Supporting Information

Two-Step Template Method for Synthesis of Axis-Length-Controlled Porphyrin-Containing Hollow Structures

Yusuke Chiba,[a,b] Yuki Oka,[c] Hiroshi Masai,[c] Wakana Matsuda,[a] Tetsuaki Fujihara,[a] Yasushi Tsuji,[a] and Jun Terao*[c,d]

[a]*Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan*

[b]*Present address: Graduate School of Pure and Applied Sciences and Tsukuba Research Center for Energy Materials Science (TREMS), University of Tsukuba, 1-1-1 Tennodai,Tsukuba, Ibaraki 305-8571*

[c]*Graduate School of Arts and Sciences, The University of Tokyo, Meguro-ku, Tokyo 153-8902, Japan*

[d]*School of Science, The University of Tokyo, Hongo, Bunkyo-ku, Tokyo, 113-0033, Japan*

* Correspondence to: Jun Terao

cterao@mail.ecc.u-tokyo.ac.jp

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1. General Comments

1.1 Materials

Solvents were purified as follows: reaction solvents were degassed through freeze-pump-thaw (three times), before use. Dry toluene (water content : < 10 ppm), THF (water content : < 10 ppm), and DMF (water content : < 50 ppm) were purchased from Kanto Chemical and further purified by passage through activated alumina under positive argon or nitrogene pressure as described by Grubbs *et al.*[1] All other reagents and solvents were purchased from commercial sources (FUJIFILM Wako Pure Chemical Corporation or Tokyo Chemical Industry Co., Ltd., Grade : Extra Pure) and used without further purification. A fluorene derivative **S1**,[2] porphyrin derivative **S4**,[3] $\mathbf{T_1}$[4] and **S10**,[5] were prepared by the reported procedures. $\mathbf{ZnP_2}$ was synthesized according to previous methods.[6]

1.2 Experimental

NMR Spectroscopy

^{1}H NMR spectra were measured on a Bruker AVANCE-500 spectrometer. The ^{1}H NMR chemical shifts are reported relative to tetramethylsilane (TMS, 0.00 ppm) or residual protonated solvents (7.26 ppm) in $CDCl_3$, or (5.32 ppm) in CD_2Cl_2. The ^{13}C NMR chemical shifts are reported relative to tetramethylsilane (TMS, 0.00 ppm), residual protonated $^{13}CDCl_3$ (77.16 ppm), or $^{13}CD_2Cl_2$ (53.84 ppm).

Preparative recycling gel permeation chromatography (GPC)

Preparative recycling GPC was performed with a JAI LC9104 System equipped with JAIGEL-1H and 2H columns, a JAI UV DETECTOR 310, and a JAI RI DETECTOR RI-5, a JAI LC9130NEXT System equipped with JAIGEL-2H and 2.5H columns, a JAI UV DETECTOR 370NEXT, and a JAI RI DETECTOR RI 700NEXT, a JAI LC9140 System equipped with JAIGEL-2.5H and -3H columns, a JAI UV DETECTOR 310, and a JAI RI DETECTOR RI-5.

Mass Spectroscopy (MS)

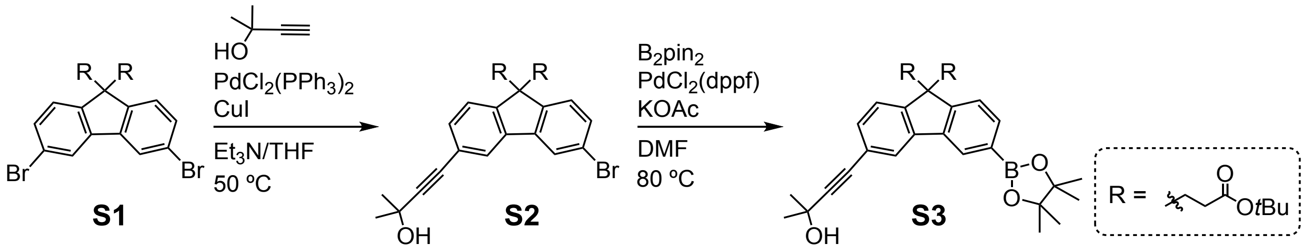
Matrix assisted laser desorption/ionization time-of-flight (MALDI-TOF) mass spectra were obtained with α-cyano-4-hydroxycinnamic acid (CHCA) and *trans*-2-[3-(4-*t*-butyl-phenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) as a matrix on Thermo Fisher Scientific LTQ orbitrapXL. ESI mass spectra were obtained on Thermo Fisher Scientific EXACTIVE and SHIMADZU Axima Performance.

Absorption spectroscopy

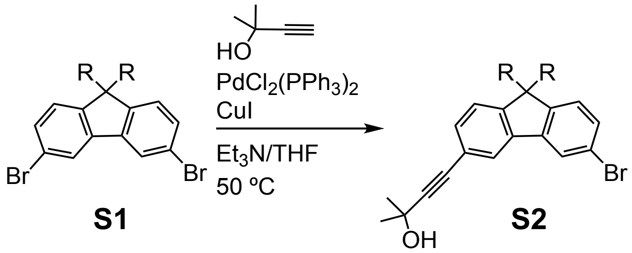
Absorption spectra were measured with SHIMADZU UV-2600 spectrophotometer. For solution measurements, concentrations of 10^{-6} M solutions were used.

2. Synthetic Procedures

Scheme S1. Synthesis of fluorene S3 from S1



2.1 Synthesis of S2



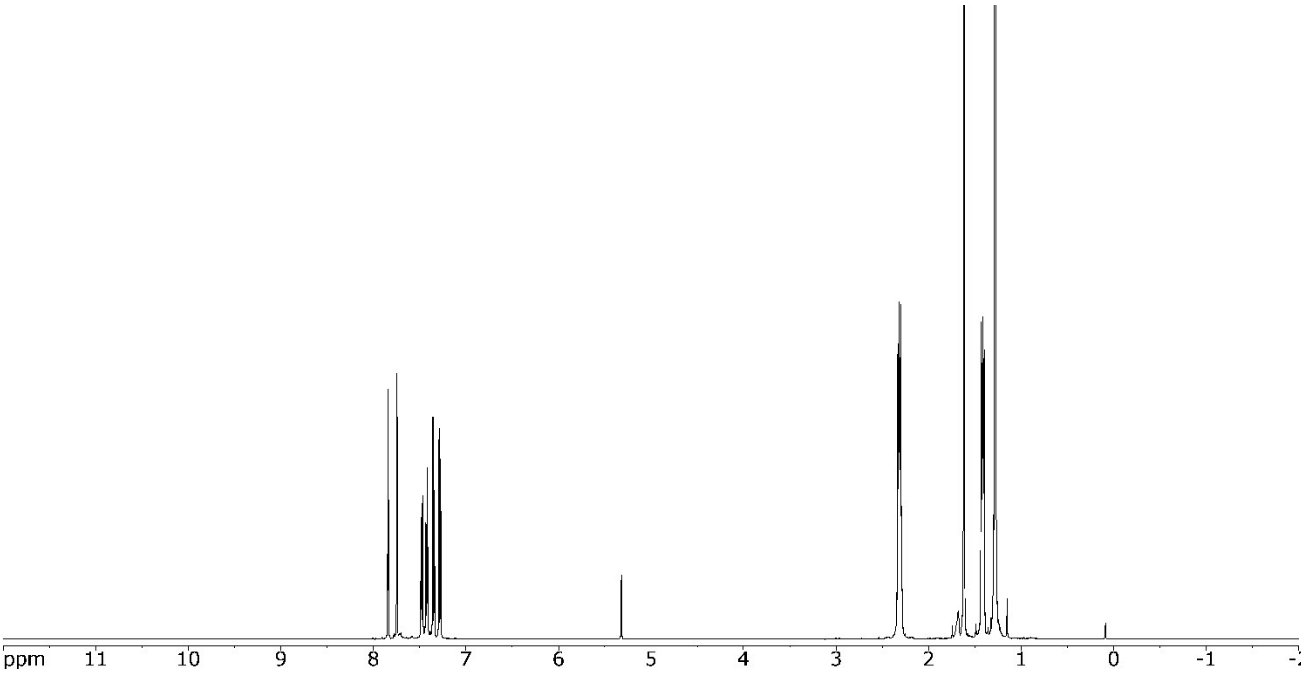
S1 (4.69 g, 8.08 mmol), $PdCl_2(PPh_3)_2$ (283 mg, 0.404 mmol), and CuI (38.5 mg, 0.202 mmol) were dissolved in degassed THF / Et_3N (4 / 1, v / v, 330 mL) under Ar. 2-Methyl-3-butyn-2-ol (0.706 mL, 7.27 mmol) was added. The solution was stirred at 50 ºC overnight, and passed through the Celite pad. The solvent was evaporated, after which the residue was purified by silica gel column chromatography (EtOAc / hexane = 1 / 4, v / v) to yield **S2** (1.62 g, 34%) as a yellow solid. Unreacted **S1** (2.50 g, 4.31 mmol) was recovered as a pure solid during the above purification process.

HR-MS (ESI-MS) (m/z) 605.1873 ([**S1** +Na]$^+$, $C_{32}H_{39}BrNaO_5$, calcd. 605.1879)

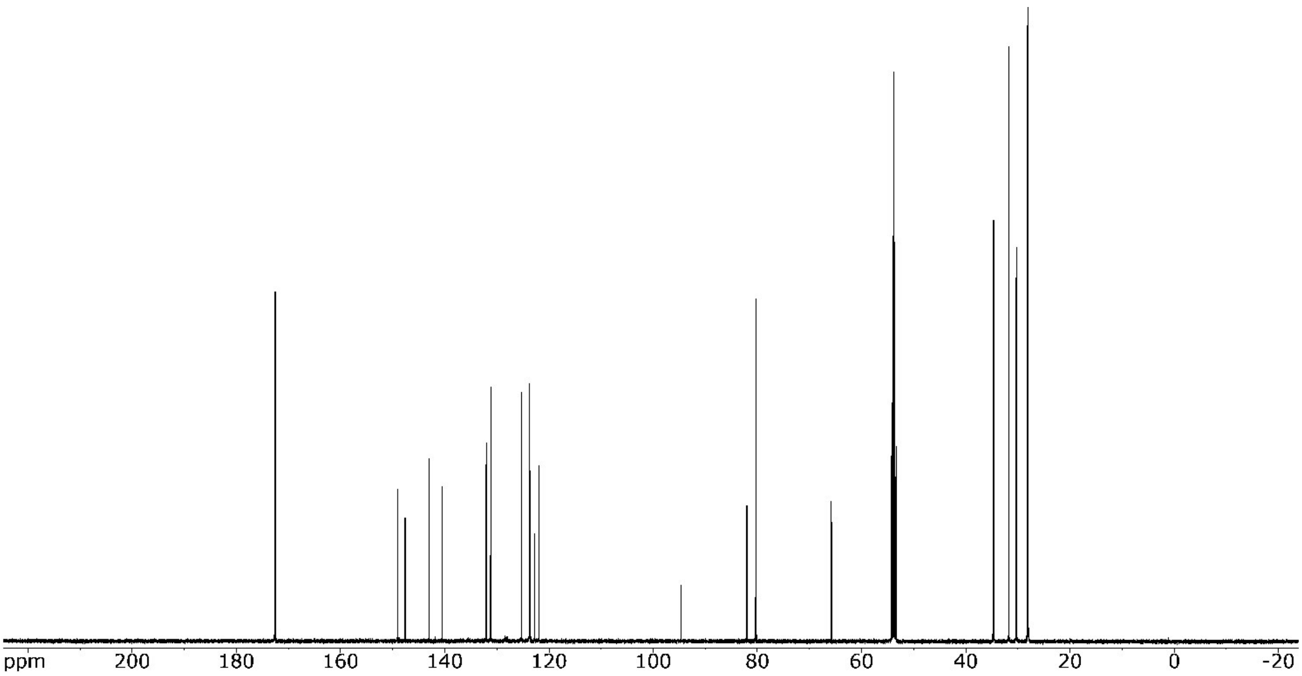
^{1}H NMR (500 MHz, CD_2Cl_2, r. t.): δ 7.84 (d, *J* = 1.5 Hz, 1H, Ar-*H*), 7.74 (s, 1H, Ar-*H*), 7.48 (dd, *J* = 8.0, 1.6 Hz, 1H, Ar-*H*), 7.42 (dd, *J* = 7.8, 1.1 Hz, 1H, Ar-*H*), 7.35 (d, *J* = 7.8 Hz, 1H, Ar-*H*), 7.28 (d, *J* = 8.0 Hz, 1H, Ar-*H*), 2.32 (t, *J* = 8.3 Hz, 4H, -CH_2CH$_2$COO^{t}Bu), 1.62 (s, 6H, -C(CH_3)$_2$OH), 1.42 (t, *J* = 8.3 Hz, 4H, -CH$_2$CH_2COO^{t}Bu), 1.28 (s, 18H, -COOC(CH_3)$_3$).

^{13}C NMR (126 MHz, CD_2Cl_2, r. t.): δ 172.5, 149.1, 147.6, 143.0, 140.5, 132.0, 131.2, 125.3, 123.8, 123.69, 123.66, 122.8, 121.9, 94.7, 82.0, 80.3, 65.8, 54.12, 34.7, 31.8, 30.3, 28.1.

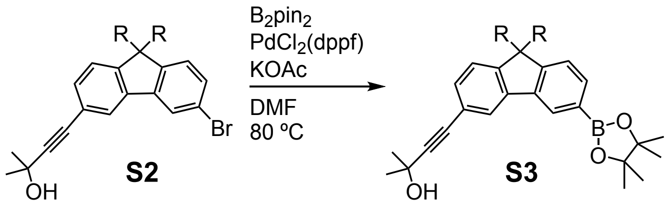
^{1}H NMR spectrum of **S2**



^{13}C NMR spectrum of **S2**



2.2 Synthesis of S3



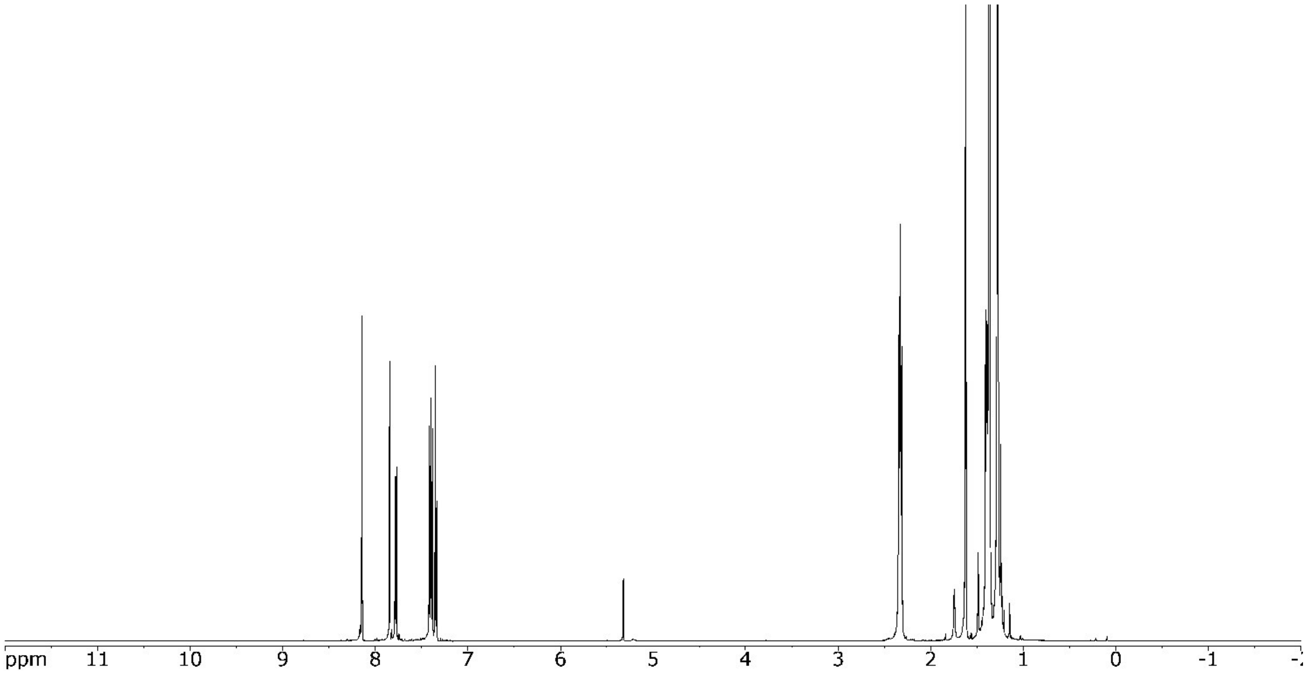
S2 (1.34 g, 2.31 mmol), bis(pinacolato)diboron (0.706 g, 2.78 mmol), $PdCl_2$(dppf) (188 mg, 0.231 mmol), and KOAc (302 mg, 3.08 mmol) were dissolved in dry DMF (54.0 mL) under Ar. The solution was stirred at 80 ºC overnight, after which the solvent was removed under vacuum. The residue was purified by silica gel column chromatography (EtOAc / hexane = 1 / 4, v / v) and GPC with $CHCl_3$ as an eluent to yield **S3** (1.01 g, 69%) as a white solid.

HR-MS (ESI-MS) (m/z) 653.3621 ([**S3**+Na]$^+$, $C_{38}H_{51}BNaO_7$, calcd. 653.3626)

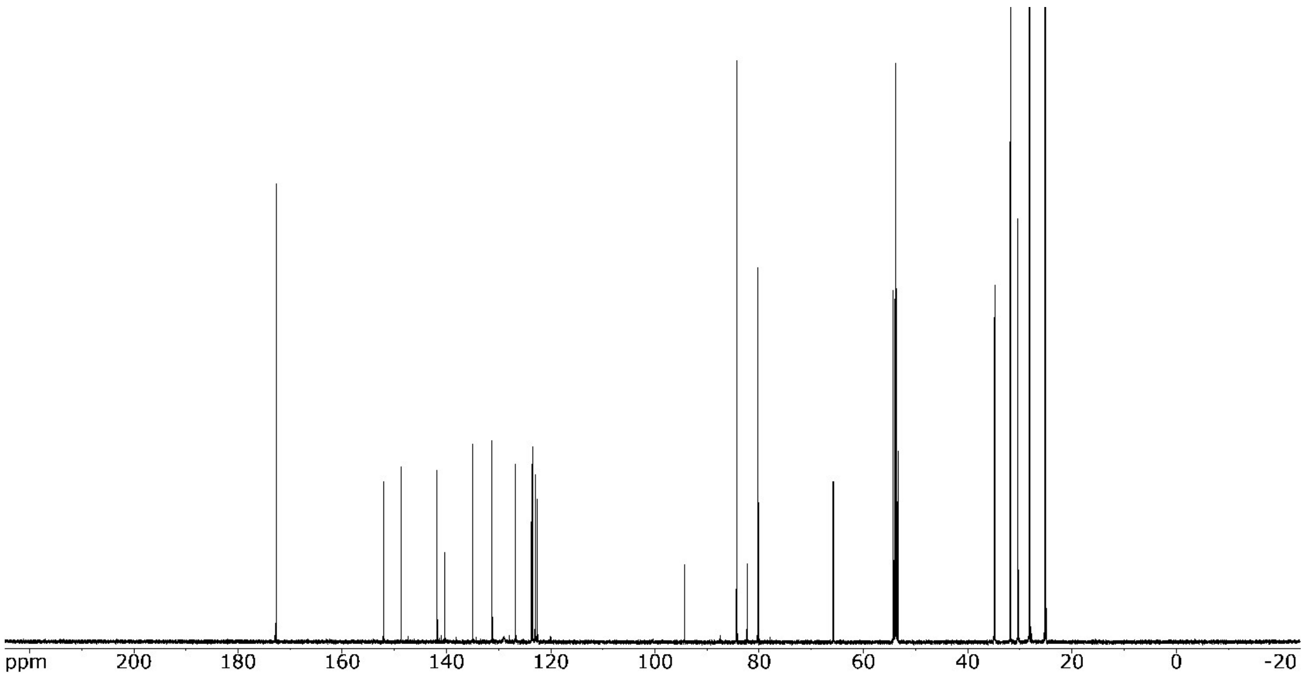
^{1}H NMR (500 MHz, CD_2Cl_2, r. t.): δ 8.14 (s, 1H, Ar-*H*), 7.84 (s, 1H, Ar-*H*), 7.78 (d, *J* = 7.5 Hz, 1H, Ar-*H*), 7.42-7.38 (m, 2H, Ar-*H*), 7.35 (s, 1H, Ar-*H*), 2.33 (t, *J* = 8.3 Hz, 4H, -C*H*$_2$CH$_2$COO^{t}Bu), 1.62 (s, 6H, -C(C*H*$_3$)$_2$OH), 1.40 (several peaks, 4H+12H, -CH$_2$C*H*$_2$COO^{t}Bu and B(pin)-*H),* 1.28 (s, 18H, -COOC(C*H*$_3$)$_3$)

^{13}C NMR (126 MHz, CD_2Cl_2, r. t.): δ 172.7, 152.0, 148.7, 141.8, 140.3, 135.0, 131.2, 126.8, 123.67, 123.49, 123.0, 122.5, 94.4, 84.3, 82.3, 80.2, 65.8, 54.3, 34.9, 31.8, 30.4, 28.1, 25.1.

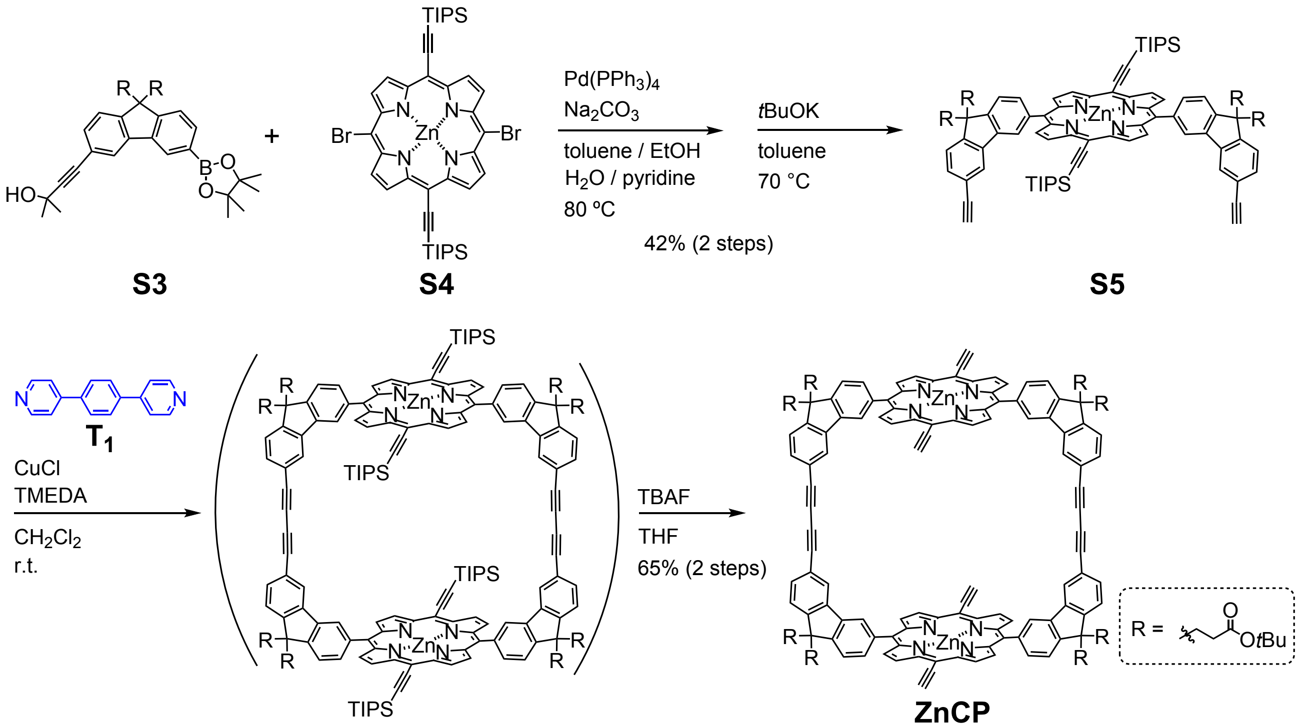
^{1}H NMR spectrum of **S3**



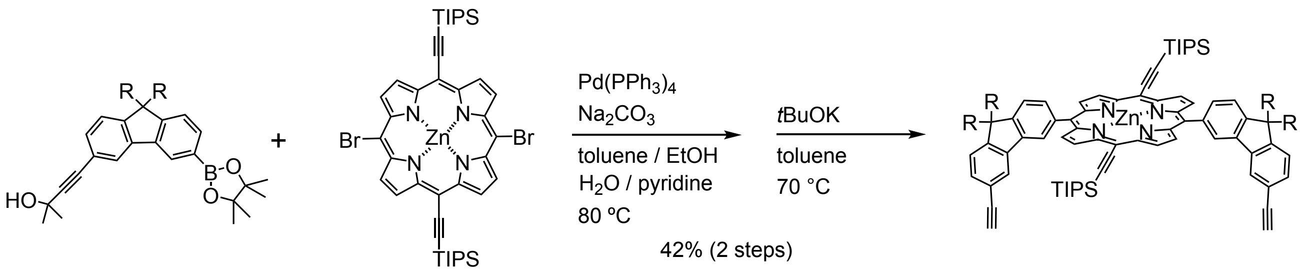
^{13}C NMR spectrum of **S3**



Scheme S2. Synthesis of ZnCP



2.3 Synthesis of S5



S3 (960 mg, 1.52 mmol), **S4** (454 mg, 0.509 mmol), $Pd(PPh_3)_4$ (119 mg, 0.103 mmol), and Na_2CO_3 (699 mg, 6.59 mmol) were dissolved in degassed toluene / EtOH / H_2O (5 / 1 / 1, v / v / v, 35.0 mL) and pyridine (2.5 mL) under Ar. The solution was stirred at 80 ºC for 2 days. The organic layer was extracted with EtOAc, after which the residue was purified by silica gel column chromatography (EtOAc / hexane = 1 / 1, v / v) and GPC with $CHCl_3$ as an eluent. The product was dissolved in degassed toluene (34 mL) before ^{t}BuOK (568 µL, 1 M in THF, 0.568 mmol) was added. The solution was stirred at 70 ºC for 30 min. The crude product was purified by silica gel column chromatography (CH_2Cl_2 / EtOAc = 4 / 1, v / v) to yield **S5** (345 mg, 42%) as a purple solid.

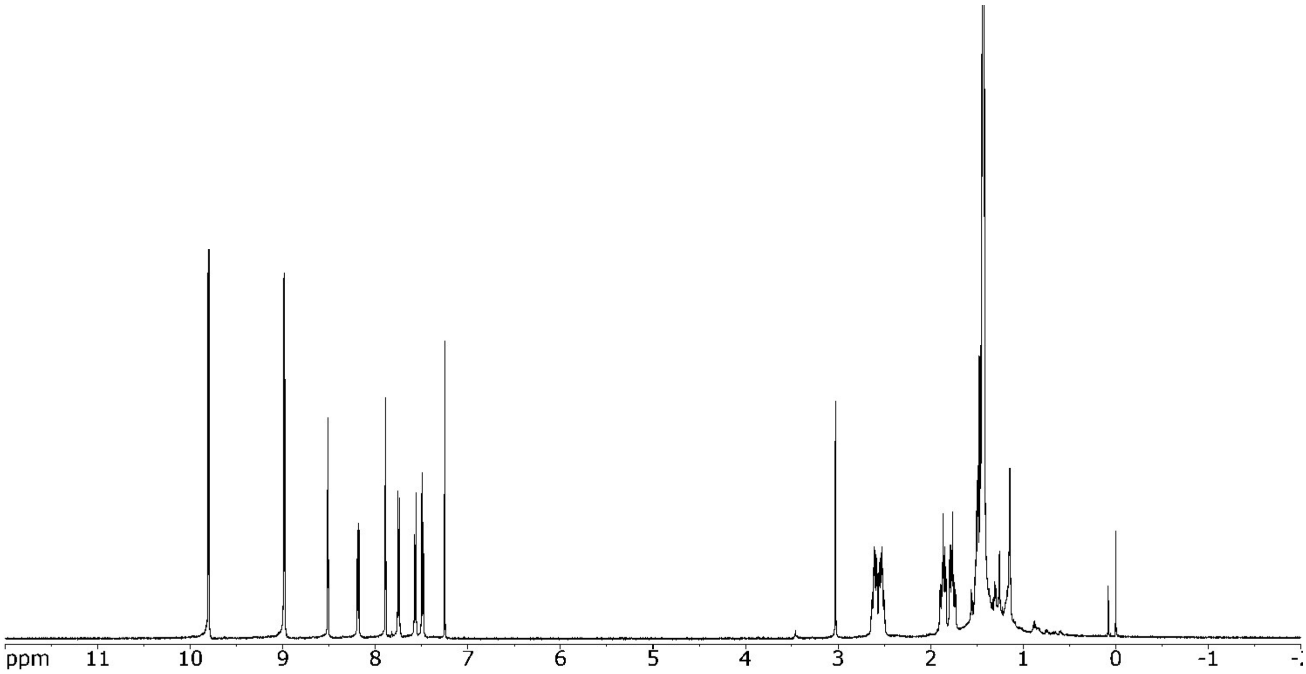
HR-MS (APCI-MS) (m/z) 1621.770 ([**S5**+H]$^+$, $C_{100}H_{117}N_4O_8Si_2Zn$, calcd. 1620.770)

^{1}H NMR (400 MHz, $CDCl_3$, r. t.): δ 9.80 (d, *J* = 4.6 Hz, 4H, β-*H*), 8.98 (d, *J* = 4.6 Hz, 4H, β-*H*), 8.51 (s, 2H, Ar-*H*), 8.19 (d, *J* = 7.6 Hz, 2H, Ar-*H*), 7.89 (s, 2H, Ar-*H*), 7.75 (d, *J* = 7.5 Hz, 2H, Ar-*H*), 7.57 (d, *J* = 8.1 Hz, 2H, Ar-*H*), 7.49 (d, *J* = 8.0 Hz, 2H, Ar-*H*), 3.03 (s, 2H, -CC*H*), 2.63-2.51 (m, 8H, -C*H*$_2$CH$_2$COO^{t}Bu), 1.90-1.73 (m, 8H, -CH$_2$C*H*$_2$COO^{t}Bu), 1.51-

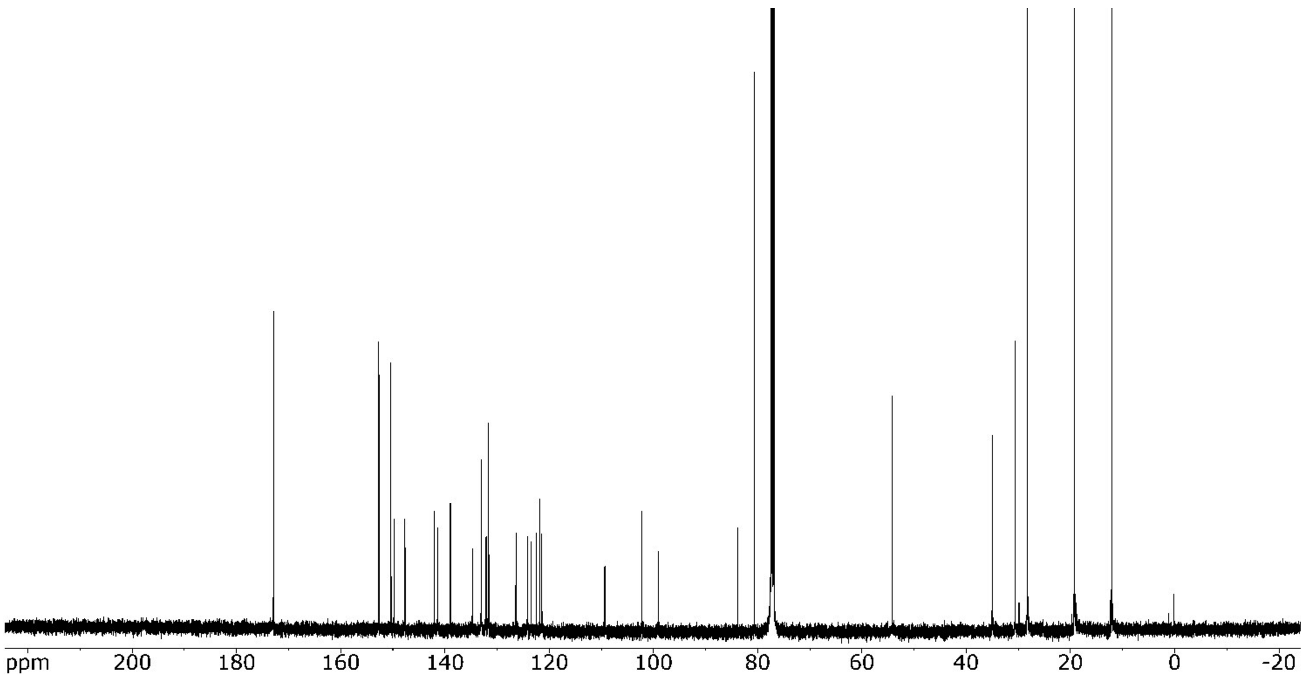
1.43 (m, 36H+42H, -COOC(CH_3)$_3$, -Si(CH(CH_3)$_2$)$_3$).

^{13}C NMR (126 MHz, CDCl$_3$, r. t.): δ 172.7, 152.5, 150.2, 149.6, 147.5, 141.9, 141.2, 138.8, 134.6, 132.9, 132.0, 131.5, 126.2, 124.0, 123.3, 122.3, 121.6, 121.3, 109.2, 102.0, 98.9, 83.7, 80.5, 54.0, 34.8, 30.5, 28.1, 19.1.

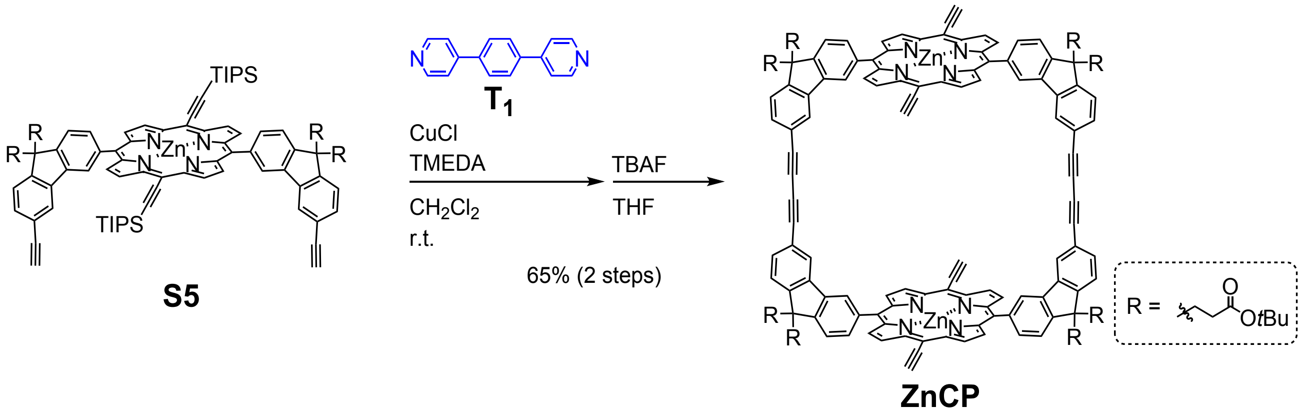
^{1}H NMR spectrum of **S5**



^{13}C NMR spectrum of **S5**



2.4 Synthesis of ZnCP



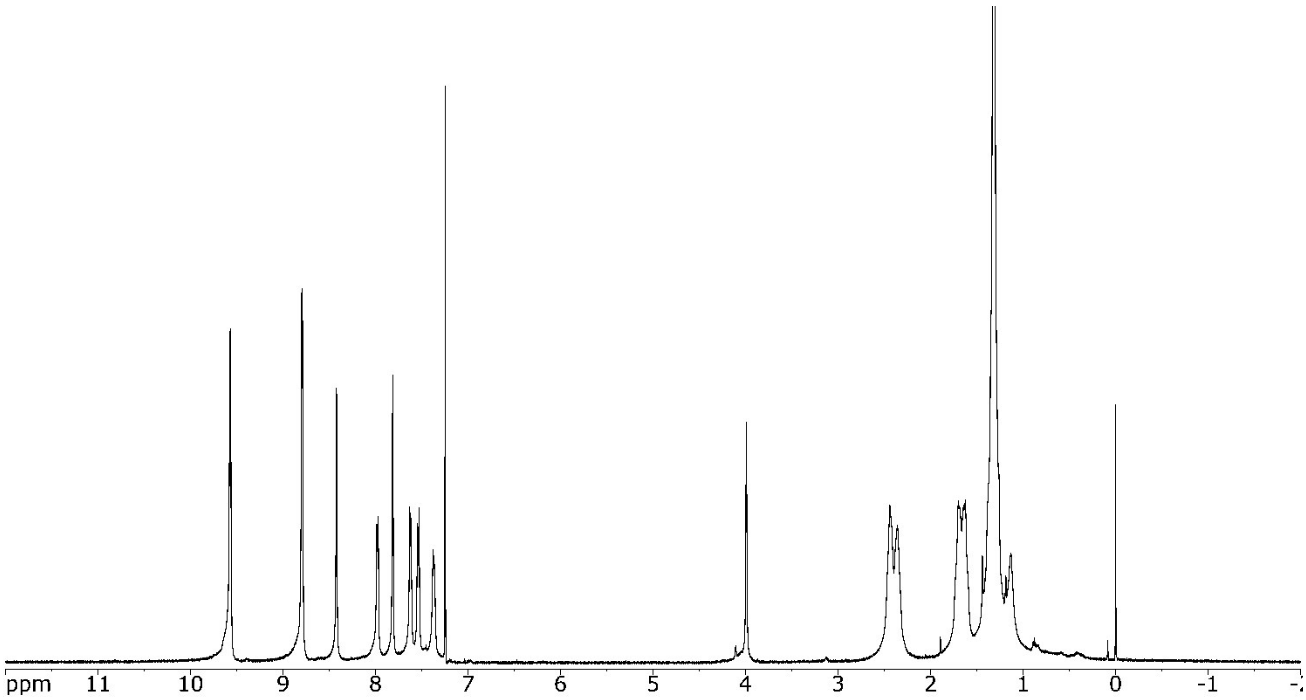
S5 (325 mg, 0.200 mmol) and $\mathbf{T_1}$ (281 mg, 1.21 mmol) were dissolved in dry CH_2Cl_2 (509 mL), and CuCl (2.46 g, 24.8 mmol) was added to the solution under Ar before TMEDA (1.8 mL) was added slowly. Ar was substituted to dry air, after which the solution was stirred at r. t. for 15 h. The solution was passed through the Celite pad before extracted with EtOAc. The residue was purified by silica gel column chromatography (EtOAc / hexane / pyridine = 1 / 1 / 0.01, v / v / v) and GPC using $CHCl_3$ as an eluent. Pyridine was added as an eluent to remove $\mathbf{T_1}$ from **ZnCP**. The product was dissolved in THF (83 mL) before addition of TBAF (0.400 mL, 0.400 mmol, 1M in THF). The solution was stirred at r. t. for 30 min. the crude mixture was purified by GPC using $CHCl_3$ as an eluent to afford **ZnCP** (169 mg, 65%) as a purple solid.

HR-MS (MALDI-TOF MS) (m/z) 2613.965 ([**ZnCP**+H]$^+$, $C_{164}H_{149}N_8O_{16}Zn_2$, calcd. 2613.967)

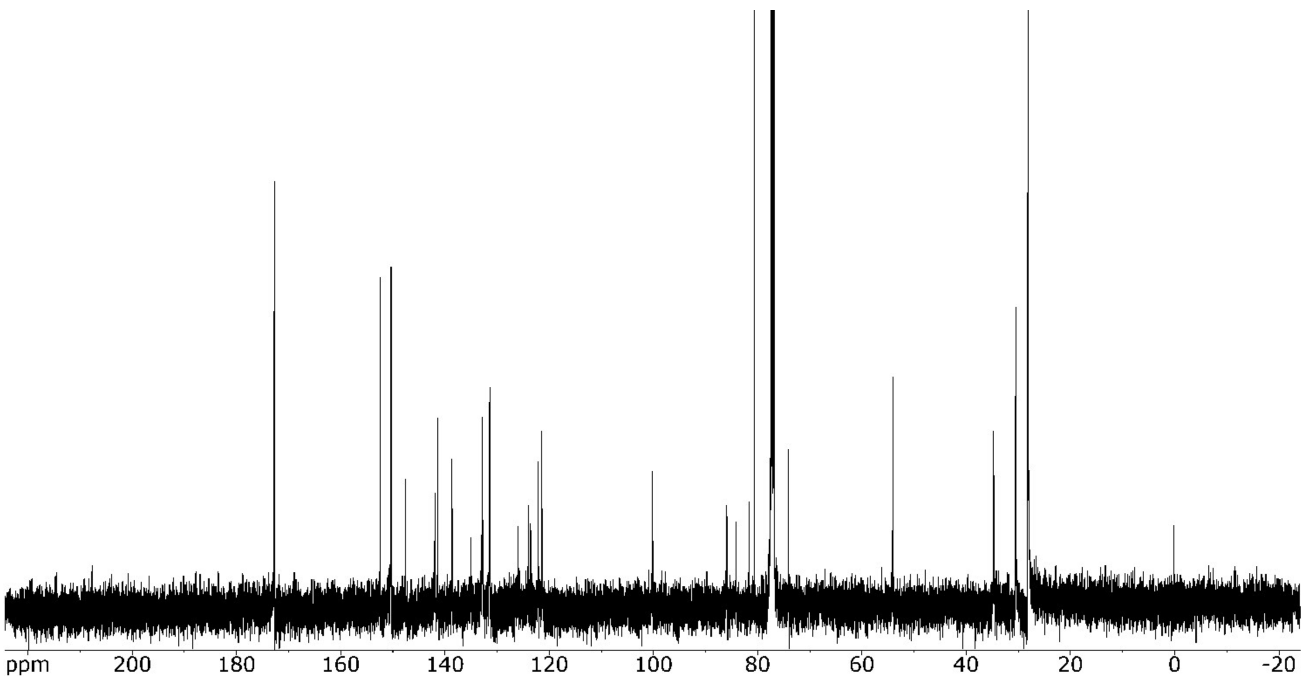
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 9.57 (d, J = 3.5 Hz, 8H, β-H), 8.79 (d, J = 3.9 Hz, 8H, β-H), 8.42 (s, 4H, Ar-H), 7.98 (d, J = 6.7 Hz, 4H, Ar-H), 7.81 (s, 4H, Ar-H), 7.62 (d, J = 6.8 Hz, 4H, Ar-H), 7.54 (d, J = 7.9 Hz, 4H, Ar-H), 7.37 (d, J = 6.9 Hz, 4H, Ar-H), 3.99 (s, 4H, -CCH), 2.44-2.35 (m, 16H, -CH_2CH$_2$COO^{t}Bu), 1.70-1.60 (m, 16H, -CH_2CH$_2$COO^{t}Bu), 1.32 (s, 72H, -CH$_2$CH$_2$COOC(CH_3)$_3$).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 172.7, 152.4, 150.3, 150.2, 147.6, 141.9, 141.4, 138.7, 135.0, 132.9, 131.4, 125.9, 124.0, 123.6, 122.1, 121.4, 121.3, 100.2, 100.1, 85.9, 84.2, 81.7, 80.6, 74.1, 54.1, 34.7, 30.5, 28.1.

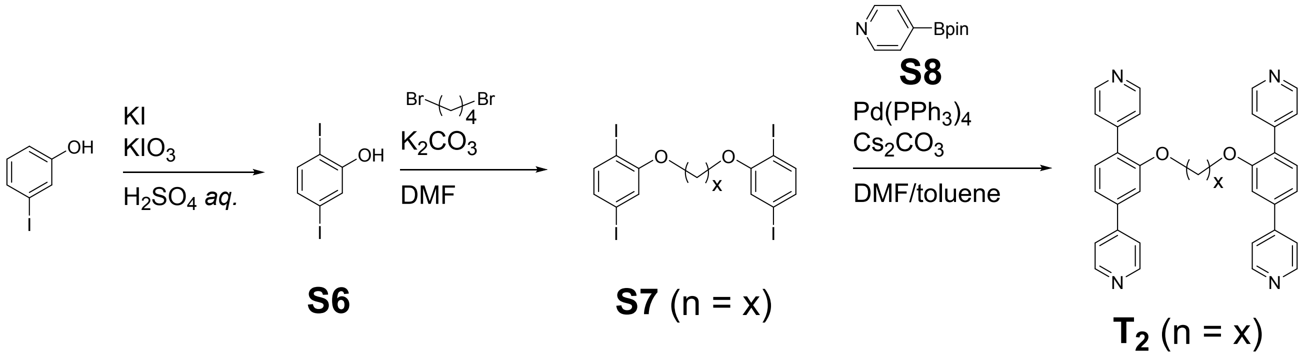
^{1}H NMR spectrum of **ZnCP**



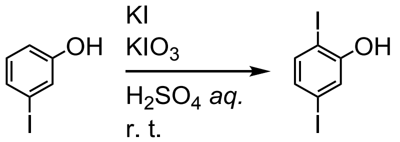
^{13}C NMR spectrum of **ZnCP**



Scheme S3. Synthesis of T_2 (n = x)



2.5 Synthesis of 2,5-diiodephenol S6



S6

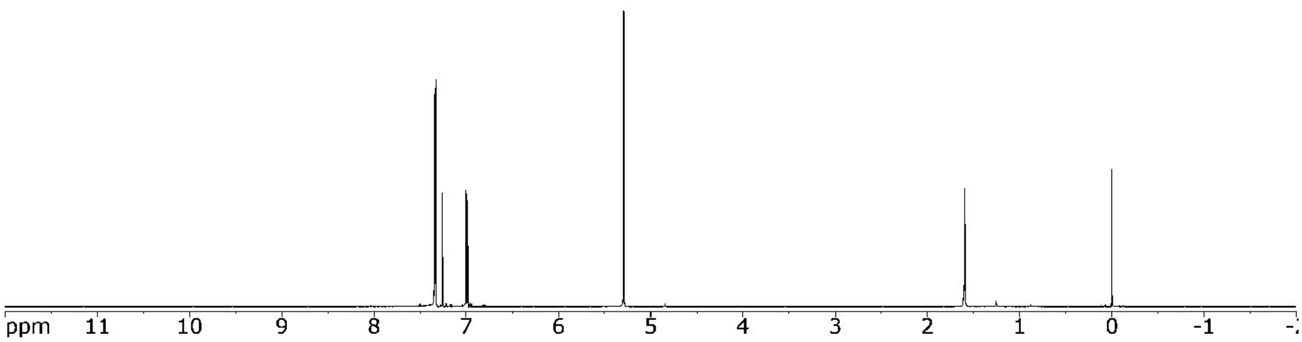
3-Iodophenol (8.46 g, 38.5 mmol), KI (4.48 g, 27.0 mmol), and KIO_3 (2.48 g, 11.6 mmol) were dissolved in 3.8% H_2SO_4 aq. (w / w, 246 mL). The solution was stirred at r. t. for 14 h, after which I_2 was quenched by $Na_2S_2O_3$. The residue was extracted by EtOAc three times and the organic layers were washed with brine. The organic layer was dried over Na_2SO_4 and evaporated to afford a brown oil. The oil was purified by silica gel column chromatography (CH_2Cl_2 / hexane = 19 / 1, v / v) to afford **S6** (7.81 g, 70%) as a white solid.

HR-MS (EI MS) (m/z) 345.8348 ([**S6**]$^+$, $C_6H_4I_2O$, calcd. 345.8352)

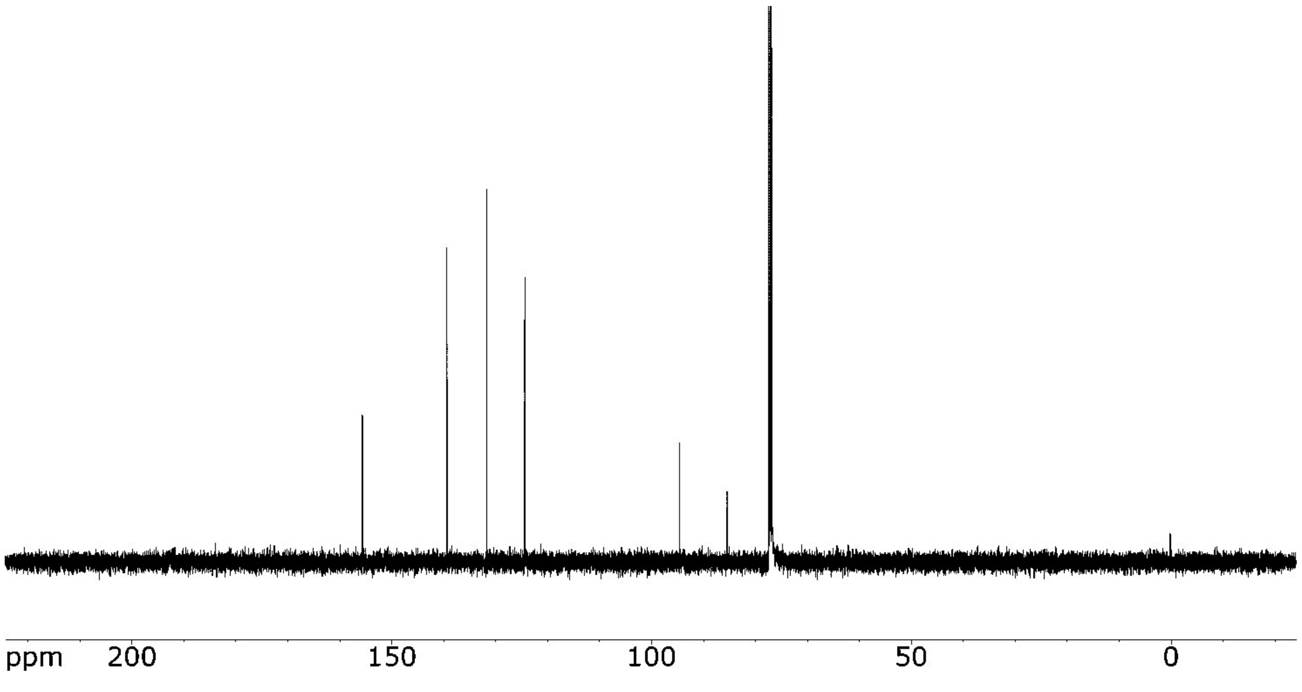
^{1}H NMR (500 MHz, CDCl$_3$, r. t.): δ 7.34 (d, *J* = 2.0 Hz, 1H, Ar-*H*), 7.34 (d, *J* = 8.3 Hz, 1H, Ar-*H*), 7.00 (dd, *J* = 8.3, 2.0 Hz, 1H, Ar-*H*), 5.29 (s, 1H, -O*H*).

^{13}C NMR (126 MHz, CDCl$_3$, r. t.): δ 155.6, 139.4, 131.7, 124.4, 94.6, 85.4.

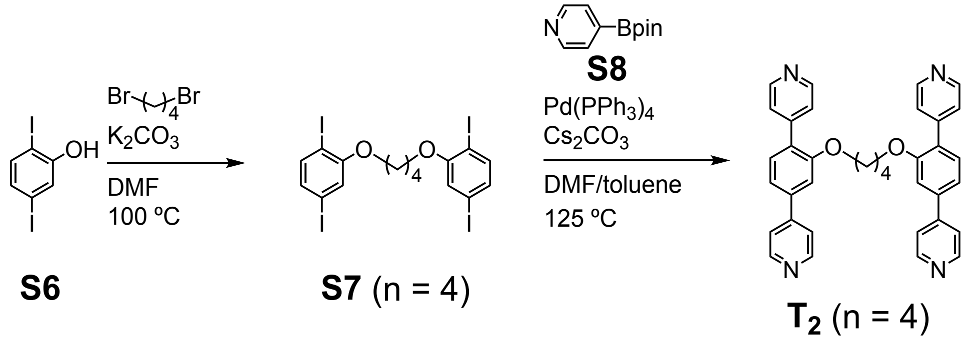
^{1}H NMR spectrum of **S6**



^{13}C NMR spectrum of **S6**



2.6 **Synthesis of $\mathbf{T_2}$** (n = 4)



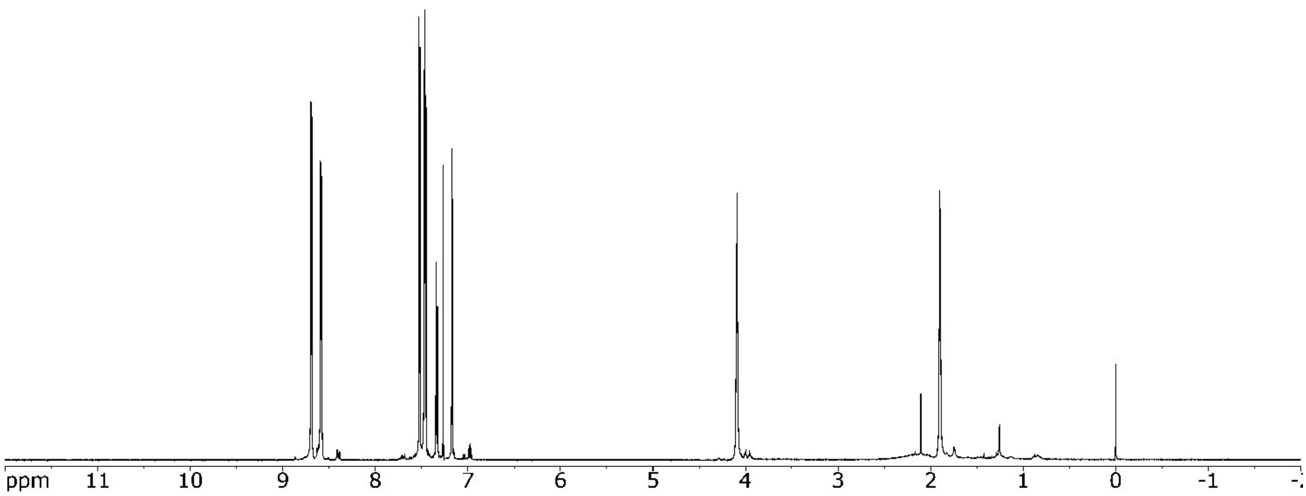
S6 (300 mg, 1.00 mmol), K_2CO_3 (222 mg, 1.61 mmol), and 1,4-dibromobutane (57.8 μL, 0.485 mmol) were dissolved in dry DMF (15 mL) under Ar. The solution was stirred at 100 ºC overnight, after which the residue was washed by water twice and brine once. The organic layer was dried by Na_2SO_4 and evaporated. The residue was purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 9, v / v) to afford **S7** (n = 4) (202 mg, 0.271 mmol) as a white solid. Half amount of **S7** (n = 4) (101 mg, 0.136 mmol), **S8** (333 mg, 1.63 mmol), Cs_2CO_3 (530 mg, 1.63 mmol), and $Pd(PPh_3)_4$ (94.0 mg, 81.3 μmol) were dissolved in DMF / toluene (1 / 1, v / v, 6.6 mL) under Ar. The solution was stirred at 125 ºC overnight. The solvents were removed under vacuum, after which the residue was passed through a Celite pad. The crude mixture was purified by silica gel column chromatography (CH_2Cl_2 / MeOH = 100 / 1 to 10 / 1, v / v) to afford $\mathbf{T_2}$ (n = 4) (34.0 mg, 25% for 2 steps) as a yellow solid.

HR-MS (APCI MS) (m/z) 551.2429 ([$\mathbf{T_2}$ (n = 4)+H]$^+$, $C_{36}H_{31}N_4O_2$, calcd. 551.2427)

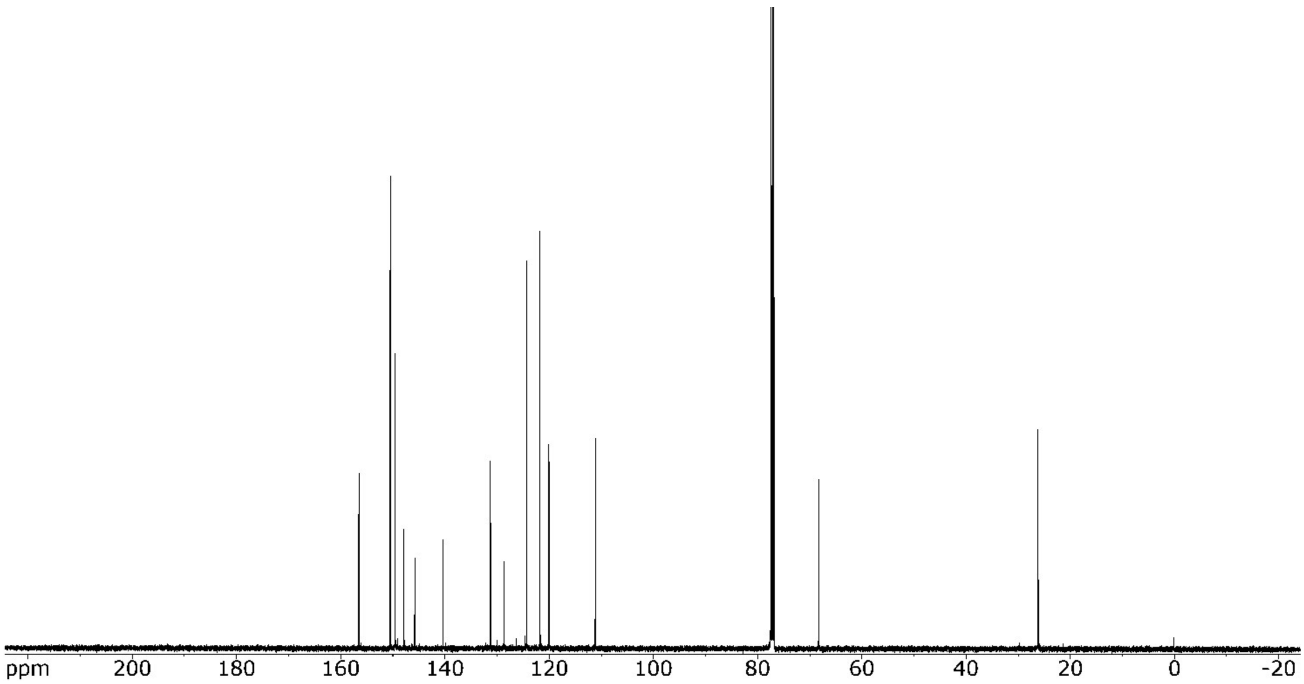
^{1}H NMR (500 MHz, CDCl$_3$, r. t.): δ 8.69 (dd, *J* = 4.5, 1.5 Hz, 4H, Ar-*H*), 8.59 (dd, *J* = 4.5, 1.5 Hz, 4H, Ar-*H*), 7.52 (dd, *J* = 4.5, 1.6 Hz, 4H, Ar-*H*), 7.47-7.45 (m, 6H, Ar-*H*), 7.33 (dd, *J* = 7.9, 1.6 Hz, 2H, Ar-*H*), 7.17 (d, *J* = 1.6 Hz, 2H, Ar-*H*), 4.09 (t, *J* = 4.5 Hz, 4H, -OCH_2CH$_2$CH$_2$-), 1.90 (m, 4H, -OCH$_2$CH_2CH$_2$-).

^{13}C NMR (126 MHz, CDCl$_3$, r. t.): δ 156.5, 150.5, 149.6, 147.8, 145.8, 140.4, 131.3, 128.7, 124.3, 121.7, 120.0, 111.1, 68.3, 26.2.

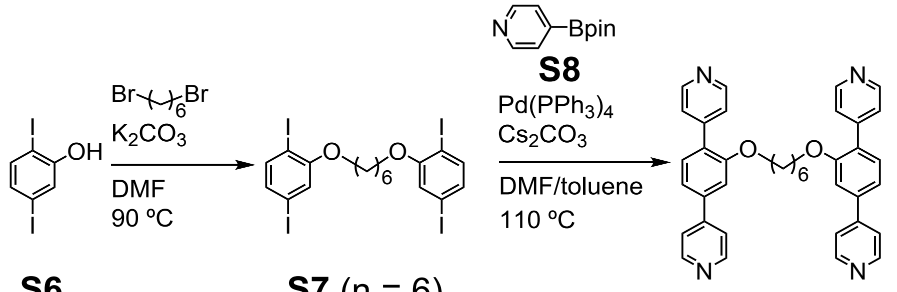
^{1}H NMR spectrum of $\mathbf{T_2}$ (n = 4)



^{13}C NMR spectrum of $\mathbf{T_2}$ (n = 4)



2.7 **Synthesis of T_2** (n = 6)



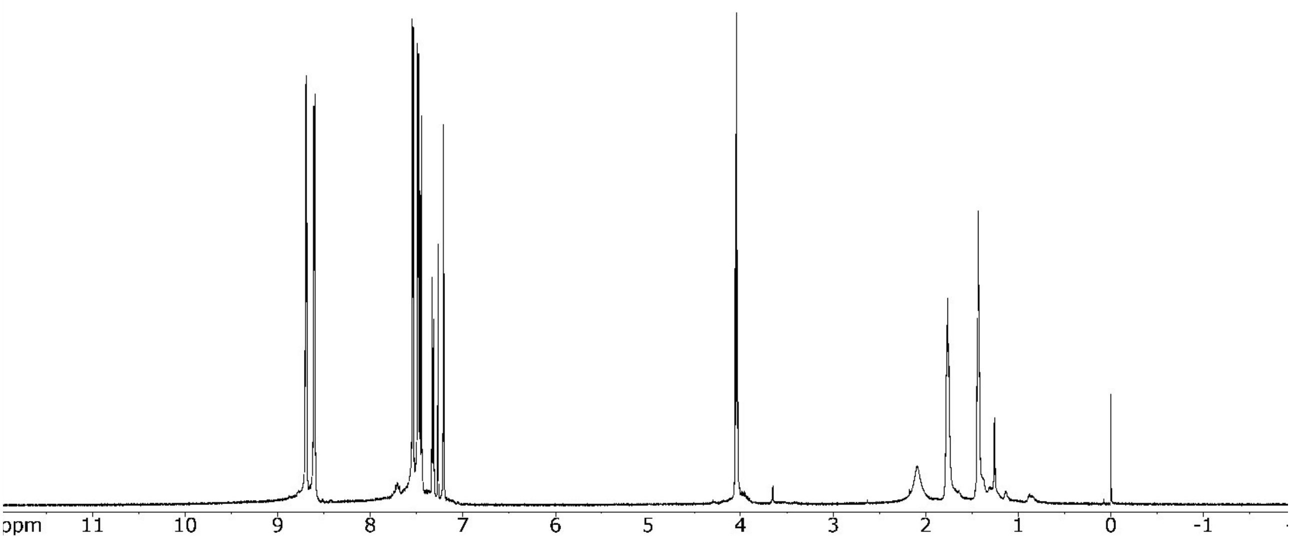
S5 (200 mg, 0.669 mmol), K_2CO_3 (105 mg, 0.760 mmol), and 1,6-dibromohexane (46.1 µL, 0.304 mmol) were dissolved in dry DMF (10 mL). The solution was stirred at 90 ºC overnight under Ar, after which the solution was extracted by EtOAc and washed by water four times and brine once. The residue was purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 10, v / v) to afford **S7** (n = 6) as a white solid (153 mg, 0.198 mmol). **S7** (n = 6) (153 mg, 0.198 mmol), **S8** (406 mg, 1.98 mmol), Cs_2CO_3 (538 mg, 1.98 mmol) and $Pd(PPh_3)_4$ (68.6 mg, 59.4 µmol) were dissolved in DMF / toluene (1 / 1, v / v, 9.6 mL) under Ar. The solution was stirred at 110 ºC overnight. The solvents were removed under vacuum, after which the residue was passed through a Celite pad. The crude mixture was purified by silica gel column chromatography (CH_2Cl_2 / MeOH = 100 / 1 to 20 / 1, v / v) to afford $\mathbf{T_2}$ (n = 6) (101 mg, 57% for 2 steps) as a yellow solid.

HR-MS (APCI MS) (m/z) 579.2739 ([$\mathbf{T_2}$ (n = 6)+H]$^+$, $C_{38}H_{35}N_4O_2$, calcd. 579.2760)

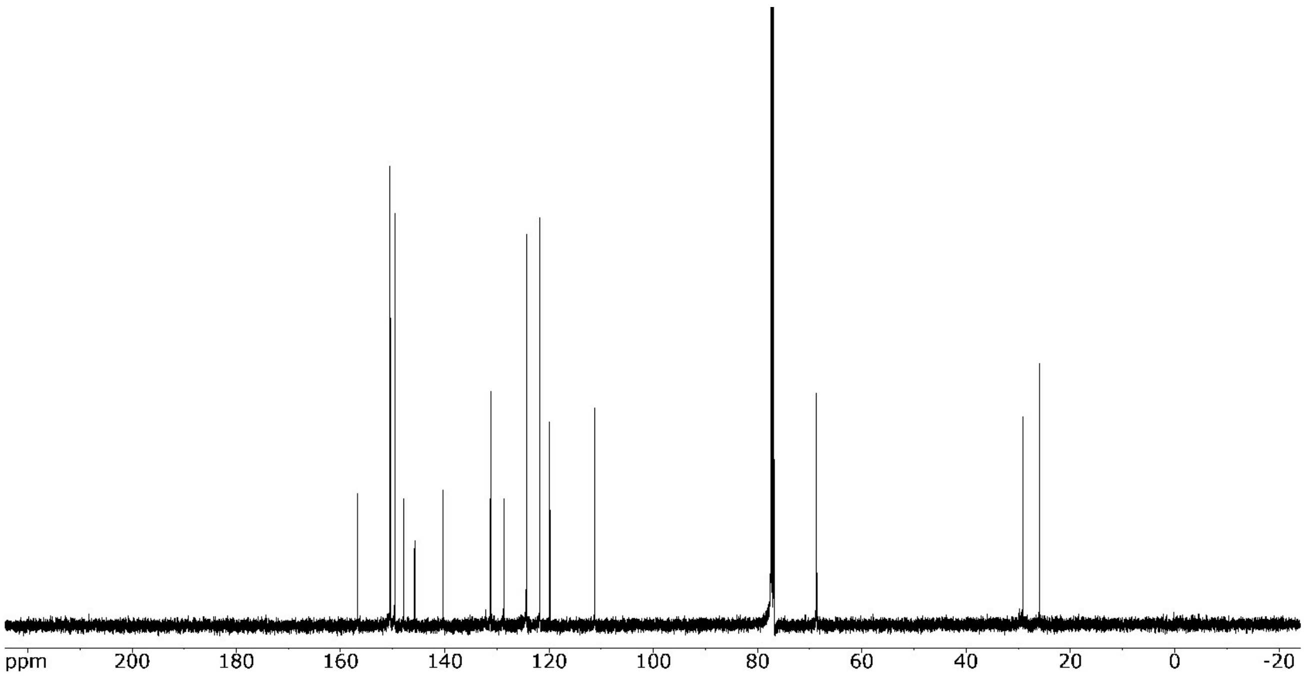
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 8.69 (dd, *J* = 4.5, 1.3 Hz, 4H, Ar-*H*), 8.61 (dd, *J* = 4.3, 1.3 Hz, 4H, Ar-*H*), 7.54 (dd, *J* = 4.6, 1.3 Hz, 4H, Ar-*H*), 7.48 (dd, *J* = 4.5, 1.3 Hz, 4H, Ar-*H*), 7.46 (d, *J* = 7.9 Hz, 2H, Ar-*H*), 7.32 (dd, *J* = 7.8, 1.1 Hz, 2H, Ar-*H*), 7.21 (d, *J* = 1.1 Hz, 2H, Ar-*H*), 4.05 (t, *J* = 6.2 Hz, 4H, -OCH_2CH$_2$CH$_2$-), 1.79-1.74 (m, 4H, -OCH$_2$CH_2CH$_2$-), 1.45-1.42 (m, 4H, -OCH$_2$CH$_2$CH_2-).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 156.7, 150.5, 149.6, 147.9, 145.8, 140.3, 131.2, 128.7, 124.3, 121.8, 119.9, 111.2, 68.7, 29.1, 25.9.

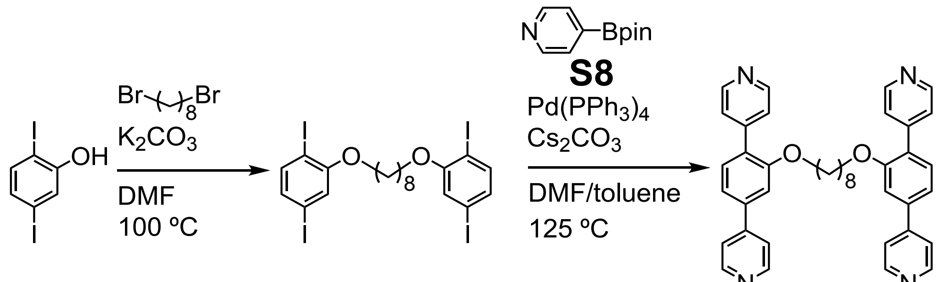
^{1}H NMR spectrum of $\mathbf{T_2}$ (n = 6)



^{13}C NMR spectrum of $\mathbf{T_2}$ (n = 6)



2.8 Synthesis of T_2 (n = 8)



S6 **S7** (n = 8) $\mathbf{T_2}$ (n = 8)

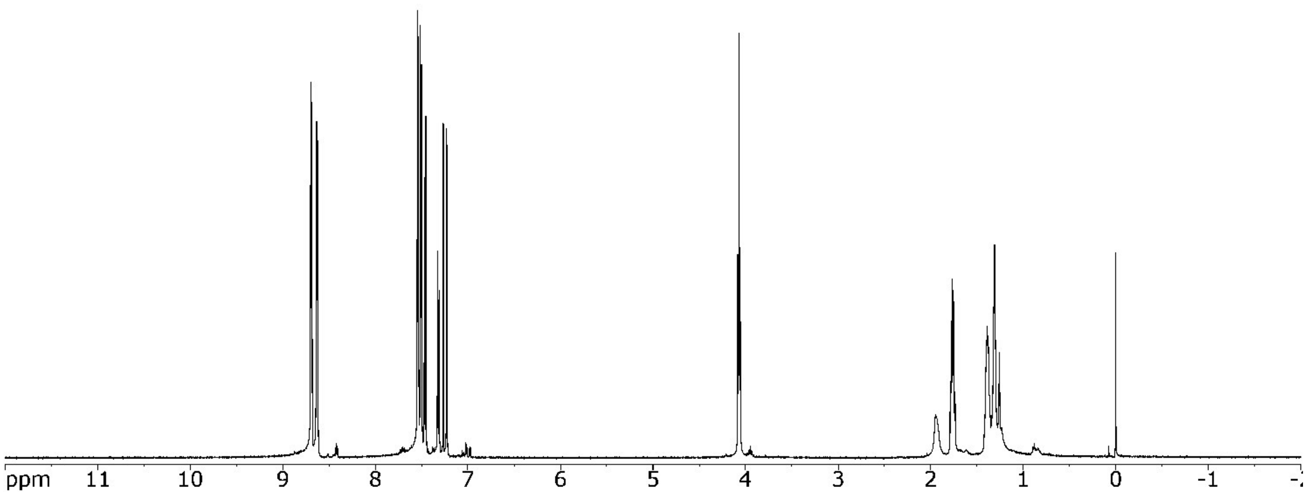
S6 (400 mg, 1.16 mmol), K_2CO_3 (216 mg, 1.56 mmol), and 1,8-dibromooctane (72.0 µL, 0.387 mmol) were dissolved in dry DMF (20 mL) under Ar. The solution was stirred at 100 ºC for 36 h, after which DMF was removed under vacuum. The residue was purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 4 to 1 / 2, v / v) to afford **S7** (n = 8) (305 mg, 0.380 mmol) as a white solid. **S7** (n = 8) (305 mg, 0.380 mmol), **S8** (624 mg, 3.04 mmol), Cs_2CO_3 (990 mg, 3.04 mmol) and $Pd(PPh_3)_4$ (87.8 mg, 76.0 µmol) were dissolved in DMF / toluene (1 / 1, v / v, 26.0 mL). The solution was stirred at 125 ºC overnight. The solvents were removed under vacuum, after which the residue was passed through a Celite pad. The crude mixture was purified silica gel column chromatography (CH_2Cl_2 / MeOH = 100 / 1 to 20 / 1, v / v) to afford $\mathbf{T_2}$ (n = 8) (168 mg, 72% for 2 steps) as a yellow solid.

HR-MS (APCI MS) (m/z) 607.3062 ([$\mathbf{T_2}$ (n = 8)+H]$^+$, $C_{40}H_{39}N_4O_2$, calcd. 607.3073)

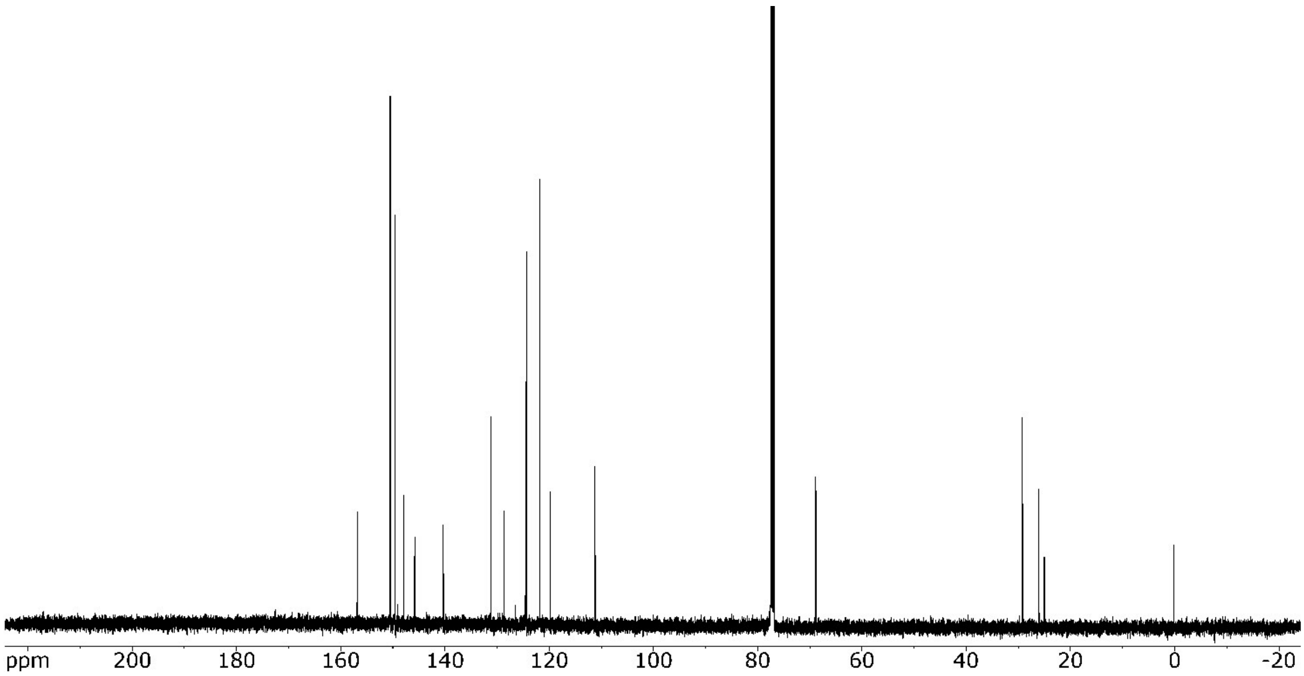
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 8.69 (dd, *J* = 4.7, 1.3 Hz, 4H, Ar-*H*), 8.63 (d, *J* = 5.9 Hz, 4H, Ar-*H*), 7.54 (dd, *J* = 4.6, 1.4 Hz, 4H, Ar-*H*), 7.51 (dd, *J* = 4.7, 1.3 Hz, 4H, Ar-*H*), 7.46 (d, *J* = 7.8 Hz, 2H), 7.32 (dd, *J* = 7.9, 1.3 Hz, 2H, Ar-*H*), 7.23 (d, *J* = 1.2 Hz, 2H, Ar-*H*), 4.07 (t, *J* = 6.3 Hz, 4H, $-OCH_2CH_2-$), 1.78-1.73 (m, 4H, $-OCH_2CH_2CH_2CH_2-$), 1.40-1.37 (m, 4H, $-OCH_2CH_2CH_2CH_2-$), 1.31 (d, *J* = 6.3 Hz, 4H, $-OCH_2CH_2CH_2CH_2-$).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 156.8, 150.5, 149.6, 148.0, 145.8, 140.3, 131.2, 128.6, 124.4, 121.8, 119.8, 111.2, 68.9, 29.2, 26.1, 25.0.

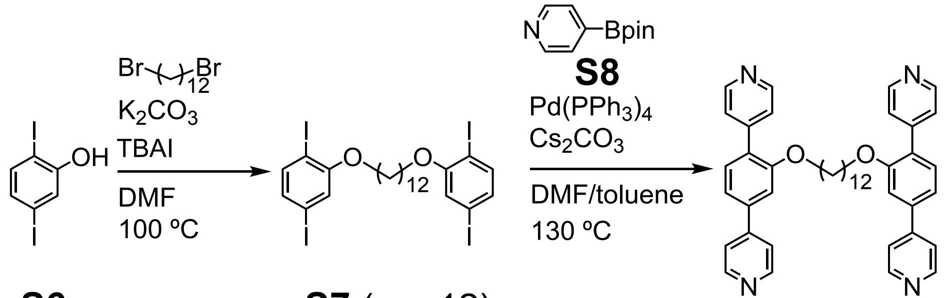
^{1}H NMR spectrum of $\mathbf{T_2}$ (n = 8)



^{13}C NMR spectrum of $\mathbf{T_2}$ (n = 8)



2.9 Synthesis of T_2 (n = 12)



S6 **S7** (n = 12) **T_2** (n = 12)

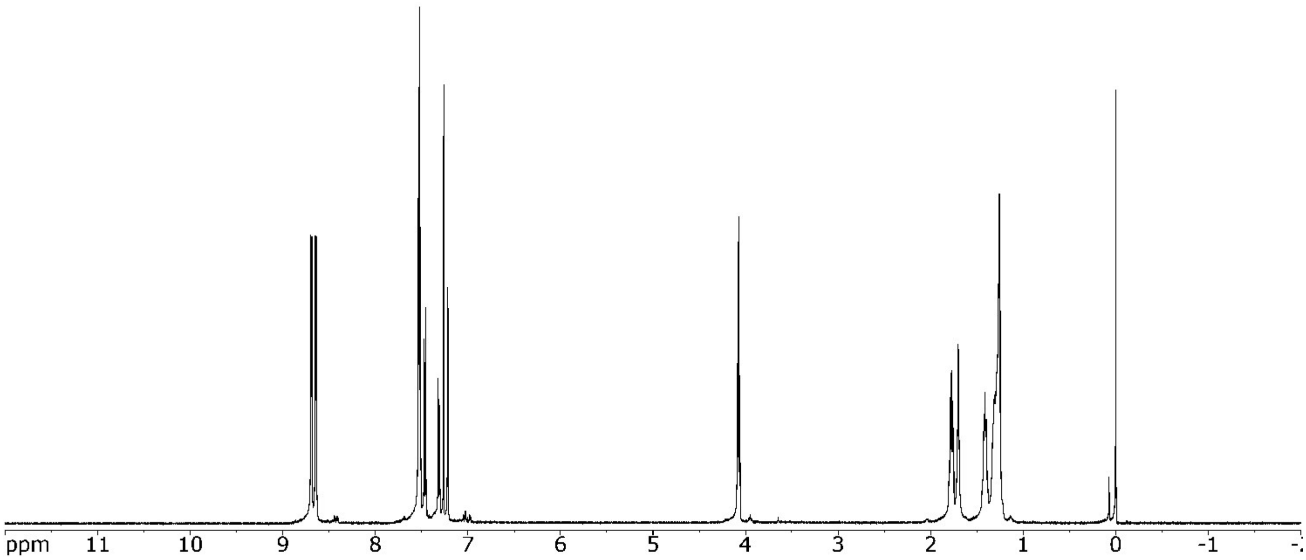
S5 (500 mg, 1.52 mmol), K_2CO_3 (210 mg, 1.52 mmol), 1,12-dibromododecane (176 mg, 0.508 mmol), and tetrabutylammonium iodide (9.38 mg, 25.4 μmol) were dissolved in dry DMF (23.0 mL) under N_2. The solution was stirred at 100 ºC overnight, after which the solution was filtered through the Celite pad. The residue was purified by silica gel column chromatography (EtOAc / hexane = 1 / 40, v / v) to afford **S7** (n = 12) (192 mg, 0.224 mmol) as a white solid. **S7** (n = 12) (172 mg, 0.200 mmol), **S8** (328 mg, 1.60 mmol), Cs_2CO_3 (521 mg, 1.60 mmol) and $Pd(PPh_3)_4$ (46.2 mg, 40.0 μmol) were dissolved in DMF / toluene (1 / 1, v / v, 13.6 mL) under N_2. The solution was stirred at 130 ºC overnight. The solvents were removed under vacuum, after which the residue was passed through a Celite pad. The crude mixture was purified by silica gel column chromatography (CH_2Cl_2 / MeOH = 100 / 1 to 10 / 1, v / v) to afford **T_2** (n = 12) (92 mg, 31% for 2 steps) as a pale yellow solid.

HR-MS (APCI MS) (m/z) 663.3675 ([**T_2** (n = 12)+H]$^+$, $C_{44}H_{47}N_4O_2$, calcd. 663.3699)

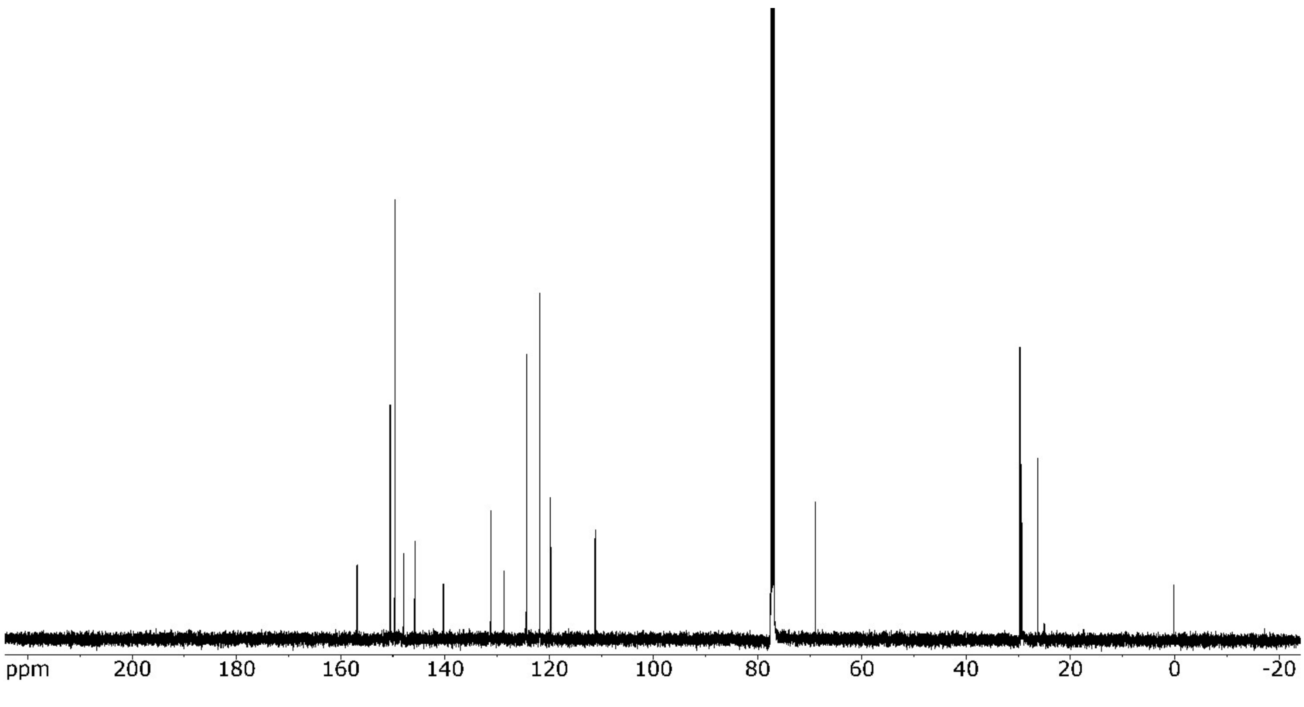
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 8.69 (dd, *J* = 4.6, 1.3 Hz, 4H, Ar-*H*), 8.64 (dd, *J* = 4.7, 1.2 Hz, 4H, Ar-*H*), 7.54-7.51 (two double doublet peaks overlapped, 8H, Ar-*H*), 7.46 (d, *J* = 7.8 Hz, 2H, Ar-*H*), 7.31 (dd, *J* = 7.9, 1.0 Hz, 2H, Ar-*H*), 7.22 (d, *J* = 1.1 Hz, 2H, Ar-*H*), 4.07 (t, *J* = 6.4 Hz, 4H, -$OCH_2CH_2CH_2CH_2CH_2CH_2$-), 1.77 (dt, *J* = 14.3, 6.9 Hz, 4H, -$OCH_2CH_2CH_2CH_2CH_2CH_2$-), 1.41 (dt, *J* = 14.5, 7.1 Hz, 4H, -$OCH_2CH_2CH_2CH_2CH_2CH_2$-), 1.33-1.26 (several peaks overlapped, 4H+4H+4H, -$OCH_2CH_2CH_2CH_2CH_2CH_2$-).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 156.9, 150.5, 149.6, 148.0, 145.8, 140.3, 131.2, 128.7, 124.4, 121.8, 119.7, 111.2, 68.9, 29.7 (two methylene carbons were overlapped), 29.4, 29.3, 26.2.

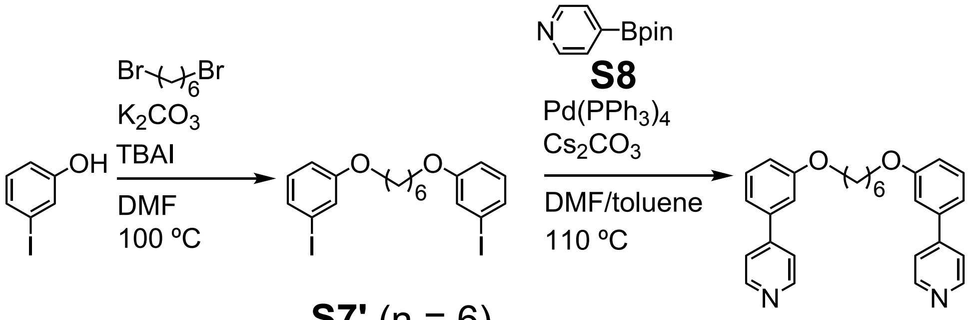
^{1}H NMR spectrum of $\mathbf{T_2}$ (n = 12)



^{13}C NMR spectrum of $\mathbf{T_2}$ (n = 12)



2.10 Synthesis of T_2' (n = 6)



S7' (n = 6)

T_2**'** (n = 6)

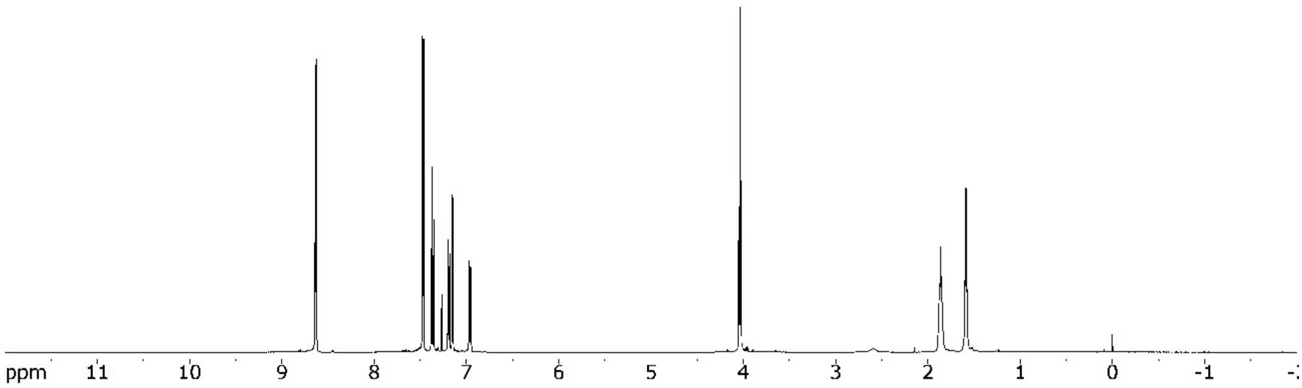
3-Iodophenol (400 mg, 1.82 mmol), K_2CO_3 (315 mg, 2.28 mmol), 1,6-dibromohexane (138 μL, 0.910 mmol), and tetrabutylammonium iodide (16.8 mg, 45.5 μmol) were dissolved in dry DMF (20.0 mL) under N_2. The solution was stirred at 100 ºC overnight, after which the solution was filtered through the Celite pad. The residue was purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 8, v / v) to afford **S7'** as a white solid (393 mg, 0.753 mmol). The half amount of **S7'** (197 mg, 0.377 mmol), **S8** (385 mg, 1.88 mmol), Cs_2CO_3 (612 mg, 1.88 mmol) and $Pd(PPh_3)_4$ (65.1 mg, 56.3 μmol) were dissolved in DMF / toluene (1 / 1, v / v, 10.6 mL) under N_2. The solution was stirred at 110 ºC overnight. The solvents were removed under vacuum, after which the residue was passed through a Celite pad. The crude mixture was purified by silica gel column chromatography (CH_2Cl_2 / EtOAc = 1 / 2, v / v) to afford T_2**'** (n = 6) (96.4 mg, 50% for 2 steps) as a pale yellow solid.

HR-MS (MALDI-TOF MS) (m/z) 425.2218 ([T_2**'** (n = 6)+H]$^+$, $C_{28}H_{29}N_2O_2$, calcd. 425.2229)

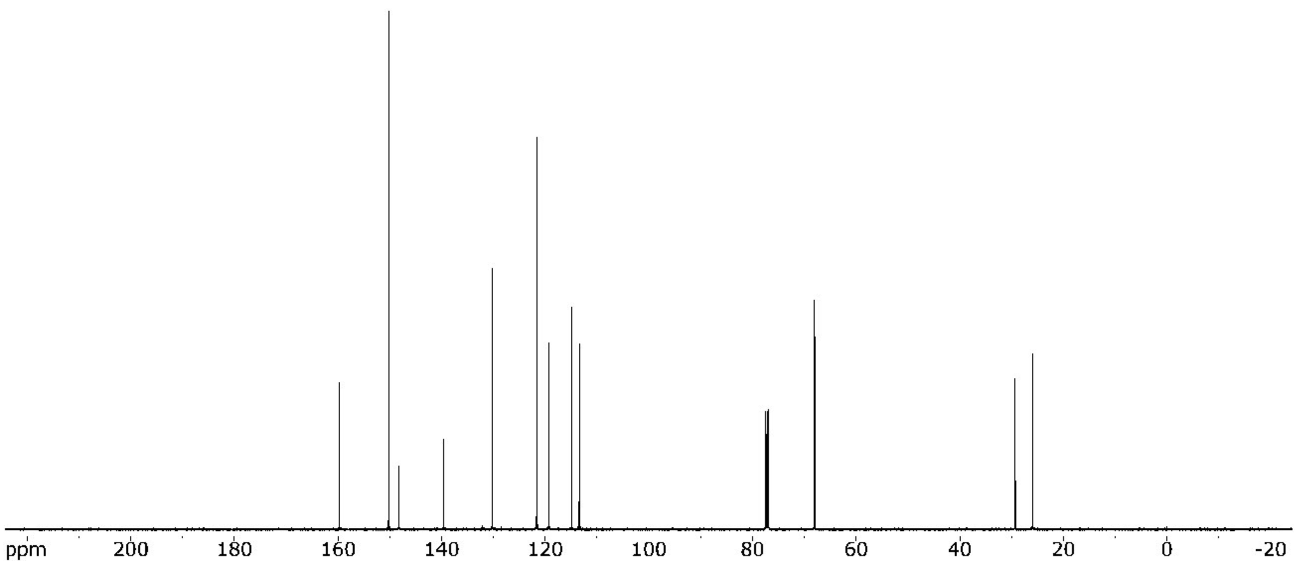
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 8.63 (dd, J = 4.5, 1.6 Hz, 4H, Ar-*H*), 7.47 (dd, J = 4.5, 1.7 Hz, 4H, Ar-*H*), 7.37 (t, J = 7.9 Hz, 2H, Ar-*H*), 7.20-7.18 (m, 2H, Ar-*H*), 7.15 (t, J = 2.1 Hz, 2*H*, Ar-*H*), 6.96 (ddd, J = 8.2, 2.5, 0.7 Hz, 2H, Ar-*H*), 4.04 (t, J = 6.4 Hz, 4H, Ar-OCH_2CH$_2$CH$_2$-), 1.89-1.84 (m, 4H, Ar-OCH$_2$CH_2CH$_2$), 1.59 (m, 4H, Ar-OCH$_2$CH$_2$CH_2-).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 159.7, 150.3, 148.3, 139.6, 130.2, 121.7, 119.3, 114.9, 113.5, 68.0, 29.3, 25.9.

^{1}H NMR spectrum of $\mathbf{T_2'}$ (n = 6)

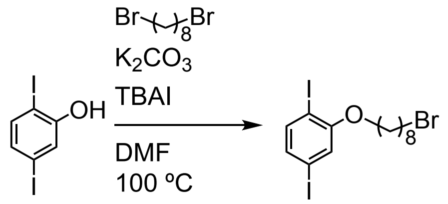


^{13}C NMR spectrum of $\mathbf{T_2'}$ (n = 6)



Scheme S4. Synthesis of T_3 (n = 8)

2.11 Synthesis of S9



S6 **S9**

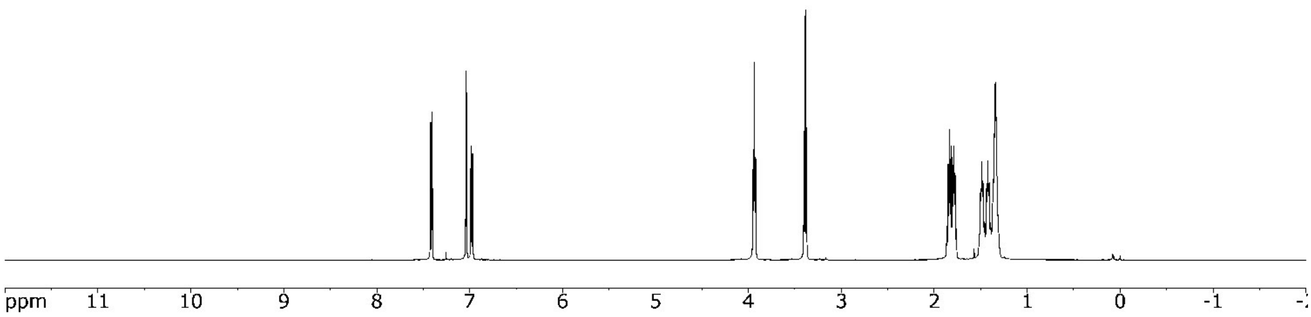
S6 (1.00 g, 2.89 mmol), K_2CO_3 (912 mg, 6.60 mmol), 1,8-dibromooctane (2.20 mL, 11.9 mmol), and tetrabutylammonium iodide (54.5 mg, 147 μmol) were dissolved in dry DMF (100 mL). The solution was stirred at 100 ºC overnight, after which DMF was removed under vacuum. The residue was filtered through the Celite pad and purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 4, v / v) to afford **S9** (638 mg, 41%) as a white solid.

HR-MS (APCI-TOF MS): (m/z) 535.8697 ([**S9**+H $]^+$, $C_{14}H_{19}BrI_2O$, calcd. 535.8709)

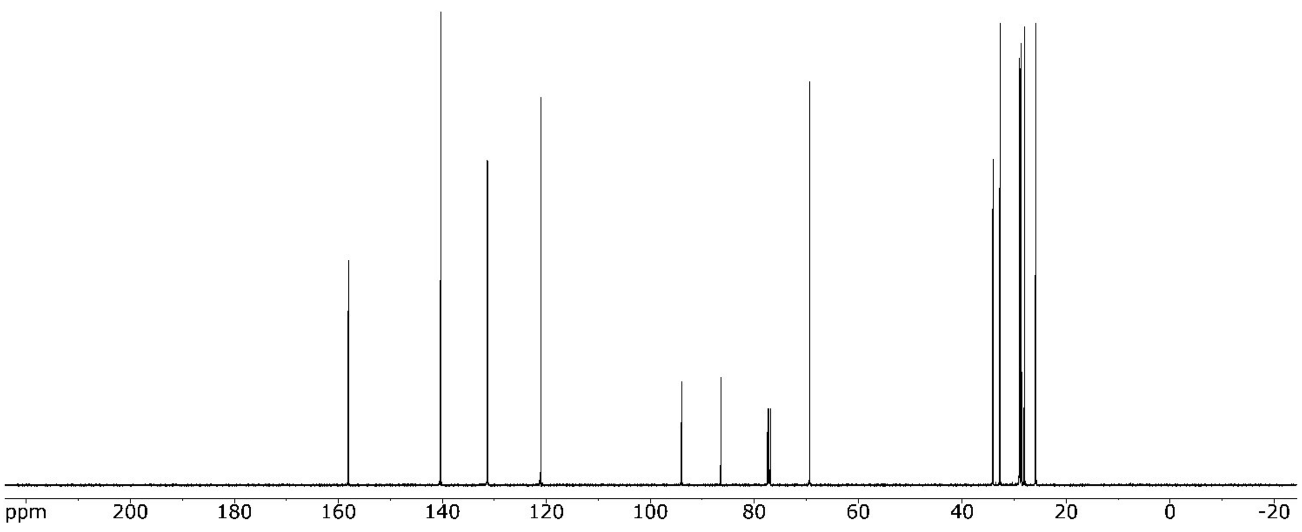
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 7.41 (dd, *J* = 8.1, 1.1 Hz, 1H, Ar-*H*), 7.04 (s, 1H, Ar-*H*), 6.98 (dt, *J* = 8.1, 1.5 Hz, 1H, Ar-*H*), 3.94 (t, *J* = 6.24 Hz, 2H, Ar-OC$H_2$$CH_2$$CH_2$-), 3.39 (t, *J* = 6.94 Hz, 2H, -CH_2-Br), 1.86-1.76 (m, 4H, methylene protons), 1.52-1.34 (m, 8H, methylene protons).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 158.1, 140.3, 131.3, 121.1, 94.0, 86.4, 69.3, 34.1, 32.7, 29.0, 28.9, 28.6, 28.1, 25.9.

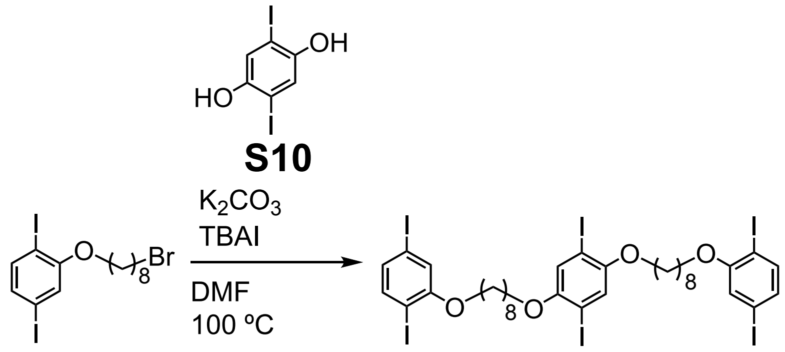
[1]H NMR spectrum of **S9**



[13]C NMR spectrum of **S9**



2.12 **Synthesis of S11**



S9 **S11**

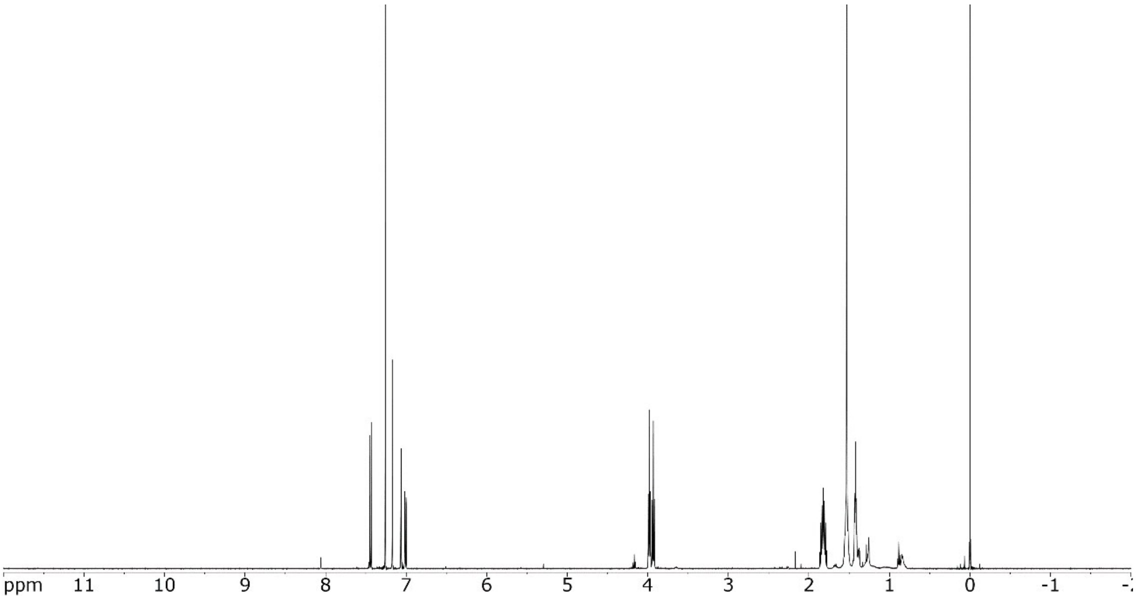
S9 (337 mg, 0.628 mmol), K_2CO_3 (107 mg, 0.775 mmol), **S10** (90.9 mg, 0.251 mmol), and tetrabutylammonium iodide (4.64 mg, 12.6 μmol) were dissolved in dry DMF (2.2 mL). The solution was stired at 100 ºC overnight, after which DMF was removed under vacuum. The residue was filtered through the Celite pad and purified by silica gel column chromatography (CH_2Cl_2 / hexane = 1 / 1, v / v) to afford **S11** (295 mg, 92%) as a white solid.

HR-MS (ESI-TOF MS): (m/z) 1273.718 ([**S11**+H]$^+$, $C_{34}H_{41}I_6O_4$, calcd. 1274.720)

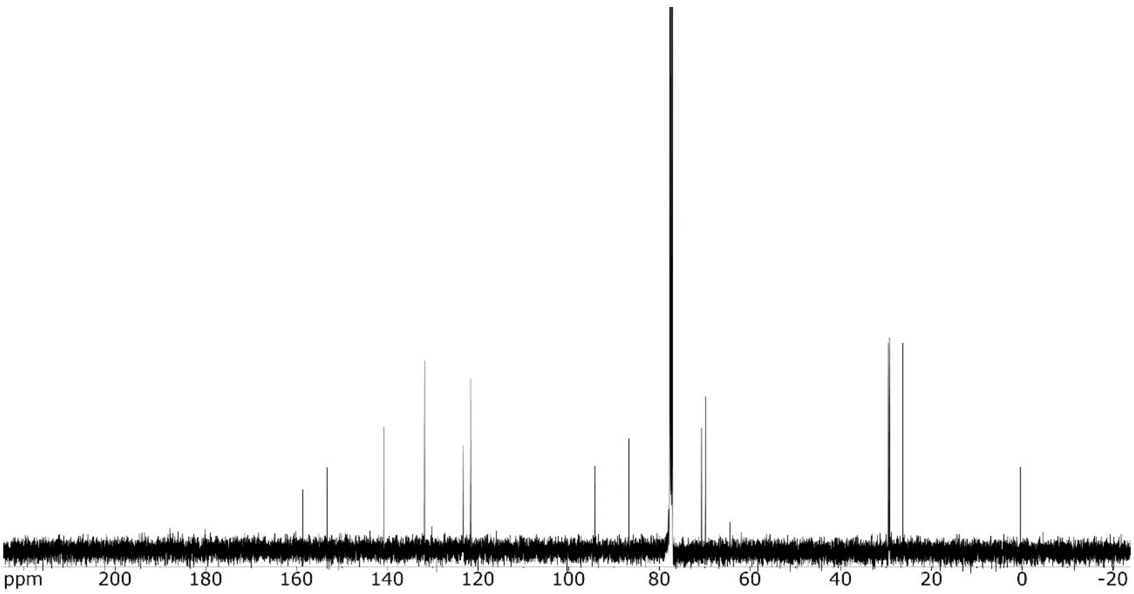
^{1}H NMR (500 MHz, CDCl$_3$, r. t.): δ 7.44 (d, *J* = 8.2 Hz, 2H), 7.17 (s, 2H), 7.06 (d, *J* = 1.8 Hz, 2H), 7.01 (dd, *J* = 8.2, 1.8 Hz, 2H), 3.98 (t, *J* = 6.4, 4H, -O-CH_2-CH_2-), 3.93 (t, *J* = 6.4 Hz, 4H, -O-CH_2-CH_2-), 1.87-1.78 (m, 8H, methylene protons), 1.57-1.50 (m, 8H, methylene protons), 1.42 (m, 8H, methylene protons).

^{13}C NMR (126 MHz, CDCl$_3$, r. t.): δ 158.6, 153.12, 140.8, 131.8, 123.1, 121.6, 94.2, 86.7 (two peaks overlapped), 70.7, 69.8, 29.5, 29.5, 29.46, 29.3, 26.3, 26.3.

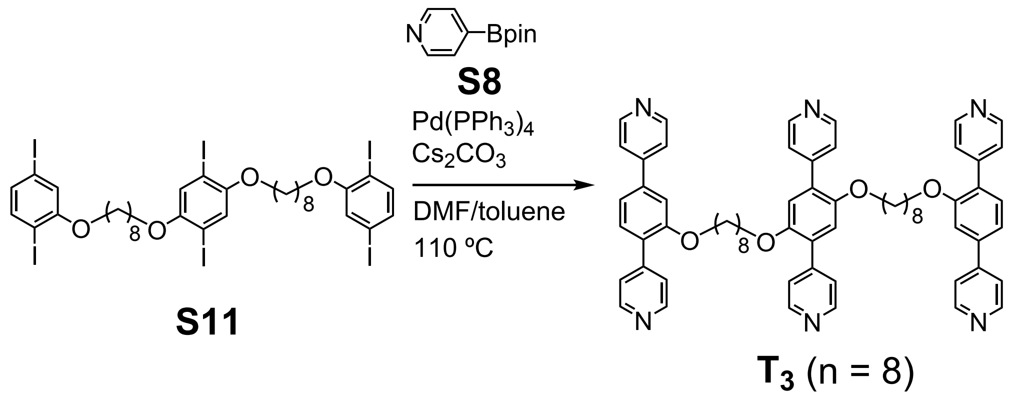
[1]H NMR spectrum of **S11**



[13]C NMR spectrum of **S11**



2.13 Synthesis of $\mathbf{T_3}$ (n = 8)



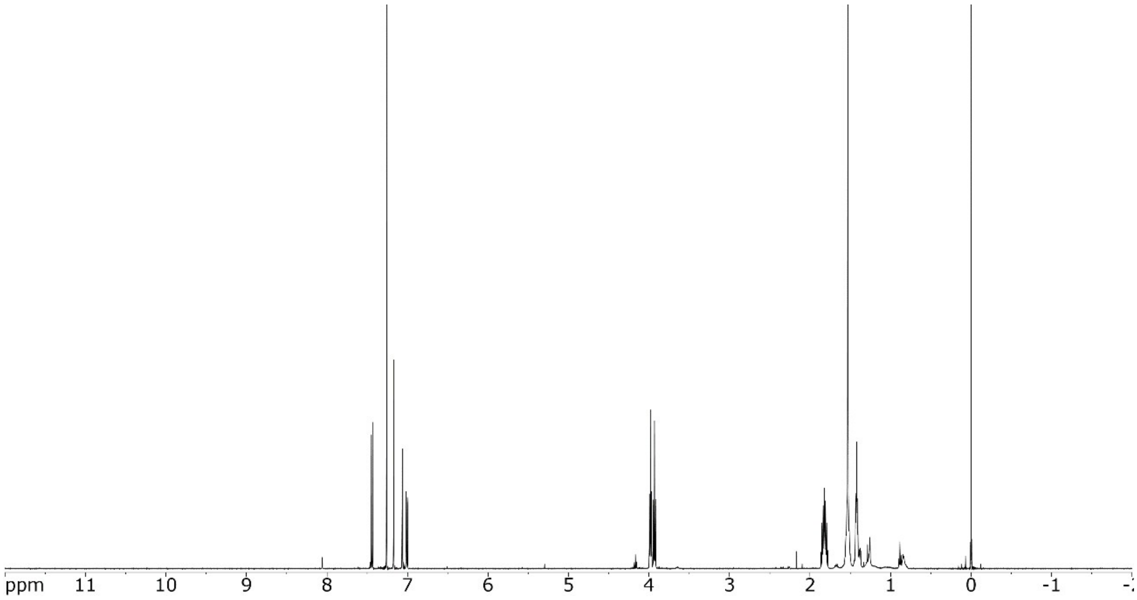
S11 (40.9 mg, 32.1 μmol), **S8** (186.8 mg, 0.910 mmol), Cs_2CO_3 (206 mg, 0.628 mmol), and $Pd(PPh_3)_4$ (7.7 mg, 6.7 μmol) were dissolved in DMF / toluene (1 / 1, v / v, 2.4 mL). The solution was stirred at 110 ºC overnight. The solvent was removed under vacuum, after which the residue was passed through a Celite pad and membrane filter. The crude mixture was purified by silica gel column chromatography (EtOAc / CH_2Cl_2 = 10 / 3, v / v to EtOAc / MeOH / Et_3N = 30 / 9 / 1, v / v / v) to afford $\mathbf{T_3}$ (n = 8) (26.6 mg, 86%) as a white solid.

HR-MS (ESI-TOF MS): (m/z) 981.5045 ([$\mathbf{T_3}$ (n = 8) +H]$^+$, $C_{64}H_{65}N_6O_4$, calcd. 981.5067)

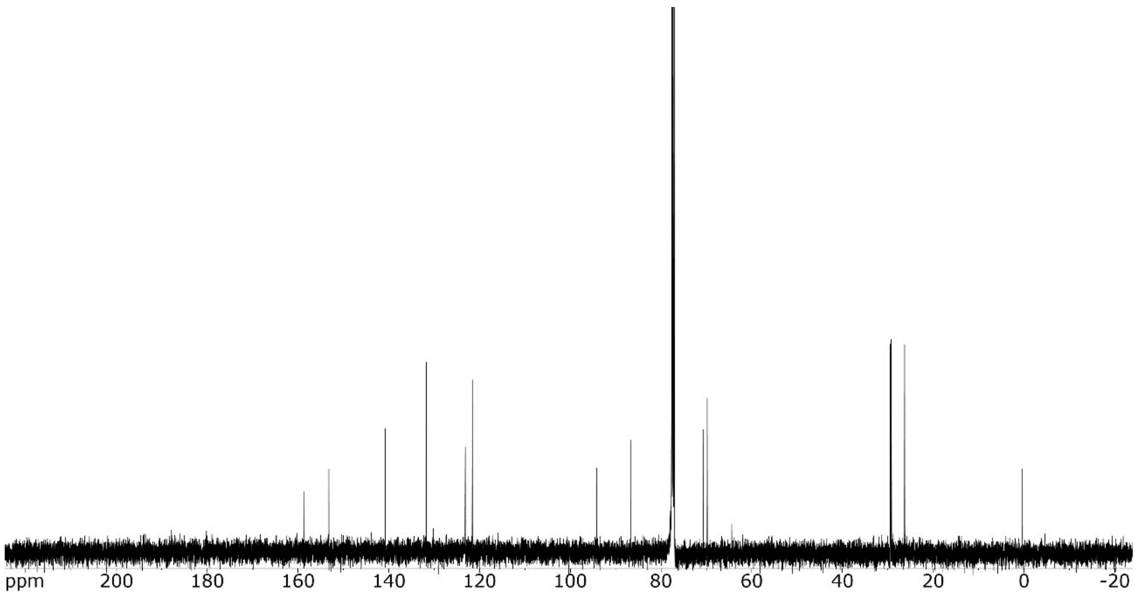
^{1}H NMR (500 MHz, $CDCl_3$, r. t.): δ 8.70-8.67 (broad, 4H, Ar-H), 8.65-8.62 (broad, 8H, Ar-H), 7.56-7.53 (broad, 4H, Ar-H), 7.53-7.50 (broad, 8H, Ar-H), 7.46 (d, J = 7.8, 2H, Ar-H), 7.32 (d, J = 7.8, 2H, Ar-H), 7.23 (s, 2H, Ar-H), 6.99 (s, 2H, Ar-H), 4.07 (t, J = 6.3 Hz, 4H), 3.95 (t, J = 6.2 Hz, 4H), 1.79-1.73 (m, 4H), 1.73-1.67 (m, 4H), 1.38-1.24 (m, 16H).

^{13}C NMR (126 MHz, $CDCl_3$, r. t.): δ 156.8 (two peaks overlapped), 150.53, 150.51, 149.65, 149.61, 147.9, 145.93, 145.78, 140.3, 131.2, 129.2, 128.6, 124.4, 121.8, 119.8, 115.6, 111.2, 69.7, 68.8, 29.35, 29.28 (two peaks overlapped), 29.20, 26.14, 26.12.

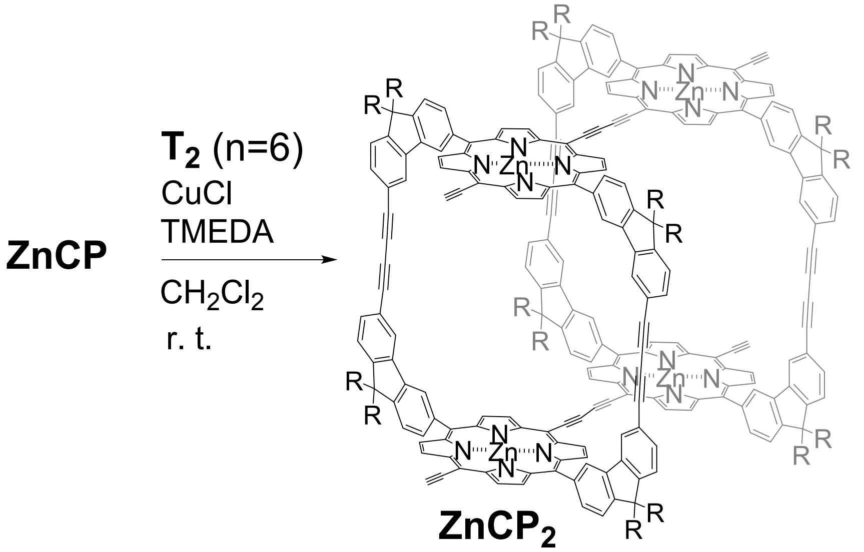
[1]H NMR spectrum of $\mathbf{T_3}$ (n = 8)



[13]C NMR spectrum of $\mathbf{T_3}$ (n = 8)



2.14 Synthesis of $ZnCP_2$

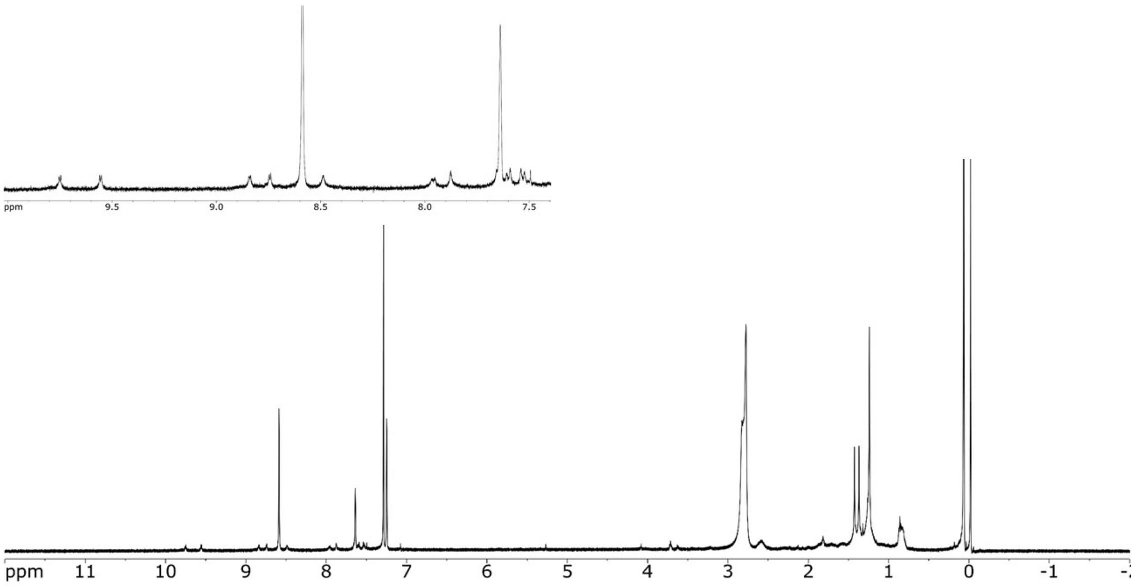


ZnCP (2.17 mg, 0.83 μmol) and **T_2 (n = 6)** (0.248 mg, 0.428 μmol) were dissolved in CH_2Cl_2 (217 mL) followed by slow additions of CuCl (171 mg, 1.73 mmol) and TMEDA (190 μL, 1.30 mmol) under air. The solution was stirred at r. t. for 18 h under air. Another tubulation of **ZnCP** was conducted under the same condition as the above. The combined reaction mixture was carefully washed with NH_4Cl aq. with TMEDA once and NH_4Cl aq. once, water once and brine once to remove copper residue from the solution. The organic layer was dried over Na_2SO_4, then the solvent was removed *in vacuo*. The residue was filtered through silica gel (CH_2Cl_2 / EtOAc / pyridine = 100 / 10 / 1, v / v / v) to remove **T_2** (n=6) from **$ZnCP_2$**. The crude product was purified by GPC (toluene / pyridine = 100 / 1, v / v) to afford **$ZnCP_2$** (1.1 mg, 25%).

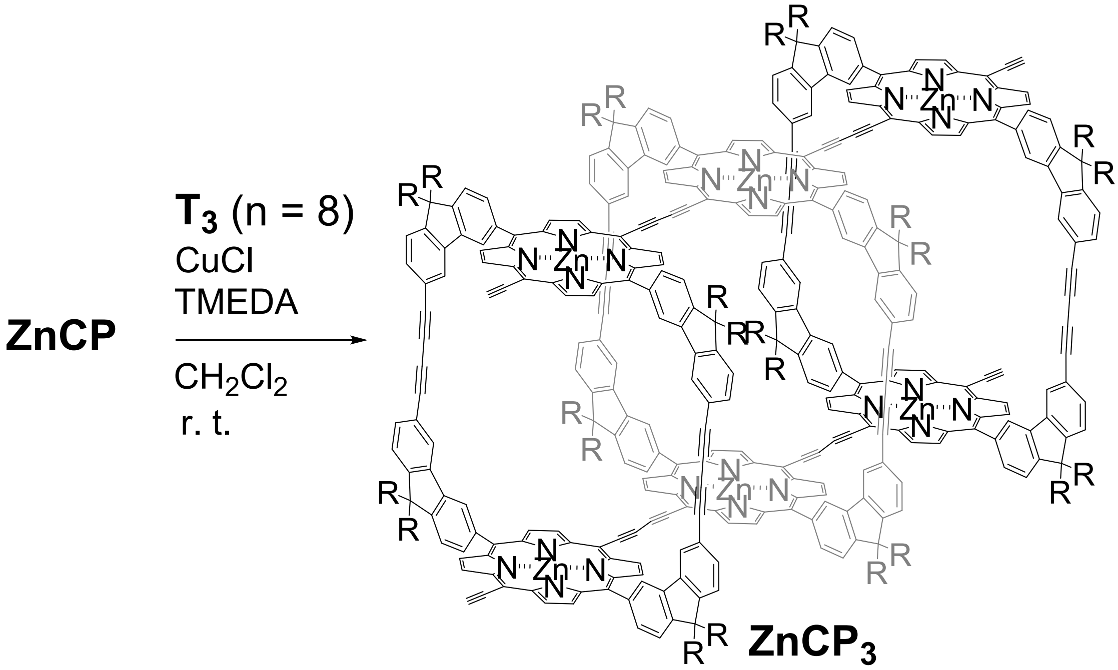
HR-MS (MALDI-TOF MS) (m/z) 5231.37 ([**$ZnCP_2$**+H]$^+$, $C_{328}H_{293}N_{16}O_{32}Zn_4$, calcd. 5231.8984)

^{1}H NMR (500 MHz, $CDCl_3$ (+ 1 % pyridine-d_5), r. t.) δ: 9.76 (d, *J* = 4.3 Hz, 8H, β-*H*), 9.56 (d, *J* = 4.4 Hz, 8H, β-*H*), 8.85 (d, *J* = 4.4 Hz, 8H, β-*H*), 8.75 (d, *J* = 4.4 Hz, 8H, β-*H*), 8.51 (s, 8H, Ar-*H*), 7.97 (d, *J* = 6.9 Hz, 8H, Ar-H), 7.67 (s, 8H, Ar-*H*), 7.62 (d, *J* = 7.9 Hz, 8H, Ar-*H*), 7.55 (d, *J* = 8.5 Hz, 8H, Ar-*H*), 4.09 (s, 4H), 2.62-2.57 (m, 32H), 1.89-1.68 (m, 32H), 1.45 (s, -$CH_2CH_2COOC(CH_3)_3$),1.42 (s, -$CH_2CH_2COOC(CH_3)_3$).

^{1}H NMR spectrum of $\mathbf{ZnCP_2}$



2.15 Synthesis of $ZnCP_3$

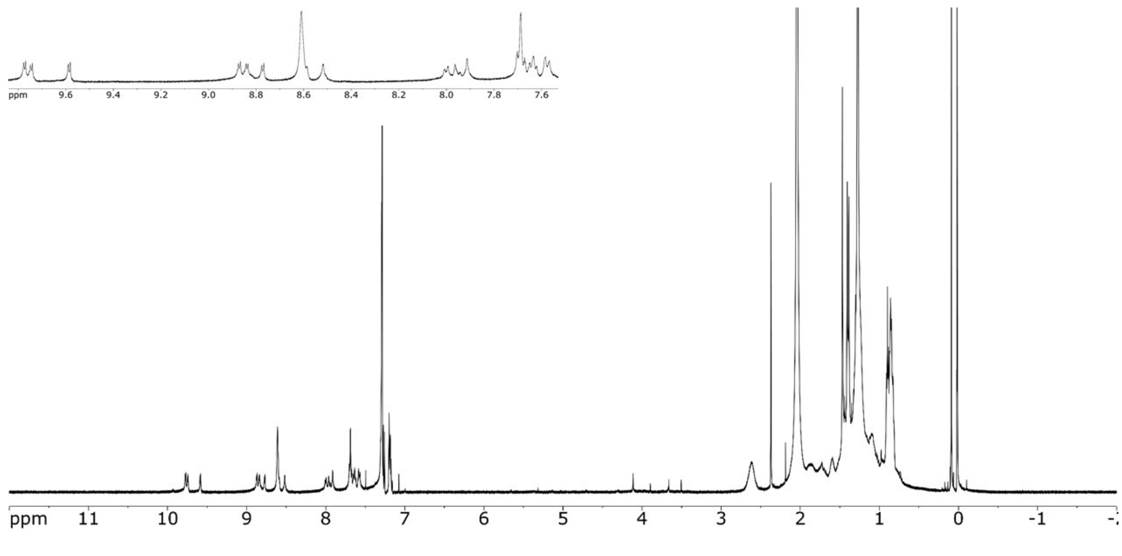


ZnCP (5.0 mg, 1.9 µmol) and $\mathbf{T_3}$ (n = 8) (0.624 mg, 0.637 µmol) from a stock solution was added to a round bottom flask, after which a solvent was removed under vacuum. These compounds were dissolved in CH_2Cl_2 (500 mL) followed by slow addition of CuCl (680 mg, 6.87 mmol) and TMEDA (790 µL, 5.15 mmol). The solution was stirred at r.t. for 45 min under air. Another tubulation of **ZnCP** (11.0 mg, 4.2 µmol) was conducted under the same condition (concentration, equivalents of reagents to **ZnCP**, and temperature) as the above. The combined reaction mixture was carefully extracted by NH_4Cl aq. with TMEDA once and NH_4Cl aq. once, water once, and brine once to remove copper residue from the solution. The organic layer was dried by Na_2SO_4, then the solvent was removed *in vacuo*. The residue was filtered through silica gel (CH_2Cl_2 / EtOAc / pyridine = 100 / 10 / 1, v / v / v) to remove $\mathbf{T_3}$ (n = 8) from $\mathbf{ZnCP_3}$. The crude product was purified by GPC (toluene / pyridine = 100 / 3, v / v) to afford $\mathbf{ZnCP_3}$ (2.4 mg, 10%).

HR-MS(MALDI-TOF MS) (m/z) 7846.62 ([$\mathbf{ZnCP_3}$+H]$^+$, $C_{492}H_{437}N_{24}O_{48}Zn_6$, calcd. 7844.8304)

^1H NMR (500 MHz, $CDCl_3$(+ 1 % pyridine-d_5), r. t.) δ :9.76 (d, J = 4.1 Hz, 8H, β-*H*), 9.73 (d, J = 4.3 Hz, 8H, β-*H*), 9.57, (d, J = 4.3 Hz, 8H, β-*H*), 8.86 (d, J = 4.3 Hz, 8H, β-*H*), 8.83 (d, J = 4.1 Hz, 8H, β-*H*), 8.76 (d, J = 4.2 Hz, 8H, β-*H*), 8.57 (s, 4H, Ar-*H*), 8.50 (s, 8H, Ar-*H*), 7.98 (d, J = 7.2, 8H, Ar-*H*), 7.95-7.92 (a double doublet peak and a singlet peak overlapped, 8H, Ar-*H*), 7.90 (s, 8H, Ar-*H*), 7.69-7.65 (two doublet peaks and residual peaks overlapped, 12H, Ar-*H*), 7.63-7.60 (two doublet peaks overlapped, 12H, Ar-*H*), 7.57-7.50 (two doublet peaks overlapped, 12H, Ar-*H*), 4.09 (s, 4H), 2.67-2.53(m, methylene protons), 1.92-1.53(m, methylene protons), 1.45 (s, -$CH_2CH_2COOC(CH_3)_3$), 1.39 (s, -$CH_2CH_2COOC(CH_3)_3$), 1.3 (s, -$CH_2CH_2COOC(CH_3)_3$).

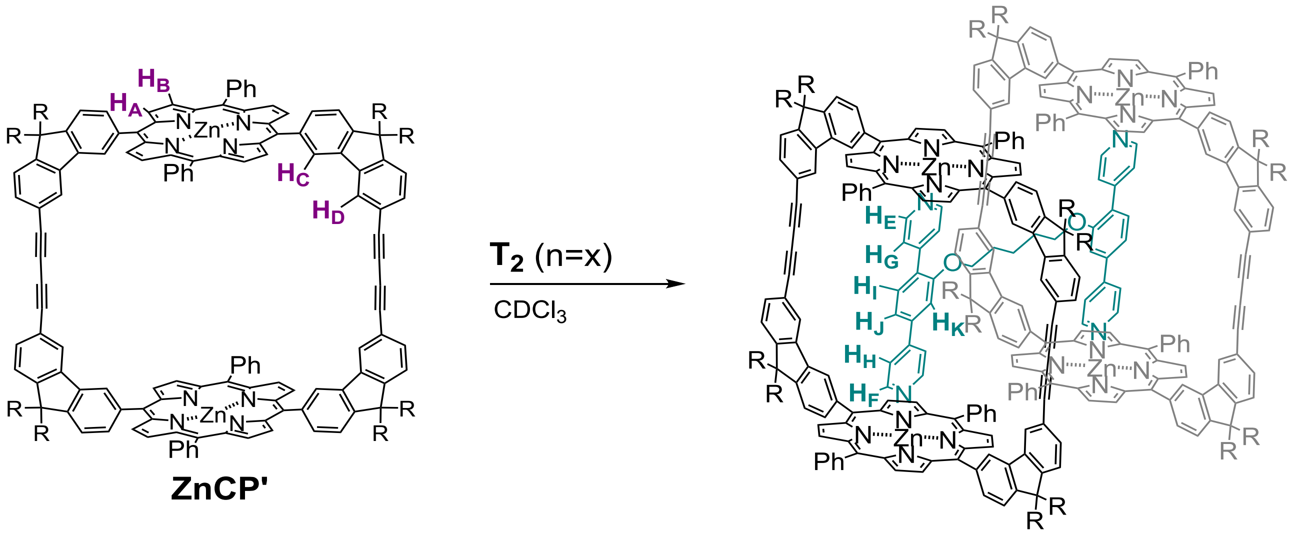
[1]H NMR spectrum of **ZnCP$_3$**



3. **Complexation study**

3.1 2:1 complexation between ZnCP and T_2 (n = x) by NMR titrations

Scheme S1. Complexation between **ZnCP'** and $\mathbf{T_2}$ (n = x).



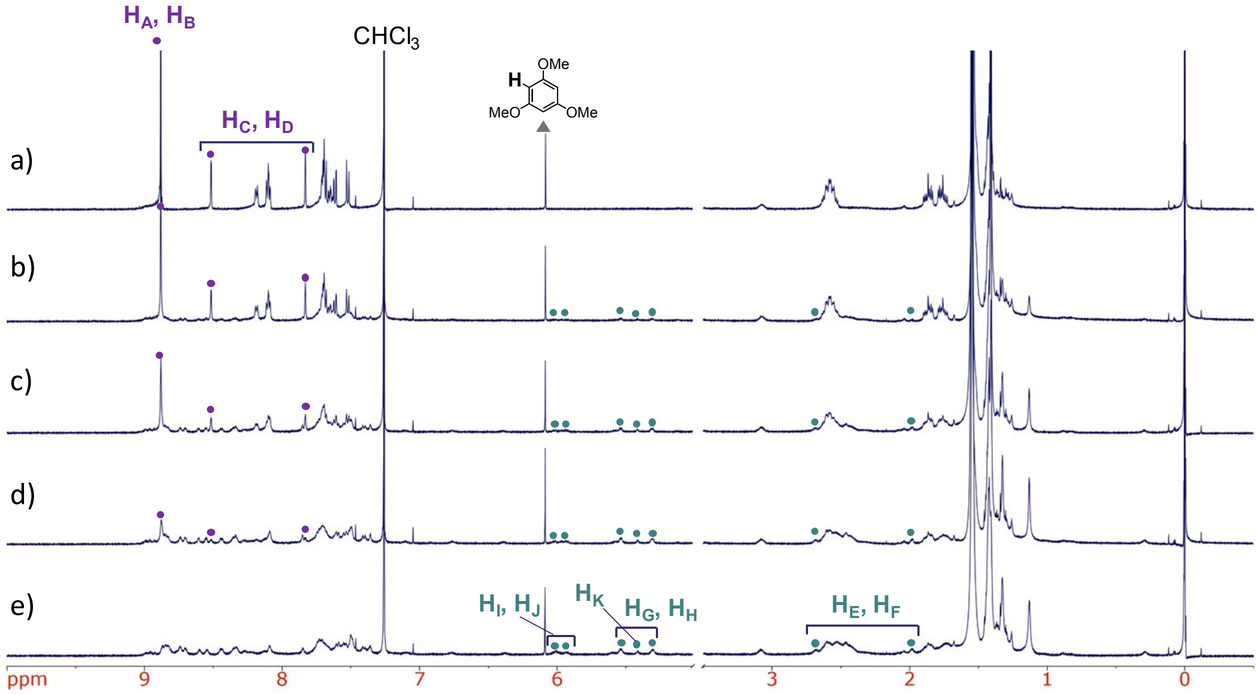


Figure S1. ^{1}H NMR titration of $\mathbf{T_2}$ (n = 4) to **ZnCP'** in $CDCl_3$.

a) 0 equiv., b) 0.125 equiv., c) 0.250 equiv., d) 0.375 equiv., e) 0.500 equiv.

1,3,5-trimethoxybenzene (gray) was added as an internal standard.

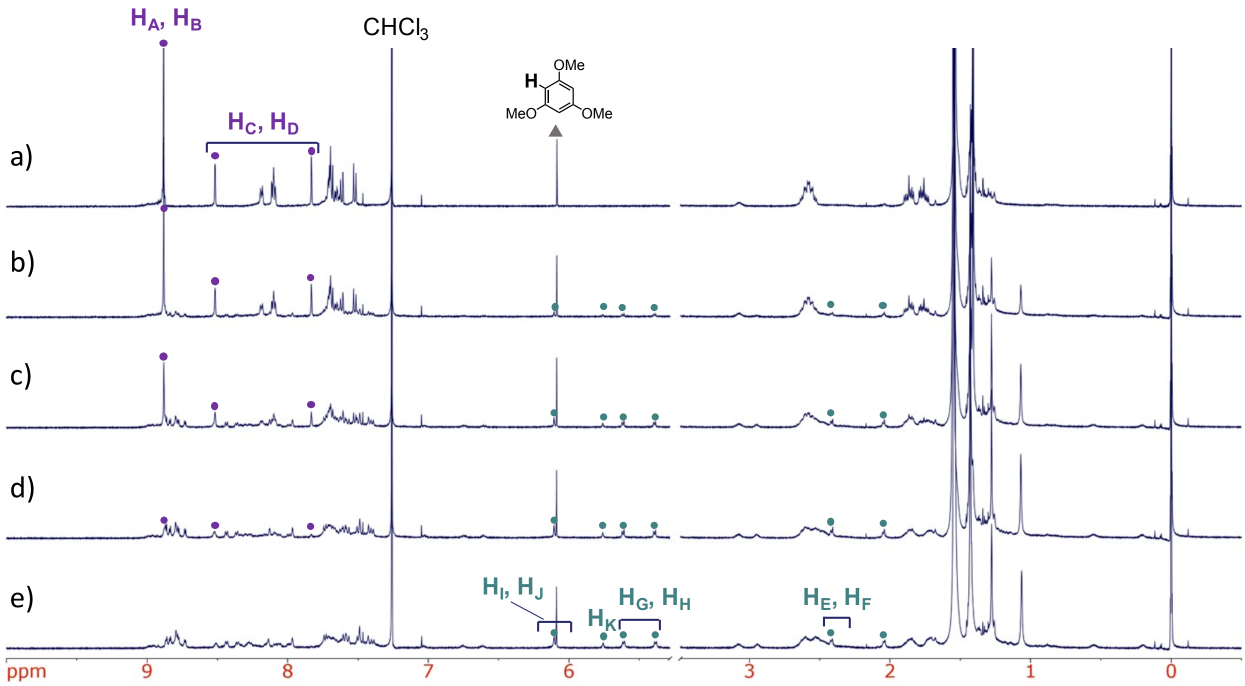


Figure S2. [1]H NMR titration of $\mathbf{T_2}$ (n = 6) to **ZnCP'** in $CDCl_3$.

a) 0 equiv., b) 0.125 equiv., c) 0.250 equiv., d) 0.375 equiv., e) 0.500 equiv.

1,3,5-trimethoxybenzene (gray) was added as an internal standard.

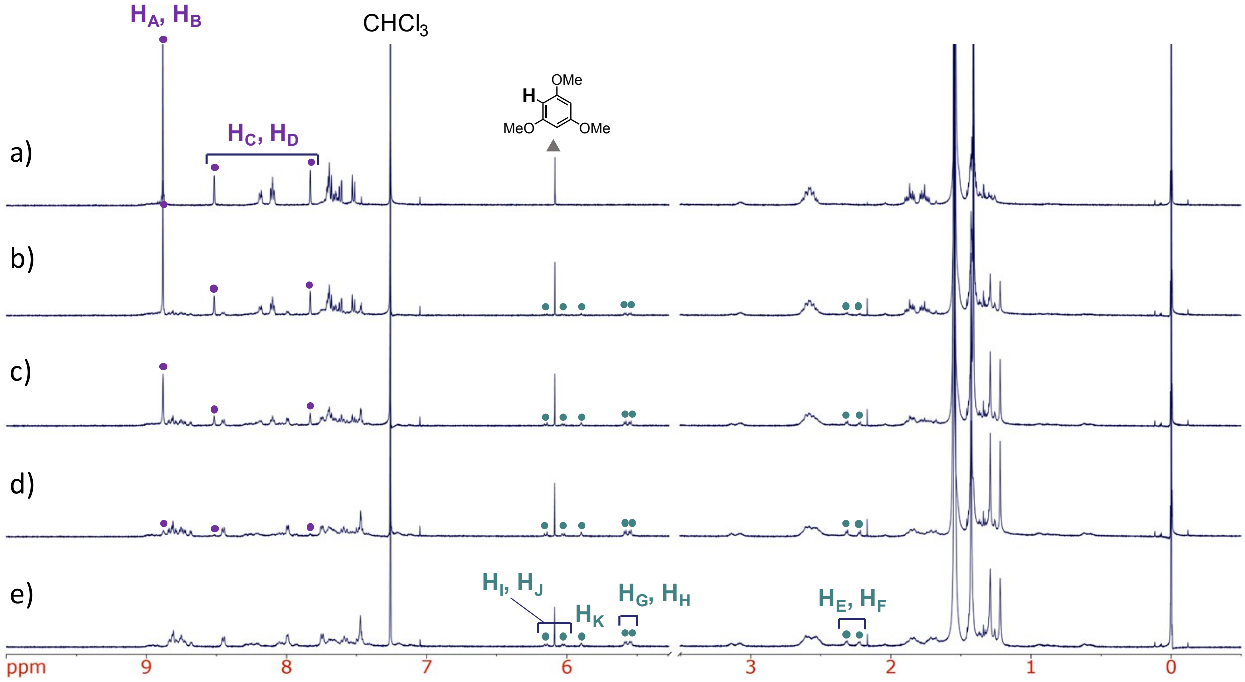


Figure S3. [1]H NMR titration of $\mathbf{T_2}$ (n = 8) to **ZnCP'** in $CDCl_3$.

a) 0 equiv., b) 0.125 equiv., c) 0.250 equiv., d) 0.375 equiv., e) 0.500 equiv.

1,3,5-trimethoxybenzene (gray) was added as an internal standard.

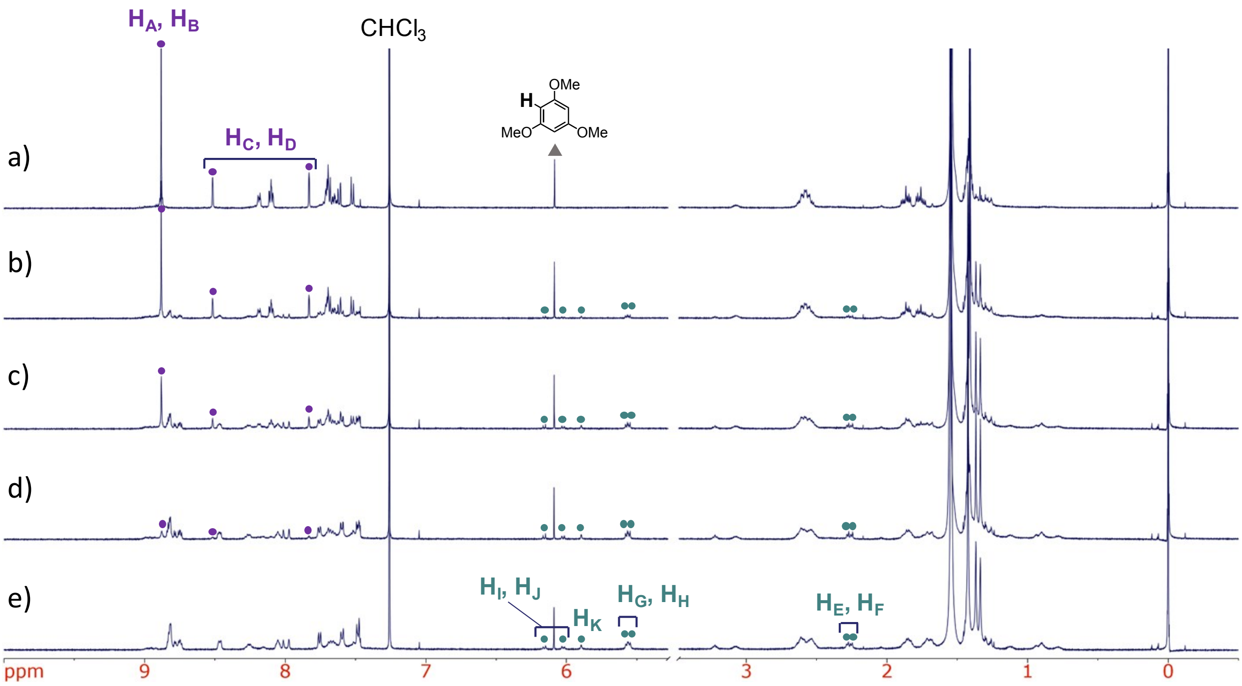


Figure S4. [1]H NMR titration of $\mathbf{T_2}$ (n = 12) to **ZnCP'** in $CDCl_3$.
a) 0 equiv., b) 0.125 equiv., c) 0.250 equiv., d) 0.375 equiv., e) 0.500 equiv.
1,3,5-trimethoxybenzene (gray) was added as an internal standard.

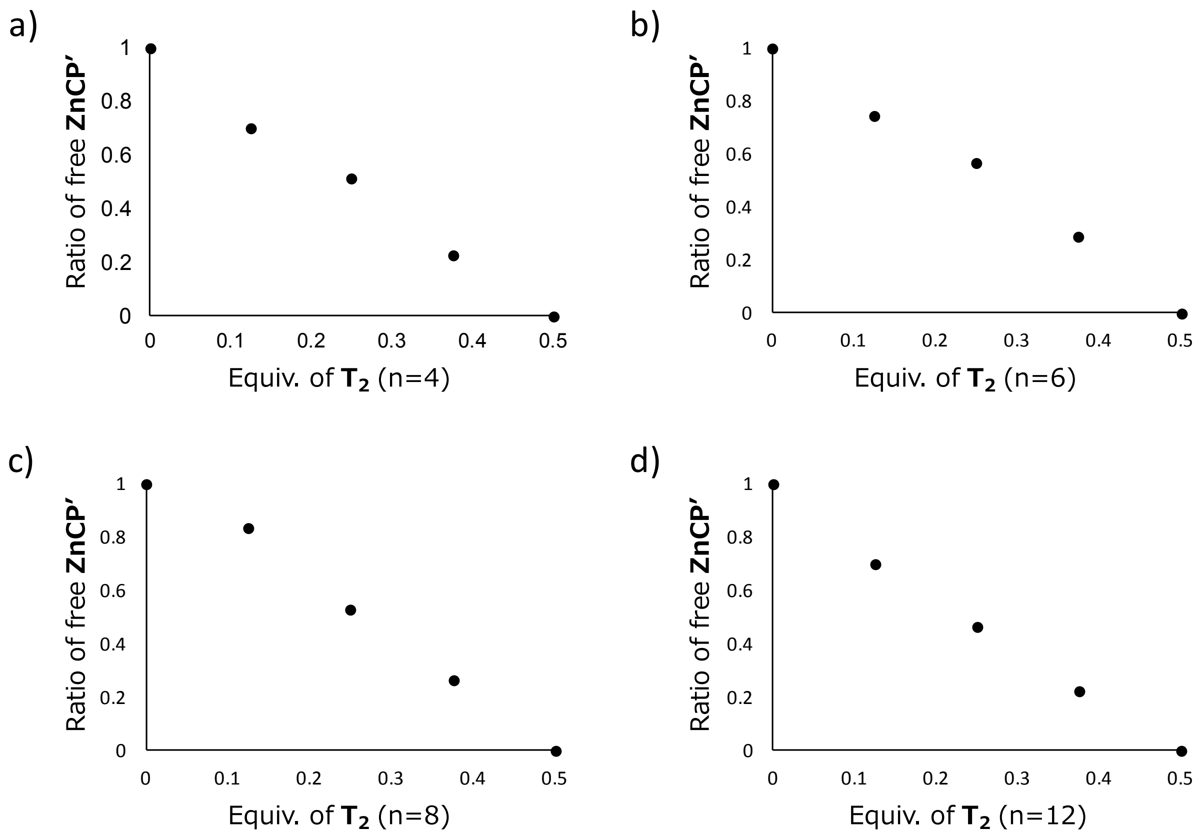
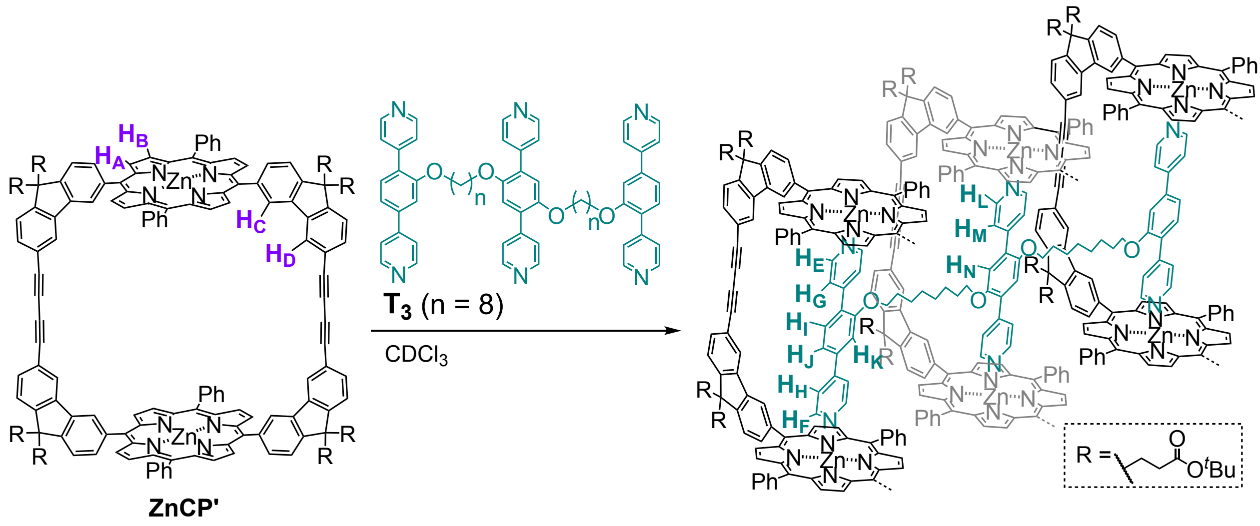


Figure S5. Conversion ratio of free **ZnCP'** in [1]H NMR titration of $\mathbf{T_2}$ (n = x) to **ZnCP'** in $CDCl_3$.
a) $\mathbf{T_2}$ (n = 4), b) $\mathbf{T_2}$ (n = 6), c) $\mathbf{T_2}$ (n = 8), d) $\mathbf{T_2}$ (n = 12)

3.2 3:1 complexation between ZnCP and T_3 (n = 8) by NMR titrations

Scheme S2. Complexation between **ZnCP'** and $\mathbf{T_3}$ (n = 8).



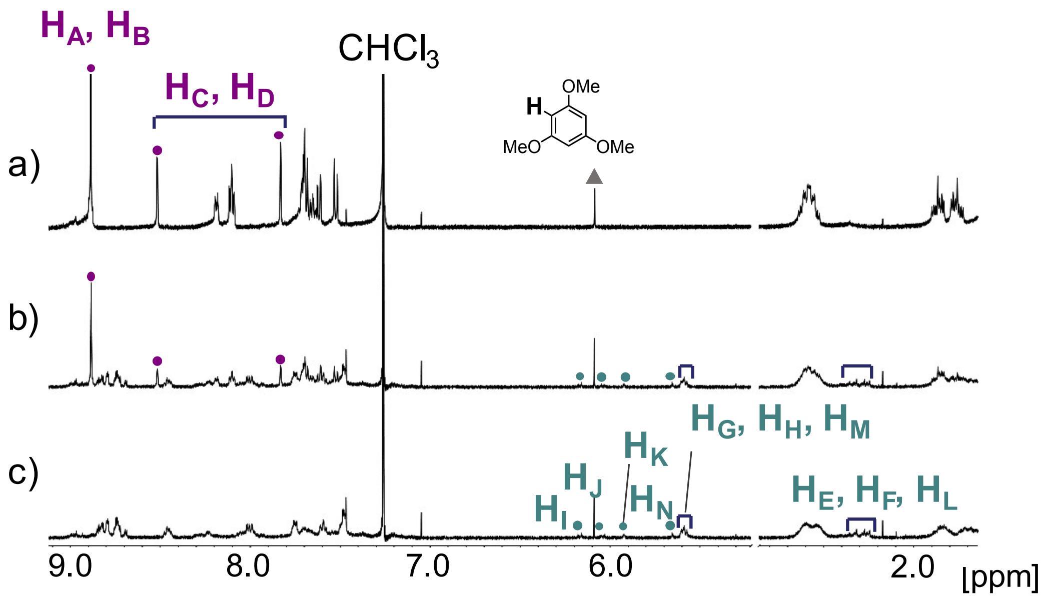


Figure S6. [1]H NMR titration of $\mathbf{T_3}$ (n = 8) to **ZnCP'** in $CDCl_3$.

a) 0 equiv., b) 0.13 equiv., c) 0.33 equiv.

1,3,5-trimethoxybenzene (gray) was added as an internal standard.

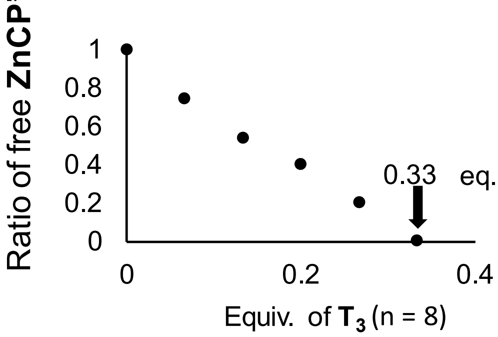


Figure S7. Conversion of **ZnCP'** in [1]H NMR titration of $\mathbf{T_3}$ (n = 8) to **ZnCP'** in $CDCl_3$.

4. Investigation of Template Synthesis

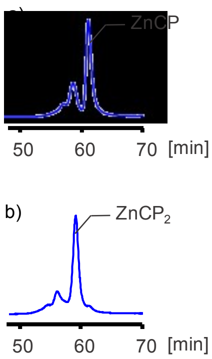


Figure S8. SEC chromatograms for synthesis of **ZnCP$_2$** in the presence of templates (Eluent : THF, detection : 420 nm). Templates: (a) **T$_2$’** (n = 6) and (b) **T$_2$** (n = 6)

5. Binding study

The simple two-state 2-site model was applied to indirectly determine the binding constant K_f for **ZnCP'(T$_1$)**. The titration of **ZnCP'(T$_1$)** with imidazole **(Im)** was analyzed assuming that each pyridyl unit of **T$_1$** binds independently, so that the equilibrium can be treated as the displacement of a 2-site ligand **T$_1$** from a 2-site receptor **ZnCP’.**

$$\mathbf{ZnCP'(T_1) + 2Im} \xrightleftharpoons{K_d} \mathbf{ZnCP'(Im)_2 + T_1}$$

$$K_d = \frac{[ZnCP'(Im)_2][T_1]}{[ZnCP'(T_1)][Im]^2} \qquad \text{(S1)}$$

The denaturation equilibrium constant, K_d, defined by equation (S1) was determined by fitting the binding isotherm to equation (S2).

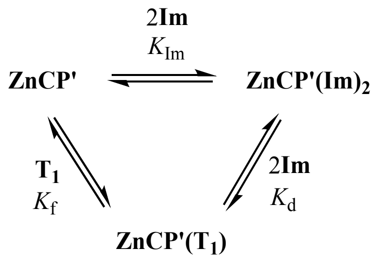
$$\Delta A = \frac{L(-K_d[Im]^2 + \sqrt{K_d^2[Im]^2 + 4K_d[Im]^2[ZnCP'(T_1)]_0})}{2[ZnCP'(T_1)]_0} \qquad \text{(S2)}$$

where ΔA is the change of absorption at any point in the titration, L is ΔA at 100 % complexation, [**Im**] is the total concentration of imidazole at each point in the titration and [**ZnCP'(T$_1$)**]$_0$ is the initial concentration of **ZnCP'(T$_1$)**. To determine the 1 : 1 formation constant between **ZnCP’** and **T$_1$**, denoted K_f, the following thermodynamic cycle was used:

Comment [A]: K の後の下付き文字は非斜体
全体的にチェックを

Comment [A]: ＋　－　×　は全て両側にスペースを入れる

Comment [A]: A の前に文字化け
Kdn が定義されていない
ZnCP ‘（T1）の’が全角？



The addition of excess imidazole, **Im** to **ZnCP'(T$_1$)** results in the displacement of the ligand **T$_1$** from **ZnCP'**, to generate **ZnCP'(Im)$_2$**. The formation constant K_f can be calculated using equation (S3),

Comment [A]: The xxx equilibrium constant, Kf can be….

$$K_f = \frac{K_{Im}^2}{K_d} \qquad \text{(S3)}$$

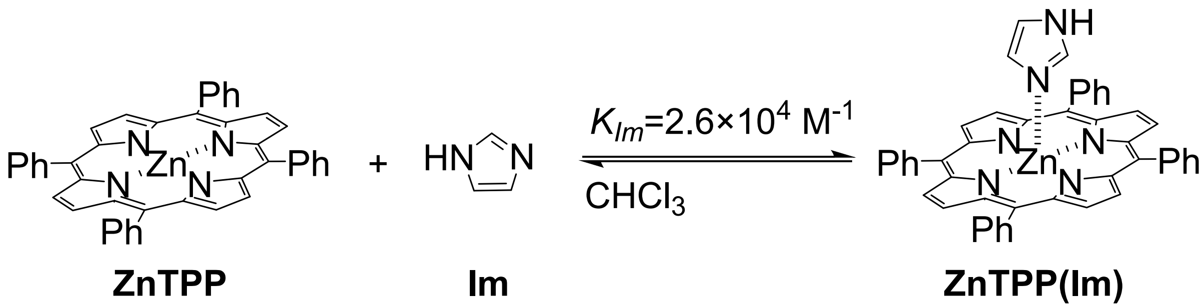
The binding constant, K_{Im} was determined by fitting the binding isotherm to equation (S4).

$$\Delta A = \frac{L(1 + K_{Im}[Im] + K_{Im}[ZnCP'(T_1)]_0 - \sqrt{L^2(K_{Im}[Im] + K_{Im}[ZnCP'(T_1)]_0)^2 - 4K_{Im}^2[Im][ZnCP'(T_1)]_0 L^2})}{2K_{Im}[Im]} \qquad \text{(S4)}$$

The value of K_{Im} obtained from fitting the binding isotherms (S4) at 423 nm to a 1 : 1 binding model for **ZnTPP** and **Im** (Scheme S3, Figure S9) instead of **ZnCP'** and **Im** is $K_{Im} = 2.6 \times 10^4$ M^{-1}.

In the case of denaturation equilibrium constant K_d obtained from fitting the binding isotherms (S2) at 436 nm is $K_d = 3.9$ M^{-1} (Scheme S4, Figure S10). The value of K_f obtained from equation (S3) was 1.7×10^8 M^{-1}.

Scheme S3. Complexation of **ZnTPP** with imidazole (**Im**) in $CHCl_3$



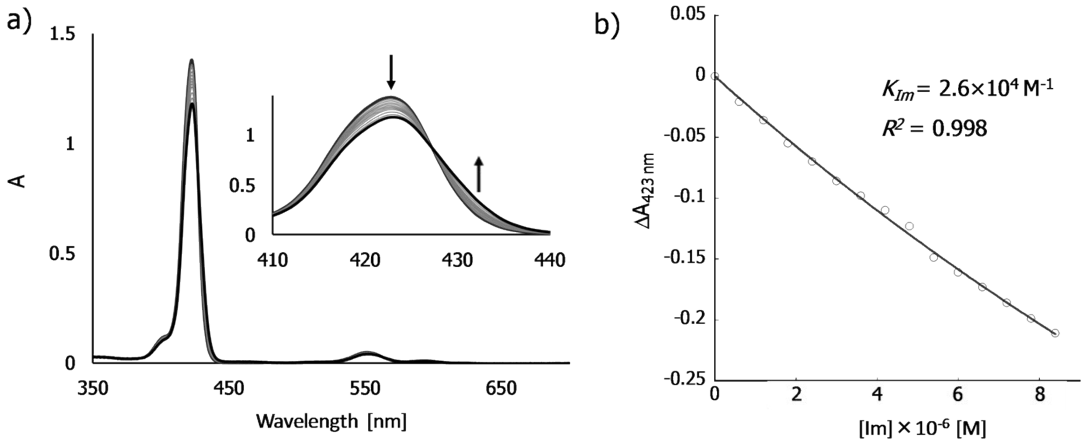
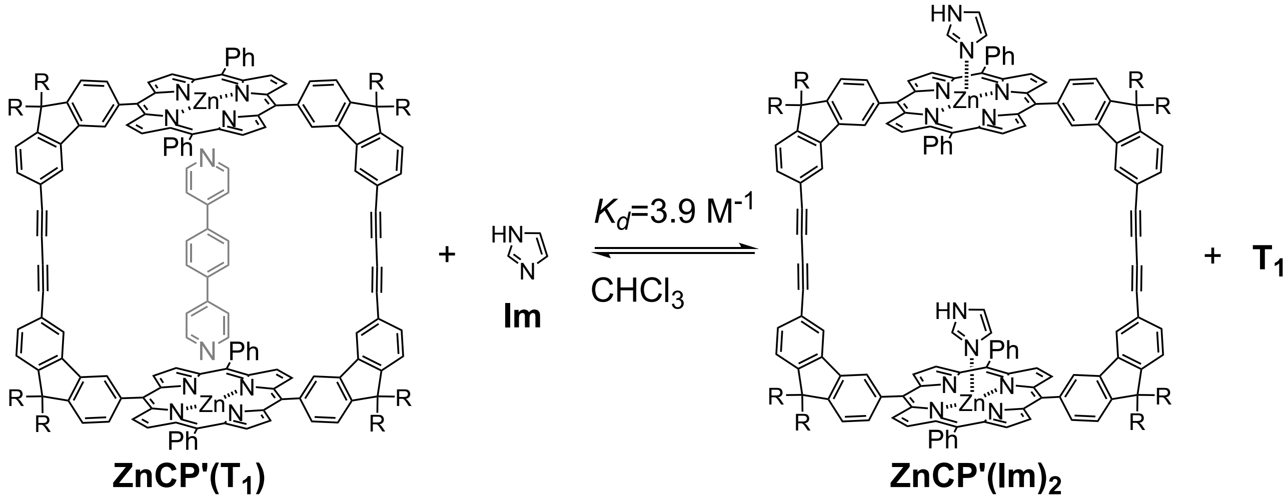


Figure S9. a) UV titration of imidazole, **Im** with 5,10,15,20-tetraphenyl-zinc-porphyrin, **ZnTPP** (6.0×10^{-6} M, r. t., $CHCl_3$). Arrows indicate areas of increasing and decreasing absorption during the titration. b) The data at 423 nm were fitted to a 1 : 1 binding isotherm to give a binding constant of $K_{Im} = 2.6 \times 10^4\ M^{-1}$.

Scheme S4. Displacement of the ligand $\mathbf{T_1}$ from **ZnCP'** by imidazole in $CHCl_3$



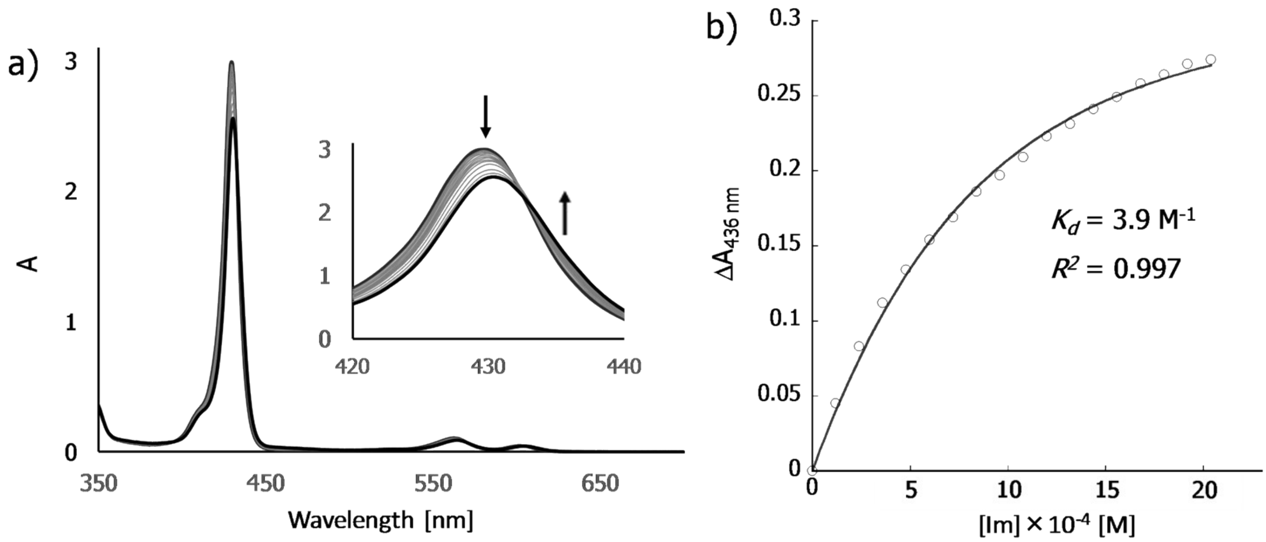


Figure S10. a) UV titration of imidazole, **Im** with **ZnCP’** (3.0×10^{-6} M, r. t., $CHCl_3$). Arrows indicate areas of increasing and decreasing absorption during the titration. b) The data at 436 nm were fitted to a 1 : 1 binding isotherm (S2) to give a binding constant of $K_d = 3.9$ M^{-1}.

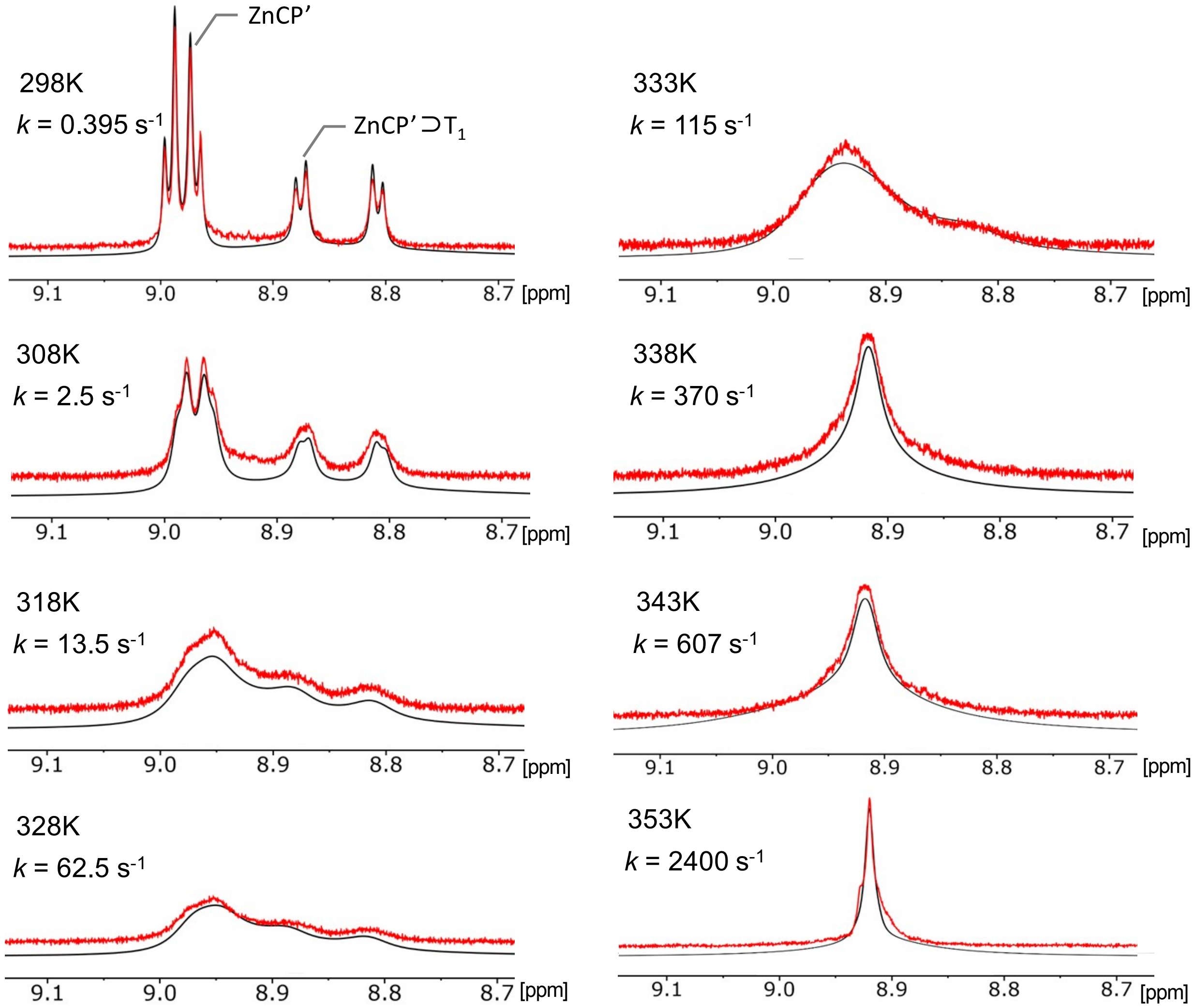


Figure S10. Experimental (red) and theoretical (black) splitting of β-H of **ZnCP'** and **ZnCP'⊃T$_1$** in ^{1}H VT-NMR in toluene-d_8. k means rate constants of ligand exchange at different temperatures.

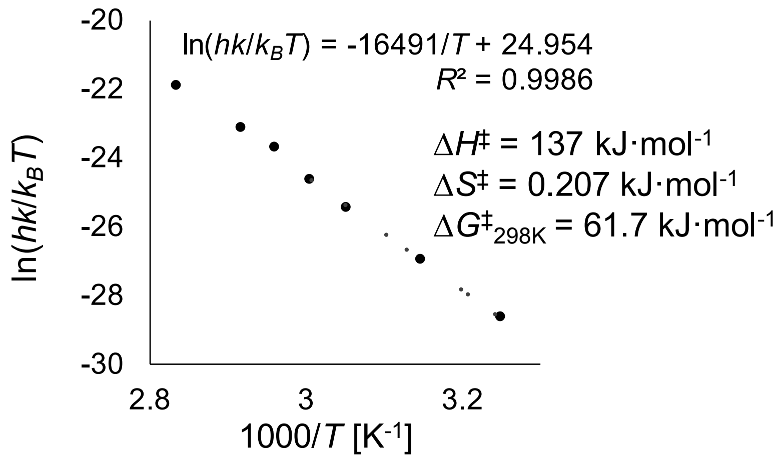


Figure S11. Eyring plot for the ligand exchange reaction between **ZnCP'** and **ZnCP'⊃T$_1$**.

6. Computational Study

Method

The optimized geometries of **ZnCP** and **ZnCP$_2$** were calculated at the B3LYP level of theory employing the 6-31G(d,p) for carbons, hydrogens, and oxygens and 6-31G+(d) for nitrogens and Lanl2DZ for zincs, neglecting ester groups and terminal alkynes of **ZnCP** and ester groups of **ZnCP$_2$** in the calculation. Stable structures of **T$_2$** (n = x) were calculated at the B3LYP level of theory using the 6-31G(d) for carbons, hydrogens and nitrogens. All DFT calculations were carried out using Gaussian 09.[7]

DFT optimized structure

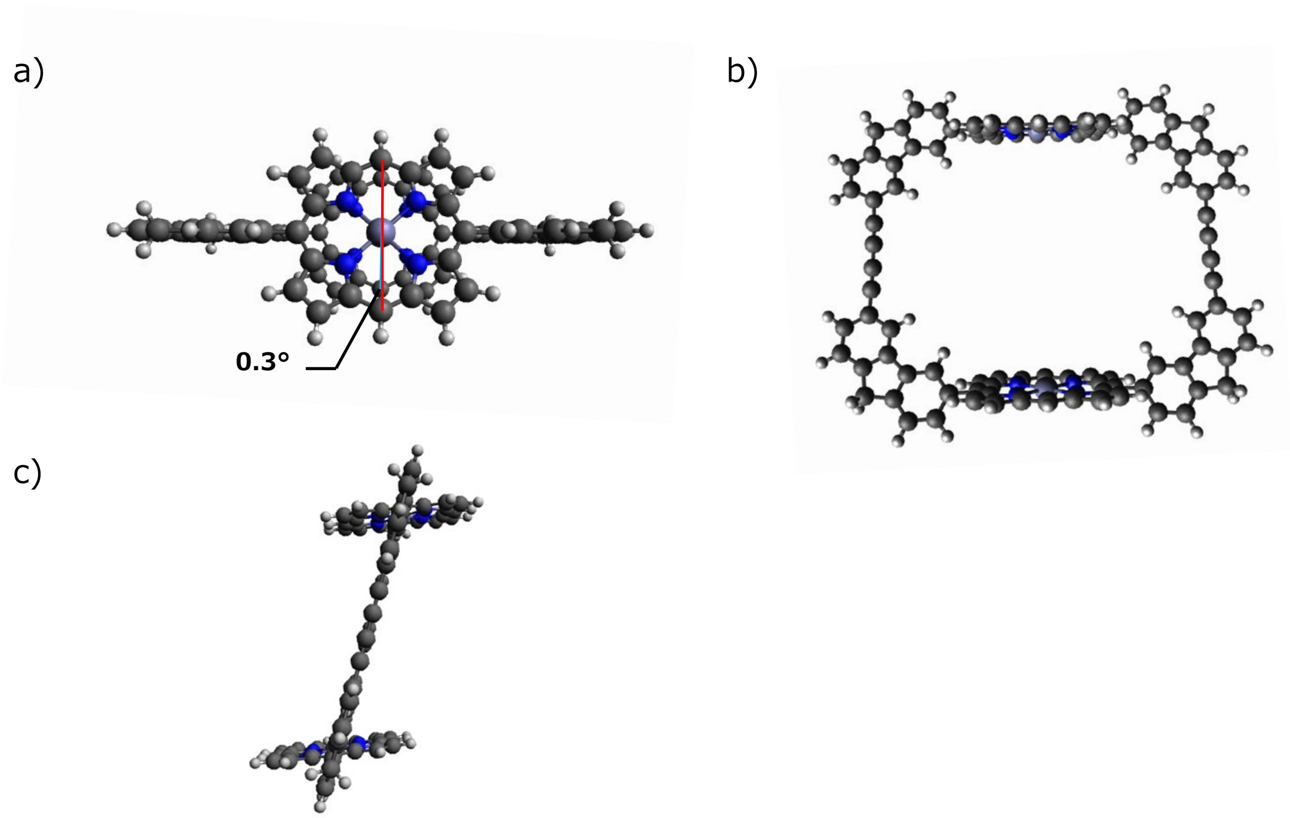


Figure S12. The optimized structure of **ZnCP**.

a) top view, b) front view, c) side view

C = dark gray; H = light gray; N = blue; Zn = purple. Hydrogen atoms are used in the calculation instead of allyl ester groups of fluorenes for simplicity.

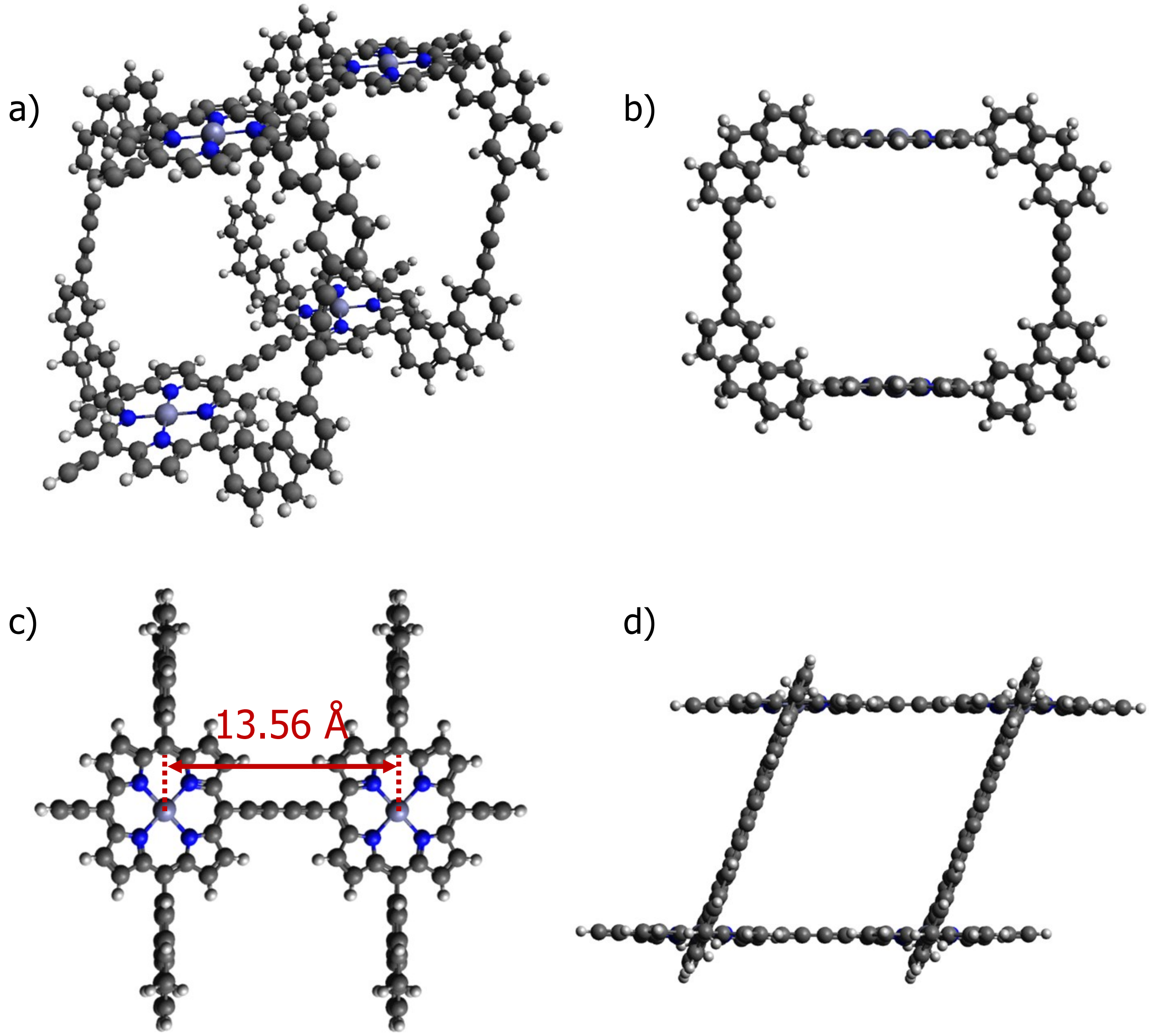


Figure S13. The optimized structure of **$ZnCP_2$**.

a) slanting view, b) front view, c) top view, d) side view

Arrow indicates the distance between two zincs. C = dark gray; H = light gray; N = blue; Zn = purple. Hydrogen atoms are used in the calculation instead of allyl ester groups of fluorenes for simplicity.

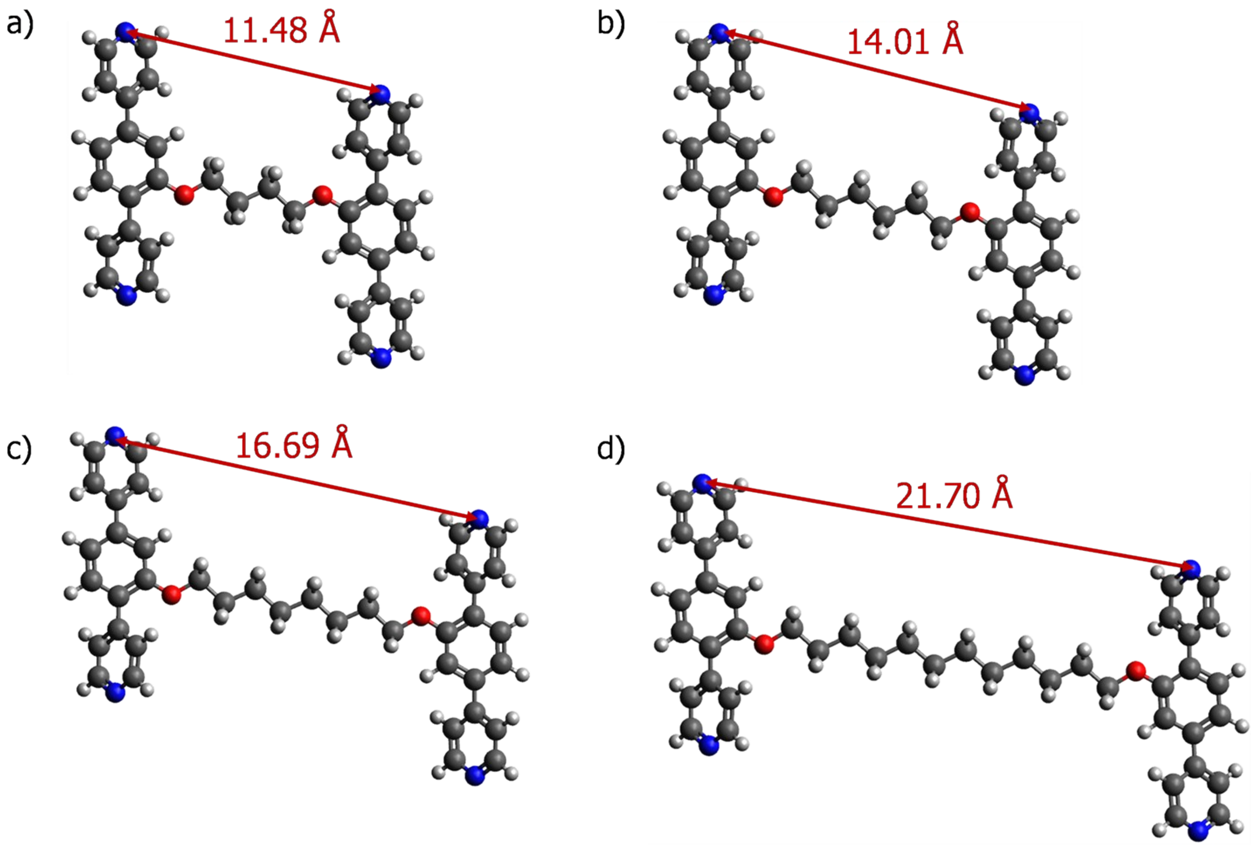


Figure S14. The optimized structures of $\mathbf{T_2}$ (n = x).

a) $\mathbf{T_2}$ (n = 4), b) $\mathbf{T_2}$ (n = 6), c) $\mathbf{T_2}$ (n = 8), d) $\mathbf{T_2}$ (n = 12)

Arrow indicates the distance between two nitrogens. C = dark gray; H = light gray; N = blue; O = red.

Computed Cartesian coordinates

1) ZnCP

B3LYP/6-31G(d) for C, H, O; 6-31G+(d) for N; Lanl2DZ for Zn

C	-2.48706	-6.58334	3.46489
C	-3.34218	-6.17822	2.48554
C	-2.67548	-6.40441	1.22766
N	-1.42529	-6.93109	1.44569
C	-1.28178	-7.04809	2.80963
C	3.09207	-8.84282	2.51074
C	2.2038	-8.49658	3.48333
C	1.00563	-8.03042	2.81643
N	1.18352	-8.09328	1.45343
C	2.44824	-8.5891	1.24632
C	-0.14964	-7.56128	3.47015

C	2.23794	-8.47745	-3.48734
C	3.11702	-8.82813	-2.508
C	2.46064	-8.58181	-1.2486
N	1.19767	-8.08564	-1.46539
C	1.03282	-8.01599	-2.82968
C	-3.32024	-6.17023	-2.53071
C	-2.45614	-6.57124	-3.50383
C	-1.25578	-7.03611	-2.83967
N	-1.41146	-6.92391	-1.47665
C	-2.66424	-6.39951	-1.26781
C	-0.11698	-7.54525	-3.49204
C	-2.2038	8.49658	3.48333
C	-3.09207	8.84282	2.51074
C	-2.44824	8.5891	1.24632
N	-1.18352	8.09328	1.45343
C	-1.00563	8.03042	2.81643
C	3.34218	6.17822	2.48554
C	2.48706	6.58334	3.46489
C	1.28178	7.04809	2.80963
N	1.42529	6.93109	1.44569
C	2.67548	6.40441	1.22766
C	0.14964	7.56128	3.47015
C	2.45614	6.57124	-3.50383
C	3.32024	6.17023	-2.53071
C	2.66424	6.39951	-1.26781
N	1.41146	6.92391	-1.47665
C	1.25578	7.03611	-2.83967
C	-3.11702	8.82813	-2.508
C	-2.23794	8.47745	-3.48734
C	-1.03282	8.01599	-2.82968
N	-1.19767	8.08564	-1.46539
C	-2.46064	8.58181	-1.2486
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C	-0.11629	-6.43089	-5.7578
C	-0.13578	-6.51912	-7.15066
C	-0.17011	-7.77497	-7.79038
C	-0.18466	-8.9416	-7.03598

C	-0.16587	-8.85073	-5.64169
C	-0.12274	-5.47112	-8.18251
C	-0.15117	-6.09088	-9.45049
C	-0.09032	-4.08331	-8.07129
C	-0.08615	-3.29972	-9.24401
C	-0.11539	-3.93353	-10.50732
C	-0.14786	-5.32337	-10.61002
C	-0.05209	-1.89336	-9.1722
C	-0.0203	-0.6442	-9.14855
C	0.13222	7.60479	-4.989
C	0.16587	8.85073	-5.64169
C	0.18466	8.9416	-7.03598
C	0.17011	7.77497	-7.79038
C	0.13578	6.51912	-7.15066
C	0.11629	6.43089	-5.7578
C	0.15117	6.09088	-9.45049
C	0.12274	5.47112	-8.18251
C	0.14786	5.32337	-10.61002
C	0.11539	3.93353	-10.50732
C	0.08615	3.29972	-9.24401
C	0.09032	4.08331	-8.07129
C	0.05209	1.89336	-9.1722
C	0.0203	0.6442	-9.14855
C	0.18069	7.60265	4.99514
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C	0.2184	6.08843	9.45616
C	0.12192	4.08181	8.07729
C	0.11795	3.29799	9.24988
C	0.16446	3.93139	10.5129
C	0.21435	5.32071	10.61553
C	0.06773	1.89132	9.17869
C	0.02298	0.64397	9.15642
C	-0.18069	-7.60265	4.99514

C	-0.23198	-8.84813	5.6475
C	-0.26366	-8.93875	7.04158
C	-0.24284	-7.77228	7.79602
C	-0.1901	-6.51693	7.15661
C	-0.15954	-6.42887	5.76393
C	-0.2184	-6.08843	9.45616
C	-0.17279	-5.46908	8.18848
C	-0.21435	-5.32071	10.61553
C	-0.16446	-3.93139	10.5129
C	-0.11795	-3.29799	9.24988
C	-0.12192	-4.08181	8.07729
C	-0.06773	-1.89132	9.17869
C	-0.02298	-0.64397	9.15642
H	-2.65171	-6.5773	4.53187
H	-4.33943	-5.77292	2.59562
H	4.09583	-9.22906	2.63001
H	2.34263	-8.53847	4.5532
H	2.38729	-8.51364	-4.556
H	4.12227	-9.21283	-2.61957
H	-4.31722	-5.7664	-2.64841
H	-2.61198	-6.56271	-4.57208
H	-2.34263	8.53847	4.5532
H	-4.09583	9.22906	2.63001
H	4.33943	5.77292	2.59562
H	2.65171	6.5773	4.53187
H	2.61198	6.56271	-4.57208
H	4.31722	5.7664	-2.64841
H	-4.12227	9.21283	-2.61957
H	-2.38729	8.51364	-4.556
H	-0.08131	-5.46654	-5.25957
H	-0.21503	-9.91625	-7.51591
H	-0.18509	-9.75559	-5.04235
H	-0.06775	-3.59371	-7.10313
H	-0.1121	-3.31802	-11.40051
H	-0.17022	-5.79297	-11.58956
H	0.18509	9.75559	-5.04235
H	0.21503	9.91625	-7.51591
H	0.08131	5.46654	-5.25957

H	0.17022	5.79297	-11.58956
H	0.1121	3.31802	-11.40051
H	0.06775	3.59371	-7.10313
H	0.11216	5.46475	5.26623
H	0.30857	9.91292	7.52134
H	0.25483	9.75279	5.04801
H	0.08432	3.59312	7.10911
H	0.1603	3.31589	11.40608
H	0.24919	5.78992	11.5949
H	-0.25483	-9.75279	5.04801
H	-0.30857	-9.91292	7.52134
H	-0.11216	-5.46475	5.26623
H	-0.24919	-5.78992	11.5949
H	-0.1603	-3.31589	11.40608
H	-0.08432	-3.59312	7.10911
C	3.23751	6.14577	-0.00126
H	4.23885	5.72582	-0.00703
C	-3.02682	8.82068	0.03496
H	-4.03663	9.21982	0.04076
C	3.02682	-8.82068	0.03496
H	4.03663	-9.21982	0.04076
C	-3.23751	-6.14577	-0.00126
H	-4.23885	-5.72582	-0.00703
C	0.17986	7.63741	-9.26659
H	1.07438	8.07936	-9.72575
H	-0.68301	8.12131	-9.74367
C	0.26668	7.59309	9.29937
H	1.1702	8.02367	9.75171
H	-0.58643	8.08397	9.78676
C	-0.26668	-7.59309	9.29937
H	0.58643	-8.08397	9.78676
H	-1.1702	-8.02367	9.75171
C	-0.17986	-7.63741	-9.26659
H	-1.07438	-8.07936	-9.72575
H	0.68301	-8.12131	-9.74367
Zn	0.11473	7.50309	0.01673
Zn	-0.11473	-7.50309	0.01673

2) **$ZnCP_2$**

B3LYP/6-31G(d) for C, H, O; 6-31G+(d) for N; Lanl2DZ for Zn

C	-2.19721	-6.50079	-3.50517
C	-3.09489	-6.17936	-2.53013
C	-2.45921	-6.45392	-1.26289
N	-1.19594	-6.94649	-1.48224
C	-1.00287	-6.99026	-2.8428
C	3.42421	-8.70946	-2.50581
C	2.53966	-8.37028	-3.48698
C	1.34833	-7.86341	-2.8325
N	1.53159	-7.90967	-1.47114
C	2.78707	-8.41824	-1.24314
C	0.17844	-7.41862	-3.4894
C	2.55069	-8.27207	3.51225
C	3.43148	-8.63905	2.53773
C	2.79003	-8.38259	1.2699
N	1.53568	-7.86698	1.48748
C	1.35748	-7.78225	2.8481
C	-3.08374	-6.10139	2.51121
C	-2.18314	-6.39439	3.49248
C	-0.99195	-6.90604	2.84118
N	-1.18978	-6.90341	1.48013
C	-2.45314	-6.41595	1.25088
C	0.19076	-7.31705	3.49624
C	-12.6047	-17.4435	-3.34052
C	-13.4895	-17.0725	-2.37115
C	-12.8527	-17.3223	-1.0995
N	-11.5971	-17.838	-1.31048
C	-11.4136	-17.9287	-2.66956
C	-6.97043	-19.602	-2.31132
C	-7.86788	-19.3126	-3.29655
C	-9.06237	-18.8017	-2.6508
N	-8.86961	-18.8011	-1.28948
C	-7.60639	-19.2862	-1.05387
C	-10.2435	-18.3947	-3.31132
C	-7.88355	-19.1904	3.70084
C	-6.98273	-19.5153	2.72986
C	-7.61303	-19.242	1.45979

N	-8.87645	-18.7474	1.67271
C	-9.07459	-18.7003	3.0329
C	-13.4979	-16.9781	2.67199
C	-12.6174	-17.3131	3.65819
C	-11.424	-17.8243	3.01066
N	-11.6019	-17.7841	1.64796
C	-12.8562	-17.2758	1.41336
C	-10.2575	-18.2681	3.67392
C	0.21983	-7.23894	4.99208
C	-0.59431	-8.07313	5.775
C	-0.54535	-7.97455	7.16682
C	0.31241	-7.04606	7.79153
C	1.12134	-6.21685	7.02337
C	1.07113	-6.31779	5.6302
C	-1.27123	-8.71463	8.21091
C	-0.85537	-8.23255	9.47121
C	-2.22132	-9.72854	8.11617
C	-2.76669	-10.2718	9.29855
C	-2.34186	-9.77985	10.55414
C	-1.39048	-8.76475	10.63995
C	-3.73819	-11.3088	9.24472
C	-4.57133	-12.2022	9.24024
C	-10.2869	-18.2973	5.1715
C	-11.1383	-19.1971	5.83917
C	-11.1888	-19.2525	7.23488
C	-10.3801	-18.3987	7.97574
C	-9.52218	-17.4911	7.32123
C	-9.4729	-17.438	5.92695
C	-9.21269	-17.1579	9.61604
C	-8.79653	-16.7173	8.34076
C	-8.67785	-16.5879	10.7669
C	-7.72644	-15.5761	10.6482
C	-7.30132	-15.1254	9.37731
C	-7.84642	-15.707	8.21318
C	-6.3298	-14.0907	9.28986
C	-5.49666	-13.198	9.2564
C	-10.2668	-18.4784	-4.80685
C	-9.45511	-17.6418	-5.58966

C	-9.49843	-17.7456	-6.98125
C	-10.3478	-18.6819	-7.60573
C	-11.1543	-19.5135	-6.83763
C	-11.11	-19.4071	-5.44467
C	-8.77386	-17.0043	-8.02533
C	-9.18175	-17.4936	-9.28542
C	-7.8315	-15.9833	-7.93046
C	-7.28569	-15.44	-9.11257
C	-7.70242	-15.9392	-10.368
C	-8.64618	-16.9615	-10.454
C	-6.32183	-14.3958	-9.05822
C	-5.49308	-13.4984	-9.0517
C	0.2021	-7.38389	-4.98687
C	1.04544	-6.47645	-5.65448
C	1.09006	-6.41564	-7.05016
C	0.28367	-7.27184	-7.79089
C	-0.56582	-8.18727	-7.13635
C	-0.60946	-8.24559	-5.74212
C	-0.88197	-8.51437	-9.43113
C	-1.29015	-8.96225	-8.15583
C	-1.41728	-9.08441	-10.5818
C	-2.36105	-10.1033	-10.4627
C	-2.77808	-10.5613	-9.19174
C	-2.23254	-9.97961	-8.02788
C	-3.74195	-11.6031	-9.10354
C	-4.5707	-12.4999	-9.06791
H	-2.32453	-6.40977	-4.57369
H	-4.09382	-5.78115	-2.65261
H	4.41617	-9.12678	-2.62131
H	2.672	-8.46339	-4.55474
H	2.68662	-8.3357	4.58172
H	4.4236	-9.05381	2.66099
H	-4.08153	-5.69758	2.6247
H	-2.30632	-6.2703	4.55813
H	-12.7368	-17.3853	-4.41078
H	-14.4815	-16.6591	-2.50044
H	-5.97146	-20.004	-2.42051
H	-7.74031	-19.4385	-4.3615

H	-7.76061	-19.2796	4.77
H	-5.98496	-19.9152	2.85671
H	-14.4901	-16.5596	2.78141
H	-12.7536	-17.2146	4.72497
H	-1.24735	-8.79185	5.2885
H	1.78389	-5.49341	7.4916
H	1.69331	-5.67005	5.02012
H	-2.5494	-10.1088	7.15411
H	-2.76996	-10.2072	11.45474
H	-1.07551	-8.39876	11.61368
H	-11.7604	-19.8645	5.25042
H	-11.8515	-19.9603	7.72634
H	-8.81975	-16.7356	5.41738
H	-8.99304	-16.9219	11.75198
H	-7.29854	-15.1196	11.53446
H	-7.51812	-15.3583	7.23929
H	-8.8084	-16.9174	-5.10313
H	-11.8106	-20.2427	-7.30579
H	-11.7305	-20.0563	-4.83438
H	-7.50991	-15.5975	-6.96839
H	-7.27421	-15.5118	-11.2686
H	-8.95487	-17.3327	-11.4277
H	1.66577	-5.80764	-5.06558
H	1.7464	-5.70209	-7.54174
H	-1.25629	-8.95373	-5.23234
H	-1.10836	-8.74512	-11.567
H	-2.78906	-10.5599	-11.3489
H	-2.55435	-10.3338	-7.0538
C	-7.03336	-19.4759	0.20814
C	-13.4245	-17.0695	0.1518
C	3.35857	-8.63004	0.01588
C	-3.03253	-6.22307	-0.00787
C	-10.2456	-18.2557	9.47734
H	-9.91772	-19.1901	9.95275
H	-11.1982	-17.9852	9.95287
C	-10.2079	-18.5928	-9.111
H	-9.87154	-19.5416	-9.55052
H	-11.1601	-18.3465	-9.59995

C	0.1441	-7.41011	-9.29247
H	1.0965	-7.67221	-9.7729
H	-0.1921	-6.47609	-9.76282
C	0.1776	-7.13995	9.29697
H	-0.15041	-6.19047	9.74154
H	1.13003	-7.39477	9.78131
Zn	-10.2351	-18.2921	0.17898
Zn	0.16921	-7.4072	0.00238
C	-14.8504	-16.488	0.13958
C	-15.9626	-16.0344	0.13004
C	-5.59942	-20.0374	0.22215
C	-4.48095	-20.4753	0.23307
H	-3.48465	-20.8654	0.2428
C	4.78451	-9.21163	0.02298
C	5.89675	-9.66527	0.02852
H	6.8875	-10.0694	0.03345
C	-4.46647	-5.66146	-0.01254
C	-5.58494	-5.2234	-0.01618
C	-7.01887	-4.66179	-0.02085
C	-8.13734	-4.22374	-0.02449
C	-9.57128	-3.66213	-0.02916
C	-10.1411	-3.4411	-1.28737
C	-10.1478	-3.43988	1.22591
C	-9.49526	-3.70601	-2.55142
N	-11.4027	-2.94706	-1.51326
C	-9.50753	-3.7047	2.49259
N	-11.4101	-2.94491	1.44567
C	-10.3809	-3.36583	-3.53129
H	-8.49712	-4.10779	-2.66878
C	-11.5816	-2.88471	-2.87455
Zn	-12.7774	-2.48398	-0.03829
C	-10.397	-3.36349	3.46862
H	-8.51014	-4.10719	2.61401
C	-11.5945	-2.88136	2.80662
H	-10.2433	-3.44242	-4.5997
C	-12.7552	-2.44736	-3.52984
N	-14.1435	-2.0221	-1.52174
N	-14.1488	-2.01958	1.44094

H	-10.2641	-3.43988	4.53764
C	-12.77	-2.44148	3.45654
C	-13.9448	-2.0445	-2.88202
C	-12.7265	-2.39177	-5.02659
C	-15.4143	-1.55032	-1.30057
C	-15.418	-1.54675	1.21348
C	-13.956	-2.03811	2.80258
C	-12.7475	-2.38349	4.9534
C	-15.1434	-1.56275	-3.54225
C	-13.5231	-3.2543	-5.79668
C	-11.8936	-1.46354	-5.67847
C	-16.0491	-1.26732	-2.56639
C	-15.9954	-1.34475	-0.04475
C	-16.0576	-1.25837	2.47554
C	-15.1566	-1.55217	3.4562
C	-11.9116	-1.45935	5.60734
C	-13.5527	-3.23966	5.7217
H	-15.2681	-1.45887	-4.60991
C	-13.4752	-3.17626	-7.1898
H	-14.1618	-3.97836	-5.29913
C	-11.8447	-1.38298	-7.07301
H	-11.2849	-0.79425	-5.07809
H	-17.0531	-0.8815	-2.68728
C	-17.4371	-0.80326	-0.04729
H	-17.0614	-0.87016	2.59068
H	-15.2854	-1.44445	4.52296
C	-11.868	-1.37684	7.00194
H	-11.2964	-0.79466	5.00858
C	-13.5103	-3.1595	7.11491
H	-14.1938	-3.9607	5.2229
C	-12.6362	-2.24014	-7.82848
C	-14.1848	-3.94724	-8.22257
H	-11.1966	-0.65363	-7.55224
C	-18.5616	-0.38089	-0.04927
C	-12.668	-2.22776	7.75556
H	-11.2174	-0.65069	7.48258
C	-14.2295	-3.92392	8.14598
C	-12.7683	-2.35973	-9.33234

C	-13.7783	-3.47624	-9.49005
C	-15.1133	-4.97936	-8.11218
H	-19.5633	-0.00466	-0.05103
C	-12.807	-2.34416	9.25905
C	-13.8251	-3.4534	9.41435
C	-15.1649	-4.94964	8.03372
H	-13.1159	-1.42415	-9.79118
H	-11.8106	-2.60186	-9.81261
C	-14.3013	-4.03788	-10.6505
C	-15.6463	-5.5526	-9.28598
H	-15.4337	-5.35137	-7.14429
H	-13.1499	-1.40555	9.71528
H	-11.8529	-2.59224	9.74354
C	-14.357	-4.00902	10.57363
C	-15.707	-5.51669	9.20644
H	-15.4841	-5.32125	7.06529
C	-15.2311	-5.07142	-10.549
H	-13.9935	-3.68082	-11.6298
C	-16.5958	-6.60893	-9.21575
C	-15.2937	-5.03607	10.47027
H	-14.0508	-3.65206	11.55347
C	-16.6636	-6.56635	9.13469
H	-15.6494	-5.52175	-11.443
C	-17.412	-7.51757	-9.19559
H	-15.7191	-5.48169	11.36328
C	-17.4841	-7.47114	9.11478
C	-18.3203	-8.52906	-9.1966
C	-18.3954	-8.47987	9.11375
C	-19.1363	-9.43781	-9.21858
C	-19.216	-9.38455	9.13179
C	-20.0852	-10.4945	-9.29092
C	-20.1732	-10.4339	9.20133
C	-20.4902	-10.9823	-10.5547
C	-20.6276	-11.0616	-8.11847
C	-20.7058	-11.007	8.02726
C	-20.5966	-10.9079	10.46428
C	-21.4192	-12.0164	-10.6583
H	-20.0648	-10.5366	-11.4476

C	-21.5552	-12.0943	-8.23093
H	-20.315	-10.6846	-7.14999
C	-21.6421	-12.0322	8.13735
H	-20.3789	-10.6405	7.0595
C	-21.5342	-11.9344	10.56547
H	-20.1784	-10.4576	11.35835
C	-21.9515	-12.5719	-9.49916
H	-21.7191	-12.3785	-11.6381
C	-22.2731	-12.8599	-7.19989
C	-22.353	-12.802	7.10454
C	-22.0567	-12.4961	9.40487
H	-21.8482	-12.2862	11.54467
C	-22.9627	-13.6876	-9.34375
C	-23.1069	-13.7994	-7.84039
C	-22.2364	-12.7746	-5.80685
C	-22.2994	-12.7291	5.71131
C	-23.2005	-13.7304	7.74325
C	-23.0736	-13.6061	9.24718
H	-23.9166	-13.4481	-9.83296
H	-22.6115	-14.6256	-9.79488
C	-23.9045	-14.6526	-7.08685
C	-23.0392	-13.6331	-5.0387
H	-21.6017	-12.0479	-5.30797
C	-23.0984	-13.5893	4.94105
H	-21.6543	-12.0107	5.21392
C	-23.9945	-14.5852	6.98767
H	-22.7343	-14.5423	9.71104
H	-24.0316	-13.3555	9.72268
C	-23.8669	-14.5648	-5.6924
H	-24.5487	-15.3845	-7.56746
C	-23.0225	-13.5697	-3.54208
C	-23.0639	-13.5391	3.44413
C	-23.9396	-14.51	5.59306
H	-24.6489	-15.3089	7.46685
H	-24.4804	-15.2309	-5.09344
C	-21.8382	-13.9692	-2.88261
C	-24.2013	-13.129	-2.89854
C	-24.2341	-13.1027	2.78249

C	-21.8727	-13.9459	2.80185
H	-24.55	-15.1778	4.99285
C	-20.6343	-14.4543	-3.53066
N	-21.6505	-13.9845	-1.52069
C	-25.3967	-12.6513	-3.56741
N	-24.3912	-13.0595	-1.53907
C	-25.4369	-12.6171	3.43232
N	-24.4076	-13.0462	1.41979
C	-20.6774	-14.4284	3.46763
N	-21.669	-13.9715	1.44192
C	-19.7365	-14.7446	-2.54602
H	-20.501	-14.5638	-4.59673
C	-20.3814	-14.455	-1.28684
Zn	-23.0284	-13.5149	-0.0507
C	-26.2902	-12.306	-2.59649
H	-25.5257	-12.5803	-4.63728
C	-25.6546	-12.5643	-1.32592
C	-26.3185	-12.281	2.4474
H	-25.5784	-12.5351	4.49982
C	-25.668	-12.5524	1.18731
C	-19.7685	-14.7273	2.49579
H	-20.5571	-14.5305	4.53593
C	-20.3979	-14.4455	1.22714
H	-18.7316	-15.1311	-2.65682
C	-19.8104	-14.654	-0.02533
H	-27.2874	-11.9049	-2.72396
C	-26.2345	-12.3368	-0.07351
H	-27.3168	-11.8779	2.55869
H	-18.7657	-15.1148	2.62103
C	-18.3688	-15.1955	-0.01345
C	-27.6684	-11.7752	-0.0833
C	-17.2444	-15.6179	-0.00419
C	-28.7868	-11.3371	-0.09094
H	-29.7831	-10.9469	-0.09775

3) **T_2** (n = 4)

B3LYP/6-31G(d)

C	-4.63793	8.25676	12.13563

C	-5.56985	8.82411	11.26617
C	-5.16416	9.78103	10.33627
C	-3.82584	10.17189	10.27633
C	-2.89411	9.60494	11.14578
H	-4.95798	7.50192	12.86843
H	-6.62431	8.5156	11.31352
H	-3.50608	10.92653	9.54303
H	-1.83936	9.91274	11.09864
C	-6.19264	10.40679	9.37602
C	-5.78685	11.36371	8.44602
C	-7.53106	10.01652	9.43666
C	-6.71867	11.92996	7.57566
H	-4.73219	11.67121	8.39787
C	-8.46259	10.58298	8.56671
H	-7.85072	9.26189	10.16996
C	-8.05639	11.53949	7.63581
H	-9.51745	10.27557	8.61415
C	-9.08508	12.16456	6.67535
C	-10.4227	11.77409	6.7354
C	-8.67878	13.12138	5.74445
C	-11.3547	12.34104	5.86574
H	-10.7433	11.02036	7.46919
C	-9.61051	13.68773	4.8747
H	-7.62402	13.42888	5.69711
H	-12.4094	12.03354	5.91359
H	-9.29065	14.44186	4.1409
N	-3.30001	8.64692	12.07518
N	-10.9487	13.29786	4.93554
O	-6.30217	12.91068	6.62196
C	-4.89722	13.14105	6.75663
H	-4.68663	13.49231	7.74508
H	-4.36774	12.2279	6.58218
C	-4.4498	14.19806	5.72993
H	-4.97898	15.11151	5.90468
H	-4.66079	13.84709	4.74148
C	-2.93667	14.4458	5.87448
H	-2.40749	13.53245	5.69982
H	-2.72558	14.79686	6.86303

C	-2.48915	15.50291	4.84798
H	-3.01843	16.41626	5.02273
H	-2.70034	15.15194	3.85953
O	-1.08416	15.73286	4.98221
C	-0.66791	16.71434	4.02914
C	0.66959	17.10561	3.96956
C	-1.59968	17.28016	3.15848
C	1.07553	18.06303	3.03949
C	-1.19401	18.2377	2.22892
H	-2.6541	16.97117	3.20541
C	0.14398	18.6295	2.16968
H	2.12992	18.37185	2.99329
H	0.46375	19.38461	1.43698
C	1.69829	16.48077	4.93027
C	1.2927	15.52356	5.86021
C	3.03614	16.87184	4.87002
C	2.22485	14.95745	6.73031
H	0.23832	15.21503	5.90754
C	3.96804	16.30626	5.7402
H	3.35571	17.62628	4.13642
H	1.90463	14.20339	7.46386
H	5.02251	16.61479	5.69347
C	-2.22233	18.86331	1.26831
C	-3.55988	18.4721	1.32704
C	-1.81603	19.82187	0.3396
C	-4.49136	19.03916	0.45683
H	-3.88026	17.71684	2.05922
C	-2.74714	20.38849	-0.53074
H	-0.76143	20.13043	0.29381
H	-5.54565	18.72996	0.50287
H	-2.42711	21.14355	-1.26339
N	3.56215	15.34901	6.67087
N	-4.08517	19.99672	-0.47231

4) **T$_2$** (n = 6)

B3LYP/6-31G(d)

C	0.1289	17.0106	5.3341
H	-0.0246	16.4126	6.208

H	-0.0224	16.4113	4.4607
C	-0.87	18.1826	5.3319
H	-0.7165	18.7806	4.458
H	-0.7187	18.7819	6.2053
C	-2.308	17.6314	5.3305
H	-2.4616	17.0333	6.2045
H	-2.4595	17.032	4.4572
C	-3.3071	18.8032	5.3284
H	-3.1535	19.4013	4.4545
H	-3.1557	19.4026	6.2017
C	-4.7451	18.252	5.327
H	-4.8987	17.654	6.2009
H	-4.8964	17.6528	4.4536
C	-5.7441	19.424	5.3248
H	-5.5905	20.022	4.4509
H	-5.5927	20.0233	6.1982
O	-7.0794	18.9122	5.3236
C	-8.0076	19.9999	5.3215
C	-7.5417	21.3145	5.3211
C	-9.3797	19.7461	5.3204
C	-8.4474	22.3758	5.3183
H	-6.4604	21.5149	5.3216
C	-10.2852	20.8071	5.3181
C	-9.8189	22.122	5.3166
H	-11.3666	20.6073	5.3172
H	-10.5329	22.9583	5.3146
C	-7.9327	23.8271	5.3172
C	-8.8378	24.8883	5.3144
C	-6.5605	24.0808	5.3185
C	-8.3715	26.2032	5.3142
H	-9.9193	24.6889	5.3137
C	-6.0944	25.3954	5.3179
H	-5.8471	23.244	5.3207
H	-9.0852	27.0397	5.3125
H	-5.013	25.5955	5.319
C	-9.8938	18.2944	5.321
C	-11.2651	18.0399	5.3198
C	-8.9873	17.2334	5.323

C	-11.7306	16.7248	5.3195
H	-11.9795	18.8758	5.3178
C	-9.4529	15.9186	5.3233
H	-7.9062	17.4343	5.324
H	-12.8118	16.5243	5.3181
H	-8.7389	15.0822	5.3249
O	1.4642	17.5225	5.3354
C	2.3924	16.4346	5.3374
C	3.7639	16.6879	5.3385
C	1.9258	15.1195	5.3379
C	4.6694	15.6265	5.3413
C	2.8312	14.0585	5.3402
H	0.8444	14.9201	5.3369
C	4.2031	14.3119	5.3423
H	5.7507	15.8264	5.3427
H	4.9166	13.4753	5.3443
C	2.3167	12.6069	5.3407
C	3.222	11.5459	5.343
C	0.9445	12.3532	5.3384
C	2.7558	10.231	5.3442
H	4.3033	11.7456	5.3451
C	0.4785	11.0385	5.3392
H	0.231	13.1899	5.3365
H	3.4697	9.3946	5.3465
H	-0.6028	10.8382	5.3374
C	4.2792	18.1391	5.3385
C	3.3746	19.2006	5.3358
C	5.6515	18.392	5.341
C	3.8415	20.5153	5.3366
H	2.2931	19.0016	5.3342
C	6.1183	19.7064	5.3413
H	6.3646	17.5549	5.3431
H	3.1282	21.3521	5.3348
H	7.1998	19.9061	5.3432
N	-6.9999	26.4567	5.3161
N	-10.8247	15.6642	5.3211
N	5.2133	20.7682	5.3395
N	1.3842	9.9773	5.3425

5) T_2 (n = 8)

B3LYP/6-31G(d)

C	-5.4872	5.4123	8.8367
C	-6.4195	5.9805	7.9682
C	-6.014	6.9375	7.0383
C	-4.6755	7.3276	6.9774
C	-3.7434	6.7598	7.8459
H	-5.8071	4.6574	9.5695
H	-7.4741	5.6726	8.0163
H	-4.3559	8.0823	6.2441
H	-2.6885	7.067	7.798
C	-7.0429	7.5642	6.0791
C	-6.6373	8.5212	5.1491
C	-8.3815	7.1747	6.1407
C	-7.5695	9.0883	4.2797
H	-5.5825	8.8281	5.1002
C	-9.3134	7.742	5.2717
H	-8.701	6.42	6.874
C	-8.9074	8.6986	4.3408
H	-10.3684	7.4352	5.3199
C	-9.9365	9.3246	3.3814
C	-11.2743	8.9349	3.4424
C	-9.5304	10.2815	2.4505
C	-12.2067	9.5027	2.5737
H	-11.5947	8.1811	4.1762
C	-10.4625	10.8487	1.5817
H	-8.4755	10.5884	2.4024
H	-13.2615	9.1958	2.6223
H	-10.1428	11.6029	0.8479
N	-4.1491	5.8017	8.7753
N	-11.8009	10.4596	1.6435
O	-7.1532	10.0691	3.326
C	-5.748	10.2986	3.4596
H	-5.5364	10.6494	4.448
H	-5.2192	9.3852	3.2844
C	-5.3008	11.3557	2.4329
H	-5.8293	12.2694	2.6084

H	-5.5128	11.0052	1.4445
C	-3.7874	11.6025	2.5763
H	-3.2589	10.6889	2.4009
H	-3.5753	11.9531	3.5648
C	-3.3401	12.6597	1.5498
H	-3.8687	13.5733	1.7253
H	-3.5523	12.3092	0.5614
C	-1.8268	12.9064	1.6932
H	-1.2983	11.9927	1.5177
H	-1.6147	13.2569	2.6816
C	-1.3794	13.9636	0.6666
H	-1.908	14.8772	0.8422
H	-1.5917	13.6131	-0.3219
C	0.1339	14.2102	0.81
H	0.6623	13.2966	0.6344
H	0.346	14.5608	1.7985
C	0.5812	15.2674	-0.2166
H	0.0527	16.1811	-0.041
H	0.369	14.917	-1.205
O	1.9865	15.4965	-0.0834
C	2.4025	16.4781	-1.0364
C	3.7401	16.8686	-1.0971
C	1.47	17.0457	-1.9056
C	4.146	17.8257	-2.0275
C	1.8758	18.0029	-2.8354
H	0.4154	16.7376	-1.8576
C	3.214	18.3927	-2.8966
H	5.2007	18.1331	-2.0754
H	3.5338	19.1472	-3.6298
C	0.8471	18.6295	-3.7949
C	1.2528	19.5867	-4.7246
C	-0.4915	18.2399	-3.7337
C	0.3209	20.1538	-5.5943
H	2.3077	19.8937	-4.7732
C	-1.4232	18.8072	-4.6029
H	-0.8112	17.4852	-3.0006
H	0.6411	20.9081	-6.3275
H	-2.4782	18.5003	-4.555

C	4.7696	16.2421	-0.1384
C	4.3645	15.2852	0.792
C	6.108	16.6321	-0.2002
C	5.2974	14.7171	1.6599
H	3.3099	14.9774	0.8407
C	7.0405	16.0645	0.6679
H	6.4271	17.3867	-0.9338
H	4.9779	13.9624	2.393
H	8.0954	16.3717	0.6194
N	6.6353	15.1066	1.5978
N	-1.017	19.7639	-5.5335

6) T_2 (n = 12)

B3LYP/6-31G(d)

C	-4.58067	8.45105	12.36072
C	-5.33452	9.61081	12.17911
C	-4.92909	10.56802	11.2494
C	-3.76838	10.36611	10.50143
C	-3.01446	9.20677	10.68317
H	-4.90082	7.69624	13.09351
H	-6.24928	9.76941	12.7685
H	-3.44877	11.12104	9.76837
H	-2.09978	9.04739	10.09374
C	-5.76155	11.84788	11.04836
C	-5.35608	12.80508	10.11851
C	-6.92171	12.05011	11.79701
C	-6.11083	13.96418	9.93601
H	-4.44205	12.64584	9.52827
C	-7.67596	13.20912	11.61471
H	-7.24125	11.29514	12.53002
C	-7.2708	14.16612	10.68386
H	-8.59038	13.36877	12.20447
C	-8.10386	15.44554	10.4827
C	-9.2638	15.64747	11.23041
C	-7.69847	16.40275	9.55182
C	-10.018	16.807	11.04866
H	-9.58331	14.89346	11.96438
C	-8.45283	17.56169	9.36978

H	-6.78402	16.24319	8.9622
H	-10.9322	16.96635	11.63864
H	-8.13362	18.31633	8.63622
N	-3.42084	8.24888	11.6125
N	-9.61255	17.7641	10.11853
O	-5.69507	14.94513	8.98223
C	-4.48726	14.51393	8.34949
H	-3.72332	14.38771	9.0879
H	-4.65859	13.58307	7.85072
C	-4.03973	15.5714	7.32331
H	-3.86789	16.50228	7.82219
H	-4.8038	15.69803	6.58514
C	-2.73932	15.10684	6.64142
H	-2.91107	14.17601	6.14263
H	-1.97509	14.98021	7.37963
C	-2.29159	16.16428	5.61536
H	-2.11987	17.09513	6.11429
H	-3.0558	16.291	4.8773
C	-0.99131	15.69969	4.93352
H	-1.16315	14.7688	4.43463
H	-0.22716	15.57301	5.67163
C	-0.54354	16.75712	3.90732
H	-0.37178	17.68793	4.40633
H	-1.30787	16.88392	3.16923
C	0.75669	16.29244	3.22547
H	0.58478	15.36172	2.72656
H	1.52093	16.16581	3.96367
C	1.20438	17.34991	2.19933
H	0.44015	17.47663	1.46123
H	1.37621	18.28073	2.69827
C	2.50466	16.88529	1.51743
H	2.33283	15.95446	1.0185
H	3.26889	16.75858	2.25553
C	2.95234	17.94275	0.49129
H	2.18811	18.06947	-0.24682
H	3.12417	18.87358	0.99022
C	4.25262	17.47814	-0.19062
H	4.08079	16.54731	-0.68954

H	5.01685	17.35143	0.54749
C	4.7003	18.5356	-1.21676
H	3.93608	18.66231	-1.95487
H	4.87213	19.46643	-0.71783
O	5.90771	18.10417	-1.84995
C	6.3238	19.08553	-2.80321
C	5.56961	20.24463	-2.9856
C	7.48453	18.88376	-3.55047
C	5.97587	21.20205	-3.91553
H	4.65492	20.40388	-2.39644
C	7.8905	19.8407	-4.48053
C	7.13569	21.00003	-4.66334
H	8.80497	19.68166	-5.07022
H	7.45563	21.75435	-5.39678
C	8.31724	17.60417	-3.34839
C	7.91121	16.64728	-2.4183
C	9.47757	17.40186	-4.09612
C	8.66563	15.488	-2.23555
H	6.9965	16.80651	-1.82916
C	10.23212	16.2431	-3.91313
H	9.79724	18.1563	-4.82967
H	8.34568	14.73416	-1.50166
H	11.14716	16.08363	-4.50182
C	5.1423	22.48113	-4.11734
C	5.54793	23.4387	-5.04689
C	3.981	22.68179	-3.37066
C	4.79249	24.5973	-5.22972
H	6.46304	23.28046	-5.63568
C	3.22595	23.84031	-3.55305
H	3.6612	21.92642	-2.63811
H	5.11297	25.3524	-5.96209
H	2.31092	23.99915	-2.96416
N	9.82617	15.28606	-2.98227
N	3.63206	24.79851	-4.48264

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