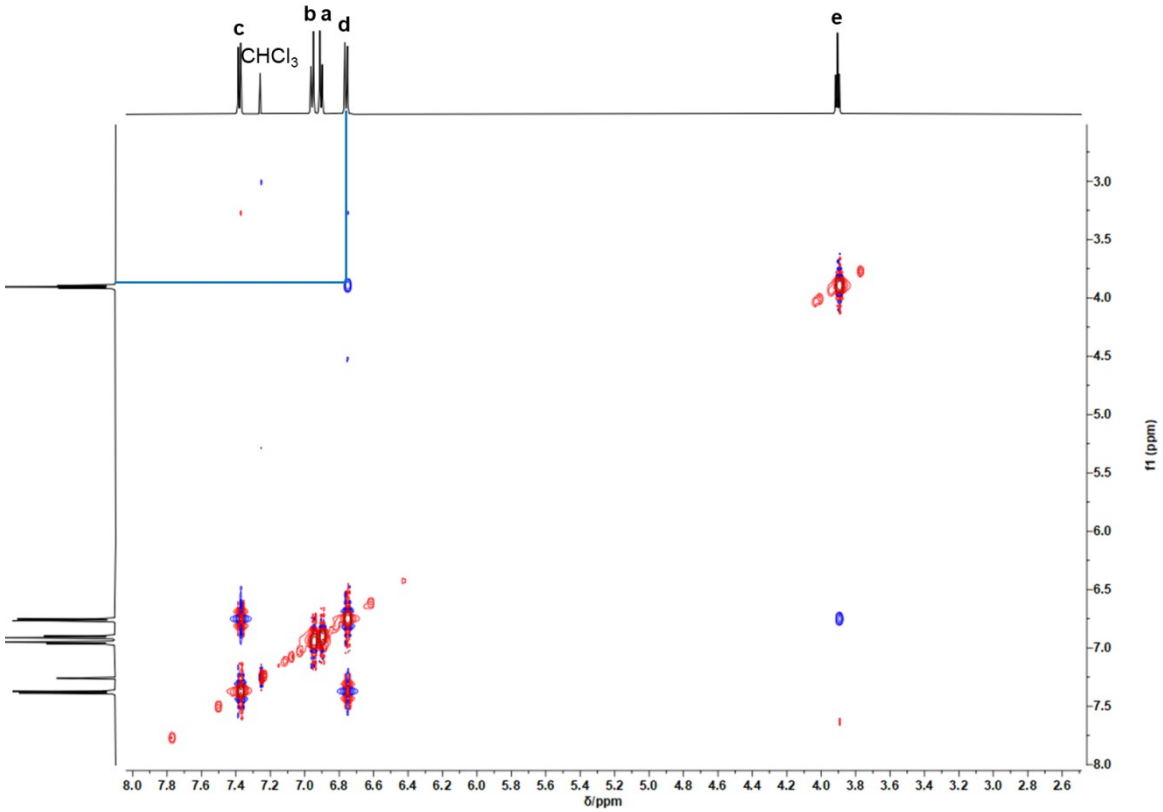


Figure S20. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CTPE**, indicating the NOEs between proton **d** and proton **e**.

3.3. 2D spectra of **[3]CTPE**

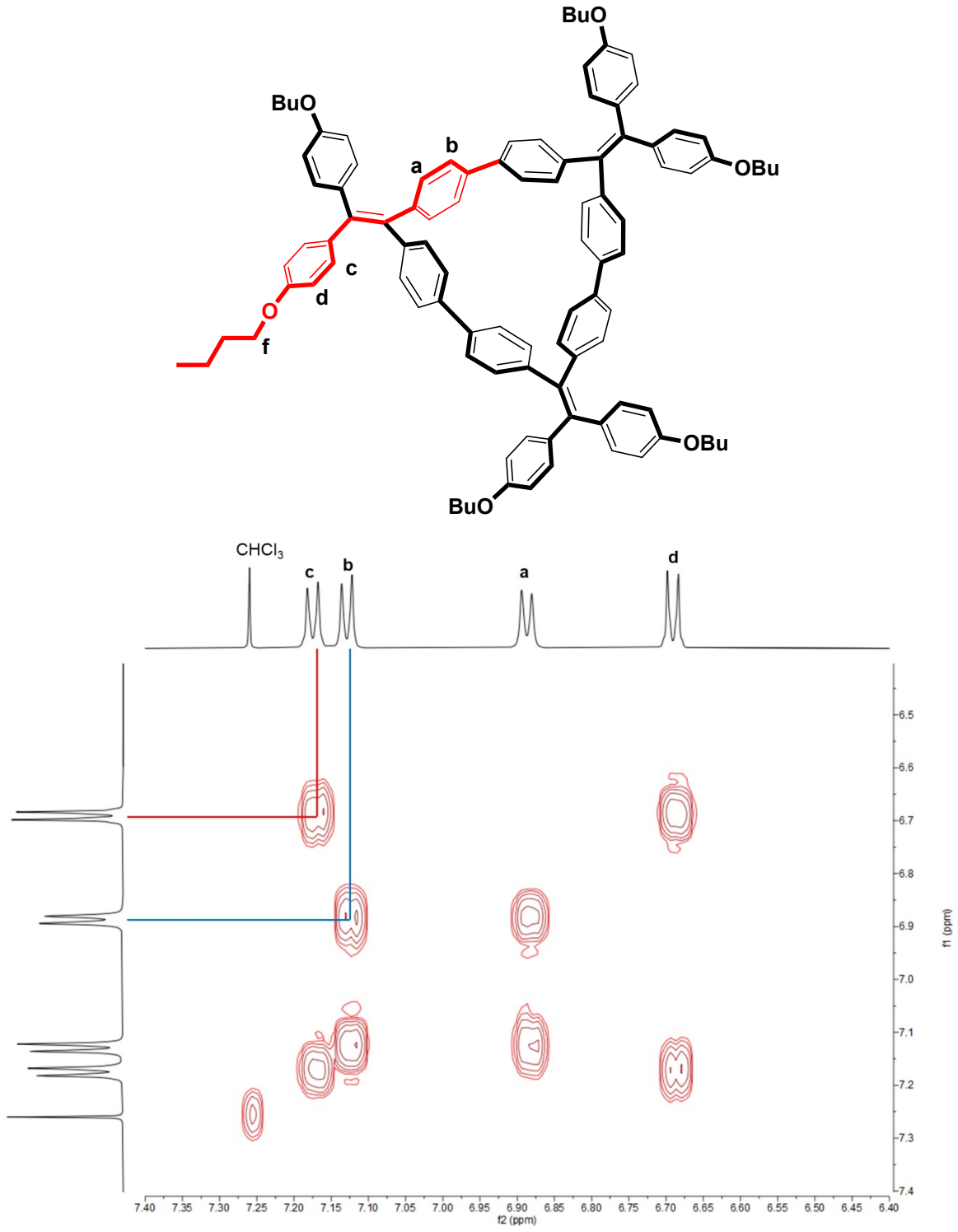


Figure S21. The COSY correlation spectrum (600 MHz, $CDCl_3$, 298 K) of **[3]CTPE**, indicating the COSY correlation between proton **a** and proton **b** , and proton **c** and proton **d**.

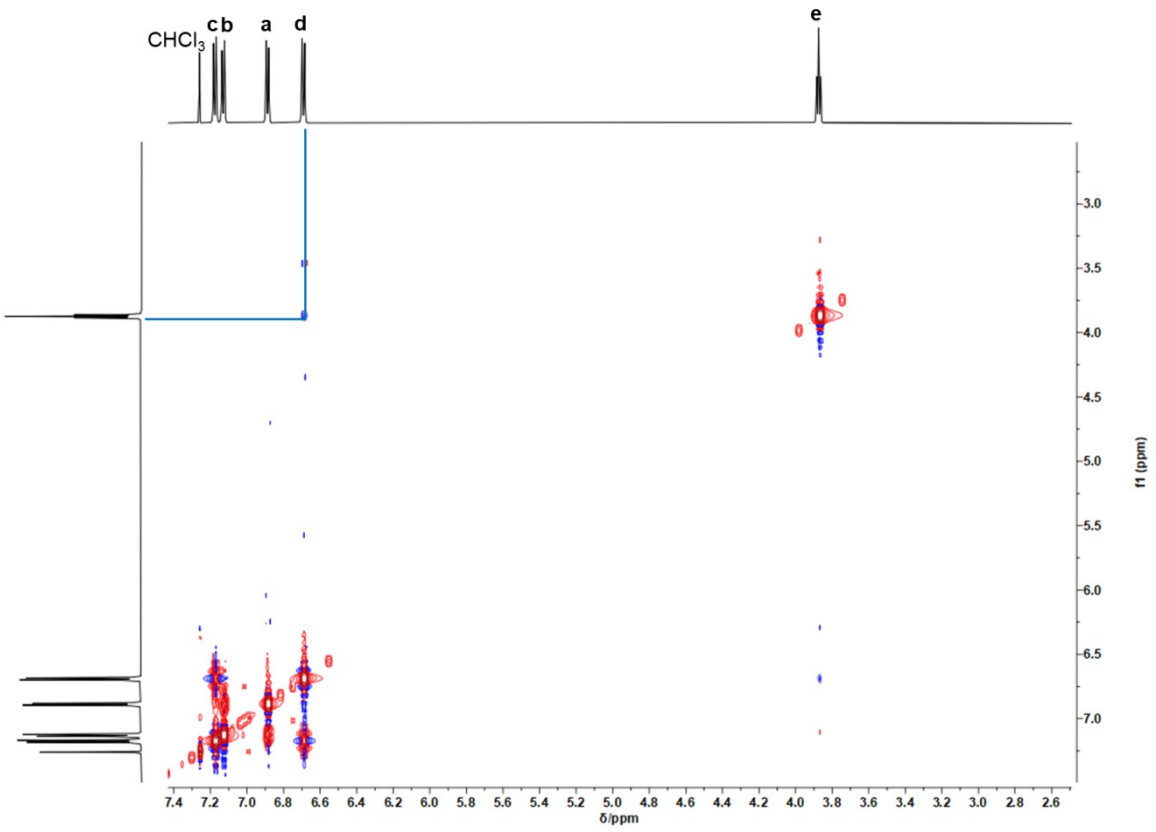
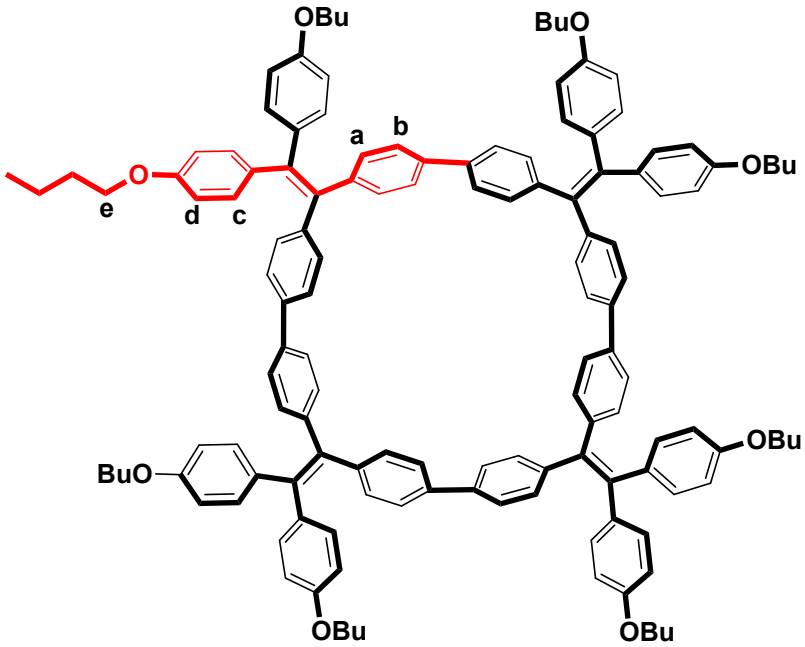


Figure S22. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[3]CTPE**, indicating the NOEs between proton **d** and protons **e**.

3.4. 2D spectra of **[4]CTPE**



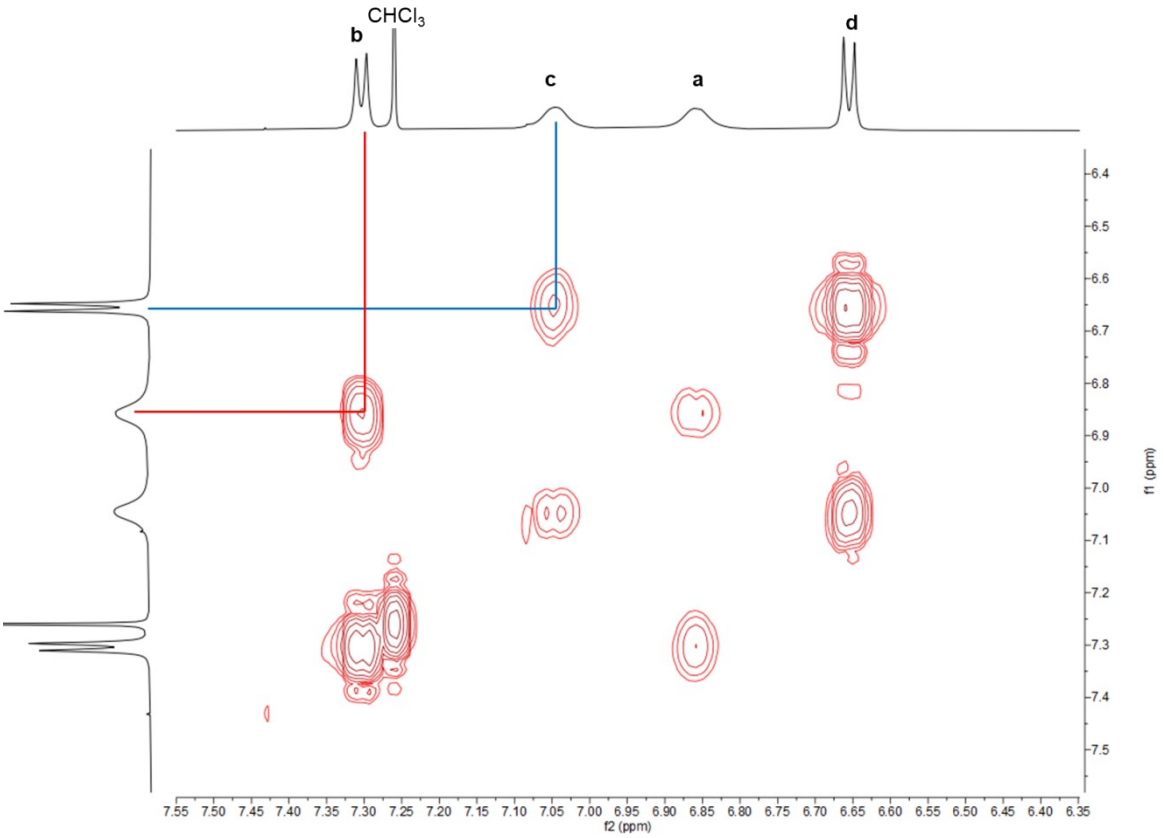


Figure S23. The COSY correlation spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the COSY correlation between proton **a** and proton **b** , and proton **c** and proton **d**.

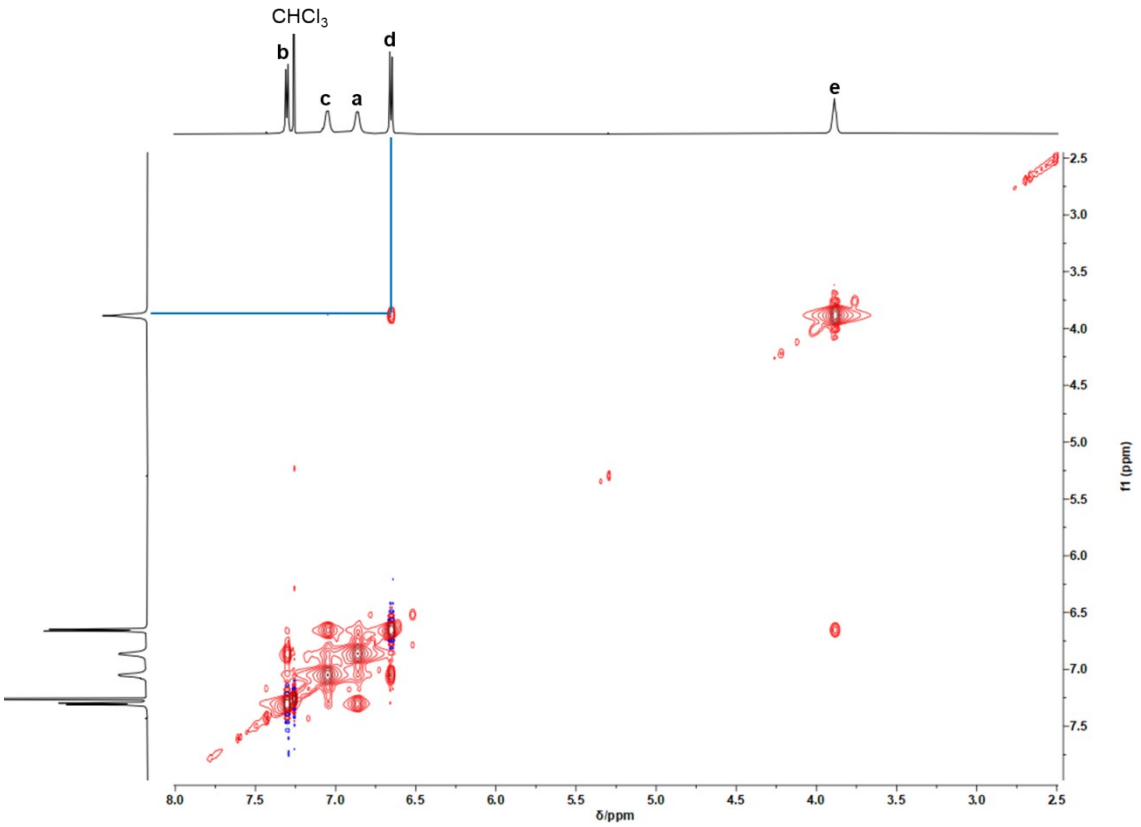


Figure S24. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the NOEs between proton **d** and protons **e**.

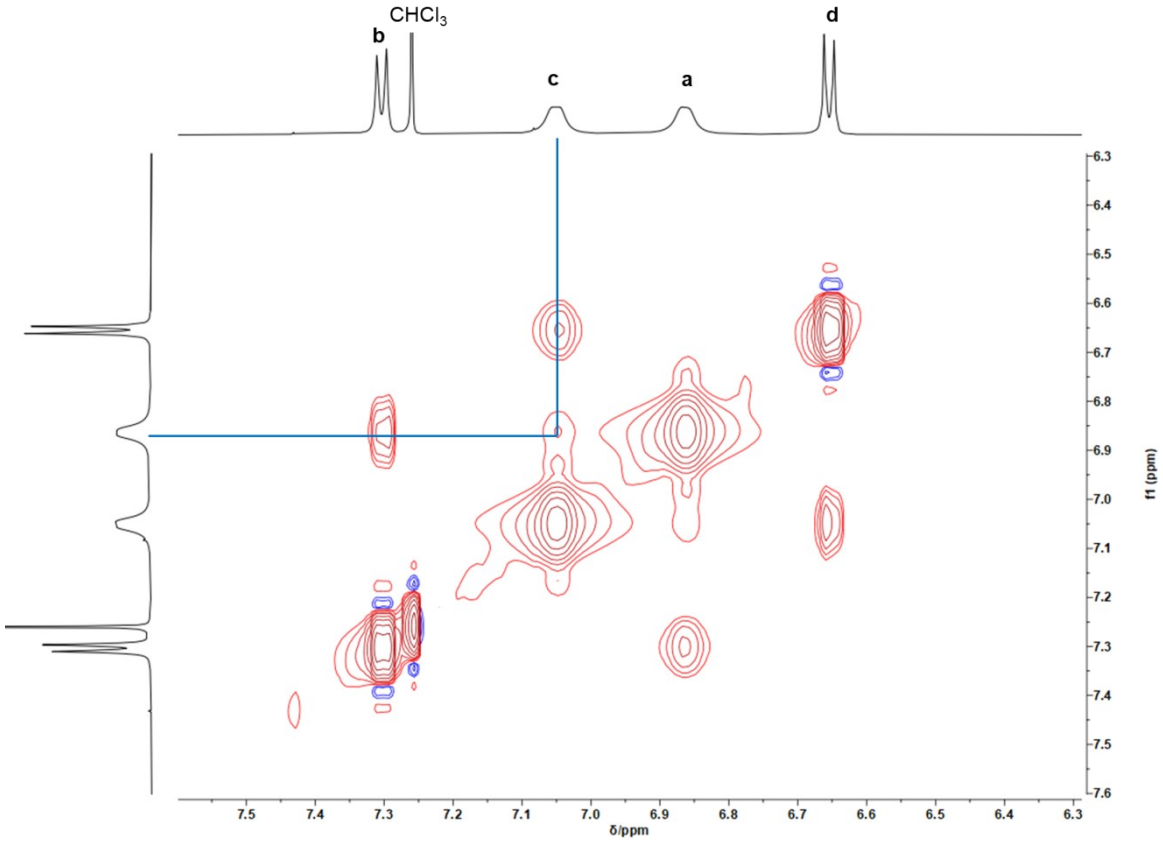
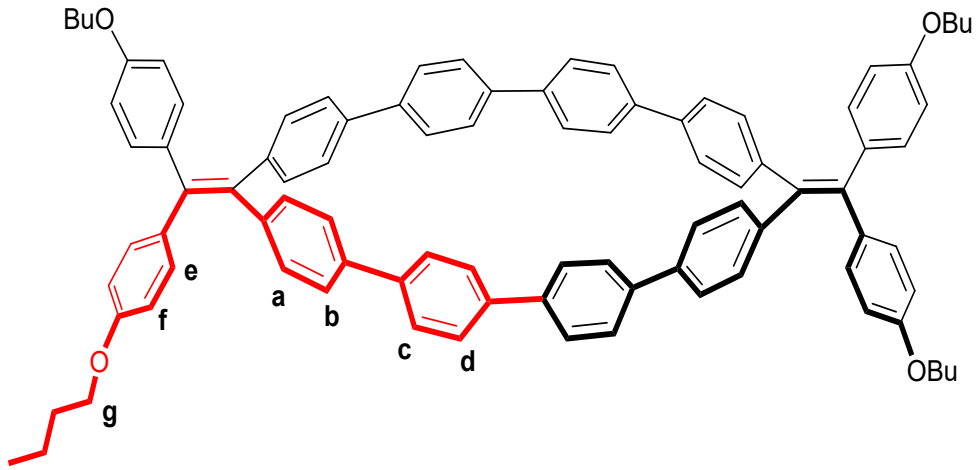


Figure S25. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the NOEs between proton **a** and protons **c**.

3.5. 2D spectra of **[2]CHPE**



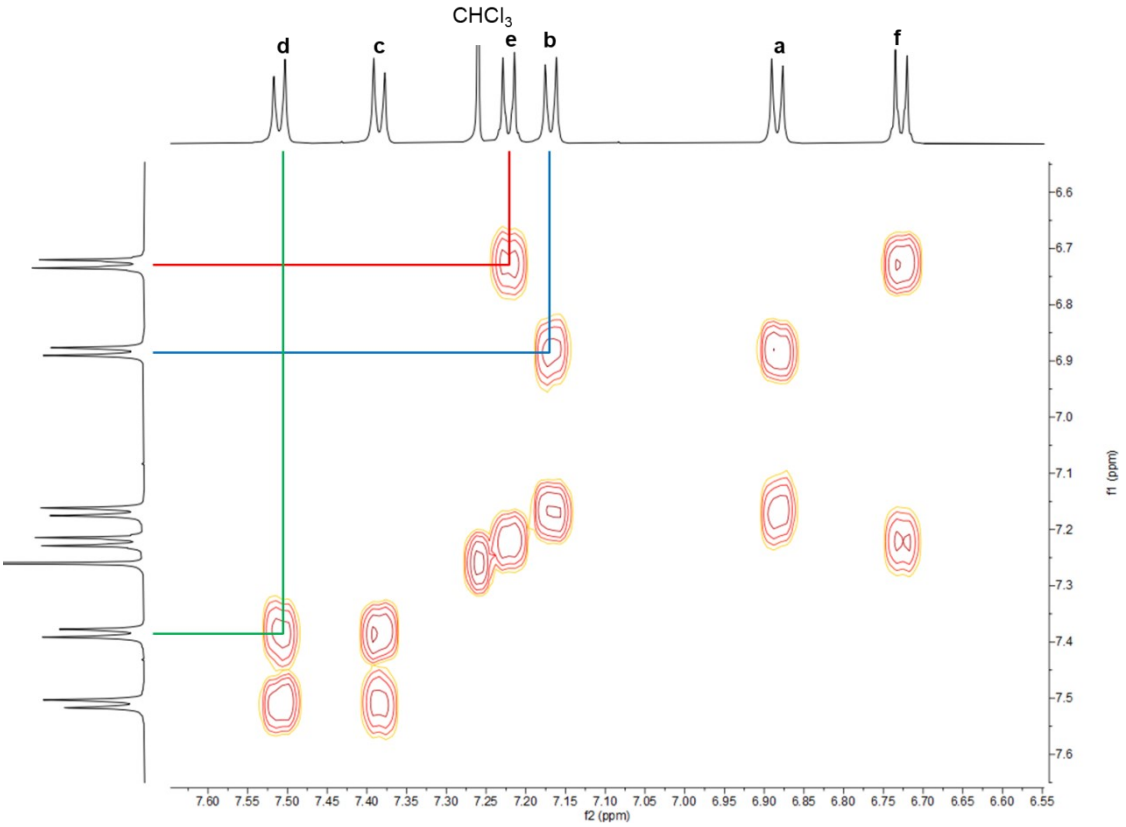


Figure S26. The COSY correlation spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the COSY correlation between proton **a** and proton **b** , and proton **c** and proton **d**, and proton **e** and proton **f**.

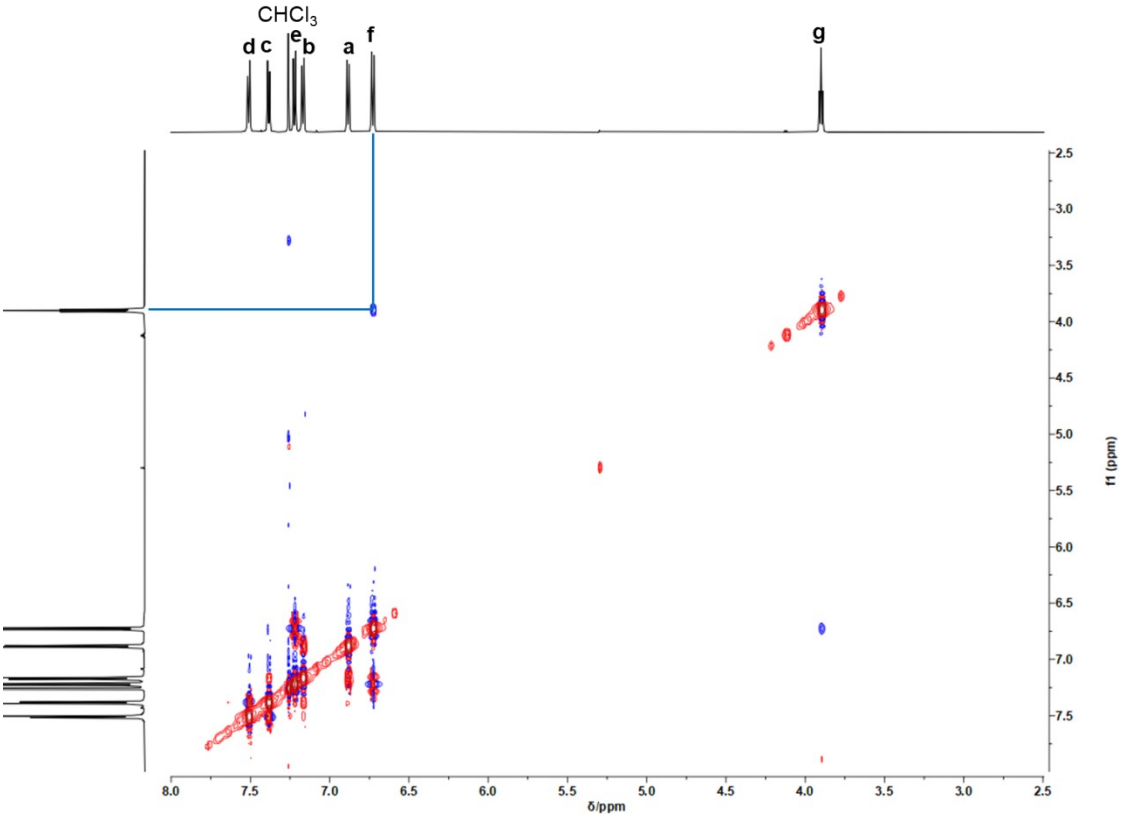


Figure S27. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the NOEs between proton **f** and protons **g**.

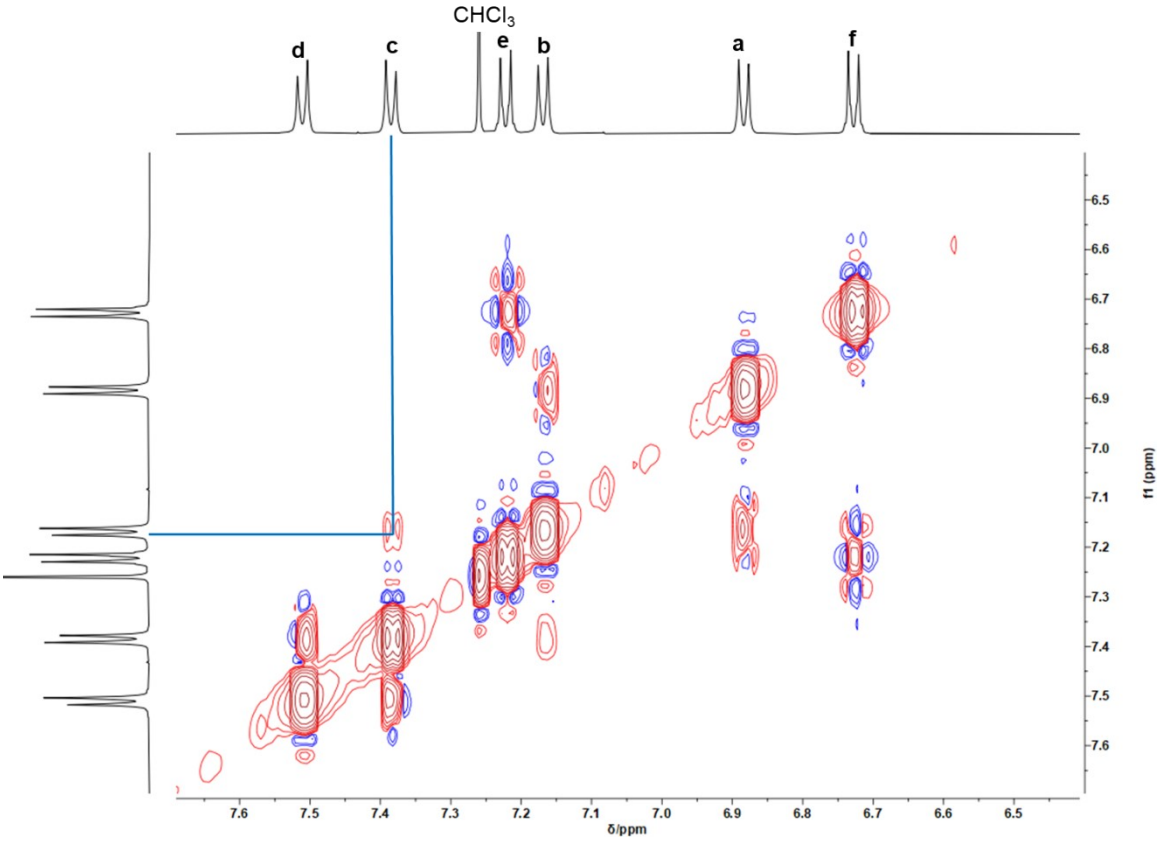
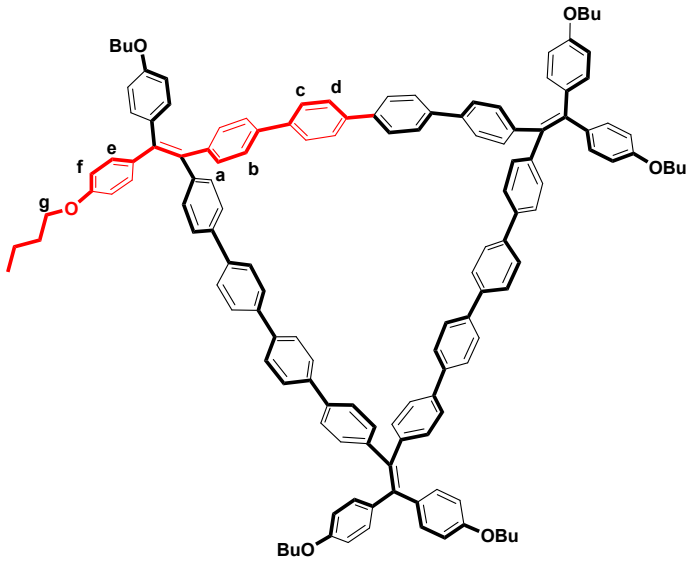


Figure S28. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[2]CHPE**, indicating the NOEs between proton **b** and protons **c**.

3.6. 2D spectra of **[3]CHPE**



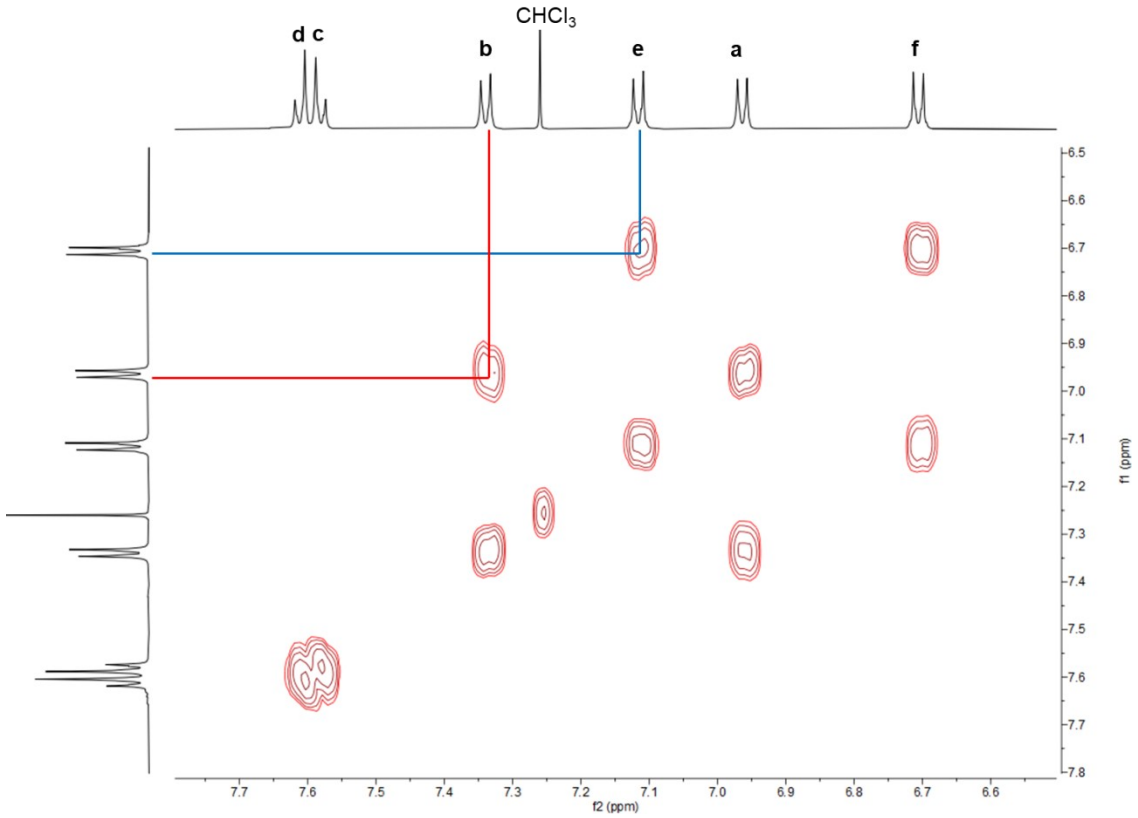


Figure S29.The COSY correlation spectrum (600 MHz, $CDCl_3$, 298 K) of **[3]CHPE**, indicating the COSY correlation between proton **a** and proton **b** and proton **e** and **f**.

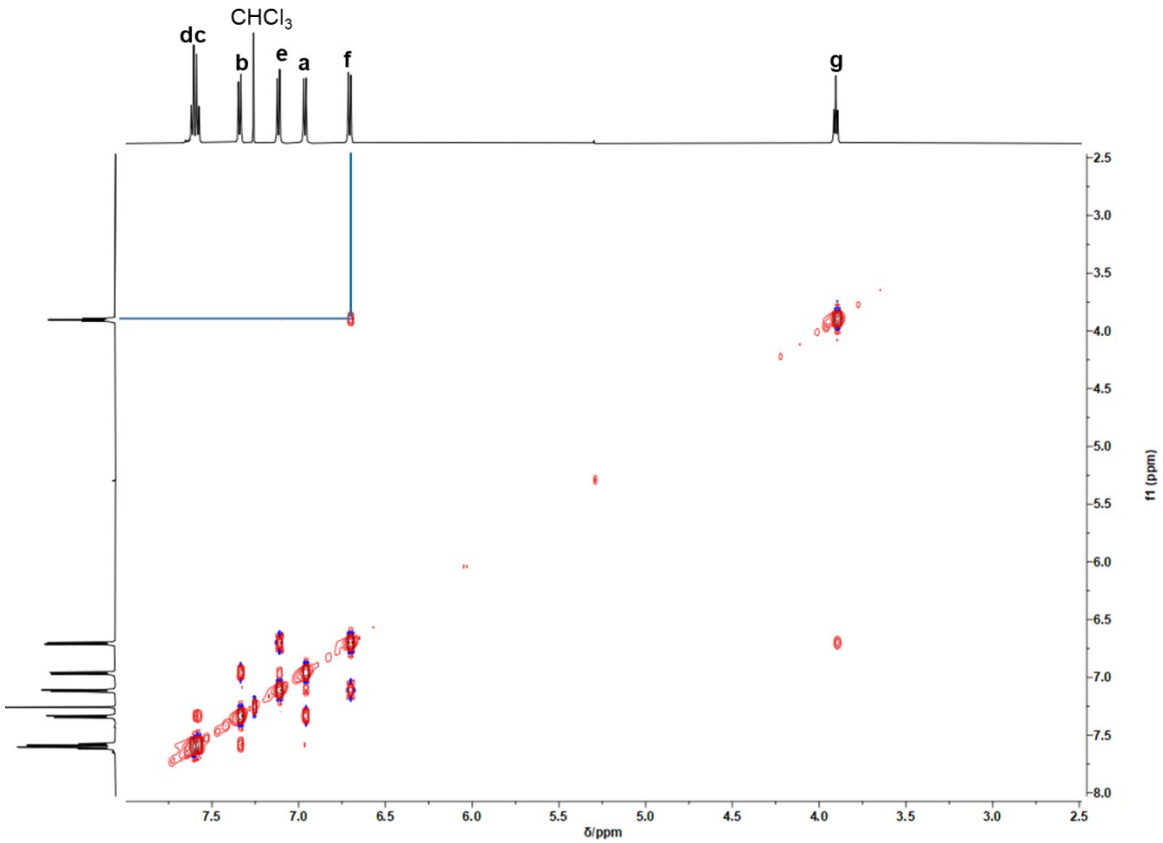


Figure S30. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[3]CHPE**, indicating the NOEs between proton **f** and protons **g**.

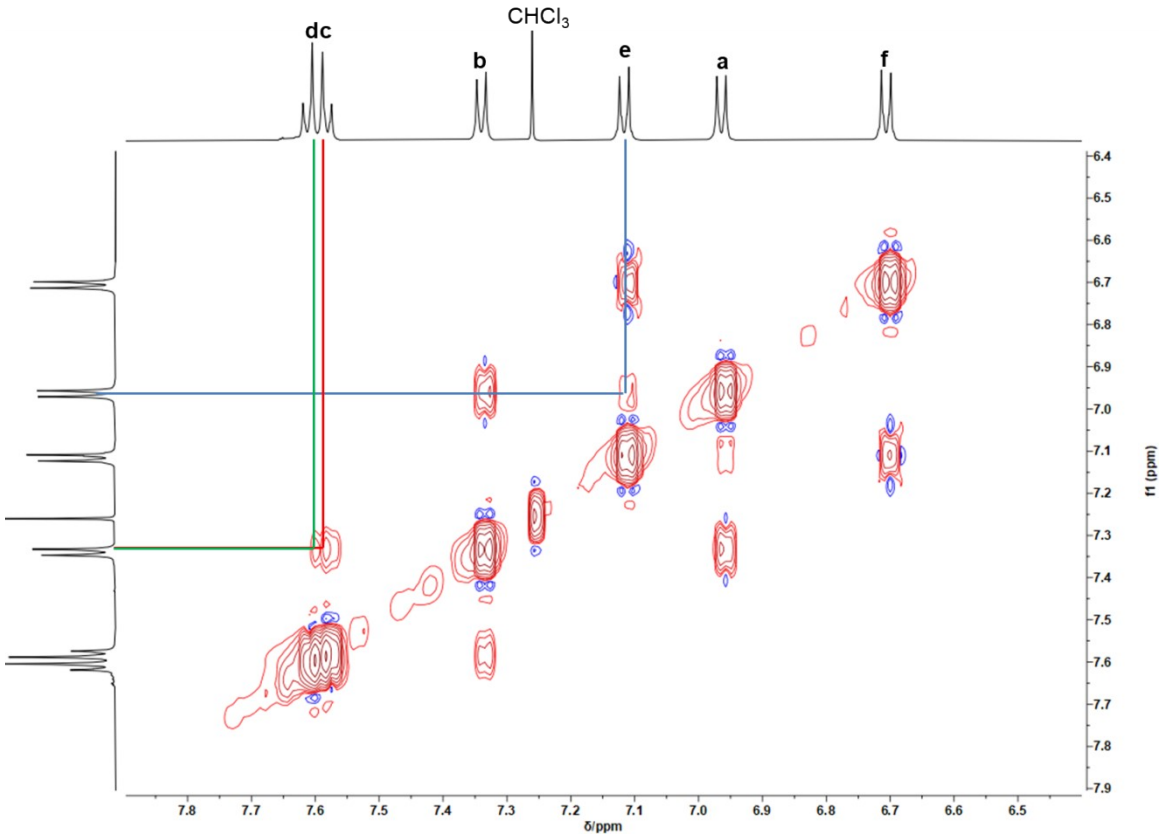


Figure S31. The NOESY spectrum (600 MHz, $CDCl_3$, 298 K) of **[3]CHPE**, indicating the NOEs between proton **a** and protons **e** and proton **b** and protons **c**, **d**.

4. Mass Spectra

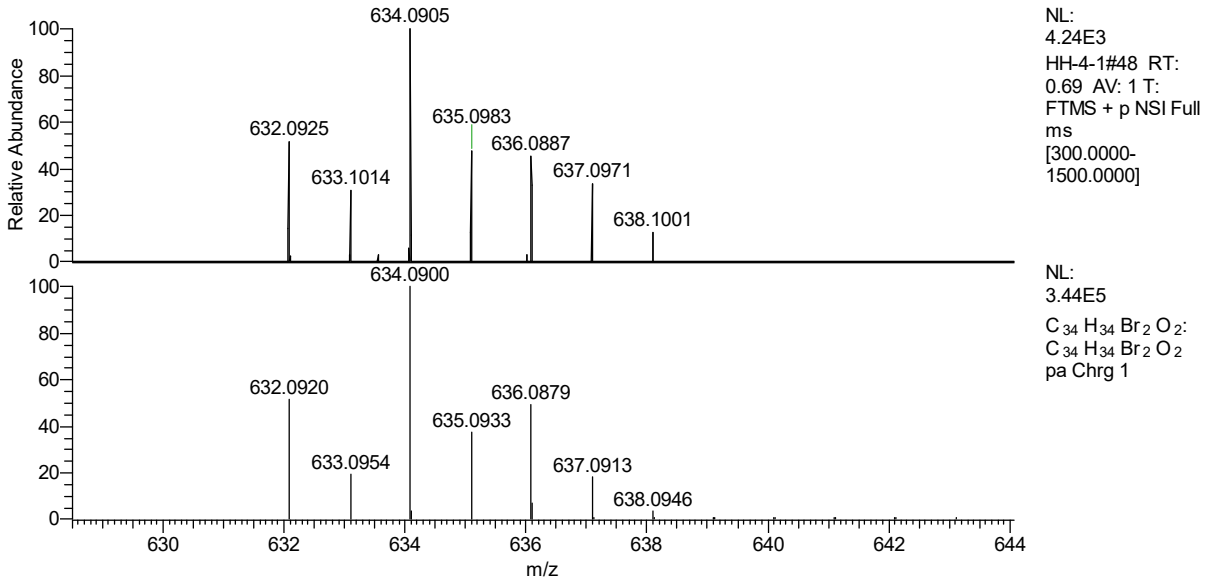


Figure S32. MALDI-TOF spectrum of **S2** (top: observed, bottom: simulated).

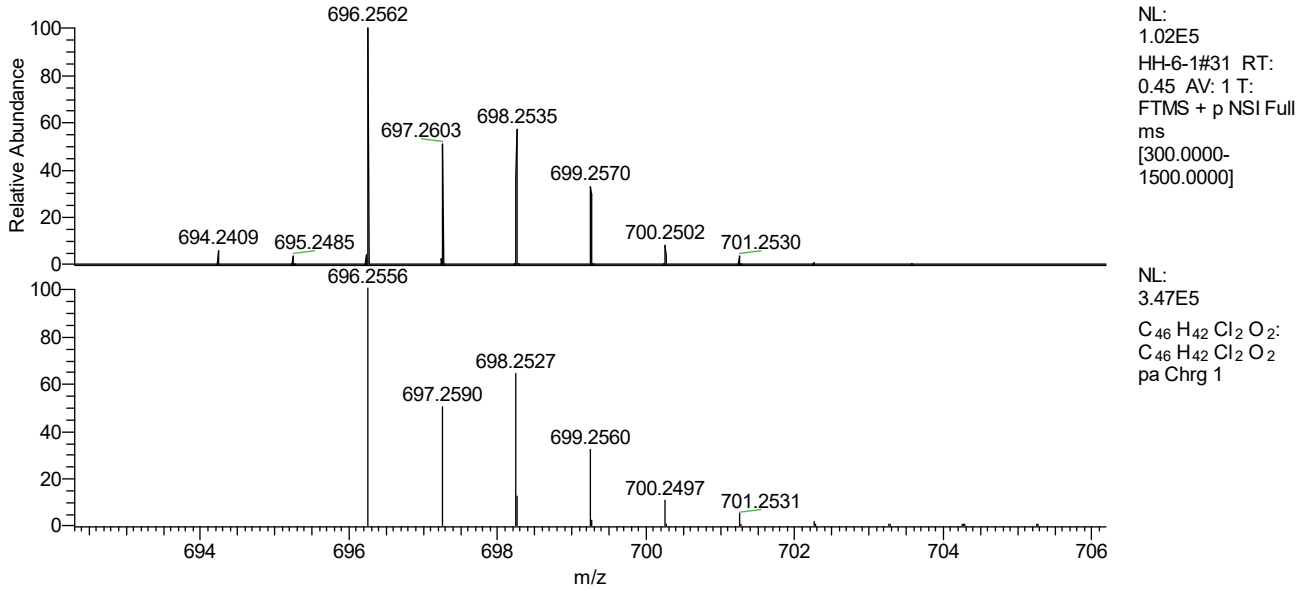


Figure S33. MALDI-TOF spectrum of **S3** (top: observed, bottom: simulated).

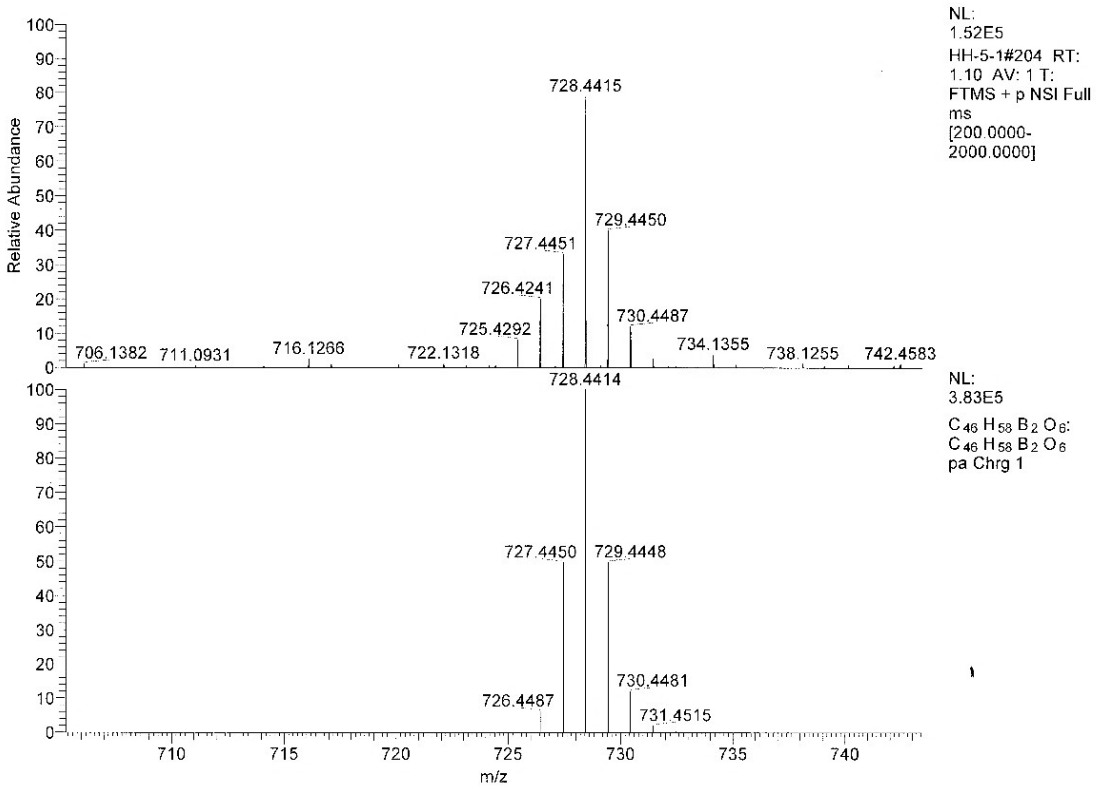


Figure S34. MALDI-TOF spectrum of **1** (top: observed, bottom: simulated).

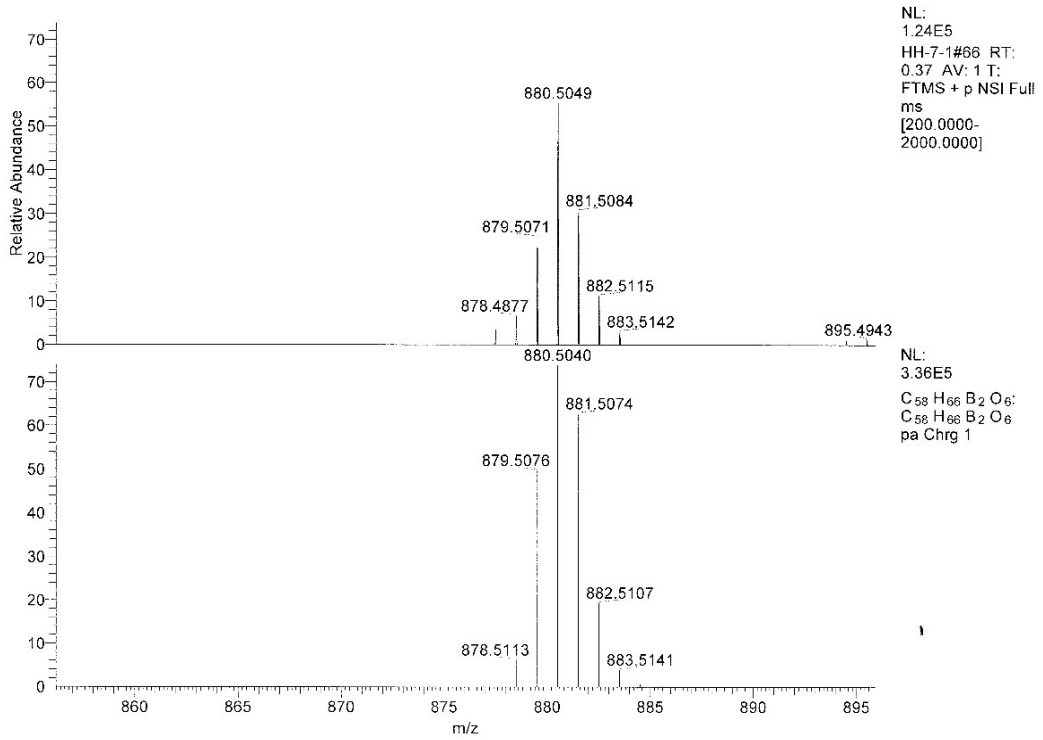
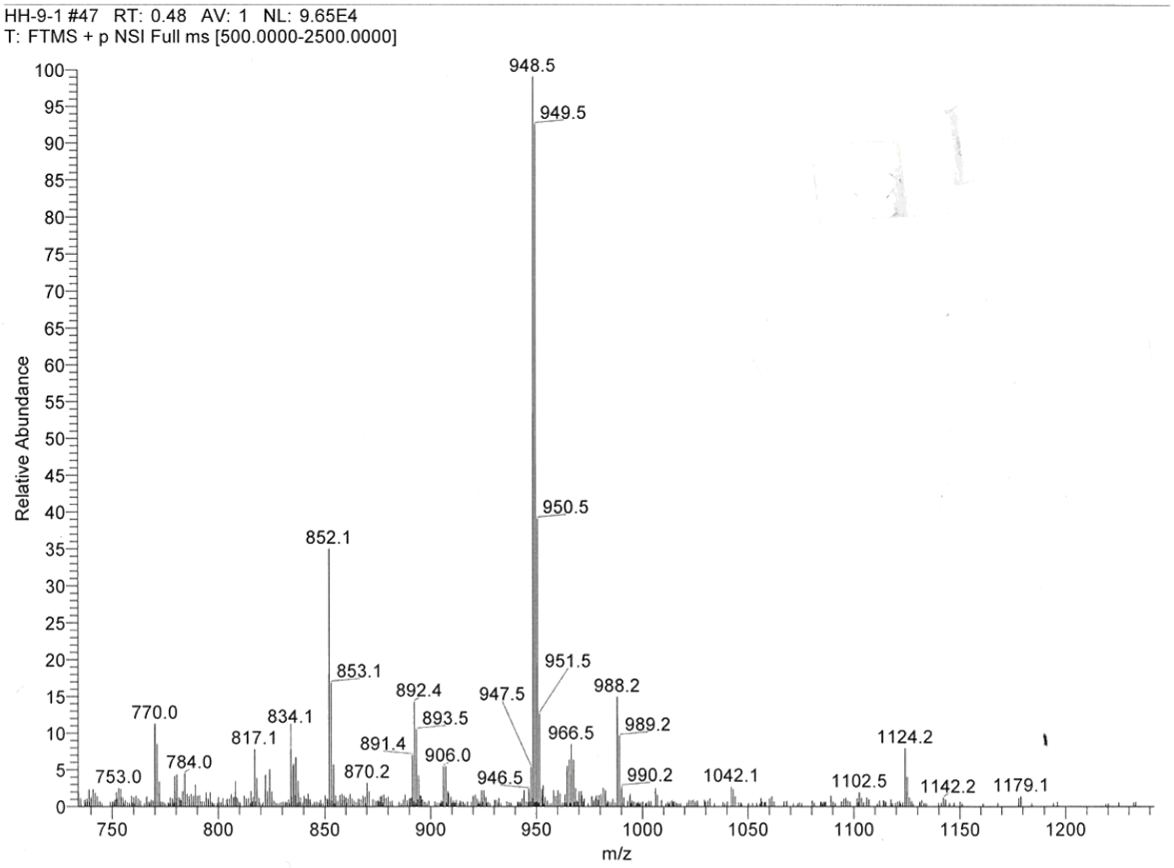


Figure S35. MALDI-TOF spectrum of **2** (top: observed, bottom: simulated).



National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MALDI-MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E210258

Sample Serial Number: HH-9-1

Operator: Songw Date: 2021/01/21

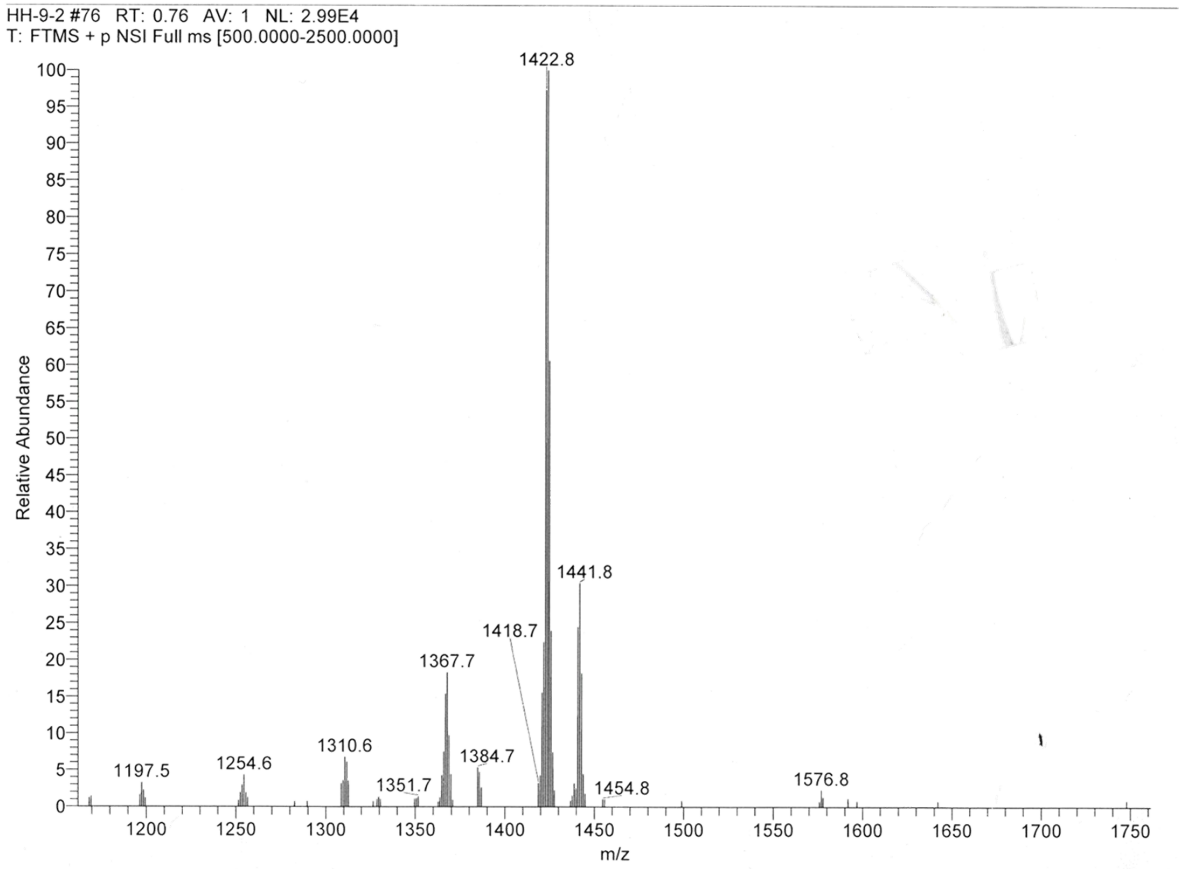
Operation Mode: MALDI Positive Ion Mode

Elemental composition search on mass 948.5111

m/z= 943.5111-953.5111

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
948.5111	948.5112	-0.11	35.0	$C_{68}H_{68}O_4$
	948.5099	1.31	35.5	$C_{66}H_{66}O_3N_3$

Figure S36. MALDI-TOF spectrum of **[2]CTPE** (top: mass spectrum, bottom: high resolution MALDI-MS report).



National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MALDI-MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E210259

Sample Serial Number: HH-9-2

Operator: Songw Date: 2021/01/21

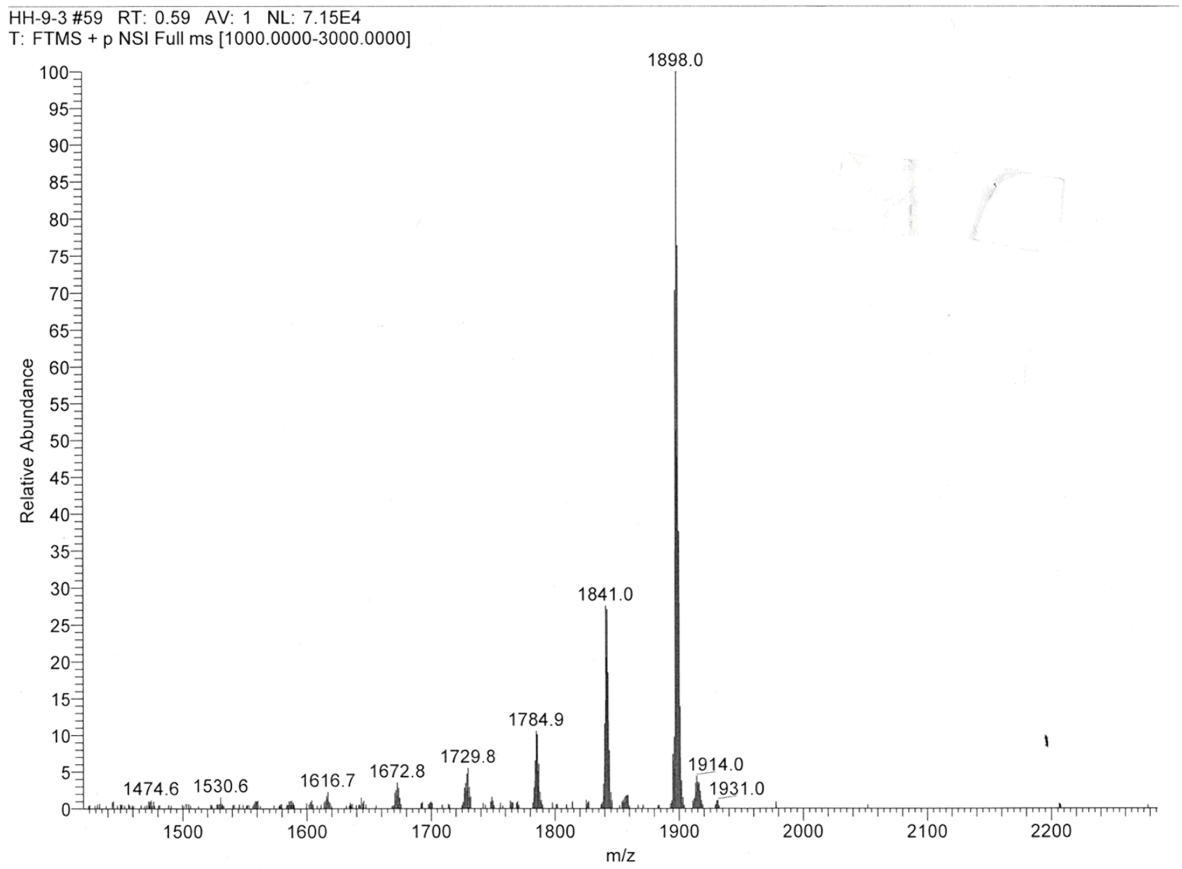
Operation Mode: MALDI Positive Ion Mode

Elemental composition search on mass 1422.7663

m/z= 1417.7663-1427.7663

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1422.7663	1422.7671	-0.55	52.0	$C_{102}H_{102}O_6$

Figure S37. MALDI-TOF spectrum of **[3]CTPE**(top: mass spectrum, bottom: high resolution MALDI-MS report).



National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MALDI-MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E210255

Sample Serial Number: HH-9-3

Operator: Songw Date: 2021/01/21

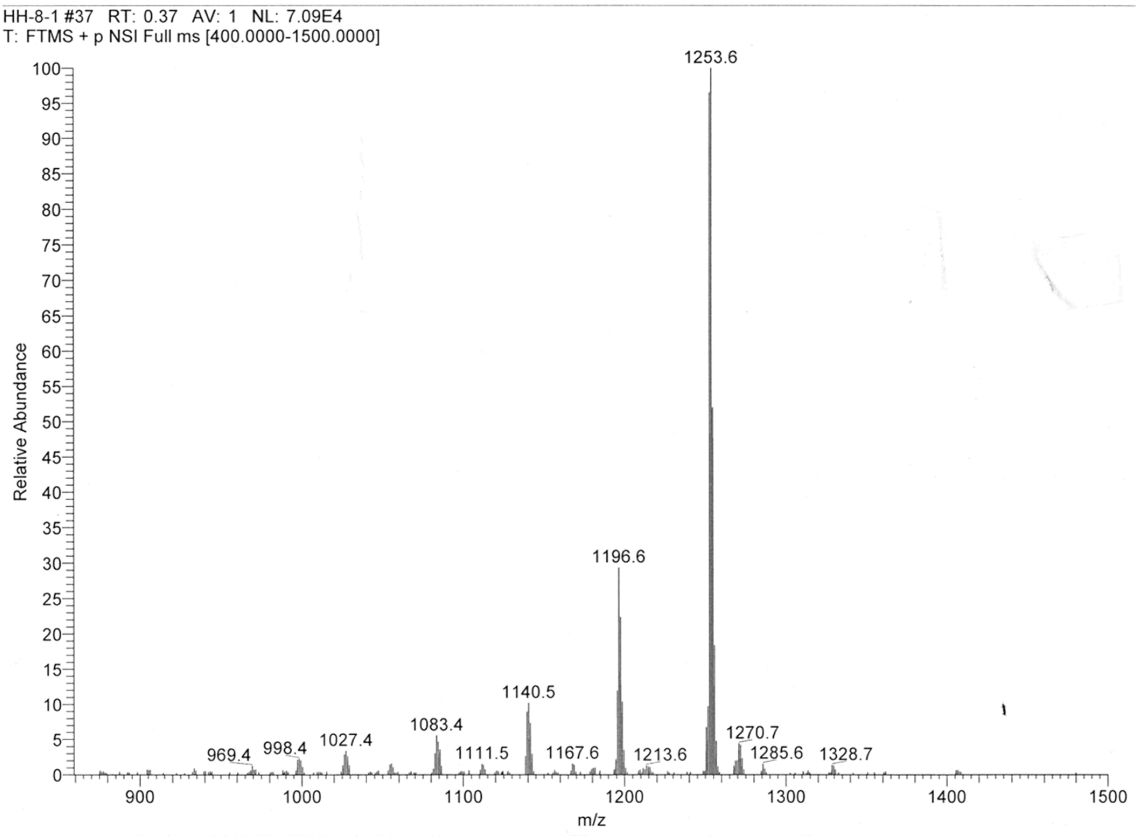
Operation Mode: MALDI Positive Ion Mode

Elemental composition search on mass 1898.0313

m/z= 1893.0313-1903.0313

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1898.0313	1898.0308	0.24	68.5	$C_{136}H_{137}O_8$

Figure S38. MALDI-TOF spectrum of **[4]CTPE**(top: mass spectrum, bottom: high resolution MALDI-MS report).



National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MALDI-MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E210256

Sample Serial Number: HH-8-1

Operator: Songw Date: 2021/01/21

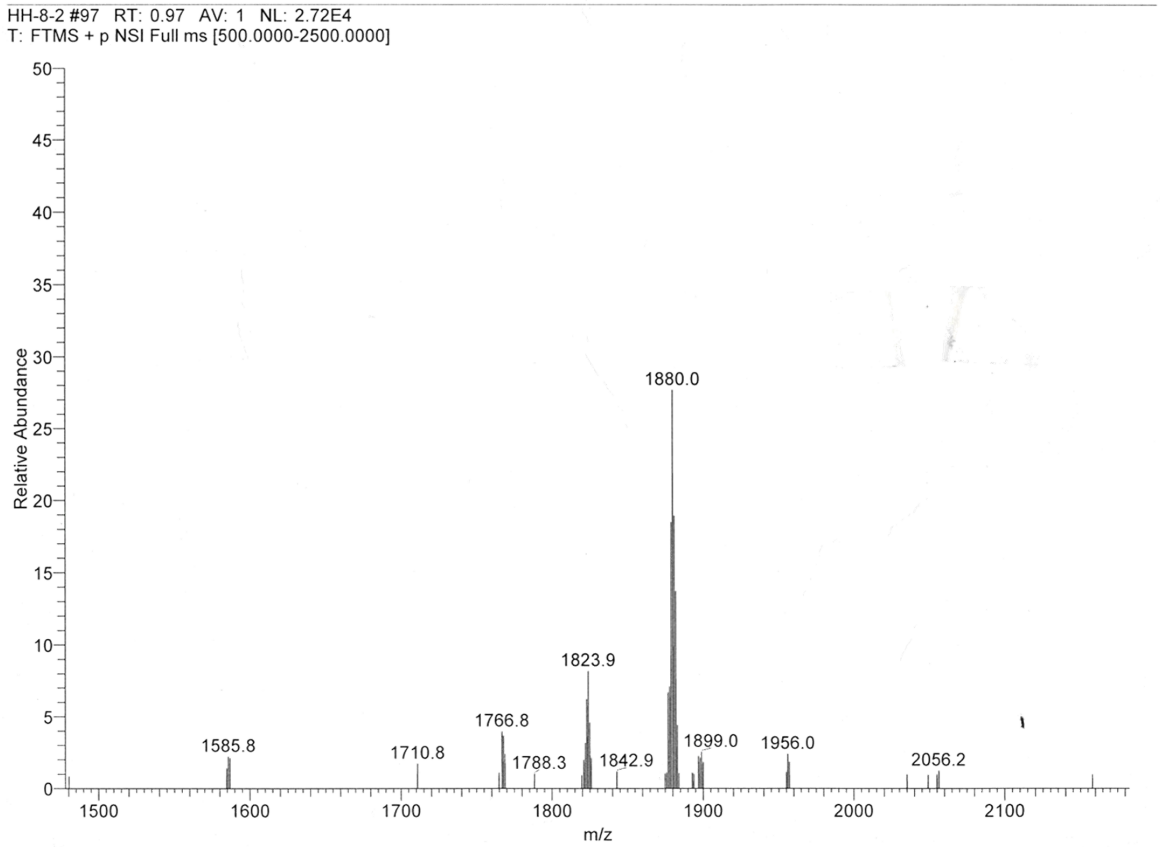
Operation Mode: MALDI Positive Ion Mode

Elemental composition search on mass 1252.6357

m/z= 1247.6357-1257.6357

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1252.6357	1252.6364	-0.54	51.0	$C_{92}H_{84}O_4$
	1252.6391	-2.68	55.5	$C_{95}H_{82}ON$

Figure S39. MALDI-TOF spectrum of **[2]CHPE**(top: mass spectrum, bottom: high resolution MALDI-MS report).



National Center for Organic Mass Spectrometry in Shanghai
Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MALDI-MS REPORT

Instrument: Thermo Scientific Q Exactive HF Orbitrap-FTMS

Card Serial Number: E210257

Sample Serial Number: HH-8-2

Operator: Songw Date: 2021/01/21

Operation Mode: MALDI Positive Ion Mode

Elemental composition search on mass 1878.9546

m/z= 1873.9546-1883.9546

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
1878.9546	1878.9549	-0.16	76.0	$C_{138}H_{126}O_6$

Figure S40. MALDI-TOF spectrum of **[3]CHPE**(top: mass spectrum, bottom: high resolution MALDI-MS report).

5. X-ray Crystallography

The diffraction intensity data of **[2]CTPE** was measured at 293 K on a Bruker APEX-II CCD diffractometer (Mo-Kα radiation, λ = 0.71073 Å) equipped with a graphite monochromator and a CCD area detector. The structure was solved by direct methods using SHELXS-97 and refined using a full-matrix least-squares technique based on F^2 using SHELXL-2013.[3] The nonhydrogen atoms were refined anisotropically. The H atoms attached to carbons were added geometrically and refined isotropically with the riding model. The butoxy in the structure is disordered. The crystal data were collected in Table S1.

Table S1. Crystal data and structure refinement for **[2]CTPE**

CCDC	2115907	
Empirical formula	$C_{68}H_{68}O_4$	
Formula weight	949.22	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 27.6563(10) Å	α= 90°.
	b = 19.8177(7) Å	β= 90°.
	c = 20.4671(9) Å	γ= 90°.
Volume	11217.7(8) $Å^3$	
Z	8	
Density (calculated)	1.124 Mg/m^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	4064	
Crystal size	0.200 x 0.110 x 0.070 mm^3	
Theta range for data collection	1.990 to 25.000°.	
Index ranges	-32<=*h*<=32, -23<=*k*<=23, -24<=*l*<=24	
Reflections collected	83833	
Independent reflections	9873 [$R_{(int)}$ = 0.1136]	
Completeness to theta = 25.242°	97.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6213	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9873 / 120 / 741	
Goodness-of-fit on F^2	1.191	
Final R indices [I>2sigma(I)]	R_1 = 0.1190, wR_2 = 0.3161	
R indices (all data)	R_1 = 0.2116, wR_2 = 0.4013	
Extinction coefficient	0.0051(12)	

Largest diff. peak and hole	0.633 and -0.385 e.Å^{-3}

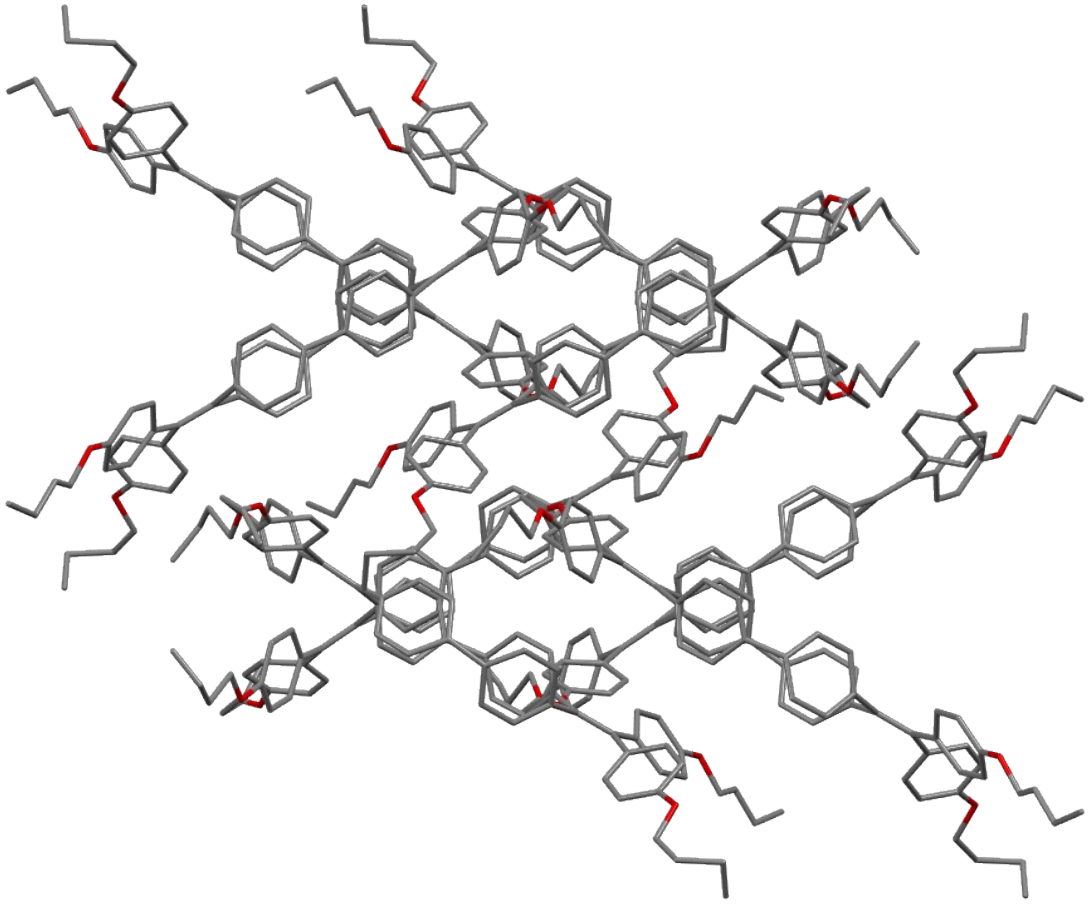


Figure S41. Molecular packing of **[2]CTPE**.

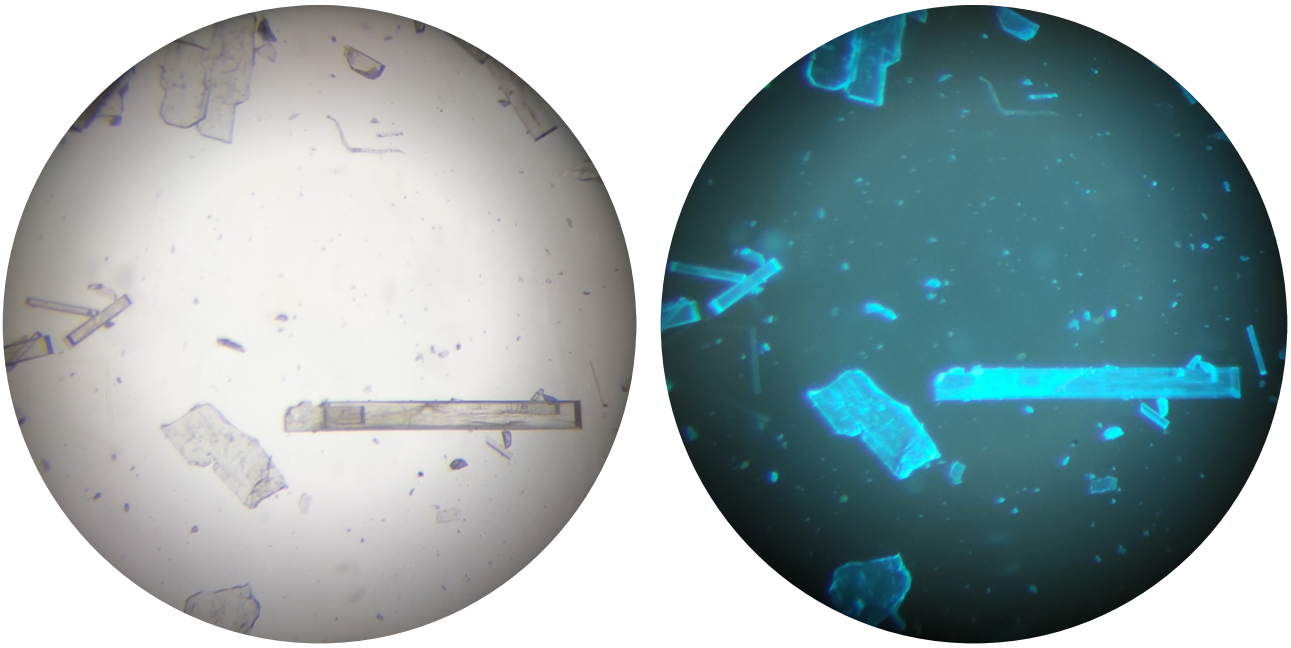


Figure S42. Magnifying glass image of **[2]CTPE** crystals without (Left) and with (Right) UV irradiation at 365 nm.

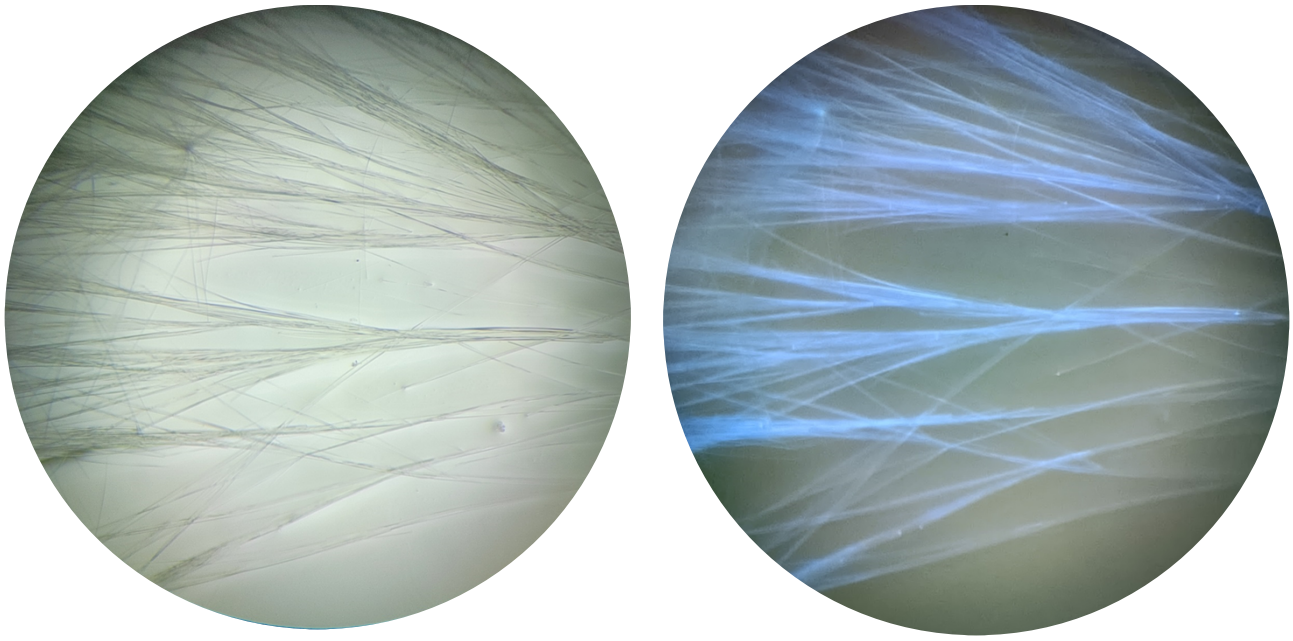


Figure S43. Magnifying glass image of **[3]CTPE** microcrystals without (Left) and with (Right) UV irradiation at 365 nm. The microcrystals were grown by slow diffusion of isopropyl alcohol into chloroform solution had very weak X-ray diffraction.

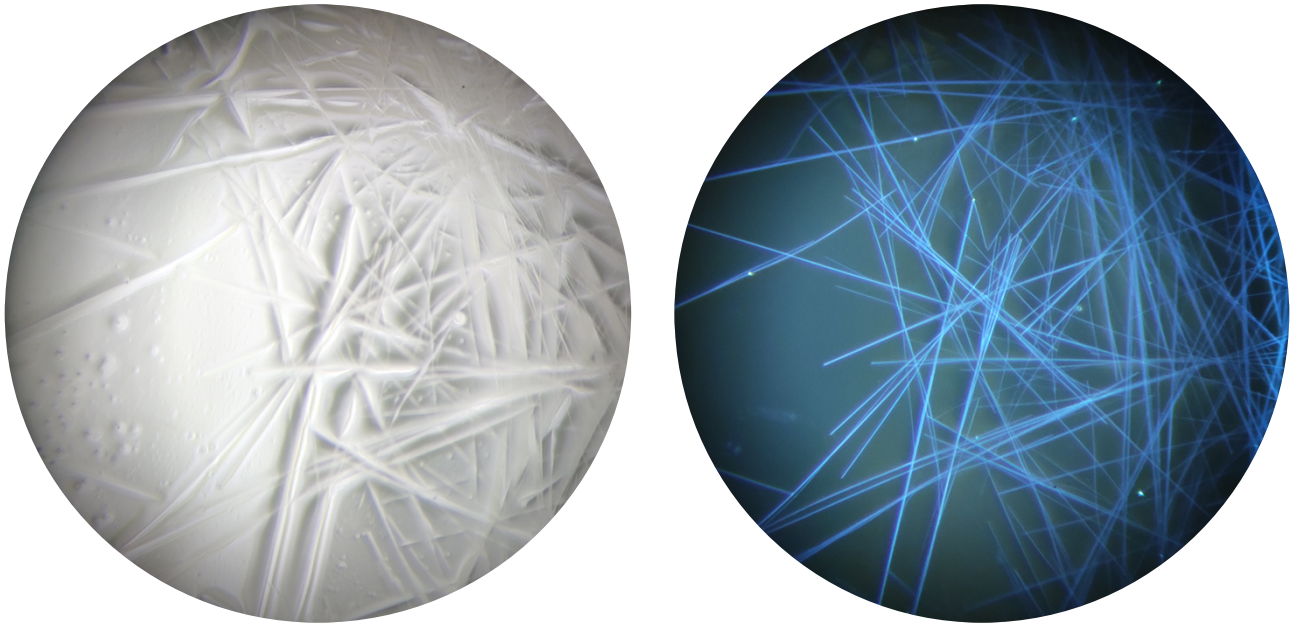


Figure S44. Magnifying glass image of **[4]CTPE** microcrystals without (Left) and with (Right) UV irradiation at 365 nm. The microcrystals were grown by slow diffusion of *n*-hexane into chloroform solution, had very weak X-ray diffraction.

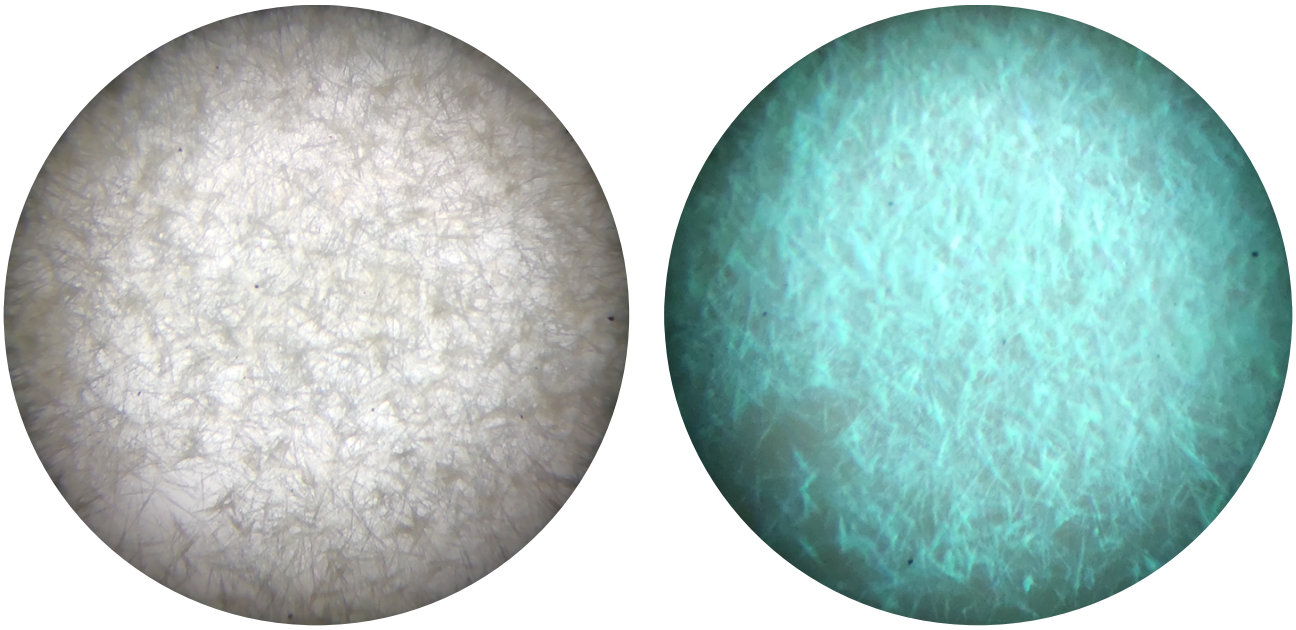


Figure S45. Magnifying glass image of **[2]CHPE** microcrystals without (Left) and with (Right) UV irradiation at 365 nm. The microcrystals were grown by slow diffusion of *n*-hexane into chloroform solution, had very weak X-ray diffraction.

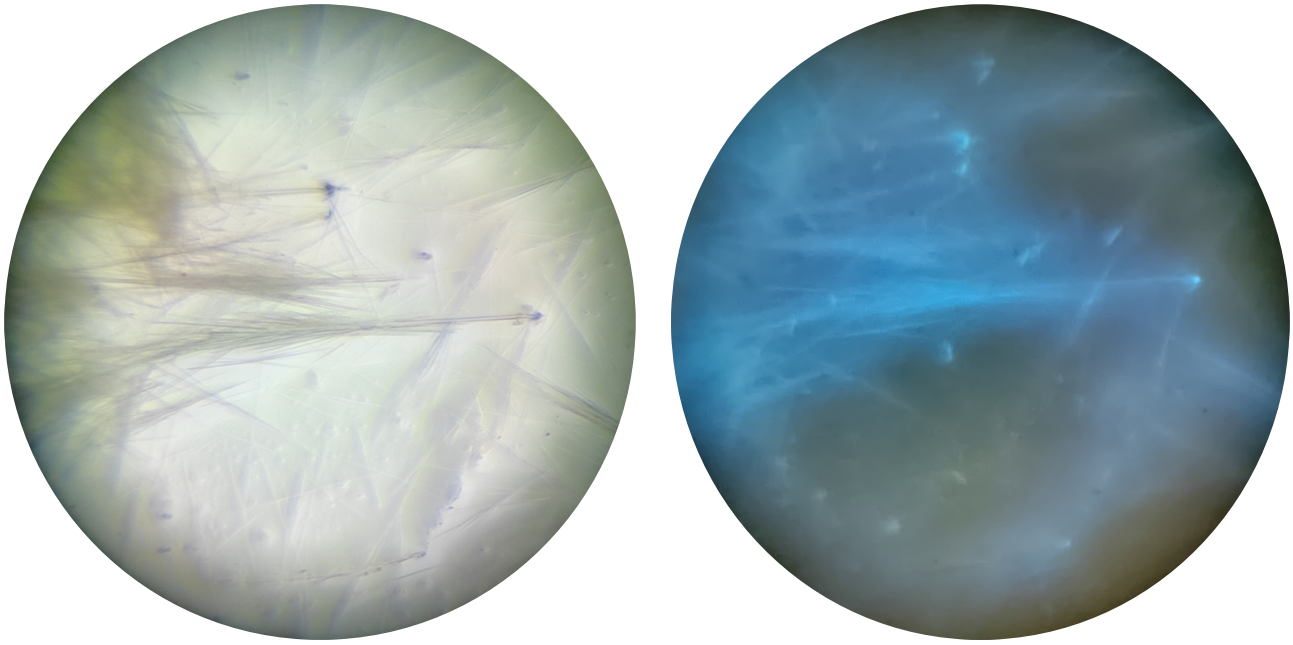
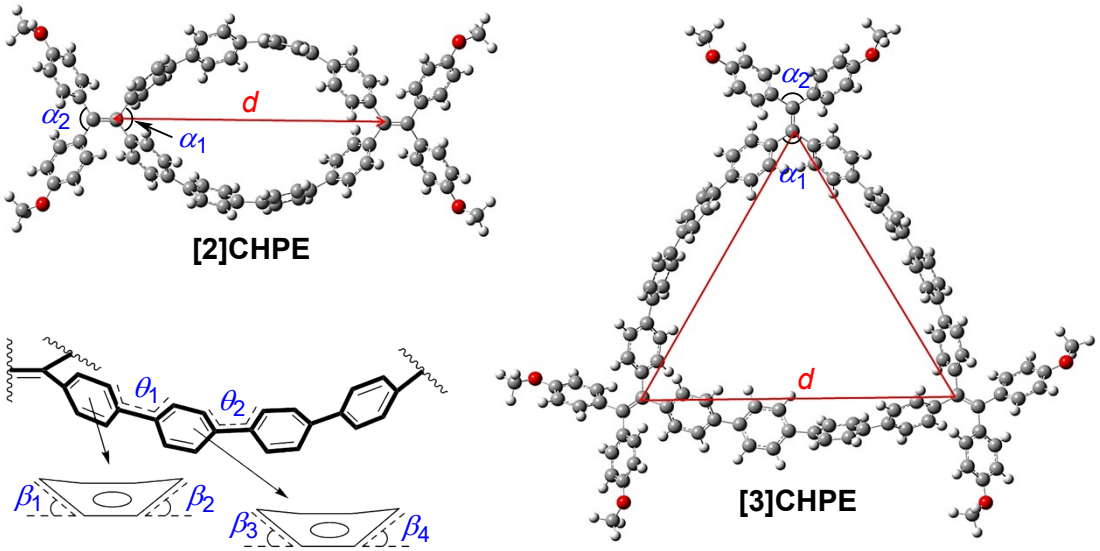


Figure S46. Magnifying glass image of **[3]CHPE** microcrystals without (Left) and with (Right) UV irradiation at 365 nm. The microcrystals were grown by slow diffusion of *n*-hexane into chloroform solution, had very weak X-ray diffraction.

6. DFT Calculations

All calculations were carried out using the Gaussian 16 program.[4] The structures of **[2]CTPE**, **[3]CTPE** and **[4]CTPE** were fully optimized without any symmetry restriction. Calculations were performed by the density functional theory (DFT) method with restricted B3LYP level, employing a basis sets 6-31G(d).[5] N-butoxy groups were replaced by methoxy due to simplify the structures and reduce the calculation costs. TD-DFT calculations were performed at the B3LYP/6-31G(d) level of theory. Nucleus independent chemical shift (NICS) values were calculated using the standard GIAO (GIAO=NMR) at the level of B3LYP/6-311+G(2d,p) with SMD ($CHCl_3$) model.[6] Visualization of molecular orbitals was performed by the use of GaussView 6.0.16 software with 0.02 of isovalue.[7]

Table S2. Calculated B3LYP/6-31G(d) distance(d(Å)), inner angle (α_1 (°)), outer angle (α_2 (°)), displacement angle (β_1, β_2, β_3, β_4 (°)) and torsion angles (θ_1, θ_2(°)) of [n]CHPEs.



	Distance(Å)	Inner/ outer angle(°)		Bending angle(°)				Torsional angle(°)	
	d	α_1	α_2	β_1	β_2	β_3	β_4	θ_1	θ_2
[2]CHPE	15.648	108.9	115.8	4.6	5.2	5.7	5.7	35.9	32.7
[3]CHPE	18.021	112.5	115.4	1.8	2.3	3.0	3.0	39.3	37.0

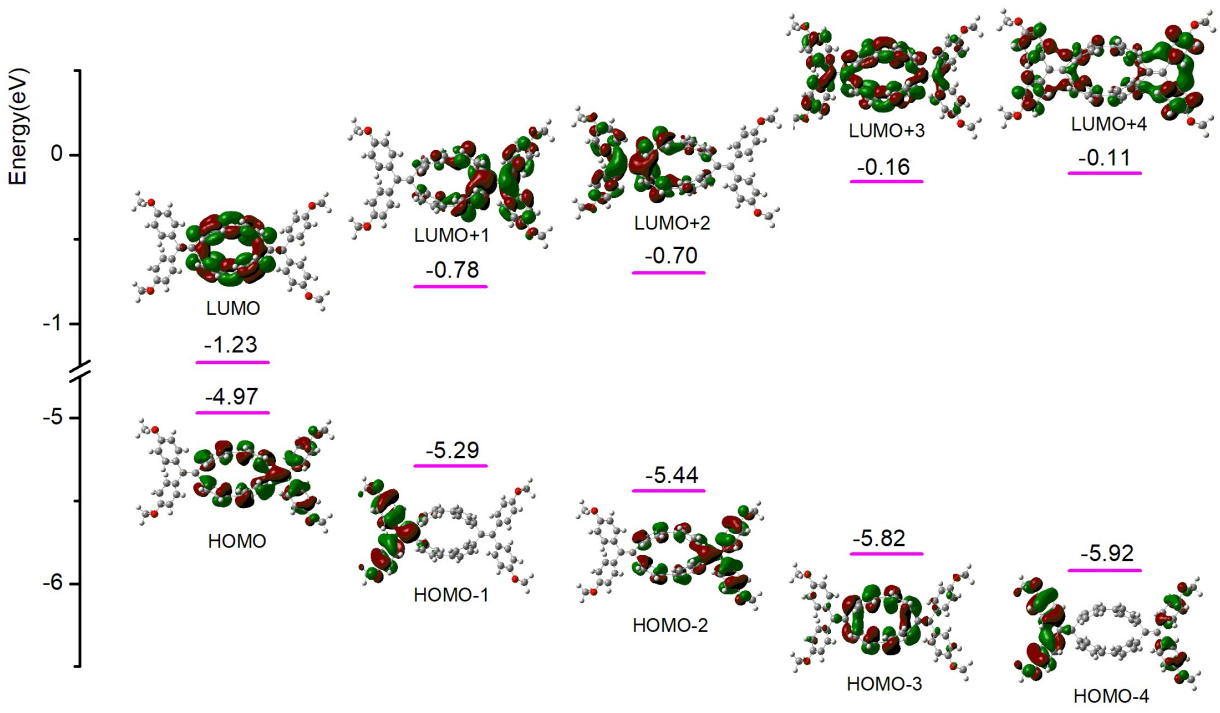


Figure S47. Frontier molecular orbitals of **[2]CTPE**.

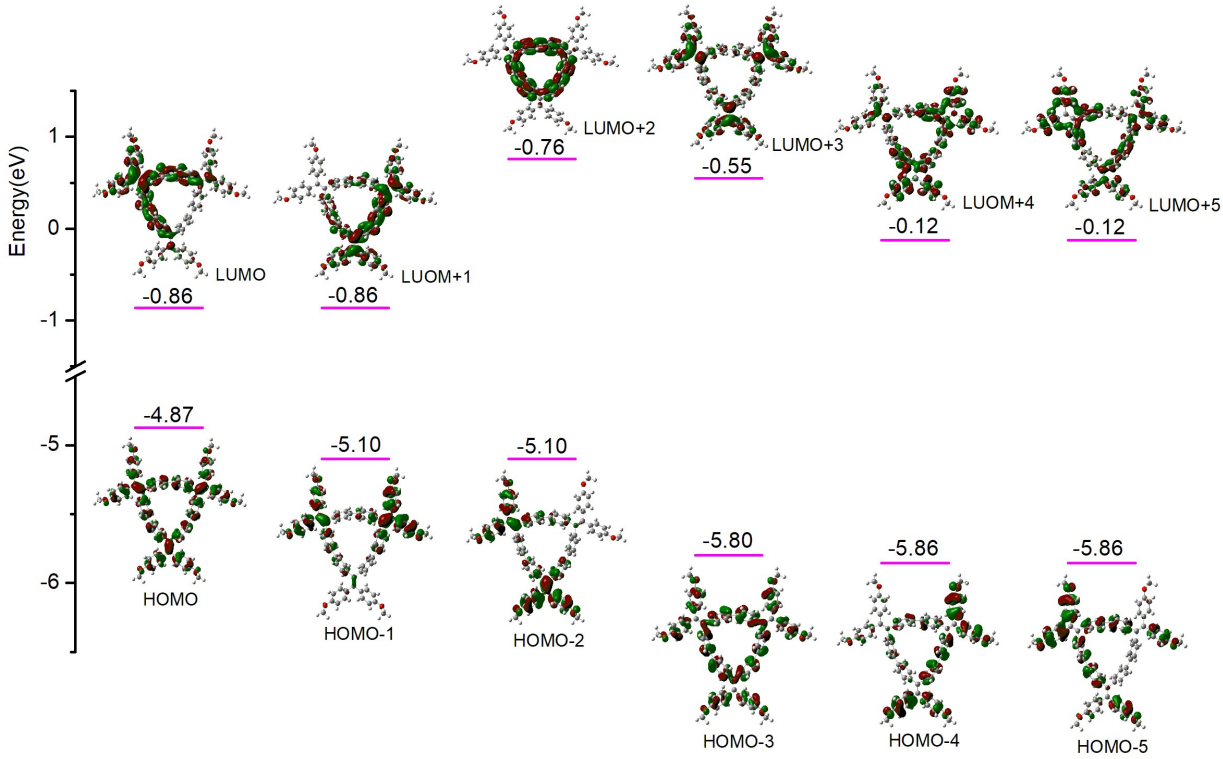


Figure S48. Frontier molecular orbitals of **[3]CTPE**.

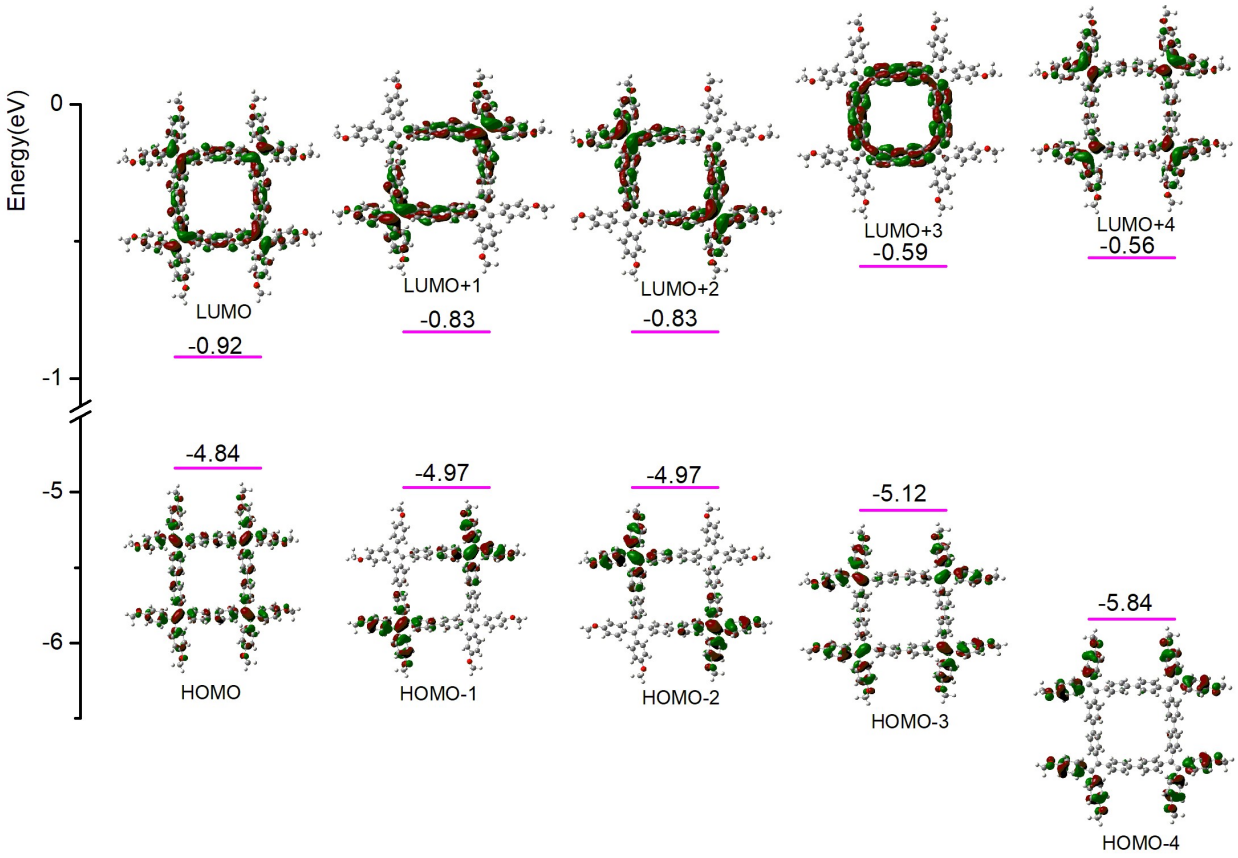


Figure S49. Frontier molecular orbitals of **[4]CTPE**.

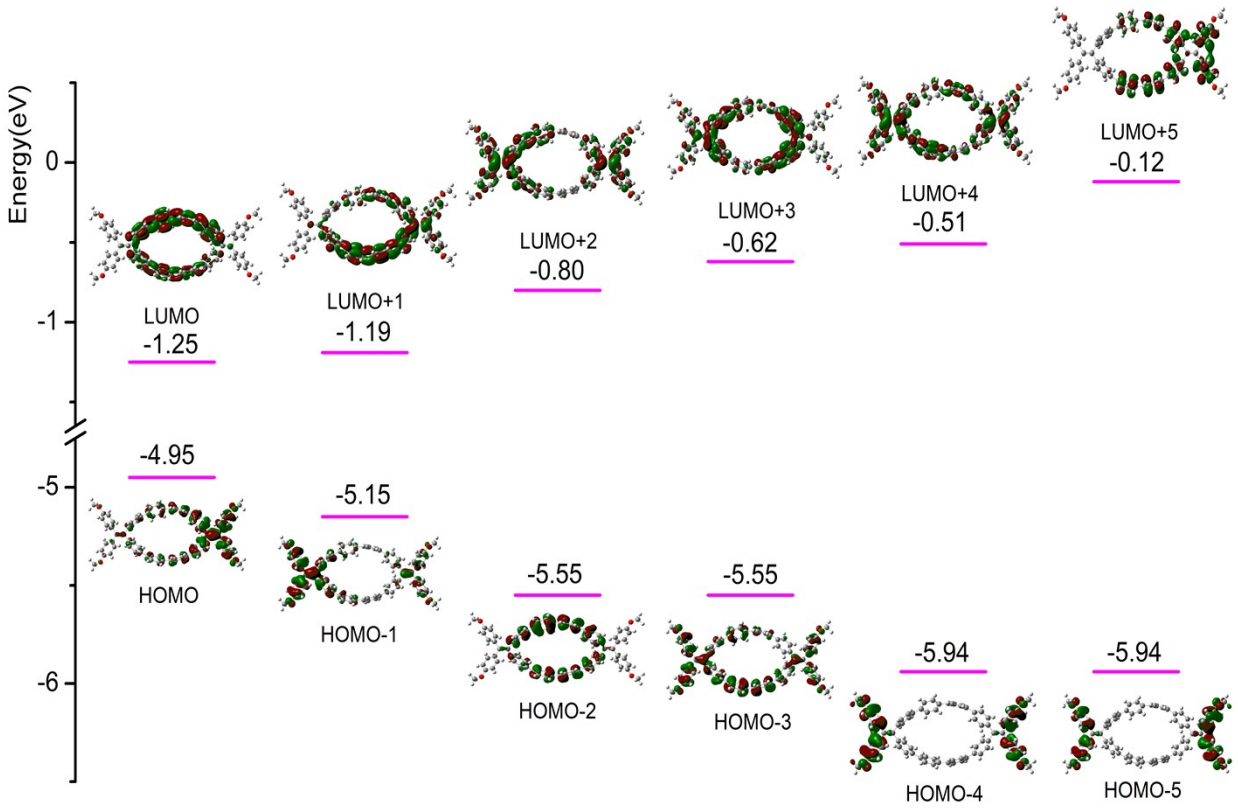


Figure S50. Frontier molecular orbitals of **[2]CHPE**.

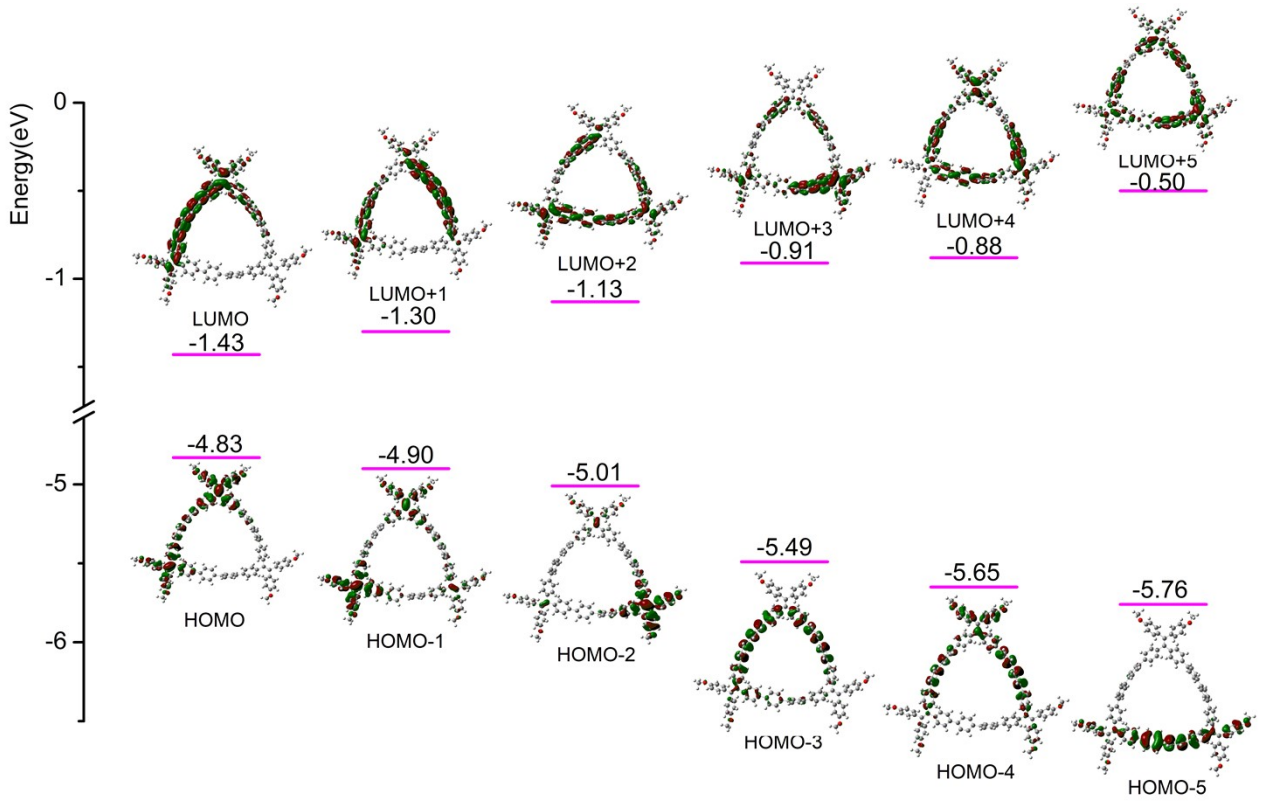


Figure S51. Frontier molecular orbitals of **[3]CHPE**.

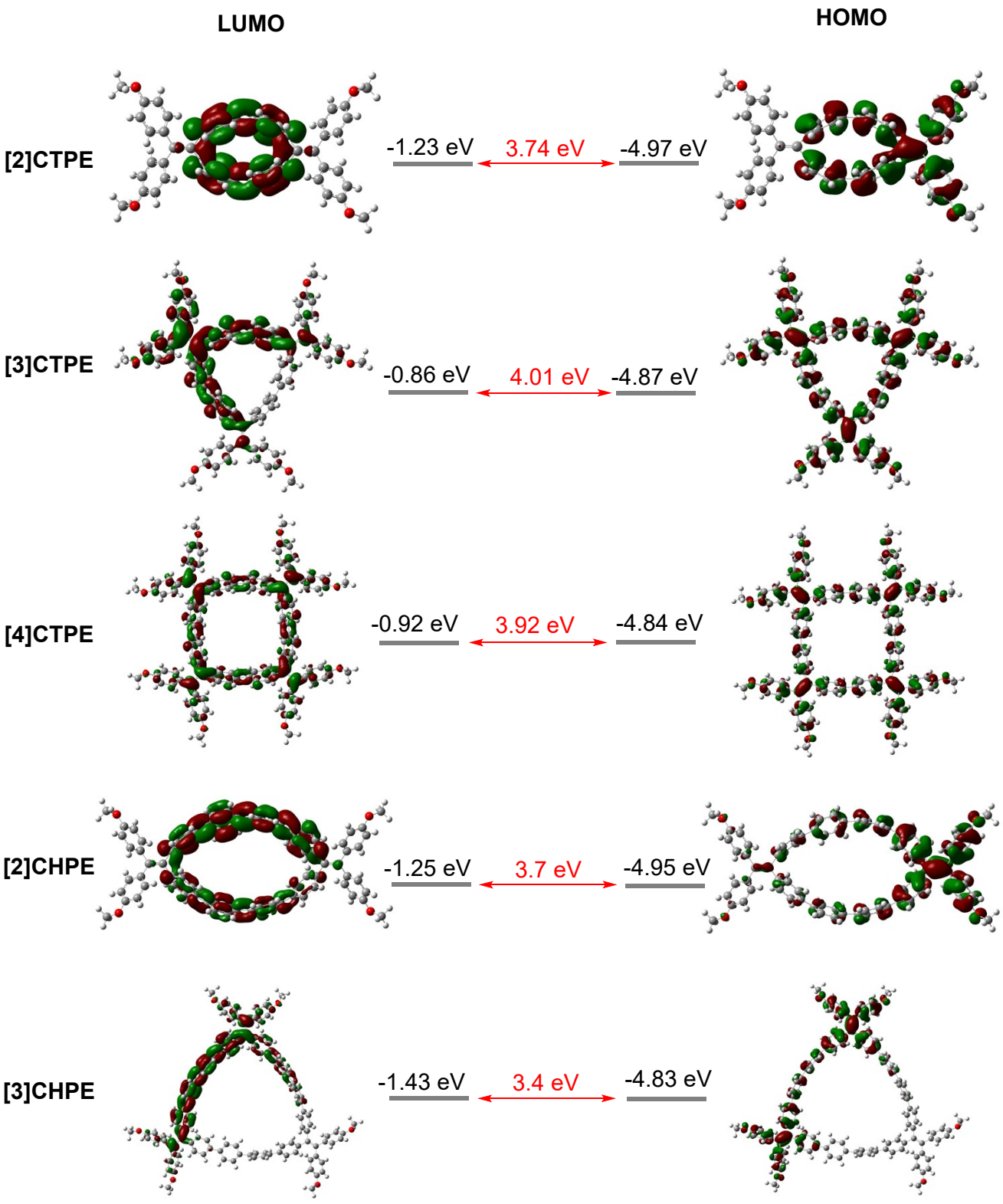


Figure S52. Calculated (B3LYP/6-31G(d)) frontier molecular orbital profiles and energy diagram of **[2]CTPE**, **[3]CTPE**, **[4]CTPE**, **[2]CHPE**, and **[3]CHPE**.

Table S3. Electronic transitions for **[2]CTPE** determined by TD-DFT methods at B3LYP/6-31G(d) level.

Excited State	Energy (eV)	Exciation (nm)	Oscillator strength (f)	Transition type
$S_0 \rightarrow S_1$	3.1160	397.89	0.0009	HOMO→LUMO (0.69849)
$S_0 \rightarrow S_2$	3.5360	350.63	0.0003	HOMO-1→LUMO (0.69725)
$S_0 \rightarrow S_3$	3.6215	342.35	0.4727	HOMO-1→LUMO+1 (0.68829)
$S_0 \rightarrow S_4$	3.6474	339.92	0.0061	HOMO-2→LUMO (0.69235)
$S_0 \rightarrow S_5$	3.7390	331.60	0.2616	HOMO-2→LUMO+2 (-0.16605)
				HOMO→LUMO+2 (0.66183)
$S_0 \rightarrow S_6$	4.0223	308.24	1.0660	HOMO-5→LUMO (0.13065)
				HOMO-3→LUMO (-0.45066)
				HOMO-2→LUMO+1 (-0.20619)
				HOMO-1→LUMO+2 (0.46649)
$S_0 \rightarrow S_7$	4.0891	303.21	0.0132	HOMO-3→LUMO (0.37571)
				HOMO-2→LUMO+1 (0.20600)
				HOMO-1→LUMO+2 (0.50049)
				HOMO→LUMO+3 (0.19100)
$S_0 \rightarrow S_8$	4.1734	297.08	0.0606	HOMO-3→LUMO (-0.16920)
				HOMO-2→LUMO+1 (0.52684)
				HOMO-1→LUMO+1 (-0.26278)
				HOMO→LUMO+3 (-0.28793)
$S_0 \rightarrow S_9$	4.2031	294.99	0.0000	HOMO-5→LUMO (-0.10183)
				HOMO-2→LUMO+1 (0.24676)
				HOMO-1→LUMO+1 (0.62928)
$S_0 \rightarrow S_{10}$	4.2454	292.04	0.0134	HOMO-6→LUMO (0.10755)
				HOMO-4→LUMO (0.20471)
				HOMO-3→LUMO (0.51241)
				HOMO-2→LUMO (0.21778)
				HOMO-1→LUMO+2 (-0.27336)
				HOMO→LUMO+3 (-0.17733)

Table S4. Electronic transitions for **[3]CTPE** determined by TD-DFT methods using B3LYP/6-31G(d).

Excited State	Energy (eV)	Exciation (nm)	Oscillator strength (f)	Transition type
$S_0 \rightarrow S_1$	3.5450	349.74	1.1871	HOMO-2→LUMO+1 (-0.14067)
				HOMO-2→LUMO+3 (0.10354)
				HOMO-1→LUMO (-0.13891)
				HOMO→LUMO (0.55338)
				HOMO→LUMO+1 (0.34628)

$S_0 \rightarrow S_2$	3.5451	349.73	1.1869	HOMO-2→LUMO (-0.14025) HOMO-1→LUMO+1 (0.13921) HOMO-1→LUMO+3 (0.10373) HOMO→LUMO (-0.34617) HOMO→LUMO+1 (0.55362)
$S_0 \rightarrow S_3$	3.5721	347.09	0.0009	HOMO-2→LUMO+1(0.13454) HOMO-1→LUMO+1(-0.13762) HOMO→LUMO+2(0.66615)
$S_0 \rightarrow S_4$	3.7943	326.76	0.0000	HOMO-2→LUMO(0.46193) HOMO-1→LUMO+1(0.46363) HOMO→LUMO+3(0.25167)
$S_0 \rightarrow S_5$	3.8153	324.97	0.0094	HOMO-2→LUMO (0.27761) HOMO-2→LUMO+1(-0.23843) HOMO-1→LUMO (-0.24011) HOMO-1→LUMO+1(-0.27510) HOMO-1→LUMO+2(0.44703) HOMO-2→LUMO (-0.10059)
$S_0 \rightarrow S_6$	3.8158	324.92	0.0091	HOMO-2→LUMO(0.23878) HOMO-2→LUMO+1(0.27504) HOMO-2→LUMO+2(0.44827) HOMO-1→LUMO (0.27661) HOMO-2→LUMO+1(-0.23891)
$S_0 \rightarrow S_7$	3.9275	315.68	0.0066	HOMO-2→LUMO+1(-0.41659) HOMO-1→LUMO (0.51436) HOMO→LUMO+2 (0.19970)
$S_0 \rightarrow S_8$	3.9285	315.60	0.2112	HOMO-2→LUMO(-0.23836) HOMO-2→LUMO+1(0.21488) HOMO-1→LUMO (0.11928) HOMO-1→LUMO+1(0.23463) HOMO-1→LUMO+2(0.50889) HOMO→LUMO(0.22373)
$S_0 \rightarrow S_9$	3.9288	315.58	0.2086	HOMO-2→LUMO(-0.16841) HOMO-2→LUMO+1(-0.29915) HOMO-2→LUMO+2(0.50632) HOMO-1→LUMO (-0.16879) HOMO-1→LUMO+1(0.17221) HOMO→LUMO+1(-0.22233)

$S_0 \rightarrow S_{10}$	3.9940	310.43	0.0000	HOMO-2→LUMO(-0.17823) HOMO-1→LUMO+1(-0.17981) HOMO→LUMO+3(0.64739)

Table S5. Electronic transitions for **[4]CTPE** determined by TD-DFT methods using B3LYP/6-31G(d).

Excited State	Energy (eV)	Exciation (nm)	Oscillator strength (f)	Transition type
$S_0 \rightarrow S_1$	3.4821	356.06	0.0000	HOMO-2→LUMO+2 (0.25546) HOMO-1→LUMO+1 (-0.25552) HOMO→LUMO (0.59603)
$S_0 \rightarrow S_2$	3.5382	350.42	1.7428	HOMO-3→LUMO+1 (-0.11953) HOMO-2→LUMO (-0.39969) HOMO-2→LUMO+4 (0.11937) HOMO→LUMO+1 (0.53981)
$S_0 \rightarrow S_3$	3.5382	350.41	1.7429	HOMO-3→LUMO+2 (0.11954) HOMO-2→LUMO (0.39969) HOMO-2→LUMO+4 (0.11939) HOMO→LUMO+2 (0.53980)
$S_0 \rightarrow S_4$	3.6833	336.61	0.0013	HOMO-2→LUMO+1 (0.33263) HOMO-1→LUMO+2 (-0.33260) HOMO→LUMO+3 (0.48573)
$S_0 \rightarrow S_5$	3.7239	332.95	0.0000	HOMO-3→LUMO (0.35353) HOMO-2→LUMO+2 (0.39850) HOMO-1→LUMO +1 (0.39857) HOMO→LUMO+4 (0.19245)
$S_0 \rightarrow S_6$	3.7622	329.55	0.0018	HOMO-3→LUMO+1 (0.20830) HOMO-2→LUMO+3 (0.16722) HOMO-1→LUMO (0.50938) HOMO→LUMO+1 (0.38734)
$S_0 \rightarrow S_7$	3.7622	329.55	0.0018	HOMO-3→LUMO+2 (0.20829) HOMO-2→LUMO (0.50938) HOMO-1→LUMO+3 (0.16725) HOMO→LUMO+2 (-0.38734)
$S_0 \rightarrow S_8$	3.7936	326.82	0.0000	HOMO-3→LUMO+3 (0.18599) HOMO-2→LUMO+1 (0.47440) HOMO-1→LUMO+2 (0.47439)
$S_0 \rightarrow S_9$	3.8250	324.14	0.0000	HOMO-3→LUMO+4 (0.10268) HOMO-2→LUMO+2 (0.41586)

				HOMO-1→LUMO+1 (-0.41582) HOMO→LUMO (-0.37618)
$S_0 \rightarrow S_{10}$	3.9191	316.36	0.0000	HOMO-2→LUMO+1 (-0.35154) HOMO-1→LUMO+2 (0.35159) HOMO→LUMO+3 (0.48106)

Table S6. Electronic transitions for **[2]CHPE** determined by TD-DFT methods using B3LYP/6-31G(d).

Excited State	Energy (eV)	Exciation (nm)	Oscillator strength (f)	Transition type
$S_0 \rightarrow S_1$	3.2389	382.80	0.1742	HOMO→LUMO+1 (0.68038)
$S_0 \rightarrow S_2$	3.3235	373.05	1.7186	HOMO→LUMO+1 (0.68038)
$S_0 \rightarrow S_3$	3.4915	355.10	0.1426	HOMO-1→LUMO (0.66737) HOMO→LUMO (-0.10219) HOMO→LUMO +3 (0.11253)
$S_0 \rightarrow S_4$	3.6060	343.83	0.2873	HOMO-1→LUMO+1 (0.64192) HOMO-1→LUMO+2 (0.17515) HOMO→LUMO+2 (0.18988)
$S_0 \rightarrow S_5$	3.7858	327.50	0.5883	HOMO-3→LUMO (-0.20745) HOMO-2→LUMO (0.57412) HOMO-2→LUMO+1 (0.27415) HOMO→LUMO (0.10909)
$S_0 \rightarrow S_6$	3.8127	325.19	0.0535	HOMO-2→LUMO+1 (-0.13428) HOMO-1→LUMO+1 (-0.18483) HOMO-1→LUMO +4 (0.10030) HOMO →LUMO+2 (0.61829)
$S_0 \rightarrow S_7$	3.8407	322.82	0.8255	HOMO-3→LUMO (-0.30516) HOMO-3→LUMO+1 (0.11777) HOMO-2→LUMO (-0.32346) HOMO-2→LUMO+1 (0.44312) HOMO-1→LUMO+1 (-0.12384) HOMO-1→LUMO+2 (0.17028) HOMO→LUMO+2 (0.14285)
$S_0 \rightarrow S_8$	3.9114	316.98	0.0895	HOMO-3→LUMO (0.45863) HOMO-2→LUMO+1 (0.34313) HOMO-1→LUMO+2 (-0.11180) HOMO→LUMO +3 (0.34986)
$S_0 \rightarrow S_9$	3.9498	313.90	0.0395	HOMO-3→LUMO (-0.31683) HOMO-2→LUMO+1 (-0.19573)

				HOMO-1→LUMO+2 (-0.15600)
				HOMO-1→LUMO+3 (0.10473)
				HOMO→LUMO+3 (0.52616)
$S_0 \rightarrow S_{10}$	3.9826	311.31	0.0381	HOMO-2→LUMO (0.18701)
				HOMO-2→LUMO+1 (-0.10329)
				HOMO-1→LUMO+2 (0.49702)
				HOMO-1→LUMO+4 (0.12273)
				HOMO→LUMO+2 (-0.10033)
				HOMO→LUMO+3 (0.18171)
				HOMO→LUMO+4 (0.31787)

Table S7. Electronic transitions for **[3]CHPE** determined by TD-DFT methods using B3LYP/6-31G(d).

Excited State	Energy (eV)	Exciation (nm)	Oscillator strength (f)	Transition type
$S_0 \rightarrow S_1$	2.9799	416.07	1.9933	HOMO-1→LUMO+1 (-0.18065)
				HOMO→LUMO (0.65760)
$S_0 \rightarrow S_2$	3.0764	403.02	0.7152	HOMO-1→LUMO (0.69725)
				HOMO-1→LUMO+1(-0.44964)
$S_0 \rightarrow S_3$	3.1865	389.09	0.2306	HOMO-2→LUMO (0.13830)
				HOMO-1→LUMO (-0.33396)
				HOMO-1→LUMO+1 (0.39746)
				HOMO→ LUMO+1 (-0.36239)
				HOMO→LUMO+2 (0.20907)
				HOMO→LUMO+3 (-0.11405)
$S_0 \rightarrow S_4$	3.3006	375.64	0.1261	HOMO-2→LUMO (0.24545)
				HOMO-2→LUMO+1 (0.24240)
				HOMO-2→LUMO+2 (-0.13603)
				HOMO-1→LUMO (0.29429)
				HOMO-1→LUMO+1 (0.29087)
				HOMO-1→LUMO+2 (0.11603)
				HOMO-1→LUMO+3 (0.10548)
				HOMO→LUMO+1 (0.30805)
				HOMO→LUMO+2 (0.21142)
$S_0 \rightarrow S_5$	3.3351	371.75	0.6135	HOMO-2→LUMO (-0.33732)
				HOMO-2→LUMO+1 (-0.30712)
				HOMO-2→LUMO+2 (0.13064)
				HOMO-2→LUMO+3 (0.10084)
				HOMO-1→LUMO+2 (0.34495)

				HOMO→LUMO+2 (0.27890)
				HOMO→ LUMO+4 (0.12058)
$S_0 \rightarrow S_6$	3.4065	363.97	0.1158	HOMO-2→LUMO (-0.29257)
				HOMO-1→LUMO+1 (0.43205)
				HOMO-1→LUMO+2 (-0.16677)
				HOMO-1→LUMO+4 (-0.12214)
				HOMO→LUMO (0.16879)
				HOMO→LUMO+1 (0.16451)
				HOMO→LUMO+2 (-0.33667)
$S_0 \rightarrow S_7$	3.4462	359.77	0.0303	HOMO-2→LUMO (-0.44578)
				HOMO-2→LUMO+1 (0.46344)
				HOMO-2→LUMO+2 (-0.14636)
				HOMO-1→LUMO (-0.13560)
				HOMO→LUMO+2 (0.13174)
$S_0 \rightarrow S_8$	3.4750	356.79	0.3749	HOMO-2→LUMO+1 (0.21285)
				HOMO-2→LUMO+2 (0.13023)
				HOMO-2→LUMO+3 (0.20785)
				HOMO-1→LUMO+2 (0.44171)
				HOMO→LUMO+1 (-0.10470)
				HOMO→LUMO+2 (-0.35980)
				HOMO→LUMO+4 (0.11874)
$S_0 \rightarrow S_9$	3.5373	350.50	0.0503	HOMO-2→LUMO+1 (0.16886)
				HOMO-2→LUMO+2 (0.47384)
				HOMO-2→LUMO+3 (0.27825)
				HOMO-1→LUMO+2 (-0.20028
				HOMO-1→LUMO+3 (0.22668)
				HOMO→LUMO+2 (0.11220)
				HOMO→LUMO+3 (-0.11192)
				HOMO→LUMO+4 (-0.13454)
$S_0 \rightarrow S_{10}$	3.6622	338.55	0.0284	HOMO-1→LUMO+2 (-0.20311)
				HOMO-1→LUMO+3 (0.19913)
				HOMO→LUMO+3 (0.31410)
				HOMO→LUMO+4 (0.53081)

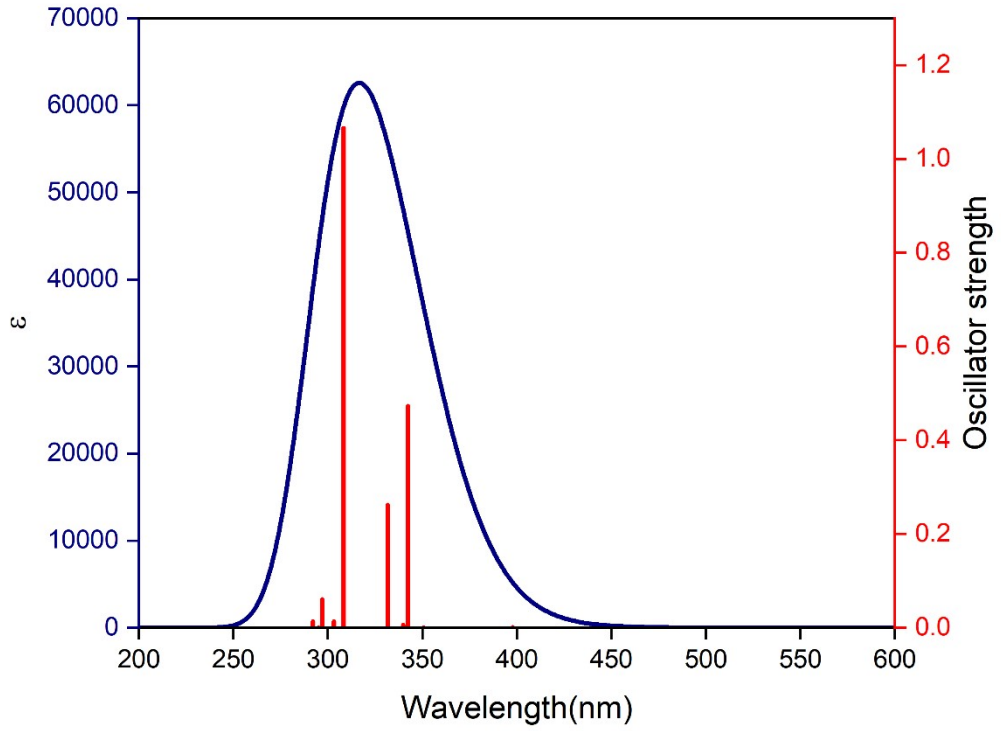


Figure S53. Calculated electronic absorption spectrum (B3LYP/6-31G(d)) of **[2]CTPE**.

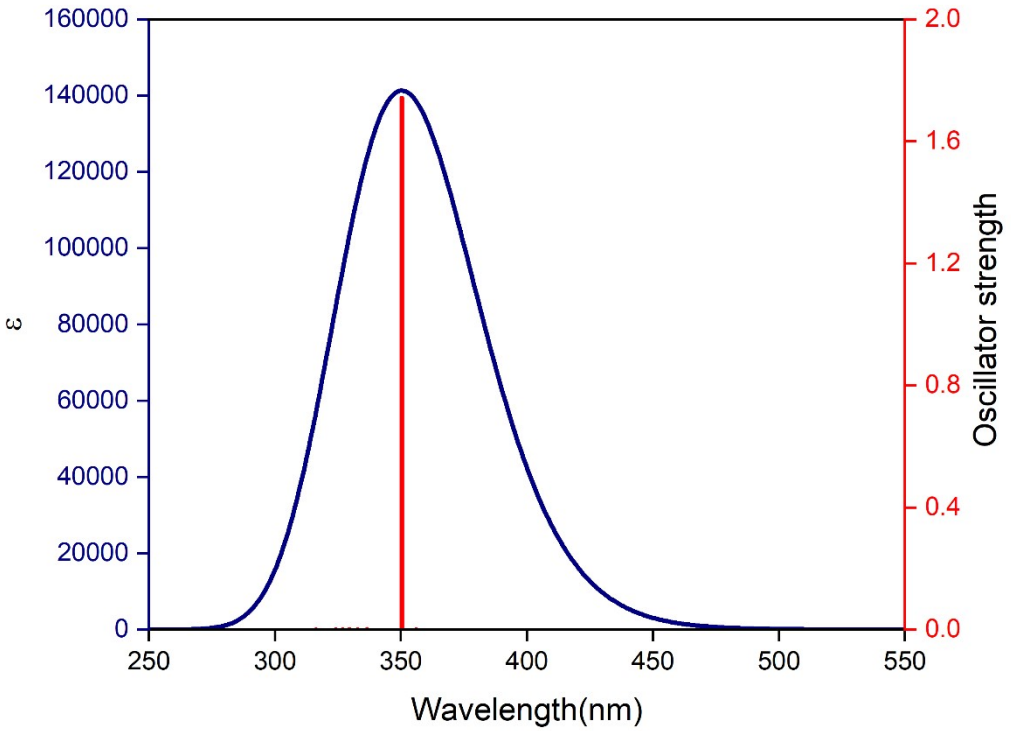


Figure S54. Calculated electronic absorption spectrum (B3LYP/6-31G(d)) of **[3]CTPE**.

Figure S55. Calculated electronic absorption spectrum (B3LYP/6-31G(d)) of **[4]CTPE**.

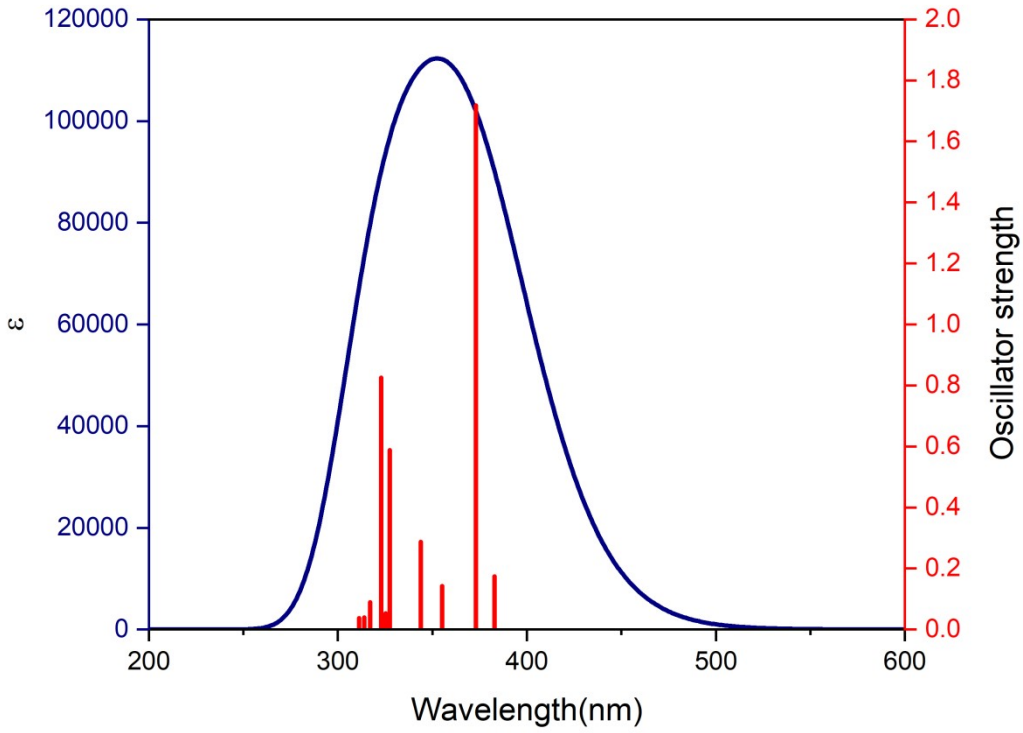


Figure S56. Calculated electronic absorption spectrum (B3LYP/6-31G(d)) of **[2]CHPE**.

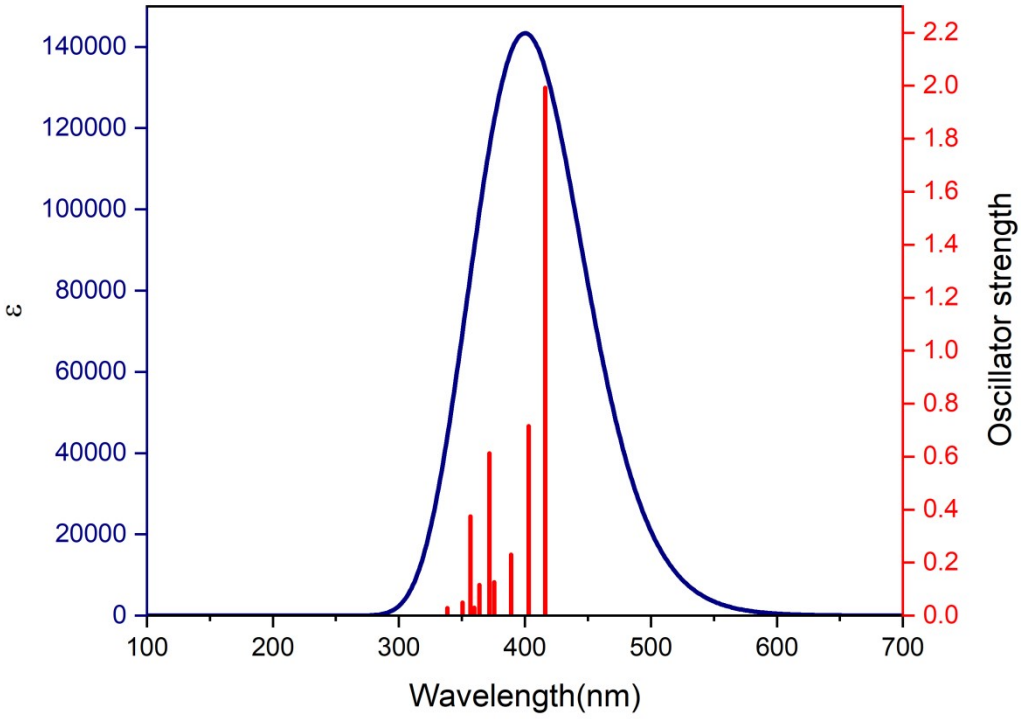
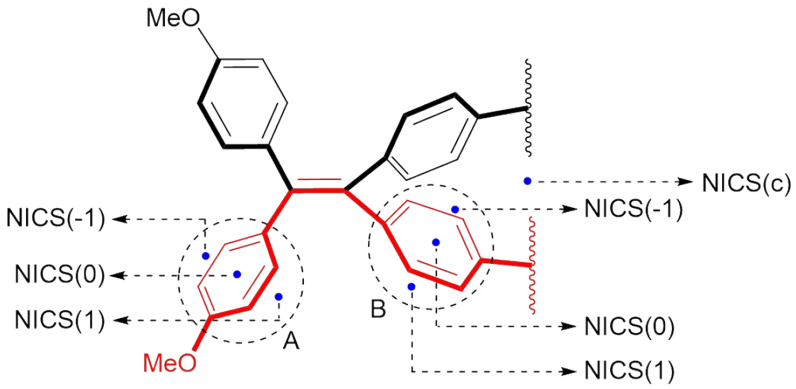
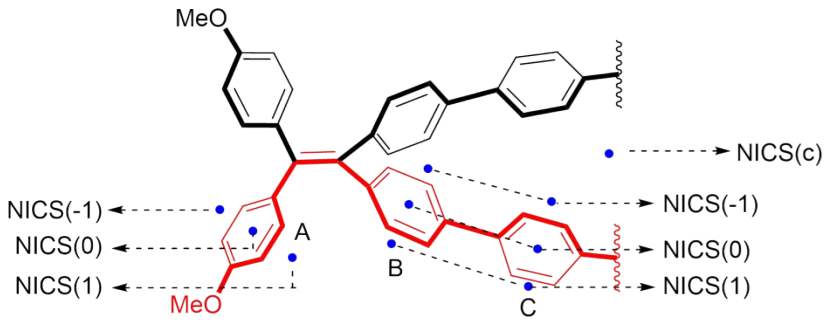


Figure S57. Calculated electronic absorption spectrum (B3LYP/6-31G(d)) of **[3]CHPE**.



molecule	ring A			ring B			geometric center
	NICS(-1)	NICS(0)	NICS(1)	NICS(-1)	NICS(0)	NICS(1)	NICS(c)
[2]CTPE	-9.1	-8.3	-9.0	-11.1	-7.6	-8.2	-5.5
[3]CTPE	-9.1	-8.2	-9.0	-10.4	-7.8	-8.6	-2.6
[4]CTPE	-9.1	-8.4	-9.2	-9.8	-7.7	-8.9	-1.6

Figure S58. Calculated NICS values (ppm) of **[2]CTPE, [3]CTPE** and **[4]CTPE**. NICS(0) means NICS value at the center of a benzene ring (A, B), NICS(1) NICS(-1)means NICS value at the position 1 Å perpendicularly to the benzene ring (A, B) as shown in the above. NICS(c) means NICS value at the geometric center of the **CTPE**.



[2]CHPE			[3]CHPE		
ring A	NICS(-1)	-9.2	ring A	NICS(-1)	-9.0
	NICS(0)	-8.2		NICS(0)	-8.0
	NICS(1')	-9.0		NICS(1)	-8.9
ring B	NICS(-1)	-10.3	ring B	NICS(-1)	-8.8
	NICS(0)	-7.6		NICS(0)	-6.4
	NICS(1)	-8.4		NICS(1)	-7.8
ring C	NICS(-1)	-9.9	ring C	NICS(-1)	-8.7
	NICS(0)	-6.7		NICS(0)	-5.9
	NICS(1)	-7.9		NICS(1)	-7.7
geometric center	NICS(c)	-2.2	geometric center	NICS(c)	-0.6

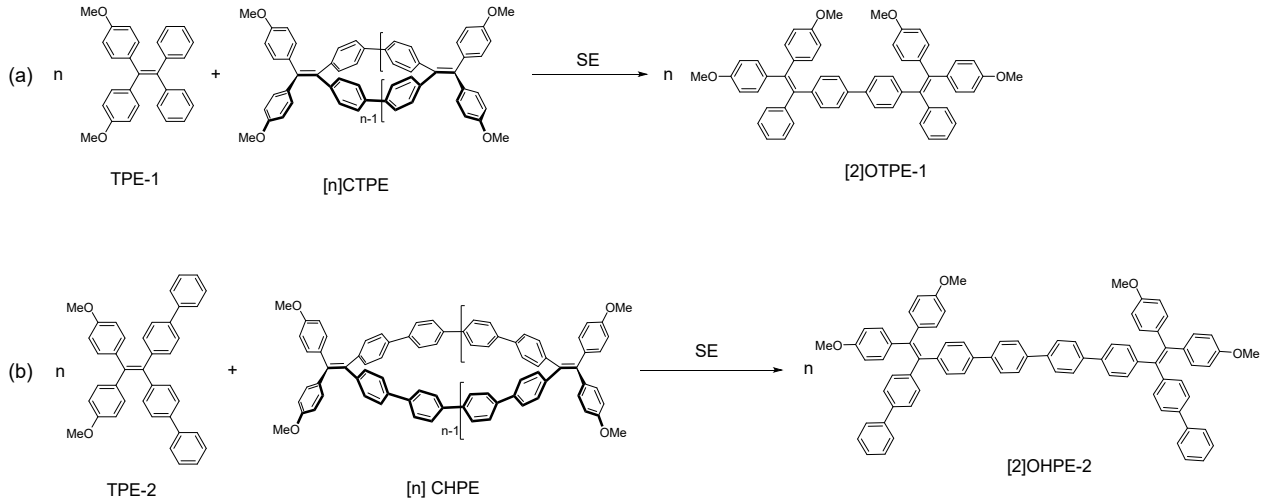
Figure S59. Calculated NICS values (ppm) of **[2]CHPE, [3]CHPE**. NICS(0) means NICS value at the center of a benzene ring (A, B), NICS(1) NICS(-1) means NICS value at the position 1 Å perpendicularly to the benzene ring (A, B, C) as shown above. NICS(c) means NICS value at the geometric center of the **CHPE**.

Table S8. Uncorrected and thermal-corrected (298K) energies of stationary points (Hartree).[a]

compound	E	E + ZPE	H	G
[2]CTPE	-2461.220097	-2460.377102	-2460.325717	-2460.466585
[3]CTPE	-3691.940968	-3690.675267	-3690.597032	-3690.800284
[4]CTPE	-4922.620514	-4920.932630	-4920.827536	-4921.094918
TPE-1	-1231.851082	-1231.408480	-1231.381759	-1231.466358
[2]OTPE-1	-2462.511709	-2461.646567	-2461.593382	-2461.741467
[2]CHPE	-3385.496128	-3384.328404	-3384.258156	-3384.441383
[3]CHPE	-5078.303968	-5076.551042	-5076.444883	-5076.711896
TPE-2	-1693.966631	-1693.362030	-1693.325850	-1693.433591
[2]OHPE-2	-3386.742619	-3385.553508	-3385.481399	-3385.675676

[a] E = electronic energy; ZPE = zero-point-energy; H (= $E+ZPE+E_{vib}+E_{rot}+E_{trans}+RT$): sum of electronic and thermal enthalpies; G(=H-TS): sum of electronic and thermal free energies.

Table S9. Strain energies (SE, kJ mol^{-1}) of **[n] CTPE**s and **[n]CHPE**s based on Homodesmotic Reaction.



[n]CTPE	Strain energy [a]
2	256.06
3	99.34
4	49.77
[n]CHPE	Strain energy [b]
2	139.00
3	57.14

[a] Calculated based on (a); [b]Calculated based on (b).

7. Photophysical Measurements

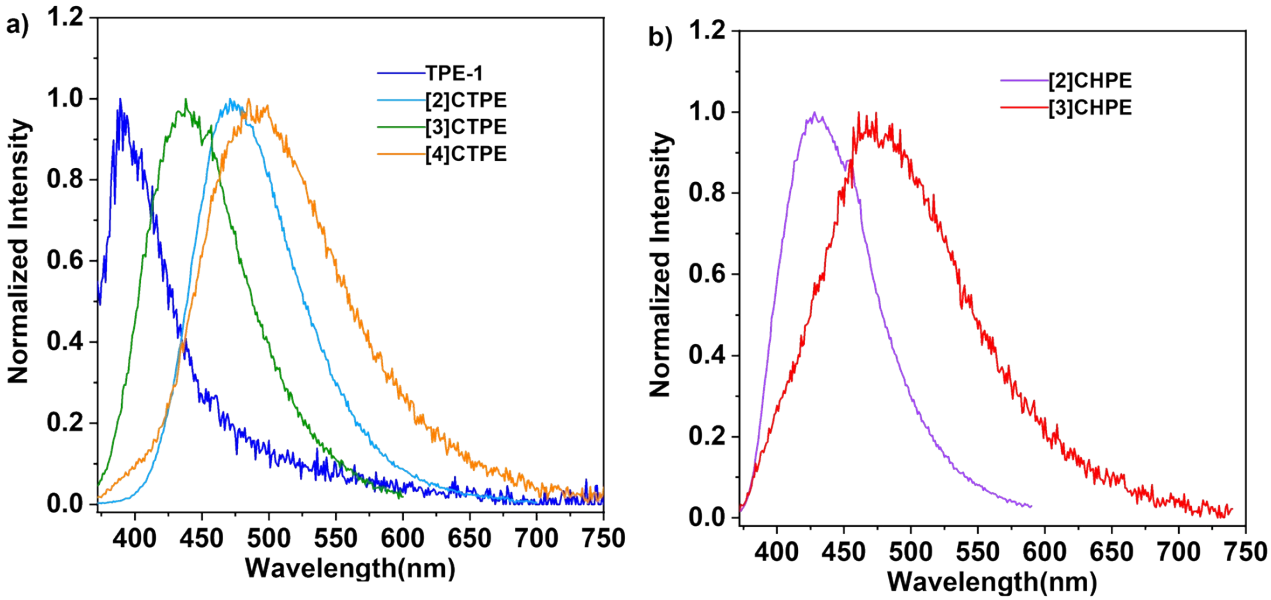


Figure S60. PL spectra of compounds in THF solution. (Concentration: 50 μM for **TPE-1**; 10 μM for **[2]CTPE**, **[3]CTPE**, **[4]CTPE**, **[2]CHPE**, and **[3]CHPE**).

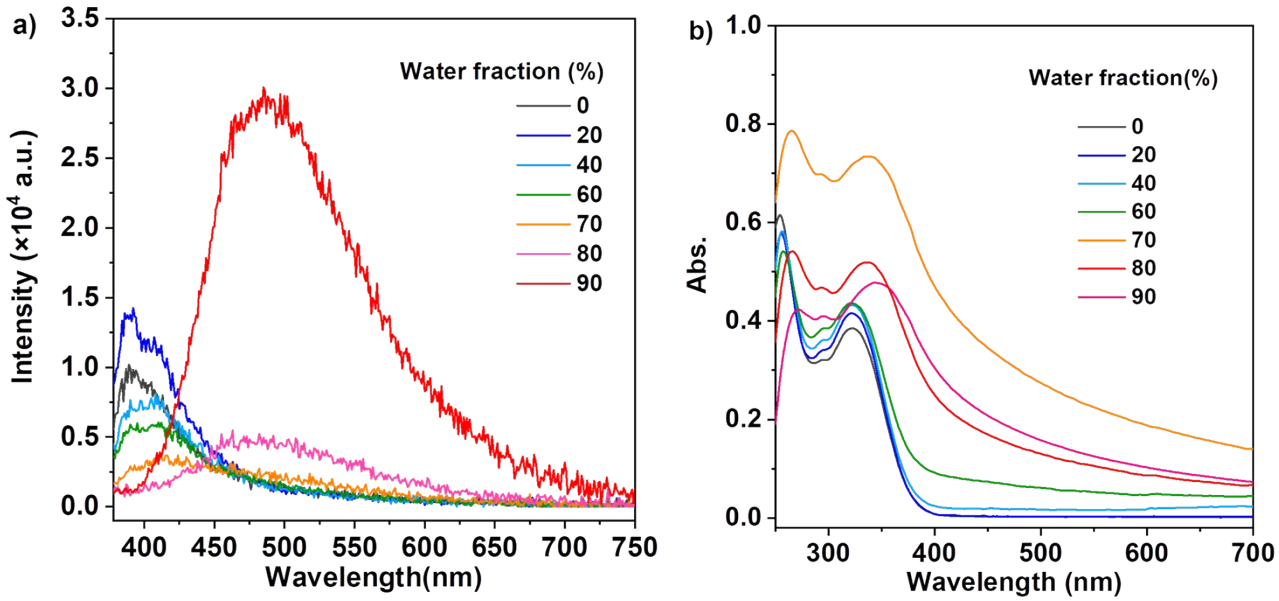


Figure S61. a) PL spectra of **TPE-1** in water/THF mixture with different water fractions. The inset is the fluorescence images of **TPE-1** in pure THF and in water/THF mixture with 90% water fraction. (Concentration: 50 μM). b) UV-Vis spectra.

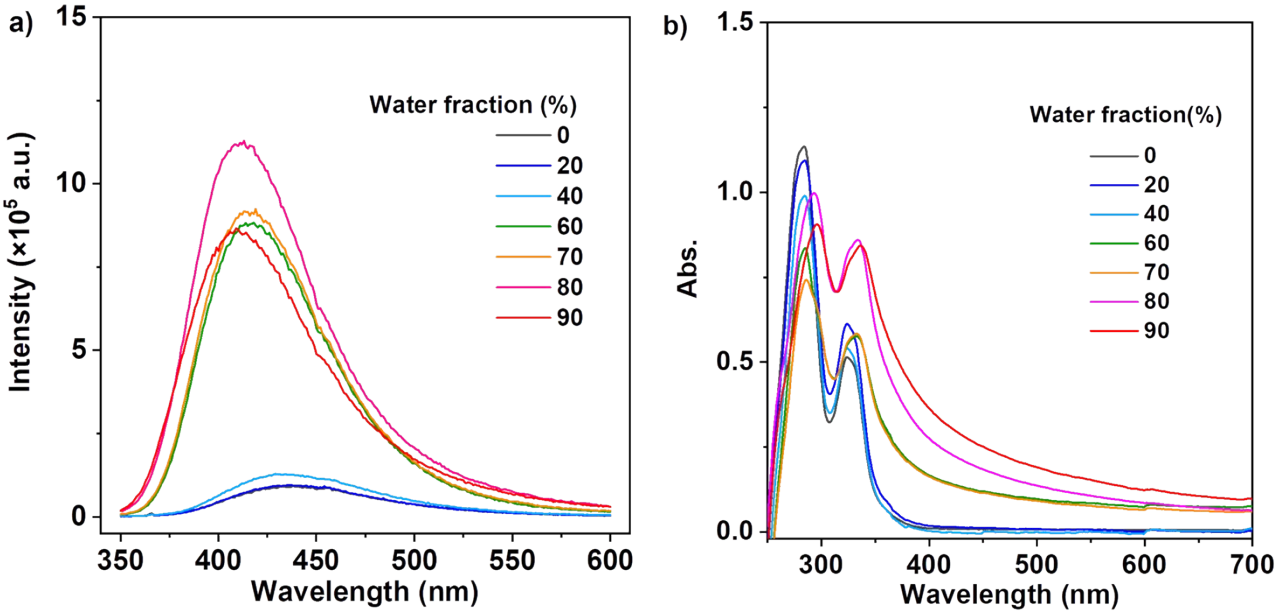


Figure 62. a) PL spectra of **[3]CTPE** in water/THF mixture with different water fractions. The inset is the fluorescence image of **[3]CTPE** in pure THF and in water/THF mixture with 90% water fraction. (Concentration: 10 μM). b) UV-Vis spectra.

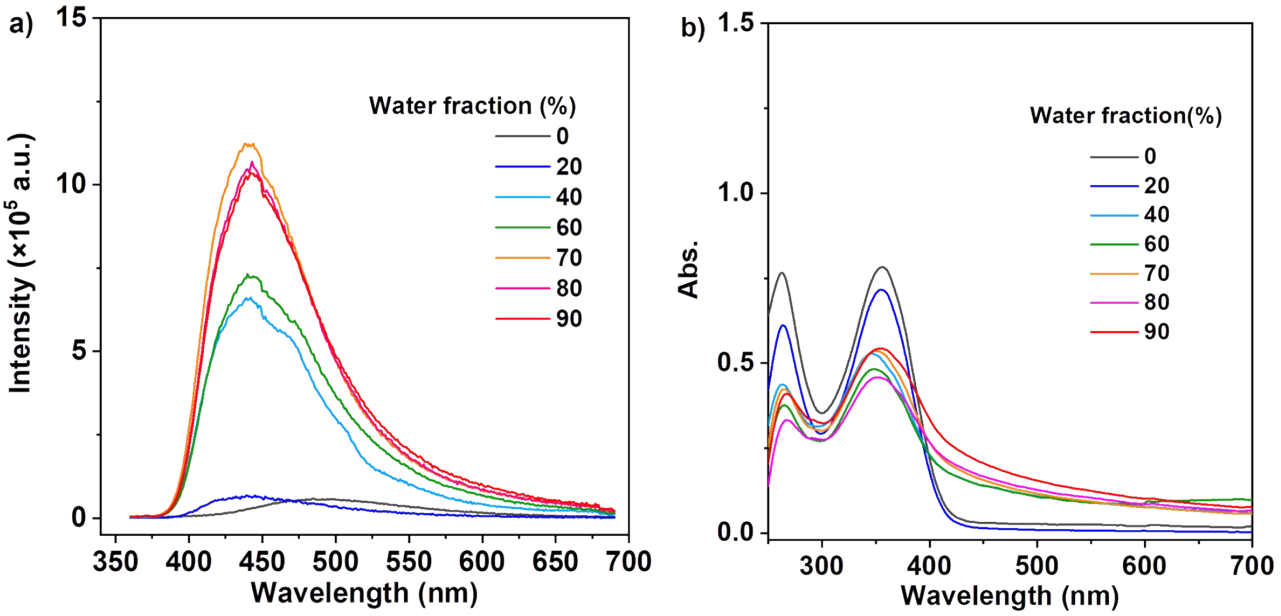


Figure S63. a) PL spectra of **[4]CTPE** in water/THF mixture with different water fractions. The inset is the fluorescence image of **[4]CTPE** in pure THF and in water/THF mixture with 90% water fraction. (Concentration: 10 μM). b) UV-Vis spectra.

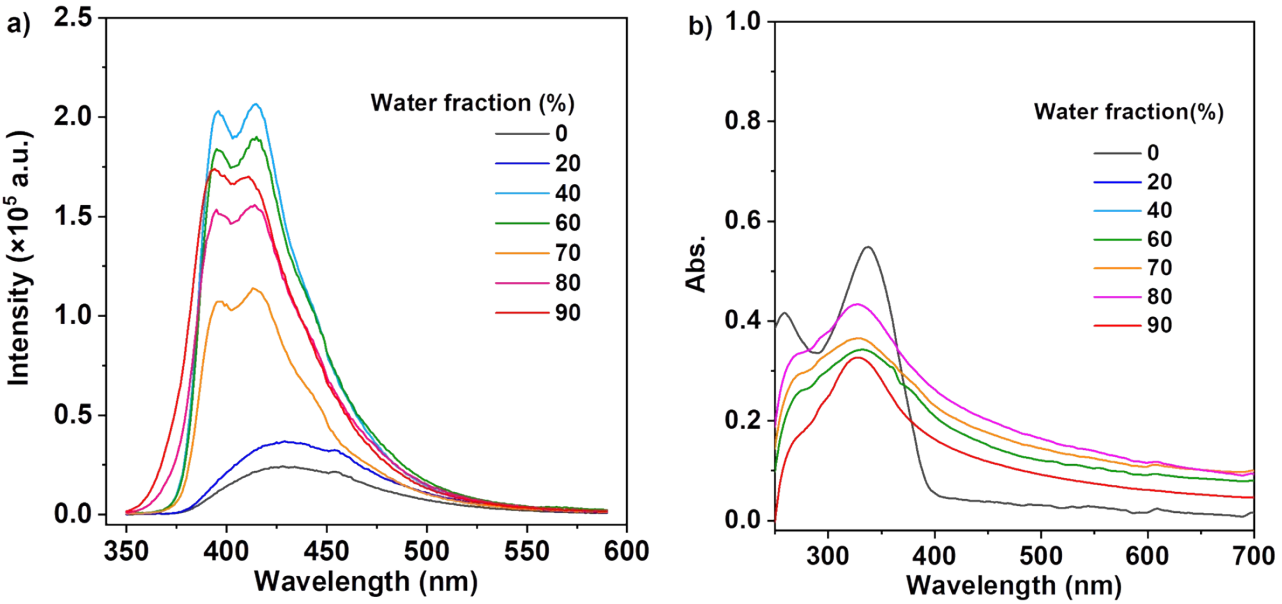


Figure S64. a) PL spectra of **[2]CHPE** in water/THF mixture with different water fractions. The inset is the fluorescence image of **[2]CHPE** in pure THF and in water/THF mixture with 90% water fraction. (Concentration: 10 μM). b) UV-Vis spectra.

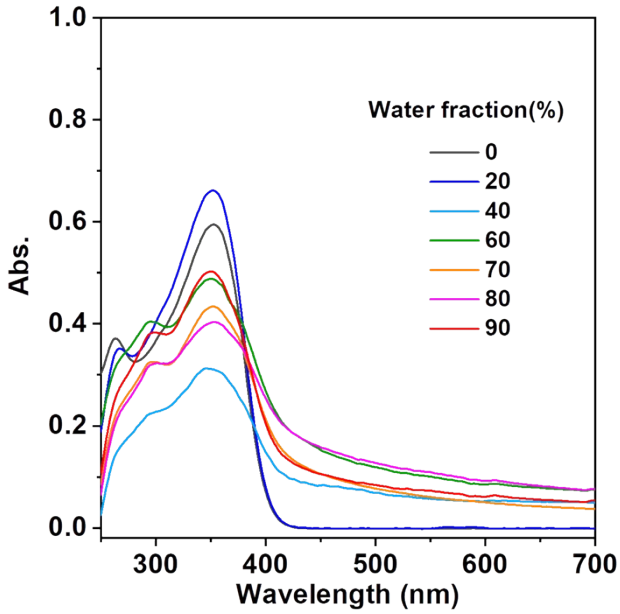


Figure S65. UV-Vis spectra of **[3]CHPE** in water/THF mixture with different water fractions. The inset is the fluorescence image of **[3]CHPE** in pure THF and in water/THF mixture with 90% water fraction. (Concentration: 10 μM).

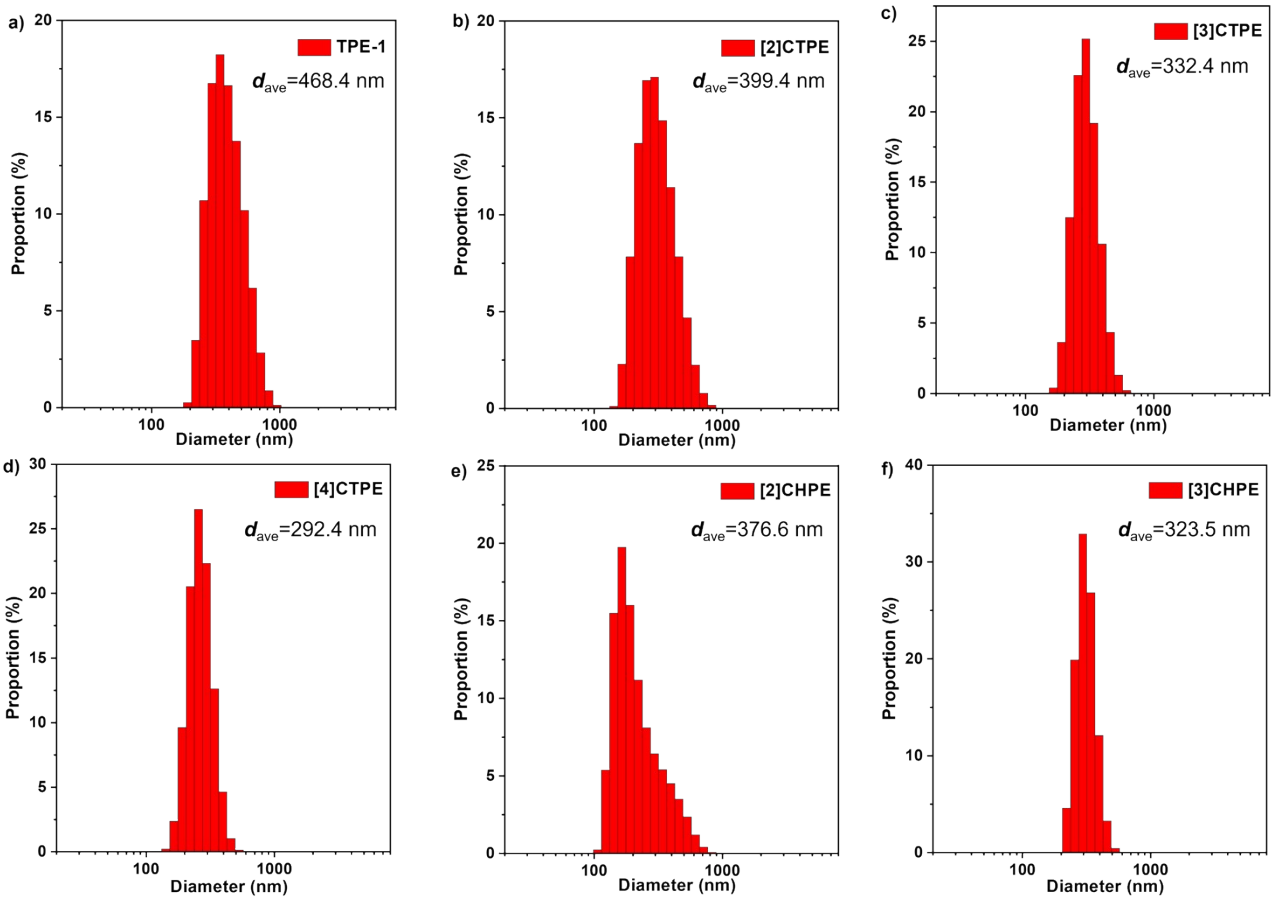


Figure S66. Effective diameters of the compounds in water/THF mixtures with 90% water fraction. Concentration: 50 μM in THF for **TPE-1**; 10 μM for **[2]CTPE**, **[3]CTPE**, **[4]CTPE**, **[2]CHPE**, and **[3]CHPE**.

Cartesian Coordinates of the Optimized Structures

[2]CTPE

C	-2.82782535	1.79892275	-1.11813886
C	-1.57861009	2.41519991	-1.16979535
C	-0.72723294	2.42037817	-0.04962170
C	-1.30474327	2.04430273	1.17764669
C	-2.56308525	1.44929372	1.23152987
C	-3.29780006	1.19782327	0.06202204
H	-3.38604424	1.67557337	-2.04287364
H	-1.21929098	2.78728332	-2.12549769
H	-0.70454320	2.06574743	2.08251762
H	-2.91130586	1.04348556	2.17748101
C	0.75743499	2.40623526	-0.18945864
C	1.64137764	2.57731075	0.89236692
C	1.29853052	1.83838974	-1.35851956
C	2.90230939	1.97374209	0.89659193
H	1.30623798	3.09332632	1.78868882
C	2.55060234	1.23829871	-1.35288157
H	0.67299670	1.71361785	-2.23636856
C	3.32658764	1.18302086	-0.18402192
H	3.50922717	2.01985448	1.79742689
H	2.86280694	0.67196448	-2.22645481
C	-2.56308348	-1.44930988	-1.23152402
C	-1.30474020	-2.04431572	-1.17763968
C	-0.72722857	-2.42038704	0.04962891
C	-1.57860499	-2.41520878	1.16980294
C	-2.82782173	-1.79893436	1.11814589
C	-3.29779863	-1.19783856	-0.06201653
H	-2.91130541	-1.04350450	-2.17747576
H	-0.70454071	-2.06576127	-2.08251078
H	-1.21928488	-2.78728965	2.12550584
H	-3.38604094	-1.67558415	2.04288064
C	0.75743902	-2.40624157	0.18946468
C	1.29853454	-1.83839494	1.35852481
C	1.64138070	-2.57731613	-0.89236132
C	2.55060557	-1.23830218	1.35288571
H	0.67300152	-1.71362365	2.23637447

C	2.90231137	-1.97374560	-0.89658798
H	1.30624105	-3.09333221	-1.78868274
C	3.32658975	-1.18302340	0.18402518
H	2.86281025	-0.67196731	2.22645858
H	3.50922820	-2.01985698	-1.79742359
C	4.25293322	-0.00000051	0.00000067
C	-4.22516707	-0.00000812	0.00000188
C	-5.57879124	-0.00000602	0.00000026
C	5.60645515	-0.00000031	-0.00000251
C	-6.38497384	1.25384748	0.14075647
C	-7.41277460	1.29949609	1.09475387
C	-6.18394321	2.40364258	-0.64369416
C	-8.18908778	2.44149603	1.29326542
H	-7.60864463	0.42168505	1.70408209
C	-6.95600096	3.54529142	-0.46815892
H	-5.42154321	2.40350482	-1.41289076
C	-7.96102609	3.57737211	0.50731249
H	-8.96295146	2.43141984	2.05253989
H	-6.80000475	4.42689840	-1.08224398
C	-6.38498612	-1.25385062	-0.14075706
C	-7.41282063	-1.29946978	-1.09472012
C	-6.18393490	-2.40366790	0.64365667
C	-8.18914694	-2.44146025	-1.29323427
H	-7.60870702	-0.42164255	-1.70401951
C	-6.95600509	-3.54530765	0.46811859
H	-5.42150849	-2.40355550	1.41282682
C	-7.96106440	-3.57735784	-0.50731863
H	-8.96303681	-2.43136000	-2.05248168
H	-6.79999258	-4.42693107	1.08217594
C	6.39577937	1.24034856	-0.26351953
C	7.48778801	1.56671881	0.55394503
C	6.09780750	2.11585950	-1.32472925
C	8.24009428	2.72495566	0.35372217
H	7.75422039	0.90421351	1.37250044
C	6.84283832	3.26632068	-1.54474903
H	5.27580378	1.88542202	-1.99332280
C	7.91762826	3.58488490	-0.70279752

H	9.06780713	2.94169074	1.01957973
H	6.61370361	3.93435042	-2.36928275
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C	7.48778023	-1.56672618	-0.55395954
C	6.09781612	-2.11585409	1.32473071
C	8.24008623	-2.72496342	-0.35373706
H	7.75420627	-0.90422580	-1.37252107
C	6.84284710	-3.26631524	1.54475016
H	5.27581898	-1.88541107	1.99333059
C	7.91762858	-3.58488605	0.70279057
H	9.06779258	-2.94170368	-1.01960109
H	6.61371901	-3.93433972	2.36928989
O	8.58504339	4.73852895	-0.99982829
O	8.58504466	-4.73852925	0.99982167
O	-8.66106250	-4.74617616	-0.60482637
O	-8.66101424	4.74619694	0.60481465
C	9.67981951	5.11013543	-0.17868288
H	9.36935043	5.26676382	0.86298637
H	10.47976655	4.35808809	-0.20562833
C	9.67981221	-5.11014203	0.17866778
H	9.36933291	-5.26677614	-0.86299755
H	10.47976062	-4.35809568	0.20560092
C	-9.68926734	-4.83201717	-1.57740391
H	-9.29731882	-4.69425421	-2.59400611
H	-10.48180123	-4.09375360	-1.39532616
C	-9.68918415	4.83206908	1.57742622
H	-9.29720066	4.69432986	2.59401816
H	-10.48172900	4.09380564	1.39539545
H	10.05563035	-6.05002242	0.58742815
H	10.05563485	6.05001776	-0.58744148
H	-10.10578407	-5.83692518	-1.48549974
H	-10.10569814	5.83697719	1.48551100

[3]CTPE

C	-3.92646862	-1.22616193	-0.05062045
C	-3.69196535	-0.42336611	-1.18007742
C	-4.04596901	0.92021051	-1.18758135

C	-4.68579319	1.51224143	-0.08594475
C	-5.02922079	0.68270497	0.99221051
C	-4.64382503	-0.65924927	1.01472310
C	-3.23654799	-2.53857467	0.05059997
C	-3.17646640	-3.45112969	-1.01458000
C	-2.28958518	-4.52947743	-0.99195709
C	-1.41141504	-4.71672018	0.08613320
C	-1.53608899	-3.85373107	1.18755670
C	-2.44211529	-2.80035949	1.17997347
H	-3.13789723	-0.83557954	-2.01897991
H	-3.76353288	1.54058749	-2.03417227
H	-5.55427520	1.10650054	1.84416743
H	-4.87236195	-1.26603289	1.88747303
H	-3.80598485	-3.29551700	-1.88727630
H	-2.23831149	-5.20244643	-1.84377447
H	-0.86477363	-3.97262154	2.03404937
H	-2.46735342	-2.11004513	2.01872394
C	3.02482161	-2.78665007	-0.04910157
C	2.21252984	-2.98546921	-1.17860941
C	1.22595695	-3.96382392	-1.18582979
C	1.03308210	-4.81356532	-0.08393536
C	1.92297968	-4.69572592	0.99433970
C	2.89236682	-3.69089477	1.01662246
C	3.81646906	-1.53292764	0.05160296
C	4.57717994	-1.02537298	-1.01361052
C	5.06773482	0.28182818	-0.99164429
C	4.79041328	1.13671660	0.08576057
C	4.10485949	0.59801993	1.18725368
C	3.64552931	-0.71326816	1.18034356
H	2.29264466	-2.29991304	-2.01781456
H	0.54757930	-4.02978216	-2.03247575
H	1.81838868	-5.36202786	1.84652340
H	3.53197448	-3.58503212	1.88943667
H	4.75745653	-1.64894331	-1.88583382
H	5.62528926	0.66209793	-1.84349056
H	3.87182499	1.23942609	2.03320924
H	3.05995801	-1.07968333	2.01909870

C	-0.58044857	4.07225805	0.04935474
C	-1.20461312	3.51513511	1.17858533
C	-2.56985489	3.25711255	1.18582542
C	-3.37937007	3.58067636	0.08426733
C	-2.77790317	4.24755912	-0.99370550
C	-1.40056616	4.47639713	-1.01604219
C	0.90112747	4.01367464	-0.05147939
C	1.75052042	4.35206102	1.01388844
C	3.10543051	4.01498797	0.99181212
C	3.65239516	3.30226365	-0.08585164
C	2.82000635	3.04353213	-1.18751641
C	1.47942629	3.40869510	-1.18050944
H	-0.59435693	3.19190782	2.01750182
H	-3.00866305	2.73515880	2.03220478
H	-3.38617094	4.53966539	-1.84564160
H	-0.95085763	4.94376092	-1.88864995
H	1.33907043	4.85373604	1.88632322
H	3.73477529	4.25827665	1.84378122
H	3.21625973	2.48828769	-2.03371220
H	0.84562808	3.13449116	-2.01942297
C	4.99125921	2.62405077	-0.00009122
C	6.19296627	3.25533899	-0.00020133
C	-0.22359676	-5.63416636	0.00111486
C	-0.27732500	-6.99055005	0.00077980
C	-4.76788683	3.01087121	-0.00079082
C	-5.91561209	3.73571852	-0.00049327
C	7.47597815	2.52118717	0.21541576
C	8.57528806	2.75626075	-0.62310492
C	7.64869086	1.59973298	1.26571934
C	9.78897042	2.08812905	-0.45428892
H	8.48079965	3.47470022	-1.43246684
C	8.85270801	0.93578873	1.45531666
H	6.82722039	1.40811714	1.94769118
C	9.93260172	1.16941290	0.59207339
H	10.60701404	2.29345775	-1.13555549
H	8.98326932	0.23142455	2.27108133
C	6.31696583	4.72830892	-0.21591907

C	7.13574988	5.49958272	0.62172238
C	5.65540664	5.39393773	-1.26538714
C	7.27495117	6.87799066	0.45286772
H	7.67434850	5.01373884	1.43042524
C	5.79255546	6.76202401	-1.45501765
H	5.03041380	4.82675270	-1.94675991
C	6.59918093	7.51809140	-0.59265298
H	7.90938051	7.43459411	1.13343836
H	5.28606252	7.26958595	-2.27018219
C	-5.92182405	5.21398978	0.21460951
C	-6.67666025	6.04779739	-0.62319578
C	-5.20920528	5.82510828	1.26379001
C	-6.70551581	7.43298176	-0.45479367
H	-7.25241807	5.60615177	-1.43164352
C	-5.23685303	7.19982335	1.45299000
H	-4.63135573	5.21011919	1.94530594
C	-5.98074820	8.01750809	0.59046634
H	-7.29362150	8.03817188	-1.13549852
H	-4.69143732	7.66565406	2.26795591
C	-7.25315886	3.10595483	-0.21490420
C	-8.32980591	3.42880274	0.62382493
C	-7.49935080	2.20002989	-1.26408802
C	-9.59298285	2.85940020	0.45628581
H	-8.17792489	4.13827170	1.43235903
C	-8.75258662	1.63400845	-1.45242022
H	-6.69616414	1.94274436	-1.94621384
C	-9.80997505	1.95395904	-0.58898980
H	-10.39168251	3.13004436	1.13769250
H	-8.93932517	0.94141809	-2.26734116
C	-1.55444659	-7.73527447	0.21514094
C	-1.89886052	-8.80527632	-0.62352831
C	-2.44035999	-7.42436448	1.26423012
C	-3.08413352	-9.52291735	-0.45605814
H	-1.22823606	-9.08250889	-1.43194999
C	-3.61718887	-8.13574110	1.45250213
H	-2.19692340	-6.61687238	1.94635699
C	-3.95310664	-9.18818601	0.58910399

H	-3.31396477	-10.33436457	-1.13738924
H	-4.29363433	-7.89682599	2.26735749
C	0.93686891	-7.83382135	-0.21425494
C	1.19561350	-8.92838427	0.62351025
C	1.84439725	-7.59326145	-1.26335190
C	2.32020236	-9.73761239	0.45509776
H	0.50530386	-9.15224726	1.43190253
C	2.96106273	-8.39556623	-1.45256807
H	1.66553444	-6.76850421	-1.94480690
C	3.21267168	-9.47206151	-0.59013201
H	2.48514699	-10.56525730	1.13573830
H	3.65406963	-8.21043019	-2.26749893
O	4.33789908	-10.19849318	-0.85737782
O	-5.13257886	-9.82319041	0.85531092
O	-11.00181297	1.34250092	-0.85524853
O	-5.94089342	9.35625969	0.85764630
O	11.07170581	0.46505201	0.85960373
O	6.66615672	8.85569628	-0.86016591
C	7.46579196	9.66849052	-0.01732606
H	7.37181257	10.68504350	-0.40405332
H	7.11349417	9.64275620	1.02251978
H	8.52135426	9.36640672	-0.04610553
C	12.19424993	0.66041375	0.01570771
H	12.97769356	0.00592928	0.40253426
H	11.97212042	0.38402723	-1.02367889
H	12.54541497	1.70071503	0.04311814
C	4.64215596	-11.29731725	-0.01449044
H	5.56980386	-11.72381564	-0.40093423
H	4.79554317	-10.97936115	1.02542805
H	3.85307901	-12.06073920	-0.04357648
C	-5.52289060	-10.89345187	0.01113880
H	-6.48172580	-11.24517688	0.39674714
H	-5.64997395	-10.56320214	-1.02849485
H	-4.79708524	-11.71727834	0.03971773
C	-12.10476113	1.62797751	-0.01117783
H	-12.93822684	1.03782992	-0.39696202
H	-11.90498619	1.33588314	1.02845019

H	-12.37157082	2.69301157	-0.03967452
C	-6.67318721	10.23002314	0.01460522
H	-6.49835964	11.23594586	0.40103067
H	-6.32415402	10.17596388	-1.02525359
H	-7.74949098	10.01315472	0.04353106

[4]CTPE

C	4.58025504	3.27649853	0.02143138
C	3.74429209	3.58766980	1.10631563
C	2.96586180	4.73986628	1.10075637
C	3.02767618	5.65444481	0.03614370
C	3.90264613	5.37058339	-1.02308397
C	4.65238194	4.19404141	-1.03764991
C	5.27766703	1.96474232	-0.02338651
C	6.07884369	1.51146887	1.03559419
C	6.63489113	0.23196944	1.02099535
C	6.38080943	-0.65221312	-0.03816122
C	5.58783637	-0.19205493	-1.10263638
C	5.06796488	1.09762532	-1.10816158
H	3.66323611	2.88614320	1.93245972
H	2.27973139	4.92723650	1.92268711
H	3.97852497	6.06938750	-1.85160560
H	5.30427467	3.98286265	-1.88160085
H	6.26850806	2.17004271	1.87946942
H	7.25678701	-0.09591300	1.84940508
H	5.35927085	-0.86563579	-1.92452999
H	4.44089600	1.42264529	-1.93421886
C	3.27652860	-4.58023397	0.02157352
C	3.58772032	-3.74427838	1.10645725
C	4.73992385	-2.96585849	1.10088728
C	5.65448793	-3.02767604	0.03626240
C	5.37060794	-3.90264217	-1.02296362
C	4.19405877	-4.65236717	-1.03751836
C	1.96476512	-5.27763348	-0.02323444
C	1.51150066	-6.07882617	1.03573857
C	0.23199871	-6.63486562	1.02114647
C	-0.65219872	-6.38075825	-0.03799345

C	-0.19204979	-5.58776688	-1.10245979
C	1.09763397	-5.06790345	-1.10799238
H	2.88620471	-3.66321992	1.93261051
H	4.92731021	-2.27973284	1.92281832
H	6.06940243	-3.97852485	-1.85149312
H	3.98286390	-5.30425552	-1.88146862
H	2.17008434	-6.26850817	1.87960219
H	-0.09587877	-7.25677272	1.84954979
H	-0.86564049	-5.35918126	-1.92433949
H	1.42264611	-4.44082008	-1.93404173
C	-5.27766438	-1.96475663	-0.02332721
C	-6.07885295	-1.51144217	1.03562686
C	-6.63489727	-0.23194207	1.02097349
C	-6.38079990	0.65220074	-0.03821269
C	-5.58781541	0.19200100	-1.10266146
C	-5.06794706	-1.09768084	-1.10813222
C	-4.58025348	-3.27651186	0.02154844
C	-3.74429326	-3.58763556	1.10644859
C	-2.96586096	-4.73983069	1.10093990
C	-3.02767162	-5.65445528	0.03636647
C	-3.90263864	-5.37064022	-1.02287561
C	-4.65237632	-4.19409979	-1.03749368
H	-6.26852844	-2.16998414	1.87952443
H	-7.25680214	0.09597317	1.84936352
H	-5.35923841	0.86555084	-1.92457724
H	-4.44086917	-1.42273354	-1.93416979
H	-3.66324142	-2.88607379	1.93256318
H	-2.27973219	-4.92716501	1.92288025
H	-3.97851475	-6.06947942	-1.85136784
H	-5.30426647	-3.98295774	-1.88145580
C	-3.27651601	4.58022408	0.02137436
C	-3.58770644	3.74430385	1.10628582
C	-4.73991001	2.96588381	1.10074318
C	-5.65447613	3.02766627	0.03611802
C	-5.37059651	3.90259638	-1.02313798
C	-4.19404781	4.65232107	-1.03771894
C	-1.96475444	5.27762432	-0.02345712

C	-1.51148185	6.07883189	1.03550117
C	-0.23198058	6.63487324	1.02089083
C	0.65220688	6.38075444	-0.03825383
C	0.19205004	5.58774916	-1.10270591
C	-1.09763255	5.06788300	-1.10822053
H	-2.88618944	3.66327132	1.93244042
H	-4.92729474	2.27978518	1.92269715
H	-6.06939179	3.97845132	-1.85166935
H	-3.98285474	5.30418180	-1.88169098
H	-2.17005878	6.26852532	1.87936746
H	0.09590174	7.25679277	1.84928285
H	0.86563374	5.35915469	-1.92458905
H	-1.42265059	4.44078851	-1.93425913
C	-6.81964987	2.08512967	-0.00093657
C	-8.12061558	2.48285283	-0.00054157
C	2.08513049	6.81961130	-0.00093051
C	2.48284749	8.12057970	-0.00052042
C	8.12062727	-2.48286169	-0.00040981
C	6.81966130	-2.08514038	-0.00082665
C	-2.48283457	-8.12058827	-0.00019582
C	-2.08511872	-6.81961865	-0.00065565
C	1.52332660	9.24933393	-0.19462944
C	1.56016510	10.36595211	0.65296581
C	0.58196543	9.26252388	-1.24158972
C	0.68352113	11.44080255	0.49688569
H	2.28769064	10.39589899	1.45921479
C	-0.28822846	10.32892923	-1.41909246
H	0.53802935	8.42447037	-1.92913712
C	-0.24970652	11.42572756	-0.54628730
H	0.74083375	12.27662420	1.18507677
H	-1.00781442	10.33753386	-2.23197849
C	3.90938983	8.51990098	0.19426475
C	4.50317687	9.46727298	-0.65222691
C	4.69701437	8.00377811	1.24101920
C	5.83077645	9.86854613	-0.49530309
H	3.91686342	9.89952756	-1.45822192
C	6.01455543	8.40159848	1.41933434

H	4.26483104	7.28374128	1.92785782
C	6.59588383	9.33348211	0.54762677
H	6.25057647	10.59441476	-1.18260472
H	6.61577391	8.00583169	2.23208498
C	8.51996263	-3.90939311	0.19438673
C	9.46743269	-4.50313847	-0.65202671
C	8.00375387	-4.69706105	1.24106790
C	9.86872272	-5.83073190	-0.49509749
H	9.89975251	-3.91679595	-1.45796507
C	8.40158843	-6.01459644	1.41938740
H	7.28363963	-4.26491591	1.92784907
C	9.33357402	-6.59588045	0.54775858
H	10.59467046	-6.25049466	-1.18233837
H	8.00575459	-6.61584482	2.23208330
C	9.24937621	-1.52332297	-0.19450619
C	10.36593084	-1.56007107	0.65317433
C	9.26261823	-0.58204631	-1.24153938
C	11.44077090	-0.68341190	0.49710598
H	10.39583554	-2.28753657	1.45947950
C	10.32901575	0.28816119	-1.41903149
H	8.42461214	-0.53818550	-1.92914959
C	11.42574888	0.24973404	-0.54614129
H	12.27654345	-0.74064846	1.18536292
H	10.33766346	1.00768480	-2.23197219
C	-1.52333693	-9.24935996	-0.19427439
C	-1.56026305	-10.36600318	0.65328641
C	-0.58190086	-9.26254976	-1.24116983
C	-0.68363978	-11.44087457	0.49723600
H	-2.28784182	-10.39595297	1.45948677
C	0.28827372	-10.32897432	-1.41864209
H	-0.53789252	-8.42448095	-1.92869361
C	0.24966073	-11.42579767	-0.54587128
H	-0.74102628	-12.27671400	1.18539935
H	1.00791461	-10.33757609	-2.23147958
C	-3.90938800	-8.51988066	0.19460537
C	-4.50322617	-9.46719102	-0.65191709
C	-4.69696090	-8.00378991	1.24141274

C	-5.83083308	-9.86843316	-0.49497249
H	-3.91694846	-9.89942098	-1.45795174
C	-6.01450875	-8.40158086	1.41974938
H	-4.26473188	-7.28380013	1.92827232
C	-6.59589098	-9.33340088	0.54801023
H	-6.25067797	-10.59425246	-1.18229868
H	-6.61569094	-8.00583957	2.23253920
C	-9.24936779	1.52331577	-0.19461140
C	-10.36594809	1.56012960	0.65303346
C	-9.26258934	0.58197046	-1.24158380
C	-11.44079307	0.68347240	0.49698928
H	-10.39586915	2.28764621	1.45929174
C	-10.32899088	-0.28823654	-1.41905152
H	-8.42456398	0.53805562	-1.92916700
C	-11.42575031	-0.24974108	-0.54619718
H	-12.27658536	0.74076288	1.18521782
H	-10.33762160	-1.00781225	-2.23194631
C	-8.51994305	3.90939639	0.19419650
C	-9.46737443	4.50312724	-0.65226949
C	-8.00376562	4.69708685	1.24087566
C	-9.86865525	5.83072994	-0.49539328
H	-9.89967070	3.91676592	-1.45820698
C	-8.40159187	6.01463205	1.41914281
H	-7.28368207	4.26495195	1.92769553
C	-9.33353698	6.59590172	0.54746129
H	-10.59457282	6.25048164	-1.18267275
H	-8.00578242	6.61589943	2.23183652
O	-1.14865847	12.42174143	-0.80204747
O	7.89787609	9.65683671	0.80415567
O	12.42176037	1.14869118	-0.80189702
O	9.65693466	-7.89787064	0.80428595
O	1.14860121	-12.42182917	-0.80159845
O	-7.89788551	-9.65673040	0.80456270
O	-9.65689259	7.89790329	0.80393924
O	-12.42176371	-1.14870375	-0.80192510
C	-8.53697282	-10.59087604	-0.04932888
H	-9.55569866	-10.69499352	0.32904269

H	-8.57105543	-10.23316021	-1.08708739
H	-8.03946064	-11.56972880	-0.02344596
C	1.15691666	-13.55269492	0.05354868
H	1.94356254	-14.20862303	-0.32427752
H	1.38527129	-13.27390794	1.09094759
H	0.19741247	-14.08661206	0.02848431
C	-13.55257019	-1.15713116	0.05329826
H	-14.20849671	-1.94376805	-0.32454969
H	-13.27370516	-1.38556395	1.09065913
H	-14.08652358	-0.19764396	0.02835173
C	-10.59115444	8.53688074	-0.04990827
H	-10.69526366	9.55563818	0.32838049
H	-10.23355440	8.57087895	-1.08770932
H	-11.56998736	8.03933776	-0.02387060
C	-1.15706002	13.55258548	0.05312690
H	-1.94369440	14.20850492	-0.32473839
H	-1.38548127	13.27376802	1.09050306
H	-0.19756658	14.08652580	0.02814330
C	8.53690953	10.59104459	-0.04970869
H	9.55564506	10.69517026	0.32863445
H	8.57096717	10.23338358	-1.08748685
H	8.03937105	11.56988211	-0.02375803
C	10.59124514	-8.53685836	-0.04950090
H	10.69535817	-9.55560108	0.32882626
H	10.23368955	-8.57089768	-1.08731594
H	11.57006716	-8.03929548	-0.02343818
C	13.55254003	1.15718748	0.05336105
H	14.20846872	1.94380808	-0.32451706
H	13.27363991	1.38568377	1.09069853
H	14.08650596	0.19770520	0.02849307

TPE-1

C	3.30116904	2.69505230	1.36118894
C	2.15846911	1.91357023	1.19780821
C	1.24813821	2.17169924	0.15844998
C	1.51304727	3.25487968	-0.69854402
C	2.66114751	4.03007791	-0.54265011

H	3.98796496	2.47859482	2.17553837
H	1.96243903	1.09284269	1.88076267
H	0.81119697	3.48442541	-1.49549671
H	2.85057748	4.85437293	-1.22561451
C	-3.56118246	3.75370838	-0.48862824
C	-2.66114965	4.03007649	0.54264950
C	-1.51304857	3.25487939	0.69854228
C	-1.24814016	2.17169803	-0.15845080
C	-2.15847264	1.91356736	-1.19780730
C	-3.30117323	2.69504854	-1.36118712
H	-2.85057911	4.85437207	1.22561339
H	-0.81119746	3.48442638	1.49549383
H	-1.96244309	1.09283961	-1.88076160
H	-3.98797013	2.47858999	-2.17553547
C	0.00000043	-0.00435570	-0.00000059
C	-0.00000062	1.36386877	-0.00000062
C	1.25240162	-0.80759579	-0.12514394
C	1.48893353	-1.90926670	0.70992884
C	2.21452987	-0.52869275	-1.11576939
C	2.64295347	-2.68674914	0.59765180
H	0.75779425	-2.16405861	1.47193672
C	3.36032919	-1.29886835	-1.24979279
H	2.05381498	0.30515064	-1.79166626
C	3.58848951	-2.38240752	-0.38850841
H	2.78872508	-3.52083280	1.27483017
H	4.09515087	-1.08420438	-2.01961590
C	-1.25240022	-0.80759672	0.12514290
C	-1.48893260	-1.90926695	-0.70993063
C	-2.21452745	-0.52869461	1.11576953
C	-2.64295205	-2.68675003	-0.59765273
H	-0.75779379	-2.16405822	-1.47193921
C	-3.36032644	-1.29887071	1.24979357
H	-2.05381206	0.30514872	1.79166646
C	-3.58848721	-2.38240940	0.38850871
H	-2.78872394	-3.52083341	-1.27483133
H	-4.09514746	-1.08420747	2.01961752
O	4.74625959	-3.07545030	-0.59839565

O	-4.74625679	-3.07545280	0.59839678
C	5.02693560	-4.18217112	0.24247715
H	5.98594863	-4.57968900	-0.09516305
H	5.11066521	-3.87976169	1.29490653
H	4.25973945	-4.96300113	0.15350838
C	-5.02693340	-4.18217338	-0.24247612
H	-5.98594594	-4.57969169	0.09516505
H	-5.11066431	-3.87976357	-1.29490527
H	-4.25973689	-4.96300317	-0.15350849
H	-4.45297323	4.36187489	-0.61529982
C	3.56117882	3.75371142	0.48862940
H	4.45296915	4.36187845	0.61530151

[2]OTPE-1

C	-7.07000887	-3.29316121	2.60756063
C	-6.63806757	-2.09943856	2.03166437
C	-5.65023769	-2.09464936	1.03186068
C	-5.09521777	-3.32745900	0.64472080
C	-5.53419272	-4.52265460	1.21238635
H	-7.83206930	-3.27084645	3.38246256
H	-7.06616688	-1.15619386	2.35651416
H	-4.31562232	-3.34386471	-0.11184793
H	-5.09873405	-5.46431248	0.88771558
C	-0.82126890	-0.50826535	0.33682754
C	-1.50032237	-0.91242145	1.49957849
C	-2.88780563	-1.00741784	1.52883326
C	-3.66656630	-0.68138415	0.40415553
C	-2.98682383	-0.28734007	-0.76130943
C	-1.59890148	-0.20322668	-0.79393582
H	-0.93086980	-1.18636285	2.38345524
H	-3.38054680	-1.34408332	2.43665219
H	-3.55863530	-0.03838870	-1.64976395
H	-1.10976730	0.12582428	-1.70657065
C	-5.99571481	0.15325096	-0.03758789
C	-5.15327465	-0.81566552	0.43713674
C	-7.45036195	-0.09037781	-0.26807482
C	-8.41302189	0.83820986	0.15414159

C	-7.90941972	-1.22700005	-0.96265756
C	-9.77698990	0.64084912	-0.06818428
H	-8.09182929	1.73533867	0.67579802
C	-9.25987101	-1.43221417	-1.20352407
H	-7.18994012	-1.95640924	-1.32074494
C	-10.20785792	-0.50206676	-0.75175539
H	-10.48522909	1.38010542	0.28876095
H	-9.60777960	-2.30611728	-1.74567177
C	-5.52940403	1.53373090	-0.36216906
C	-5.92252642	2.16756712	-1.54994328
C	-4.72685226	2.27212280	0.52988609
C	-5.51470984	3.46512230	-1.86447004
H	-6.55748732	1.63351535	-2.25118702
C	-4.32353244	3.56695693	0.23910032
H	-4.42078426	1.81890648	1.46740612
C	-4.70874093	4.17356670	-0.96575389
H	-5.83274415	3.90886012	-2.80119304
H	-3.71102133	4.13427687	0.93309798
O	-11.51109073	-0.79602304	-1.03451724
O	-4.25770402	5.44763488	-1.16086417
C	-12.51184603	0.11094793	-0.60257877
H	-13.46307171	-0.31540627	-0.92680103
H	-12.51670287	0.21769668	0.49042484
H	-12.38466727	1.10165345	-1.05923662
C	-4.61707439	6.10937595	-2.36237393
H	-4.15384685	7.09656182	-2.31111349
H	-4.23924279	5.57755191	-3.24580195
H	-5.70569097	6.22443855	-2.45120397
C	-6.52423842	-4.51110195	2.19709606
H	-6.86221324	-5.44178069	2.64522019
C	0.65776080	-0.41630148	0.30335736
C	1.38710338	0.01084090	1.42705826
C	1.38489297	-0.74465150	-0.85391498
C	2.77433664	0.10572568	1.39348869
H	0.85673159	0.30239932	2.32943623
C	2.77312746	-0.66108072	-0.88357215
H	0.85650016	-1.09230082	-1.73728228

C	3.50297175	-0.24430624	0.24271732
H	3.30688167	0.45977081	2.27168655
H	3.30531474	-0.92861017	-1.79106129
C	4.99040453	-0.11419668	0.20853609
C	5.80358849	-1.10224673	-0.27750831
C	5.51833941	1.17518287	0.74510275
C	6.58046657	1.21133911	1.67026309
C	4.93298906	2.39883648	0.38900057
C	7.04317741	2.40885105	2.19497298
H	7.04416592	0.28078486	1.98177739
C	5.39423295	3.61426012	0.89825600
H	4.09887657	2.40604842	-0.30703453
C	6.45741270	3.62365288	1.80826324
H	7.85690930	2.43087241	2.91334899
H	4.91714423	4.53594458	0.58469660
C	5.30945034	-2.48859873	-0.54161298
C	5.61269251	-3.13881664	-1.75130536
C	4.58138467	-3.20054623	0.42699271
C	5.17497596	-4.43926336	-1.99671568
H	6.19233829	-2.61273994	-2.50468825
C	4.15313852	-4.50543144	0.18711924
H	4.35346851	-2.72240345	1.37459518
C	4.44283650	-5.12918306	-1.02790968
H	5.40958359	-4.91611615	-2.94509596
H	3.59482204	-5.03698486	0.95349729
H	4.10719947	-6.14570910	-1.21566269
C	7.24833319	-0.88436608	-0.58189136
C	8.21780491	-1.81744481	-0.18608928
C	7.68841694	0.22921455	-1.32486535
C	9.57166177	-1.64660062	-0.48125876
H	7.91099360	-2.69799461	0.37133622
C	9.02776678	0.40795058	-1.63718616
H	6.96218953	0.96125176	-1.66341527
C	9.98399912	-0.52648706	-1.21191821
H	10.28597268	-2.38906139	-0.14364094
H	9.36066531	1.26379917	-2.21633781
O	6.98593758	4.74647345	2.37804065

O	11.27536935	-0.25904948	-1.56641041
C	6.42834632	6.00210399	2.02683342
H	6.99344698	6.74866043	2.58813371
H	6.53023627	6.20361686	0.95208384
H	5.36785003	6.06600310	2.30498340
C	12.28324050	-1.17213067	-1.16488514
H	13.22300336	-0.76823891	-1.54628017
H	12.34194986	-1.25474603	-0.07136005
H	12.11830728	-2.17046957	-1.59182946

[2]CHPE

C	-5.76065428	-3.01443142	-1.03758973
C	-6.82196312	-2.10730886	-0.99522810
C	-6.95266466	-1.19862119	0.06591145
C	-6.04848394	-1.31184021	1.13439352
C	-5.00799706	-2.23125792	1.10571278
C	-4.80314400	-3.06011820	-0.01128615
H	-5.65596508	-3.67164999	-1.89738601
H	-7.52711324	-2.06752164	-1.82128464
H	-6.12213960	-0.62049376	1.96954894
H	-4.28357550	-2.23995854	1.91512800
C	-3.50331717	-3.76736737	-0.13749500
C	-2.86510187	-4.36296273	0.96463457
C	-2.76656906	-3.66313449	-1.32880303
C	-1.51832421	-4.71076035	0.91669298
H	-3.42299865	-4.51985051	1.88424871
C	-1.41679270	-3.99747621	-1.37174116
H	-3.22683604	-3.20676208	-2.20082868
C	-0.74092286	-4.46416505	-0.23009205
H	-1.05366845	-5.14197997	1.79917178
H	-0.85652001	-3.78732051	-2.27782152
C	0.74396189	-4.47215511	-0.19784317
C	1.52245814	-4.61376159	-1.36155748
C	1.42093041	-4.12366043	0.98460770
C	2.87267226	-4.27546627	-1.37305533
H	1.05651262	-4.95347584	-2.28253620
C	2.77318568	-3.79844599	0.97657999

H	0.86025224	-3.99632573	1.90566366
C	3.51306957	-3.79382422	-0.21759397
H	3.43134259	-4.34864558	-2.30262054
H	3.23365373	-3.43115268	1.88950300
C	4.81658966	-3.08432088	-0.26883100
C	5.75384006	-3.12087125	0.77697787
C	5.04043402	-2.16517208	-1.30953440
C	6.80575648	-2.20423131	0.83676884
H	5.63595472	-3.84794203	1.57668124
C	6.06987011	-1.23638047	-1.23527932
H	4.33380466	-2.11020190	-2.13273550
C	6.94528587	-1.20231769	-0.13661859
H	7.49053476	-2.22588613	1.68028010
H	6.15267048	-0.47185735	-2.00324905
C	-5.32677746	2.27337924	-1.71116817
C	-6.38450499	1.39254754	-1.52803359
C	-6.98285549	1.22059732	-0.26920259
C	-6.54393101	2.05066625	0.77217579
C	-5.45470479	2.90627808	0.59816165
C	-4.77671601	2.98803177	-0.63034291
H	-4.88704869	2.36616253	-2.69962050
H	-6.72076919	0.78488655	-2.36448035
H	-7.00622486	1.96756896	1.75231083
H	-5.07444375	3.44833214	1.45943294
C	-3.43617514	3.61944811	-0.73921333
C	-2.97233149	4.61916251	0.13595951
C	-2.50353558	3.08851469	-1.64826299
C	-1.62661446	4.98355971	0.17497626
H	-3.66674349	5.10228064	0.81817868
C	-1.16743545	3.45964943	-1.61902361
H	-2.80325848	2.29626388	-2.32597176
C	-0.68149835	4.37522621	-0.66980208
H	-1.30229429	5.73529303	0.89027838
H	-0.46818168	2.94987259	-2.27459418
C	0.78739543	4.47989410	-0.48479224
C	1.67282641	4.33964775	-1.56819530
C	1.34559032	4.47748102	0.80542348

C	3.01488912	4.03415722	-1.36698597
H	1.28981630	4.39869078	-2.58340073
C	2.68997649	4.17835496	1.00635741
H	0.69858549	4.60950892	1.66840530
C	3.53503343	3.86125575	-0.07214653
H	3.64355405	3.82529639	-2.22810311
H	3.07201849	4.11834126	2.02185736
C	4.81475514	3.13429036	0.12545556
C	4.87667453	2.15497882	1.13366527
C	5.89766091	3.20944027	-0.76741922
C	5.89922283	1.21802974	1.16317862
H	4.05623420	2.06081702	1.83854075
C	6.93691714	2.27744348	-0.72540826
H	5.90954518	3.98046727	-1.53378193
C	6.92634328	1.22478923	0.20406017
H	5.86197944	0.41622204	1.89534623
H	7.73696223	2.33246937	-1.45857477
C	7.80361078	0.01281460	0.07583360
C	-7.84421275	0.01236173	-0.01467115
C	-9.19282997	0.01222570	0.12321715
C	9.16103679	0.01195416	0.14746586
C	-9.95732752	-1.22551823	0.46573767
C	-9.58142144	-2.07919119	1.51983449
C	-11.11237615	-1.56117921	-0.25530777
C	-10.31343466	-3.21874365	1.82402239
H	-8.70671060	-1.84032109	2.11488239
C	-11.85248863	-2.70971523	0.02882402
H	-11.44030713	-0.91299349	-1.06308618
C	-11.45262982	-3.54818994	1.07614364
H	-10.02383902	-3.87017568	2.64280088
H	-12.73159201	-2.93486196	-0.56440230
C	-10.01111829	1.25083391	-0.04854943
C	-9.86427303	2.10996158	-1.15361186
C	-10.98773432	1.58394259	0.90140944
C	-10.64145068	3.25214879	-1.29078498
H	-9.13678639	1.87324535	-1.92209112
C	-11.76855001	2.73466139	0.78561964

H	-11.13901038	0.93213520	1.75719847
C	-11.59662138	3.57865605	-0.31802519
H	-10.52952450	3.90756347	-2.14899329
H	-12.50230131	2.95733840	1.55207390
C	9.96838415	-1.20874090	-0.14613062
C	9.73621711	-2.00510111	-1.28416646
C	11.01841909	-1.58836916	0.70288381
C	10.50269956	-3.13133517	-1.54808471
H	8.94687436	-1.72938650	-1.97544405
C	11.79094003	-2.72481992	0.45887922
H	11.23511294	-0.98600100	1.58051769
C	11.53385852	-3.50553262	-0.67435471
H	10.32492950	-3.73770050	-2.43088920
H	12.58394452	-2.98598221	1.15054210
C	9.93539323	1.22971724	0.52938435
C	9.58537519	2.02111235	1.64045748
C	11.07098613	1.60967512	-0.20083690
C	10.32284676	3.14305955	1.99082431
H	8.72523588	1.74492285	2.24132992
C	11.81664756	2.74209620	0.13043642
H	11.37835418	1.01060545	-1.05331906
C	11.44267350	3.51776019	1.23415114
H	10.05380659	3.74566330	2.85285583
H	12.67981112	3.00376158	-0.47116479
O	12.09876995	4.63769043	1.65753110
O	12.22700822	-4.63006013	-1.01928689
O	-12.10081606	-4.69009251	1.45087130
O	-12.30693664	4.72323945	-0.54155814
C	-13.25902769	-5.07210257	0.72728976
H	-13.03265418	-5.25426697	-0.33175416
H	-13.60646393	-5.99985457	1.18582909
H	-14.05025832	-4.31390301	0.79999777
C	-13.28646526	5.10148860	0.41154313
H	-12.84223075	5.27733826	1.40035076
H	-13.72094587	6.03210009	0.04155938
H	-14.07656489	4.34408677	0.50251902
C	13.23900214	5.06295129	0.92939370

H	12.98686288	5.30582209	-0.11147902
H	13.59719200	5.96313199	1.43241554
H	14.03184650	4.30304683	0.93884702
C	13.27999173	-5.05589666	-0.17014407
H	12.91577946	-5.29170829	0.83867014
H	13.68607425	-5.96043568	-0.62683778
H	14.07285192	-4.29938404	-0.09796346

[3]CHPE

C	-8.73848346	-4.22257241	0.37416224
C	-8.47798077	-5.58997239	0.42186060
C	-7.52347101	-6.18072576	-0.42398203
C	-6.89767367	-5.34726620	-1.36773014
C	-7.15765745	-3.98361541	-1.41586500
C	-8.05398211	-3.37676947	-0.51708329
H	-9.47031787	-3.80356879	1.05925490
H	-8.99528911	-6.20667365	1.15053045
H	-6.15291448	-5.76856966	-2.03683511
H	-6.59742797	-3.36922185	-2.11403722
C	-8.14748058	-1.89819863	-0.44243209
C	-7.86784401	-1.08241061	-1.55318739
C	-8.38969702	-1.24728384	0.78061627
C	-7.73143852	0.29516781	-1.42511003
H	-7.72147692	-1.53498251	-2.52960604
C	-8.27163065	0.13275326	0.90480007
H	-8.61505679	-1.83455701	1.66590300
C	-7.88654603	0.93649007	-0.18294541
H	-7.43887214	0.87406702	-2.29603446
H	-8.45185111	0.58888401	1.87394864
C	-7.52852074	2.36582279	-0.01310533
C	-6.99524263	2.82843324	1.20352112
C	-7.58800074	3.28663709	-1.07431261
C	-6.48269621	4.11359046	1.32973911
H	-6.92685494	2.15379609	2.05145724
C	-7.05974050	4.56833127	-0.95271418
H	-8.03066444	2.98936284	-2.02078390
C	-6.45721463	5.00305916	0.24124567

H	-6.06999262	4.42287427	2.28552986
H	-7.06696811	5.22352018	-1.81913414
C	-5.72634253	6.29114124	0.31738220
C	-6.07076284	7.40653517	-0.46661825
C	-4.58034951	6.40269741	1.12552264
C	-5.28231533	8.55488346	-0.48019130
H	-6.96446161	7.37442078	-1.08394679
C	-3.79258261	7.54618240	1.10940614
H	-4.26454763	5.55739867	1.72931502
C	-4.11131548	8.64541489	0.29244035
H	-5.56460379	9.38836287	-1.11608858
H	-2.88897082	7.57598582	1.71122176
C	-3.44588147	-6.67149818	0.52180418
C	-4.83397152	-6.70203198	0.55104031
C	-5.56055294	-7.69032388	-0.13913829
C	-4.82318589	-8.67673589	-0.81862104
C	-3.42862037	-8.65457601	-0.83676892
C	-2.71324003	-7.63328656	-0.19256979
H	-2.91463484	-5.88797824	1.05551541
H	-5.36953768	-5.93197102	1.09756152
H	-5.35027415	-9.45075620	-1.36745223
H	-2.88926005	-9.40645919	-1.40749835
C	-1.23811808	-7.48682856	-0.30259673
C	-0.33576211	-8.50231266	0.04940966
C	-0.71104798	-6.26266399	-0.74572510
C	1.04258584	-8.28410182	0.00485175
H	-0.71779920	-9.45964791	0.39491320
C	0.66079333	-6.05490636	-0.81670244
H	-1.39181448	-5.46777208	-1.03782258
C	1.56604494	-7.05370481	-0.42211321
H	1.72178926	-9.07870120	0.30362204
H	1.04265356	-5.09126167	-1.14247841
C	4.57382624	5.95434903	-0.12557111
C	4.14846842	6.67744190	1.00275135
C	3.82390394	6.11199611	-1.30480839
C	2.99169243	7.45075095	0.97483457
H	4.71879012	6.61873789	1.92550788

C	2.67817619	6.89733759	-1.33723803
H	4.11142678	5.56996795	-2.20064189
C	2.20662604	7.55443947	-0.18721280
H	2.66646315	7.94244012	1.88723426
H	2.12716141	6.98423342	-2.26906720
C	0.88996675	8.23687238	-0.17715452
C	-0.15799458	7.75984258	-0.98509985
C	0.60039319	9.31164180	0.68221223
C	-1.43645683	8.29582511	-0.90245165
H	0.01453954	6.91573010	-1.64585738
C	-0.68130576	9.85118579	0.76302597
H	1.38744111	9.73000282	1.30374206
C	-1.73704936	9.34436569	-0.01477679
H	-2.22977720	7.87041052	-1.51003429
H	-0.87442836	10.66596074	1.45406342
C	-3.15396016	9.78798641	0.16747475
C	-7.05107480	-7.58729085	-0.22590449
C	-7.89918437	-8.65421320	-0.10883913
C	-3.53508002	11.10080288	0.21297158
C	-9.34381752	-8.56292193	-0.46800481
C	-9.77183095	-7.96533486	-1.67033823
C	-10.33028668	-9.11336205	0.36396520
C	-11.11484815	-7.90469697	-2.01109719
H	-9.03347036	-7.54923713	-2.34822474
C	-11.68708825	-9.04963916	0.04237981
H	-10.03365584	-9.59733401	1.29012334
C	-12.08679975	-8.44110993	-1.15323902
H	-11.43870076	-7.45041873	-2.94242160
H	-12.41442735	-9.47702016	0.72339908
C	-7.44932556	-9.98480204	0.39377818
C	-6.67378931	-10.10865015	1.56362050
C	-7.82784879	-11.16825859	-0.25689814
C	-6.28176433	-11.34922054	2.04417933
H	-6.38099421	-9.21337274	2.10299133
C	-7.43099422	-12.42423639	0.20578040
H	-8.44159386	-11.10897311	-1.15128956
C	-6.65154958	-12.51969812	1.36454806

H	-5.69100667	-11.44020992	2.95048544
H	-7.73649550	-13.31097839	-0.33810876
C	-4.89162915	11.52206771	0.66859353
C	-5.46924637	11.00939577	1.84716400
C	-5.62345560	12.48578188	-0.04092435
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TPE-2

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[2]OHPE-2

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H	-16.68186980	-1.41319854	-1.04897131
H	-16.46232919	-3.04565338	-0.35070452

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