Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Dithienopicenocarbazole as the kernel module of low-energy-gap organic dyes for efficient conversion of sunlight to electricity

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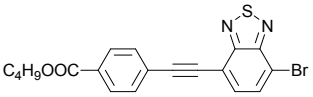
1. Experimental section

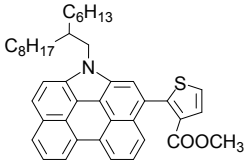
Materials: Palladium(II) acetate ($Pd(OAc)_2$), bis(triphenylphosphine)palladium(II) chloride ($Pd(PPh_3)_2Cl_2$), copper(I) iodide (CuI), triphenylphosphine (PPh_3), 4,7-dibromobenzo[*c*][1,2,5]thiadiazole, *N*-bromosuccinimide (NBS), *n*-butyllithium (*n*-BuLi), chlorotrimethylstannane (Me_3SnCl), methyl thiophene-3-carboxylate, tricyclohexylphosphinetetrafluroborate ($PCy_3{\cdot}HBF_4$), trimethylacetic acid (PivOH), 1-bromo-4-hexylbenzene, magnesium, Amberlyst 15, potassium hydroxide (KOH), potassium carbonate (K_2CO_3), phosphoric acid, lithium bis(trifluoromethanesulfonyl)imide (LiTFSI), 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide (EMITFSI), decamethylferrocene (DMFC), ferrocene (FC), and 4-*tert*-butylpyridine (TBP) were purchased from Sigma-Aldrich and used without further purification. Toluene, diisopropylamine, ethanol, acetonitrile, chloroform, and tetrahydrofuran (THF) were dried and distilled prior to use. Butyl 4-ethynylbenzoate,[S1] 3-bromo-1-(2-hexyldecyl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole (**1**),[S2] (4-hexylphenyl)magnesium bromide,[S3] 1-(2-hexyldecyl)-3,10-di(thiophen-2-yl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole (**7**),[S4] and 1-((2-hexyldecyl)oxy)-4-iodobenzene[S5] were synthesized according to the respective literature procedures. The synthetic routes to **C279, C280**, and **C281** are respectively illustrated in Scheme S1, Scheme 1, and Scheme S2. The preparation details are described as follows.

Butyl 4-((7-bromobenzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoate



In a dried Schlenk tube were dissolved butyl 4-ethynylbenzoate (850 mg, 4.21 mmol), 4,7-dibromobenzo[*c*][1,2,5]thiadiazole (1.49 g, 5.05 mmol), PPh_3 (48 mg, 0.18 mmol), CuI (17 mg, 0.09 mmol), and diisopropylamine (2 mL) in toluene (10 mL). Then $Pd(PPh_3)_2Cl_2$ (63 mg, 0.09 mmol) was added to the reaction mixture, which was refluxed for 2 h under argon. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/petroleum ether 60–90 °C, 3/1, *v*/*v*) on silica gel to yield a yellow solid as the desired product butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate (1.45 g, 83% yield). M. p. 103–104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.05 (d, J = 8.0 Hz, 2H), 7.84 (d, J = 8.0 Hz, 1H), 7.71–7.67 (m, 3H), 4.34 (t, J = 6.6 Hz, 2H), 1.80–1.73 (m, 2H), 1.53–1.44 (m, 2H), 0.99 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 166.10, 154.18, 153.25, 133.28, 132.06, 131.95, 130.80, 129.67, 126.98, 116.28, 115.47, 95.95, 87.24, 65.27, 30.88, 19.40, 13.89. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{19}H_{15}BrN_2O_2S$): 414.004. Found: 414.003. Anal. Calcd. for $C_{19}H_{15}BrN_2O_2S$: C, 54.95%; H, 3.64%; N, 6.75%. Found: C, 54.94%; H, 3.65%; N, 6.74%.

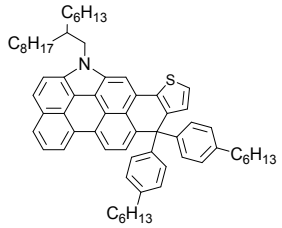
*Methyl 2-(1-(2-hexyldecyl)-1H-phenanthro[1,10,9,8-cdefg]carbazol-3-yl)thiophene-3-carboxylate (**2**)*



In a dried Schlenk tube were dissolved **1** (4.50 g, 7.91 mmol), methyl thiophene-3-carboxylate (1.35 g, 9.50 mmol), K_2CO_3 (1.64 g, 11.87 mmol) in toluene (30 mL). Then $Pd(OAc)_2$ (130 mg, 0.47 mmol), $PCy_3{\cdot}HBF_4$ (350 mg, 0.95 mmol), and PivOH (242 mg, 2.37 mmol) were added to the reaction mixture in a nitrogen-filled glovebox, which was refluxed for 24 h. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/50, *v*/*v*) on silica gel to yield a yellow solid as the desired product **2** (3.24 g, 65% yield). M. p. 122–123 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.68–8.66 (m, 2H), 8.14 (d, J = 8.0 Hz, 1H), 7.93 (d, J = 8.7 Hz, 1H), 7.87–7.80 (m, 3H), 7.78–7.74 (m, 2H), 7.73 (dd, J_1 = 9.2 Hz, J_2 = 5.1 Hz, 1H), 7.43 (dd, J_1 = 5.4 Hz, J_2 = 0.4 Hz, 1H), 4.53 (d, J = 6.4 Hz, 2H), 3.42–3.42 (m, 3H), 2.29–2.26 (m, 1H), 1.39–1.19 (m, 24H), 0.87–0.81 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.80, 150.14, 132.84, 130.56, 129.64, 128.61, 127.58, 124.71, 124.64, 124.47, 123.64, 121.01, 120.94, 117.99, 117.36, 115.63, 113.55, 51.51, 50.16, 40.05, 31.95, 31.88, 29.71, 29.61, 29.36, 26.56, 22.72, 14.21, 14.17. HR-MS (MALDI-TOF) *m*/*z* calcd. for

($C_{42}H_{47}NO_2S$): 629.33275. Found: 629.33115. Anal. Calcd. for $C_{42}H_{47}NO_2S$: C, 80.08%; H, 7.52%; N, 2.22%. Found: C, 80.10%; H, 7.51%; N, 2.19%.

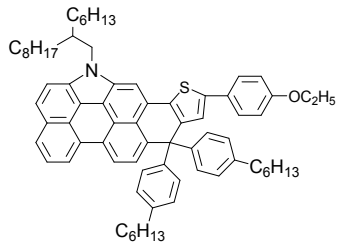
*11-(2-Hexyldecyl)-6,6-bis(4-hexylphenyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-bcdefg]carbazole (**3**)*



In a dried Schlenk tube was dissolved **2** (3.15 g, 5.00 mmol) in THF (10 mL). Then (4-hexylphenyl)magnesium bromide (12.50 mL, 2 M in THF, 25.00 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred at reflux under argon for 6 h. Water was slowly added to terminate the reaction and the mixture was poured into cold 1 M hydrochloric acid aqueous solution. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the residue tertiary alcohol was used in the next reaction directly.

In a dried Schlenk tube were dissolved the above tertiary alcohol, Amberlyst 15 (1.00 g) in 20 mL toluene, which was refluxed for 6 h. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/20, *v*/*v*) on silica gel to yield a yellow solid as the desired product **3** (4.07 g, 90% yield). M. p. 101–102 °C. ^{1}H NMR (400 MHz, THF-d_8) δ: 8.57 (d, J = 8.0 Hz, 1H), 8.56 (d, J = 8.0 Hz, 1H), 8.02 (d, J = 8.0 Hz, 1H), 7.97 (s, 1H), 7.80 (d, J = 8.7 Hz, 1H), 7.75 (d, J = 8.8 Hz, 1H), 7.73–7.69 (m, 1H), 7.62 (d, J = 8.1 Hz, 1H), 7.22–7.19 (m, 5H), 7.04 (d, J = 8.0 Hz, 4H), 6.89 (d, J = 5.1 Hz, 1H), 4.59 (d, J = 7.1 Hz, 2H), 2.54 (t, J = 7.6 Hz, 4H), 2.33–2.30 (m, 1H), 1.61–1.55 (m, 4H), 1.44–1.40 (m, 6H), 1.35–1.26 (m, 12H), 1.23–1.20 (m, 16H), 0.88–0.85 (m, 8H), 0.82–0.79 (m, 6H). ^{13}C NMR (100 MHz, THF-d_8) δ: 147.30, 145.07, 142.24, 141.58, 137.74, 133.72, 133.49, 131.61, 131.20, 130.69, 130.20, 129.27, 128.73, 127.86, 127.02, 125.70, 125.65, 125.54, 125.03, 124.40, 123.97, 123.21, 122.77, 121.31, 118.81, 118.23, 114.54, 106.96, 59.20, 50.63, 41.00, 36.49, 32.97, 32.94, 32.85, 32.80, 32.64, 31.04, 30.74, 30.65, 30.38, 30.26, 27.56, 23.66, 23.63, 14.59, 14.57. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{65}H_{77}NS$): 903.57767. Found: 903.57547. Anal. Calcd. for $C_{65}H_{77}NS$: C, 86.32%; H, 8.58%; N, 1.55%. Found: C, 86.33%; H, 8.57%; N, 1.57%.

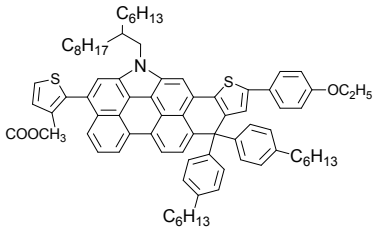
*8-(4-Ethoxyphenyl)-11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-bcdefg]carbazole (**4**)*



In a three-neck flame-dried round-bottom flask was dissolved **3** (3.62 g, 3.00 mmol) in THF (20 mL) and cooled to −78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (2.25 mL, 1.6 M in hexanes, 3.60 mmol) was added dropwise to the reaction mixture, which was stirred at −78 °C for 0.5 h. After trimethylstannyl chloride (0.72 g, 3.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for another 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product 11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-8-(trimethylstannyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-*bcdefg*]carbazole was used to synthesize **4** without further purification.

In a dried Schlenk tube were dissolved 11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-8-(trimethylstannyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-*bcdefg*]carbazole and 1-ethoxy-4-iodobenzene (893 mg, 3.60 mmol) in toluene (10 mL). Then $Pd(PPh_3)_2Cl_2$ (154 mg, 0.22 mmol) was added to the reaction mixture, which was refluxed for 6 h under argon. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/10, *v*/*v*) on silica gel to yield a yellow oil as the desired product **4** (2.58 g, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.59 (br, 2H), 8.03 (s, 1H), 7.77–7.70 (m, 4H), 7.50 (br, 2H), 7.43–7.41 (m, 5H), 7.19 (d, J = 9.9 Hz, 4H), 7.12 (s, 1H), 6.87 (d, J = 8.5 Hz, 2H), 4.11–4.03 (m, 4H), 2.66–2.63 (m, 4H), 2.15 (br, 1H), 1.69–1.63 (m, 4H), 1.48–1.45 (m, 4H), 1.41–1.35 (m, 18H), 1.31–1.26 (m, 17H), 0.95–0.93 (m, 6H), 0.92–0.90 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 158.57, 146.41, 144.80, 141.15, 140.88, 135.62, 132.34, 130.12, 129.85, 128.96, 128.07, 127.23, 126.77, 125.25, 124.49, 123.91, 123.06, 121.85, 120.34, 117.67, 117.01, 114.73, 113.01, 105.63, 63.60, 49.66, 39.84, 35.67, 32.01, 31.85, 31.44, 30.05, 29.73, 29.45, 29.32, 26.61, 22.78, 22.73, 14.93, 14.23. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{73}H_{85}NOS$): 1023.63519. Found: 1023.63203. Anal. Calcd. for $C_{73}H_{85}NOS$: C, 85.58%; H, 8.36%; N, 1.37%. Found: C, 85.56%; H, 8.37%; N, 1.39%.

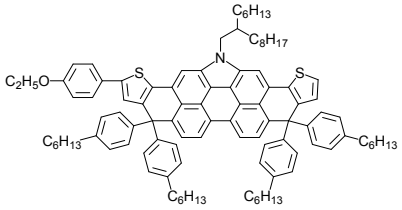
*Methyl 2-(8-(4-ethoxyphenyl)-11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-bcdefg]carbazol-13-yl)thiophene-3-carboxylate (**5**)*



In a three-neck round-bottom flask was dissolved **4** (2.05 g, 2.00 mmol) in THF (10 mL) and cooled to 0 °C using an ice/water cold bath. NBS (493 mg, 2.20 mmol) was added to the reaction mixture, which was stirred at 0 °C for 0.5 h. Chloroform was added before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/5, *v*/*v*) on silica gel to yield a yellow oil as the intermediate product 13-bromo-8-(4-ethoxyphenyl)-11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-*bcdefg*]carbazole, which was used for the next reaction directly.

In a dried Schlenk tube were dissolved 13-bromo-8-(4-ethoxyphenyl)-11-(2-hexyldecyl)-6,6-bis(4-hexylphenyl)-6,11-dihydrothieno[3',2':8,9]chryseno[10,11,12,1-*bcdefg*]carbazole, methyl thiophene-3-carboxylate (0.34 g, 2.40 mmol), and K_2CO_3 (0.41 g, 3.00 mmol) in toluene (20 mL). Then $Pd(OAc)_2$ (33 mg, 0.12 mmol), $PCy_3{\cdot}HBF_4$ (88 mg, 0.24 mmol), and PivOH (61 mg, 0.60 mmol) were added to the reaction mixture in a nitrogen-filled glovebox, which was refluxed for 24 h. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/5, *v*/*v*) on silica gel to yield an orange oil as the desired product **5** (1.61 g, 69% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.64 (d, J = 8.1 Hz, 1H), 8.61 (d, J = 7.4 Hz, 1H), 7.89–7.86 (m, 2H), 7.81 (s, 1H), 7.78–7.73 (m, 3H), 7.49 (d, J = 8.5 Hz, 2H), 7.43 (d, J = 5.4 Hz, 1H), 7.38 (d, J = 8.2 Hz, 4H), 7.17 (d, J = 8.2 Hz, 4H), 7.10 (s, 1H), 6.88 (d, J = 8.6 Hz, 2H), 4.40 (d, J = 6.7 Hz, 2H), 4.06 (q, J = 6.8 Hz, 2H), 3.45 (s, 3H), 2.65–2.61 (m, 4H), 2.31 (br, 1H), 1.68–1.62 (m, 4H), 1.51–1.42 (m, 12H), 1.38–1.34 (m, 12H), 1.29 (br, 15H), 0.95–0.91 (m, 6H), 0.90–0.87 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.87, 158.70, 150.17, 146.08, 145.39, 141.54, 141.26, 140.98, 135.40, 133.32, 131.91, 130.62, 130.43, 129.85, 128.81, 127.89, 127.20, 127.09, 126.90, 125.40, 125.09, 124.61, 124.26, 123.91, 123.49, 122.95, 122.33, 120.69, 118.62, 117.22, 115.63, 114.82, 105.67, 63.68, 58.22, 51.50, 50.05, 40.00, 35.71, 32.08, 32.04, 31.91, 31.48, 30.16, 29.78, 29.51, 29.36, 26.61, 22.82, 22.78, 14.98, 14.28. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{79}H_{89}NO_3S_2$): 1163.62839. Found: 1163.62515. Anal. Calcd. for $C_{79}H_{89}NO_3S_2$: C, 81.47%; H, 7.70%; N, 1.20%. Found: C, 81.46%; H, 7.71%; N, 1.20%.

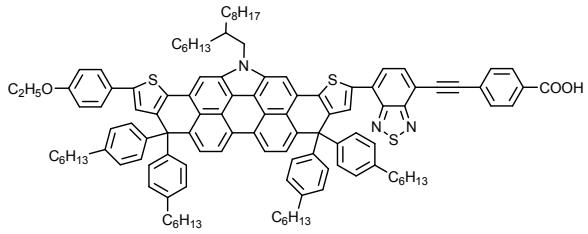
*2-(4-Ethoxyphenyl)-14-(2-hexyldecyl)-4,4,9,9-tetrakis(4-hexylphenyl)-9,14-dihydro-4H-dithieno[2',3':2,3;3'',2'':10,11]piceno[1,14,13,12-bcdefgh]carbazole (**6**)*



In a dried Schlenk tube was dissolved **5** (1.16 g, 1.00 mmol) in THF (10 mL). Then (4-hexylphenyl)magnesium bromide (2.50 mL, 2 M in THF, 5.00 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred at reflux for 6 h under argon. Water was slowly added to terminate the reaction and the mixture was poured into cold 1 M hydrochloric acid aqueous solution. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the residue tertiary alcohol was used in the next reaction directly.

In a dried Schlenk tube were dissolved the above tertiary alcohol, Amberlyst 15 (0.50 g) in toluene (20 mL), which was refluxed for 6 h. The mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/20, *v*/*v*) on silica gel to yield a red oil as the desired product **6** (1.27 g, 88% yield). ^{1}H NMR (400 MHz, THF-d_8) δ: 8.45 (d, J = 8.0 Hz, 2H), 7.79 (br, 2H), 7.57–7.55 (m, 2H), 7.44–7.42 (m, 2H), 7.28 (d, J = 7.4 Hz. 4H), 7.19 (d, J = 7.8 Hz, 4H), 7.14 (s, 1H), 7.12–7.05 (m, 9H), 6.90–6.88 (d, J = 5.1 Hz, 1H), 6.83 (d, J = 8.4 Hz, 2H), 4.39 (br, 2H), 4.00 (q, J = 6.8 Hz, 2H), 2.55 (br, 8H), 2.30 (br, 1H), 1.58 (br, 8H), 1.36–1.26 (m, 44H), 1.19 (br, 6H), 0.87 (br, 13H), 0.80 (br, 6H). ^{13}C NMR (100 MHz, THF-d_8) δ: 159.91, 147.29, 146.14, 144.96, 142.12, 141.87, 141.59, 141.55, 137.88, 136.39, 134.01, 133.92, 131.42, 130.79, 130.72, 129.02, 128.80, 128.72, 128.01, 127.51, 126.84, 126.06, 124.70, 124.66, 124.07, 123.31, 122.57, 118.72, 118.61, 115.53, 106.84, 106.56, 64.24, 59.19, 50.51, 40.83, 36.52, 33.21, 32.84, 32.62, 31.11, 30.79, 30.74, 30.47, 30.29, 27.48, 23.74, 23.64, 15.31, 14.60. HR-MS (MALDI-TOF) m/z calcd. for ($C_{102}H_{119}NOS_2$): 1438.87666. Found: 1438.86905. Anal. Calcd. for $C_{102}H_{119}NOS_2$: C, 85.12%; H, 8.33%; N, 0.97%. Found: C, 85.13%; H, 8.31%; N, 0.98%.

*4-((7-(11-(4-Ethoxyphenyl)-14-(2-hexyldecyl)-4,4,9,9-tetrakis(4-hexylphenyl)-9,14-dihydro-4H-dithieno[2',3':2,3;3'',2'':10,11]piceno[1,14,13,12-bcdefgh]carbazol-2-yl)benzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoic acid (**C280**)*



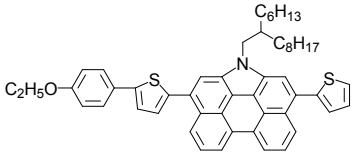
In a three-neck flame-dried round-bottom flask was dissolved **6** (720 mg, 0.50 mmol) in THF (10 mL) and cooled to −78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.38 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred at −78 °C for 0.5 h. After trimethylstannyl chloride (119 mg, 0.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product 2-(4-ethoxyphenyl)-14-(2-hexyldecyl)-4,4,9,9-tetrakis(4-hexylphenyl)-11-(trimethylstannyl)-9,14-dihydro-4*H*-dithieno[2',3':2,3;3'',2'':10,11]piceno[1,14,13,12-*bcdefgh*]carbazole was used to synthesize **C280** without further purification.

In a dried Schlenk tube were dissolved 2-(4-ethoxyphenyl)-14-(2-hexyldecyl)-4,4,9,9-tetrakis(4-hexylphenyl)-11-(trimethylstannyl)-9,14-dihydro-4*H*-dithieno[2',3':2,3;3'',2'':10,11]piceno[1,14,13,12-*bcdefgh*]carbazole and butyl 4-((7-

bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate (415 mg, 1.00 mmol) in toluene (10 mL). Then $Pd(PPh_3)_2Cl_2$ (22 mg, 0.03 mmol) was added to the reaction mixture, which was refluxed for 6 h under argon. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/1, *v*/*v*) on silica gel to yield a black powder as the desired butyl ester.

In a three-neck round-bottom flask were dissolved butyl ester (780 mg, 0.44 mmol) and KOH (246 mg, 4.40 mmol) in a solvent mixture of THF/H_2O (8 mL, 3/1, *v*/*v*). The reaction mixture was refluxed overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M phosphoric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 10/1, *v*/*v*) on silica gel to yield a black powder as the desired product **C280** (750 mg, 84% yield). M. p. 259–261 °C. ^{1}H NMR (400 MHz, THF-d_8) δ: 8.67 (d, J = 5.8 Hz, 2H), 8.35 (s, 1H), 8.13 (br, 2H), 7.83–7.77 (m, 4H), 7.55 (br, 9H), 7.30 (br, 8H), 7.07 (s, 1H), 6.92–6.87 (m, 2H), 6.51 (s, 1H), 6.36 (br, 2H), 6.15 (br, 2H), 3.87 (br, 2H), 2.64 (br, 8H), 2.08 (br, 1H), 1.69–1.64 (m, 6H), 1.34–1.14 (m, 48H), 1.02–0.75 (m, 25H). ^{13}C NMR (100 MHz, THF-d_8) δ: 158.53, 155.97, 151.90, 147.86, 146.34, 145.83, 142.83, 142.54, 141.92, 141.87, 139.92, 137.78, 136.16, 134.78, 134.73, 134.07, 133.84, 132.45, 131.00, 130.83, 129.06, 128.74, 128.56, 128.47, 128.09, 127.34, 126.63, 126.41, 125.76, 125.21, 124.94, 124.49, 124.43, 124.29, 124.16, 122.84, 122.68, 118.82, 117.89, 114.37, 114.02, 107.98, 106.52, 95.85, 90.07, 63.76, 59.01, 49.75, 40.48, 36.60, 33.01, 32.83, 32.64, 32.47, 31.17, 30.79, 30.50, 30.31, 27.01, 23.73, 23.62, 15.38, 14.56. HR-MS (MALDI-TOF) *m/z* calcd. for ($C_{117}H_{125}N_3O_3S_3$): 1716.89116. Found: 1716.89228. Anal. Calcd. for $C_{117}H_{125}N_3O_3S_3$: C, 81.82%; H, 7.34%; N, 2.45%. Found: C, 81.80%; H, 7.32%; N, 2.47%.

*3-(5-(4-Ethoxyphenyl)thiophen-2-yl)-1-(2-hexyldecyl)-10-(thiophen-2-yl)-1H-phenanthro[1,10,9,8-cdefg]carbazole (**8**)*

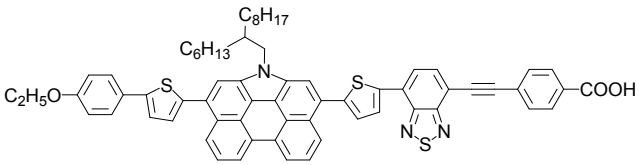


In a three-neck flame-dried round-bottom flask was dissolved **7** (654 mg, 1.00 mmol) in THF (10 mL) and cooled to −78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.75 mL, 1.6 M in hexanes, 1.20 mmol) was added dropwise to the reaction mixture, which was stirred at −78 °C for 0.5 h. After trimethylstannyl chloride (239 mg, 1.20 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product 1-(2-hexyldecyl)-3-(thiophen-2-yl)-10-(5-(trimethylstannyl)thiophen-2-yl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole was used to synthesize **8** without further purification.

In a dried Schlenk tube were dissolved 1-(2-hexyldecyl)-3-(thiophen-2-yl)-10-(5-(trimethylstannyl)thiophen-2-yl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole and 1-ethoxy-4-iodobenzene (496 mg, 2.00 mmol) in toluene (10 mL). Then $Pd(PPh_3)_2Cl_2$ (44 mg, 0.06 mmol) was added to the reaction mixture, which was refluxed for 6 h under argon. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (toluene/petroleum ether 60–90 °C, 1/5, *v*/*v*) on silica gel to yield an orange solid as the desired product **8** (550 mg, 71% yield). M. p. 123 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.65–8.64 (m, 2H), 8.53 (d, J = 5.5 Hz, 1H), 8.42 (d, J = 5.4 Hz, 1H), 7.87 (s, 1H), 7.84–7.82 (m, 2H), 7.79 (d, J = 7.6 Hz, 1H), 7.65 (d, J = 8.6 Hz, 2H), 7.49 (d, J = 4.9 Hz, 1H), 7.45 (br, 1H), 7.39 (s, 1H), 7.36 (d, J = 3.5 Hz, 1H), 7.30–7.28 (m, 1H), 6.96 (d, J = 8.7 Hz, 2H), 4.43 (d, J = 6.8 Hz, 2H), 4.10 (q, J = 7.0 Hz, 2H), 2.26–2.20 (m, 1H), 1.47 (t, J = 5.6 Hz, 3H), 1.36–1.33 (m, 8H), 1.28 (br, 2H), 1.20–1.18 (m, 14H), 0.84–0.78 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 147.71, 145.29, 142.66, 142.01, 138.17, 134.15, 133.92, 132.05, 131.64, 131.14, 130.64, 129.71, 129.17, 128.31, 127.46, 126.15, 126.09, 125.99, 125.48, 124.85, 123.66, 123.22, 121.77, 119.27, 118.68, 115.00, 107.43, 63.81,

50.11, 39.99, 32.11, 32.08, 31.97, 30.21, 29.98, 29.90, 29.80, 29.55, 26.67, 22.90, 15.15, 14.35. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{52}H_{55}NOS_2$): 773.37251. Found: 773.37056. Anal. Calcd. for $C_{52}H_{55}NOS_2$: C, 80.68%; H, 7.16%; N, 1.81%. Found: C, 80.67%; H, 7.18%; N, 1.80%.

*4-((7-(5-(10-(5-(4-Ethoxyphenyl)thiophen-2-yl)-1-(2-hexyldecyl)-1H-phenanthro[1,10,9,8-cdefg]carbazol-3-yl)thiophen-2-yl)benzo[c][1,2,5]thiadiazol-4-yl)ethynyl)benzoic acid (**C279**)*



In a three-neck flame-dried round-bottom flask was dissolved **8** (387 mg, 0.50 mmol) in THF (10 mL) and cooled to −78 °C using a dry ice/acetone cold bath. Under argon, *n*-BuLi (0.38 mL, 1.6 M in hexanes, 0.60 mmol) was added dropwise to the reaction mixture, which was stirred at −78 °C for 0.5 h. After trimethylstannyl chloride (119 mg, 0.60 mmol) was added in one portion *via* syringe, the mixture was slowly warmed up and stirred for 2 h at room temperature. Water was slowly added to terminate the reaction and the mixture was extracted three times with diethyl ether before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product 3-(5-(4-ethoxyphenyl)thiophen-2-yl)-1-(2-hexyldecyl)-10-(5-(trimethylstannyl)thiophen-2-yl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole was used to synthesize **C279** without further purification.

In a dried Schlenk tube were dissolved 3-(5-(4-ethoxyphenyl)thiophen-2-yl)-1-(2-hexyldecyl)-10-(5-(trimethylstannyl)thiophen-2-yl)-1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole and butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate (415 mg, 1.00 mmol) in toluene (10 mL). Then $Pd(PPh_3)_2Cl_2$ (22 mg, 0.03 mmol) was added to the reaction mixture, which was refluxed for 6 h under argon. Water was added to terminate the reaction and the mixture was extracted three times with chloroform before the organic phase was washed with water and dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/petroleum ether 60–90 °C, 1/1, *v*/*v*) on silica gel to yield a black powder as the desired butyl ester.

In a three-neck round-bottom flask were dissolved butyl ester (476 mg, 0.43 mmol) and KOH (241 mg, 4.30 mmol) in a solvent mixture of THF/H_2O (7 mL, 3/1, *v*/*v*). The reaction mixture was refluxed overnight and then cooled to room temperature. Chloroform was added before the organic phase was washed with 0.1 M phosphoric acid and deionized water in turn and then dried over anhydrous sodium sulfate. After solvent removal under reduced pressure, the crude product was purified by column chromatography (chloroform/methanol, 15/1, *v*/*v*) on silica gel to yield a black solid as the desired product **C279** (452 mg, 86% yield). M. p. 239–241 °C. ^{1}H NMR (400 MHz, THF-d_8) δ: 8.88–8.66 (m, 2H), 8.55 (d, J = 8.2 Hz, 1H), 8.51 (d, J = 8.2 Hz, 1H), 8.32 (d, J = 2.9 Hz, 1H), 8.08 (d, J = 7.9 Hz, 2H), 7.98 (s, 1H), 7.92–7.90 (m, 2H), 7.82–7.75 (m, 3H), 7.72 (d, J = 7.8 Hz, 2H), 7.63 (d, J = 8.3 Hz, 2H), 7.55 (d, J = 3.0 Hz, 1H), 7.40 (br, 2H), 6.92 (d, J = 8.4 Hz, 2H), 4.50 (d, J = 6.2 Hz, 2H), 4.04 (q, J = 6.7 Hz, 2H), 2.28 (br, 1H), 1.41–1.37 (m, 6H), 1.28 (br, 7H), 1.17–1.11 (m, 14H), 0.74–0.73 (m, 6H). ^{13}C NMR (100 MHz, THF-d_8) δ: 167.23, 160.02, 156.27, 152.69, 147.55, 145.25, 142.78, 139.57, 134.14, 133.51, 133.23, 132.54, 132.08, 131.65, 131.50, 130.94, 130.78, 130.21, 130.02, 129.06, 129.00, 128.68, 128.48, 128.35, 128.16, 127.66, 126.04, 125.91, 125.71, 125.65, 125.26, 125.19, 124.92, 123.39, 122.35, 122.30, 118.25, 117.82, 115.96, 115.79, 115.72, 115.36, 96.16, 89.45, 64.29, 50.46, 40.84, 32.97, 32.95, 32.76, 32.71, 31.10, 30.79, 30.67, 30.43, 27.43, 23.69, 23.63, 15.35, 14.59, 14.57, 14.44. HR-MS (MALDI-TOF) *m*/*z* calcd. for ($C_{67}H_{61}N_3O_3S_3$): 1051.38750. Found: 1051.38743. Anal. Calcd. for $C_{67}H_{61}N_3O_3S_3$: C, 76.46%; H, 5.84%; N, 3.99%. Found: C, 76.45%; H, 5.85%; N, 3.40%.

Theoretical Calculations: By selecting the 6-311G(d, p) basis set, all quantum chemical calculations were conducted with the Gaussian 09 software package. The simulation of solvent (THF) effects was performed by unitizing the conductor-like polarized continuum model (C-PCM).[S6] The optimized ground-state geometries were achieved by virtue of the general B3LYP exchange-correlation functional.[S7] The TD-MPW1K hybrid functional, [S8] which includes 42% of Hartree-Fock exchange was carried out for the vertical electron transition calculations.[S9]

Device Fabrication: The negative electrode of DSCs consists of a titania coated fluorine doped tin oxide (FTO) conducting glass (NSG, Solar, 4.0 mm), which was described in a previous paper[S10] In brief, by using of screen-printing and sintering, a bilayer titania film was deposited on a sheet of conducting glass. The semiconducting bilayer film is composed of a 4.5-μm-thick translucent layer of small particles (25 nm) and a 5.0-μm-thick light-scattering layer of large particles (350–450 nm). Dye-loading was conducted by immersing a titania electrode into a solution of 150 μM dye in the solvent mixture of chloroform/ethanol (*v*/*v*, 4/6) for 10 h. A 25-μm-thick Surlyn ring was heated at 130 °C to adhere a dyed titania electrode and an Au/Cr coated FTO (NSG, TEC7, 2.2 mm) electrode. The internal space of a partly sealed cell was infiltrated with a cobalt electrolyte. The Co-bpy electrolyte is composed of 0.25 M tris(2,2'-bipyridine)cobalt(II) di[bis(trifluoromethanesulfonyl)imide], 0.05 M tris(2,2'-bipyridine)cobalt(III) tris[bis(trifluoromethanesulfonyl)imide], 0.5 M TBP, and 0.1 M LiTFSI in acetonitrile. An antireflection film (ASAHI, ARKTOP, λ<380 nm) was laminated onto the photoanode of DSCs.

Instrumentation: Nonaqueous electrochemical measurements of dye molecules were carried out in a nitrogen-filled glovebox with THF as the solvent and 1-ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide as the supporting electrolyte. A CHI660C electrochemical workstation was employed in conjunction with a three-electrode electrolytic cell equipped with a glassy carbon working electrode, a platinum gauze counter electrode, and a silver wire quasi-reference electrode. To obtain a well-defined cyclic voltammograms, the potential scan rate was kept low, i.e. 5 mV s^{-1}. In addition an *iR* drop was compensated in consideration of a low conductivity of our electrolyte. Decamethylferrocene (DMFC) characteristic of an electrochemically reversible behavior was utilized as the internal reference, because it has a larger redox potential difference with respect to a high HOMO DSC dye, in contrast to the routinely used ferrocene (FC) reference. We measured the difference in formal redox potentials of DMFC and FC to be 0.489 V. After voltammetric measurements, all potentials were calibrated with respect to Fc. Electronic absorption measurements were performed on an Agilent G1103A spectrometer. TCSPC measurements were performed on a LifeSpec-II fluorescence spectrometer employing an EPL485 pulsed laser diode and a Hamamatsu H5773-04 photomultiplier. The EQE, *J*–*V*, charge extraction (CE), and transient photovoltage decay (TPD) measurements have been detailed in our previous papers.[S11,S12] A black metal mask with an aperture area of 0.160 cm^2 was covered on a testing cell during EQE and *J*–*V* measurements.

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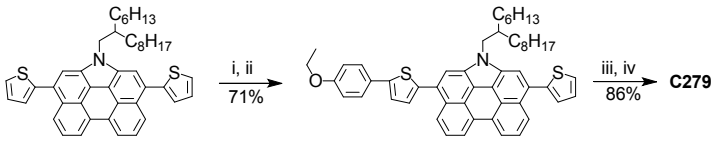
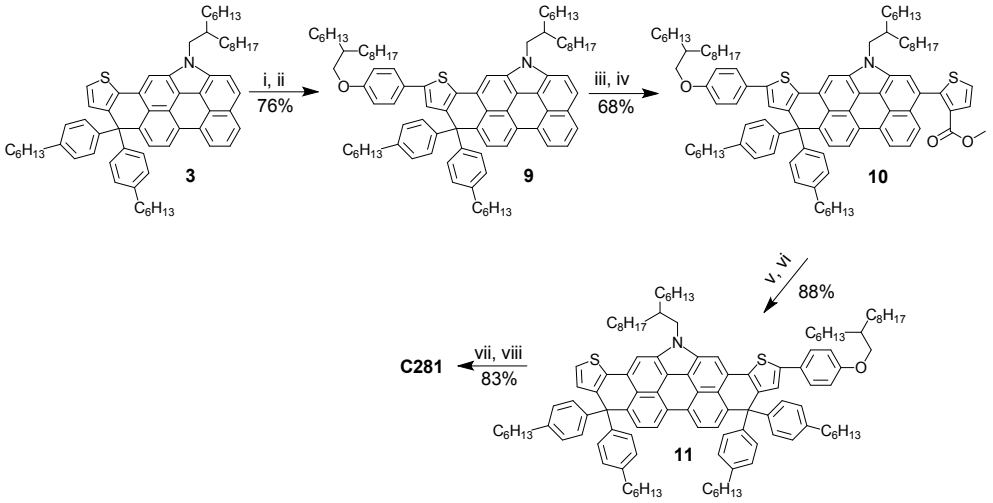


7 8

Scheme S1. Synthetic routes of **C279** characteristic of a T-PC-T moiety. Reagents and conditions: (i) *n*-BuLi, THF, −78 °C, 0.5 h; then $Sn(CH_3)_3Cl$, RT, 2 h; (ii) 1-ethoxy-4-iodobenzene, $Pd(PPh_3)_2Cl_2$, toluene, reflux, 6 h; (iii) *n*-BuLi, THF, −78 °C, 0.5 h; $Sn(CH_3)_3Cl$, RT, 2 h; then **2**, $Pd(PPh_3)_2Cl_2$, toluene, reflux, 6 h; (iv) KOH, THF/H_2O (3/1, *v*/*v*), reflux, overnight; phosphoric acid.



Scheme S2. Synthetic routes of **C281**. Reagents and conditions: (i) *n*-BuLi, THF, −78 °C, 0.5 h; then $Sn(CH_3)_3Cl$, RT, 2 h; (ii) 1-((2-hexyldecyl)oxy)-4-iodobenzene, $Pd(PPh_3)_2Cl_2$, toluene, reflux, 6 h; (iii) NBS, THF, 0 °C, 0.5 h; (iv) methyl thiophene-3-carboxylate, $Pd(OAc)_2$, $PCy_3{\cdot}HBF_4$, PivOH, K_2CO_3, toluene, reflux, 24 h; (v) (4-hexylphenyl)magnesium bromide, THF, reflux, 6 h; (vi) Amberlyst 15, toluene, reflux, 6 h; (vii) *n*-BuLi, THF, −78 °C, 0.5 h; $Sn(CH_3)_3Cl$, RT, 2 h; then **2**, $Pd(PPh_3)_2Cl_2$, toluene, reflux, 6 h; (viii) KOH, THF/H_2O (3/1, *v*/*v*), reflux, overnight; phosphoric acid.

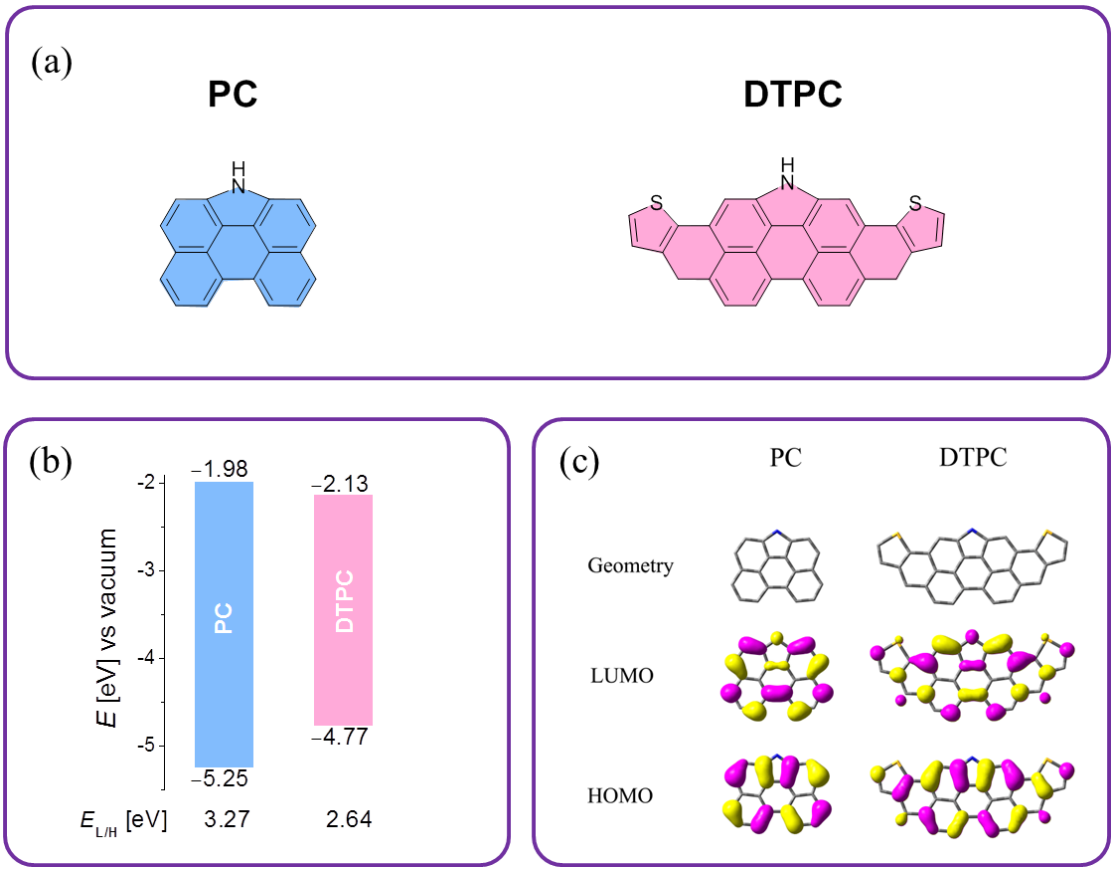


Figure S1. (a) Chemical structures of two polycyclic aromatic hydrocarbons derived from carbazole: 1*H*-phenanthro[1,10,9,8-*cdefg*]carbazole (PC) and 9,14-dihydro-4*H*-dithieno[2',3':2,3;3",2":10,11]piceno[1,14,13,12-*bcdefgh*]carbazole (DTPC). (b) LUMO energy levels (values above color bars), HOMO energy levels (value under color bars), and LUMO/HOMO energy gaps ($E_{L/H}$). (c) Optimized molecular geometries and contour plots of frontier molecular orbitals at the B3LYP/6-311G(d,p) level. The values of isodensity surface are fixed at 0.03.

Table S1. Energy levels and electronic absorption properties

Dye	E_L^{B3LYP} [eV] [a]	E_L^{CV} [eV] [b]	E_H^{B3LYP} [eV] [a]	E_H^{CV} [eV] [b]	$\lambda_{ABS,MAX}^{TD\text{-}MPW1K}$ [nm] [c]	$\lambda_{ABS,MAX}^{MEAS}$ [nm] [d]	Transition[c]
C279	−3.06	−3.33	−5.10	−5.07	535	470	H−1→L (11%) H→L (78%) H→L+1 (6%)
C280	−3.09	−3.32	−4.83	−4.84	630	609	H−1→L (6%) H→L (88%) H→L+1 (6%)

[a] Molecular orbital energy levels (E_L^{B3LYP} and E_H^{B3LYP}) vs vacuum were calculated at the B3LYP/6-311G(d,p) level of theory for dyes in THF. [b] Molecular orbital energy levels (E_L^{CV} and E_H^{CV}) vs vacuum were derived from cyclic voltammograms (CV) shown in Figure 1a of the main text. H and L denote HOMO and LUMO, respectively. [c] Maximum absorption wavelengths ($\lambda_{MAX}^{TD\text{-}MPW1K}$) and transitions were calculated at the TD-MPW1K/6-311G(d,p) level of theory for dyes in THF. [d] Maximum absorption wavelength (λ_{MAX}^{MEAS}) were derived from electronic absorption spectra in Figure 1b of the main text.

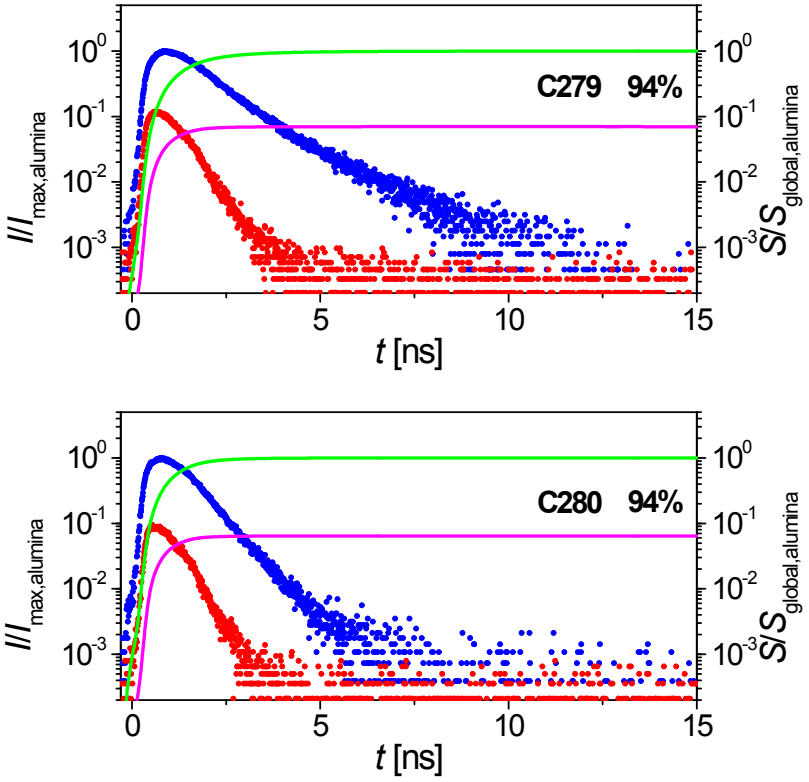


Figure S2. PL decay traces of dye-grafted alumina (blue line) and titania (red line) films immersed in a cobalt electrolyte: (a) **C279**, (b) **C280**. The PL intensity (I) was corrected in term of the absorbance at 482 nm and further normalized with respect to the PL maximum of a corresponding dye-grafted alumina film ($I_{max,alumina}$). The PL integral areas (S) of the alumina (green line) and titania (magenta line) films were normalized with respect to the global PL integral area ($S_{global,alumina}$) of a corresponding dye-grafted alumina film. Excitation wavelength: 482 nm; probe wavelength: 815 nm.

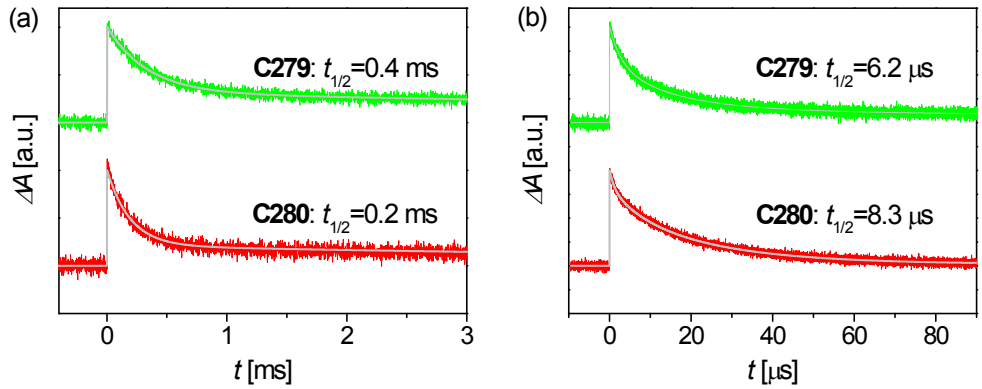


Figure S3. Transient absorption traces upon nanosecond pulsed laser excitation of 4.5-μm-thick titania films grafted with **C279** and **C280** immersed in the inert (panel a) and Co-bpy (panel b) electrolytes. Pulse fluence: 19 μJ cm^{-2}. Excitation wavelength: 629 nm for **C279**; 694 nm for **C280**. Probe wavelength: 850 nm. The excitation wavelengths were carefully selected according to a 0.5 optical density of dye-grafted titania films to ascertain a similar excited state distribution in the testing films. The solid gray lines are fittings of normalized absorption (ΔA) via a multi-exponential function: $\Delta A = \sum_i A_i \exp(-t/\tau_i)$.

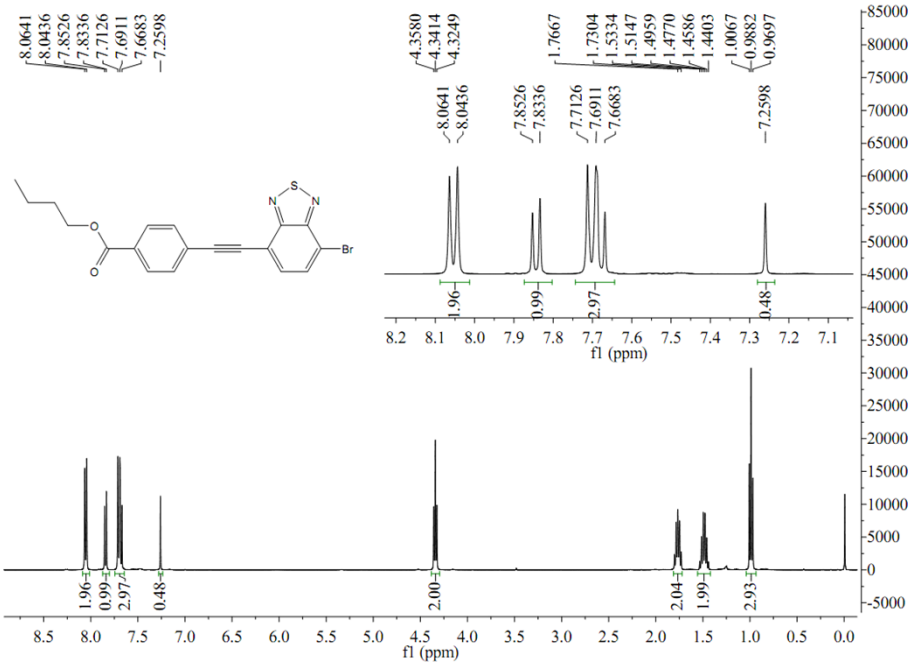


Figure S4. The ^{1}H NMR (400 MHz) spectrum of butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate in $CDCl_3$.

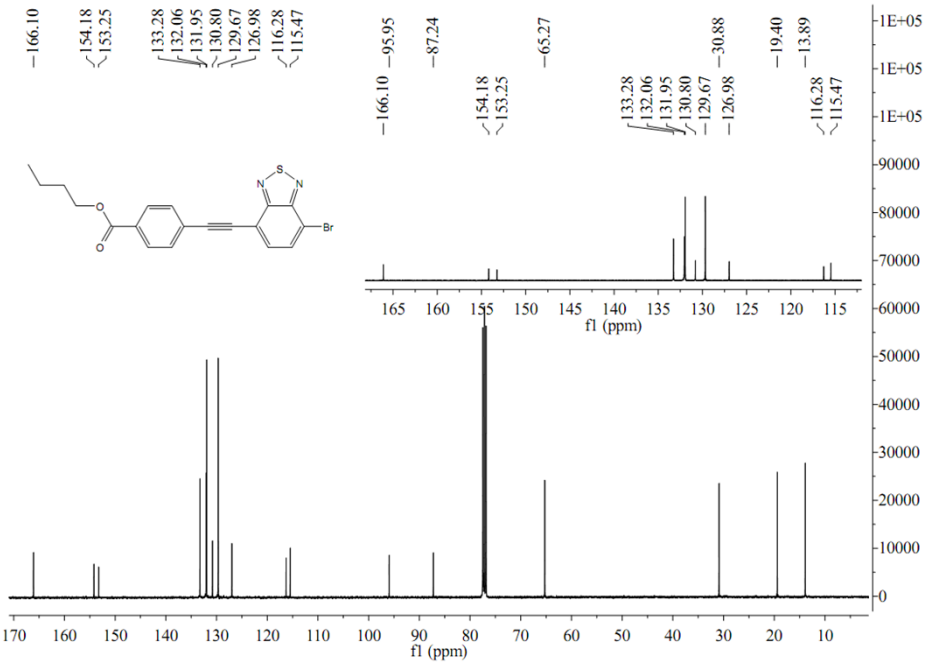


Figure S5. The ^{13}C NMR (100 MHz) spectrum of butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate in $CDCl_3$.

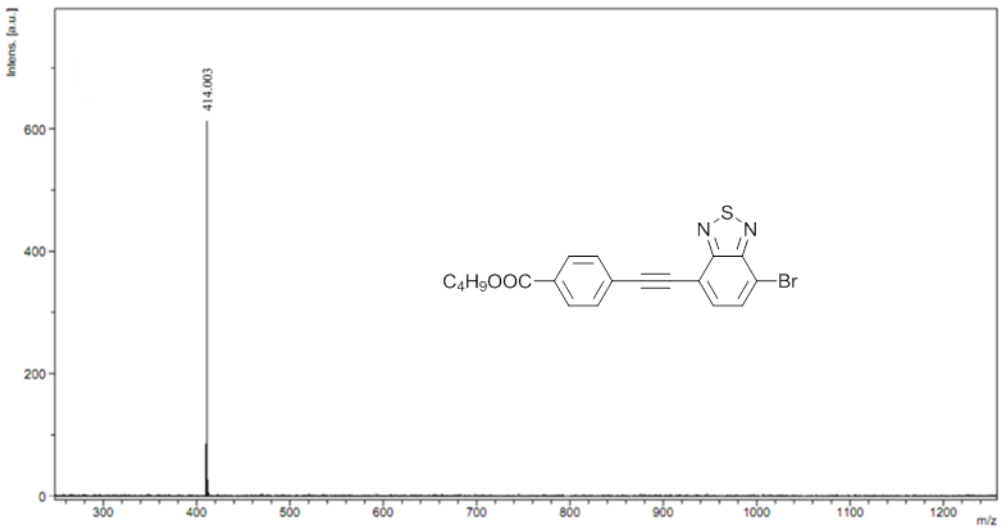


Figure S6. The high resolution mass spectrum (MALDI-TOF) of butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate.

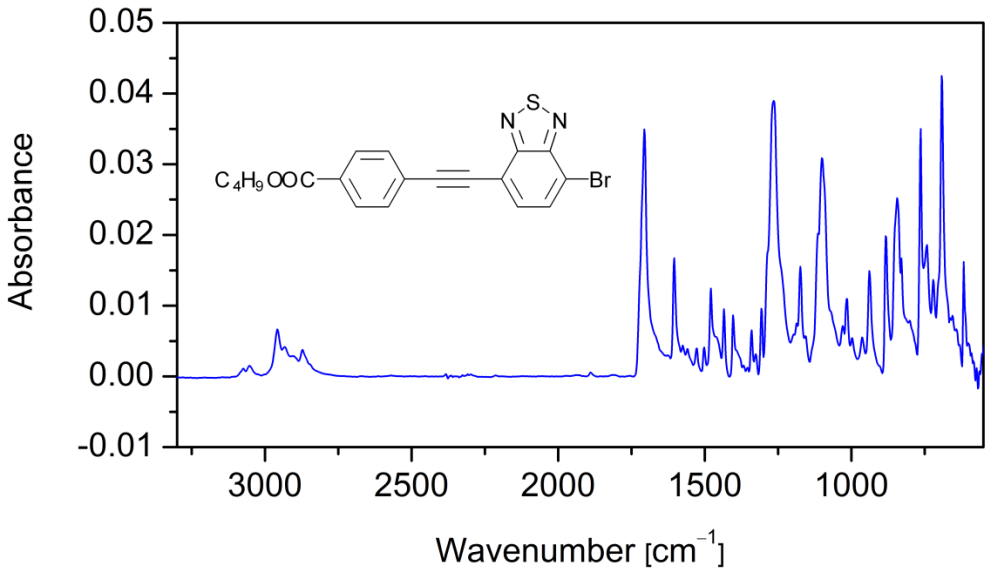


Figure S7. The ATR-IR spectrum of butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate.

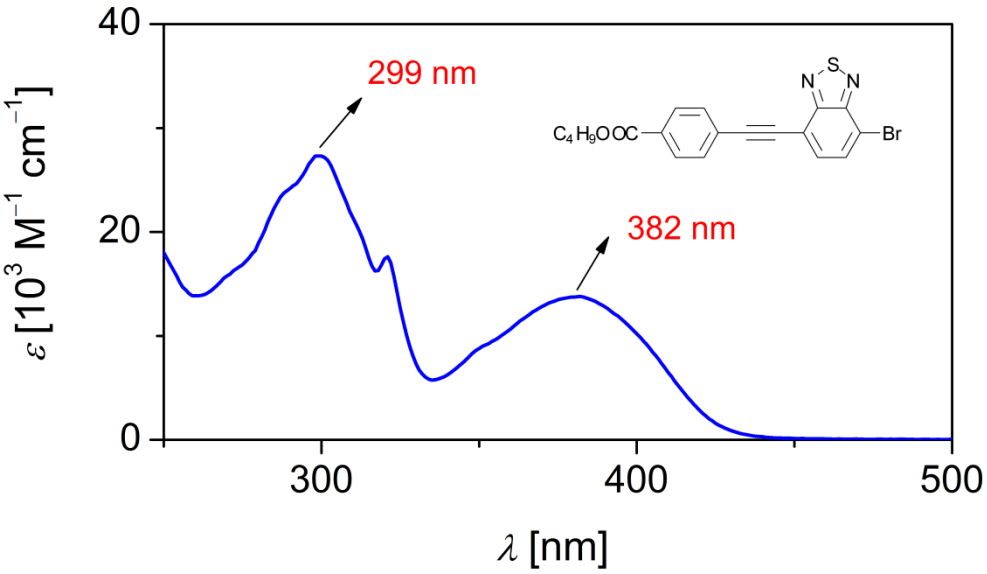


Figure S8. Electronic absorption spectrum of 10 μM butyl 4-((7-bromobenzo[*c*][1,2,5]thiadiazol-4-yl)ethynyl)benzoate dissolved in THF.

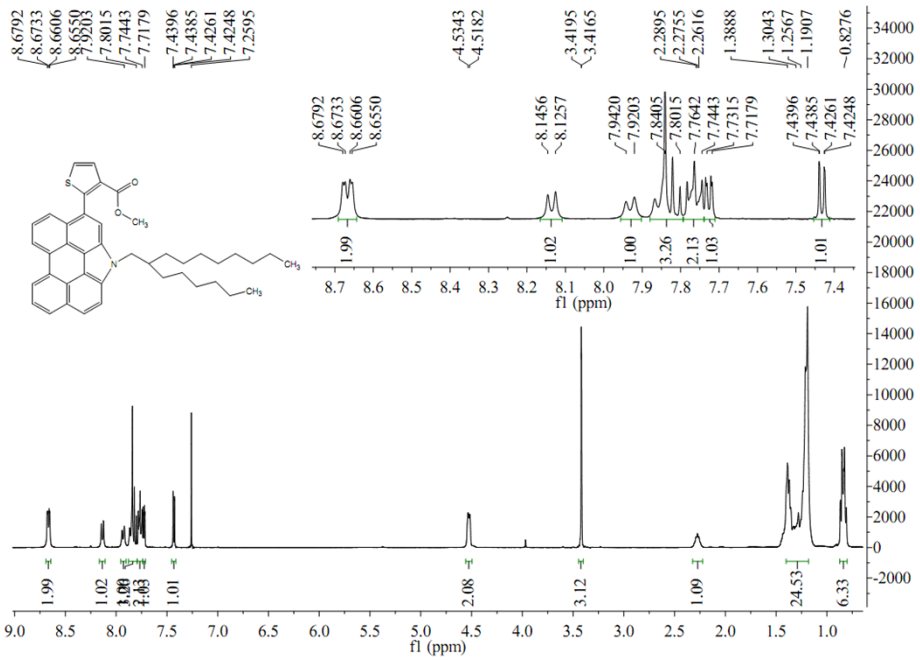


Figure S9. The ^{1}H NMR (400 MHz) spectrum of **2** in $CDCl_3$.

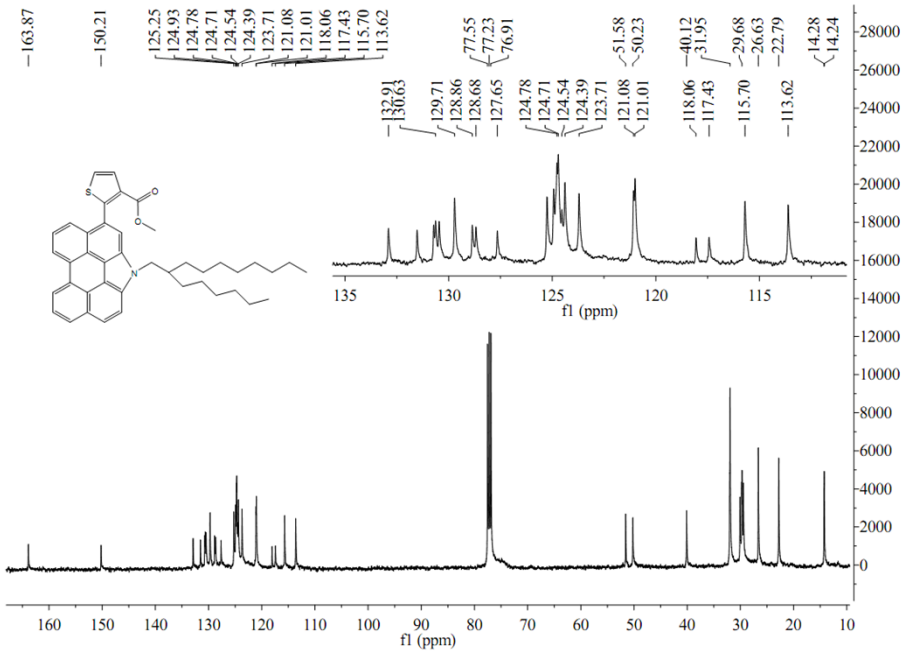


Figure S10. The ^{13}C NMR (100 MHz) spectrum of **2** in $CDCl_3$.

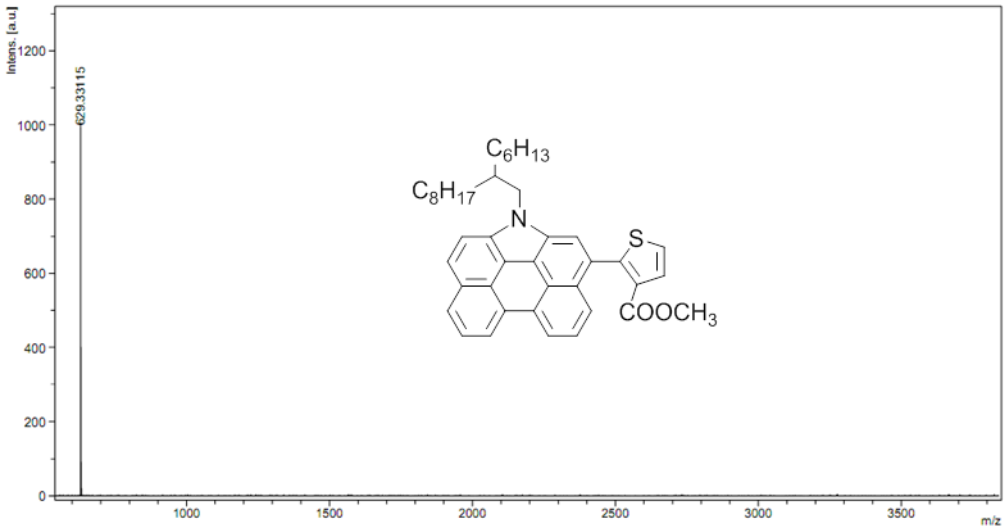


Figure S11. The high resolution mass spectrum (MALDI-TOF) of **2**.

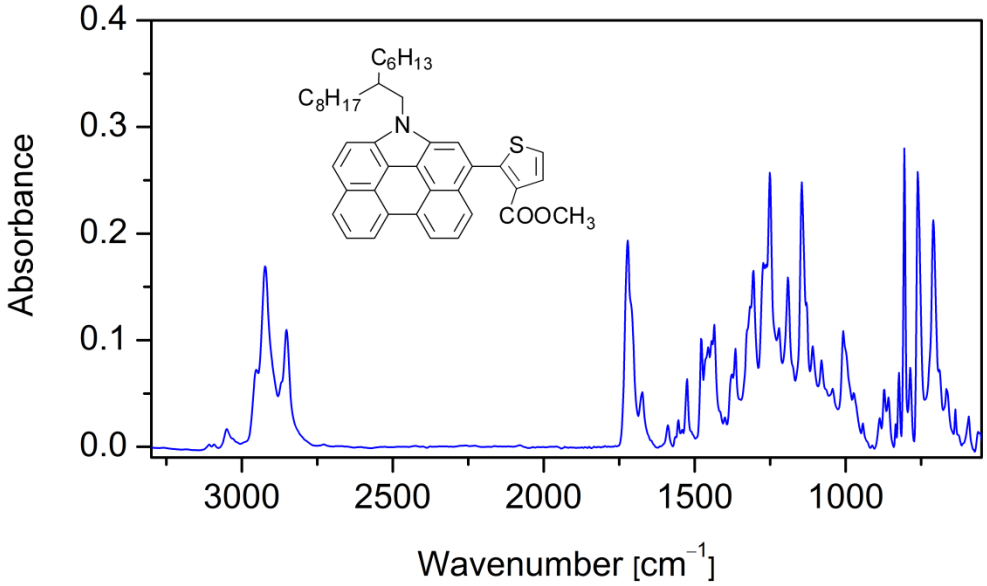


Figure S12. The ATR-IR spectrum of **2**.

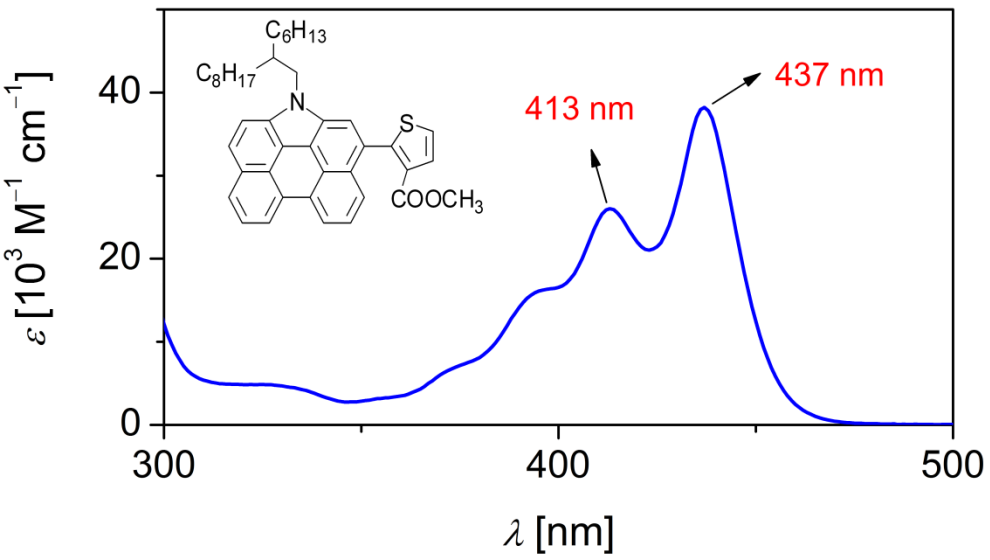


Figure S13. Electronic absorption spectrum of 10 μM **2** dissolved in THF.

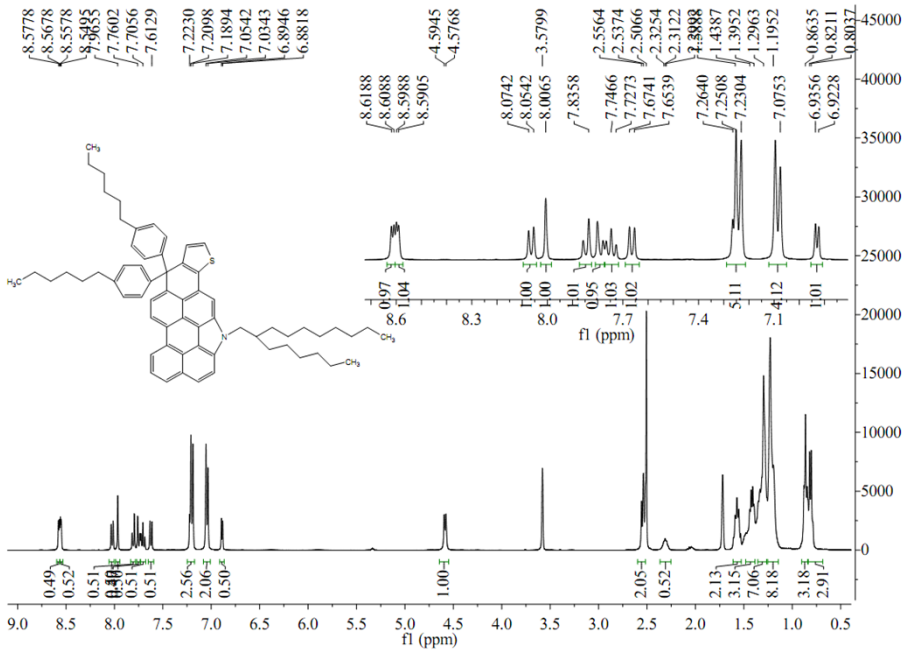


Figure S14. The ^{1}H NMR (400 MHz) spectrum of **3** in THF.

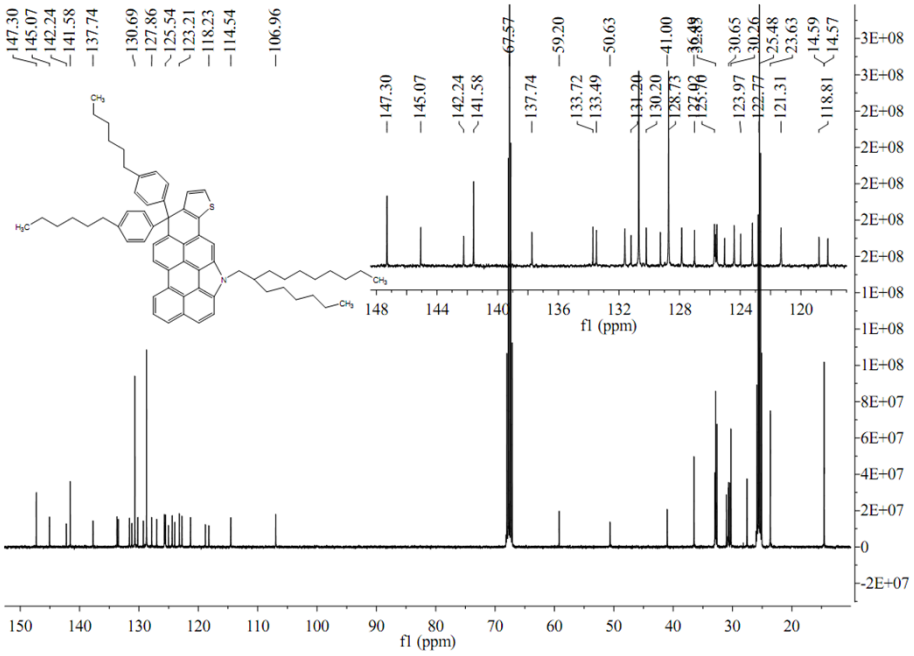


Figure S15. The ^{13}C NMR (100 MHz) spectrum of **3** in THF.

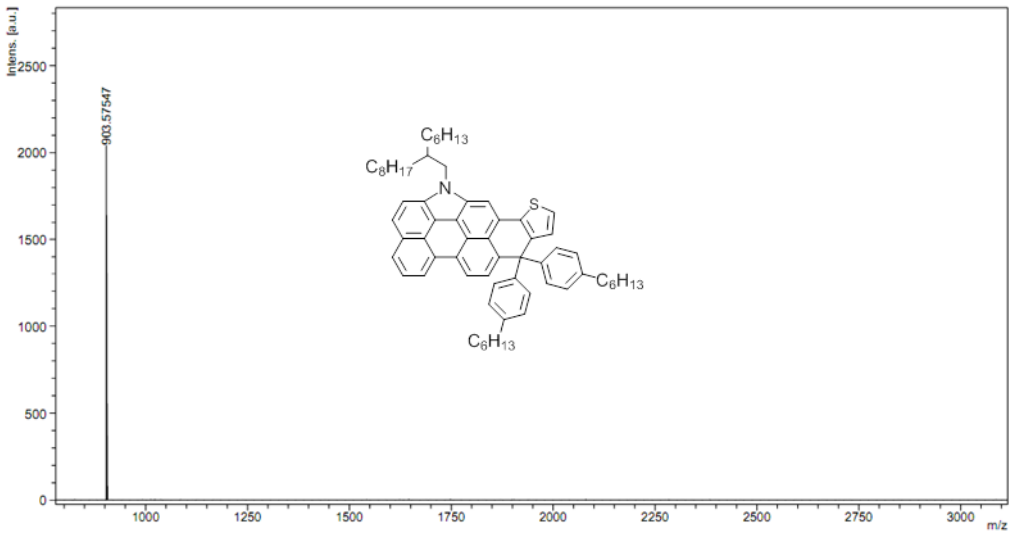


Figure S16. The MALDI-TOF high resolution mass spectrum of **3**.

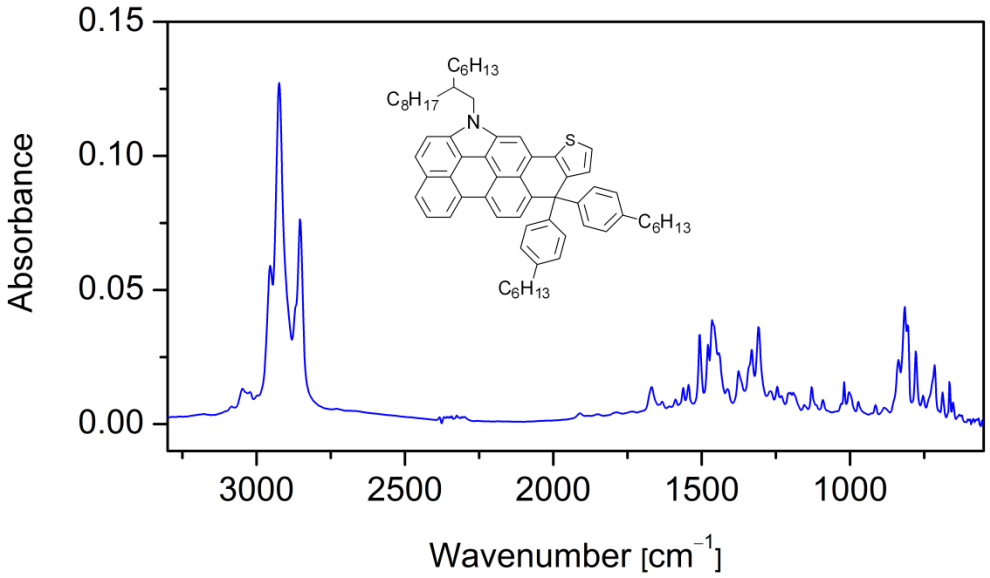


Figure S17. The ATR-IR spectrum of **3**.

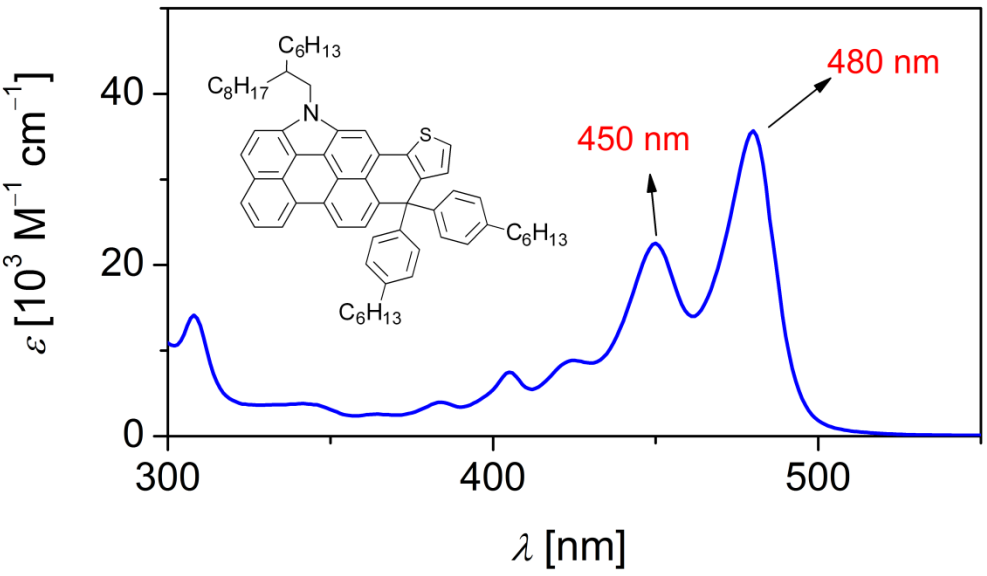


Figure S18. Electronic absorption spectrum of 10 μM **3** dissolved in THF.

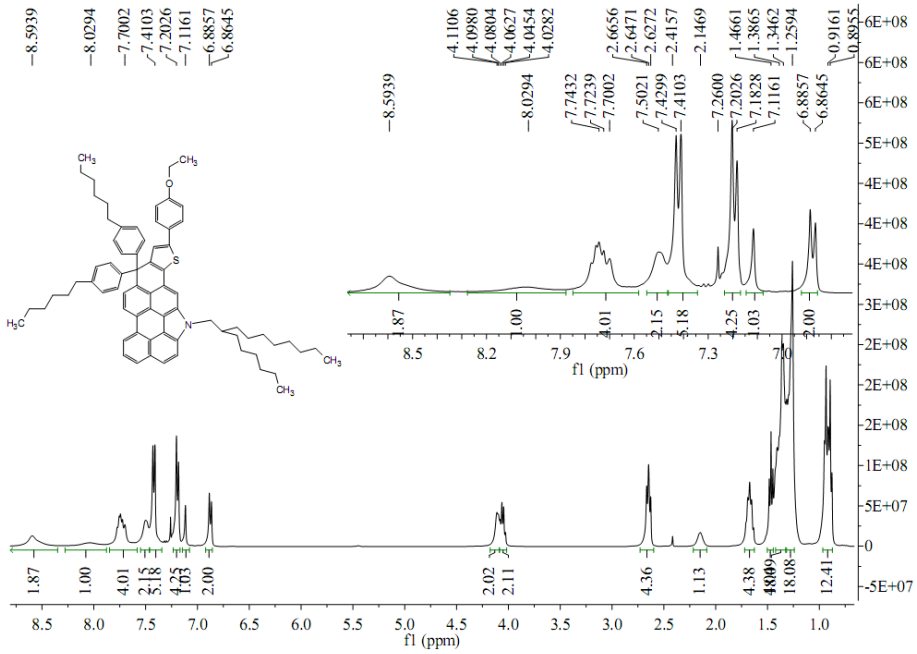


Figure S19. The ^{1}H NMR (400 MHz) spectrum of **4** in $CDCl_3$.

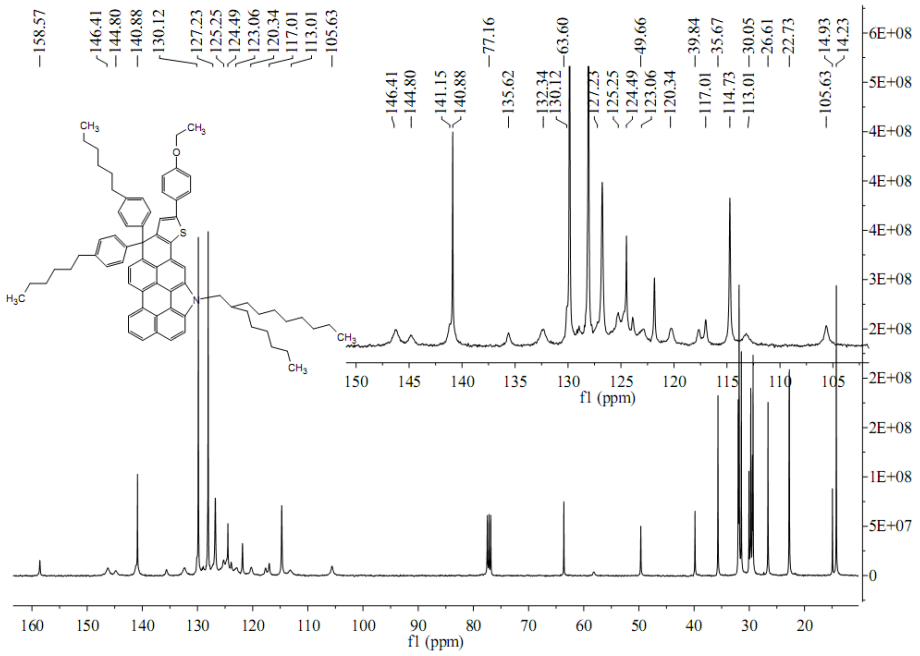


Figure S20. The ^{13}C NMR (100 MHz) spectrum of **4** in $CDCl_3$.

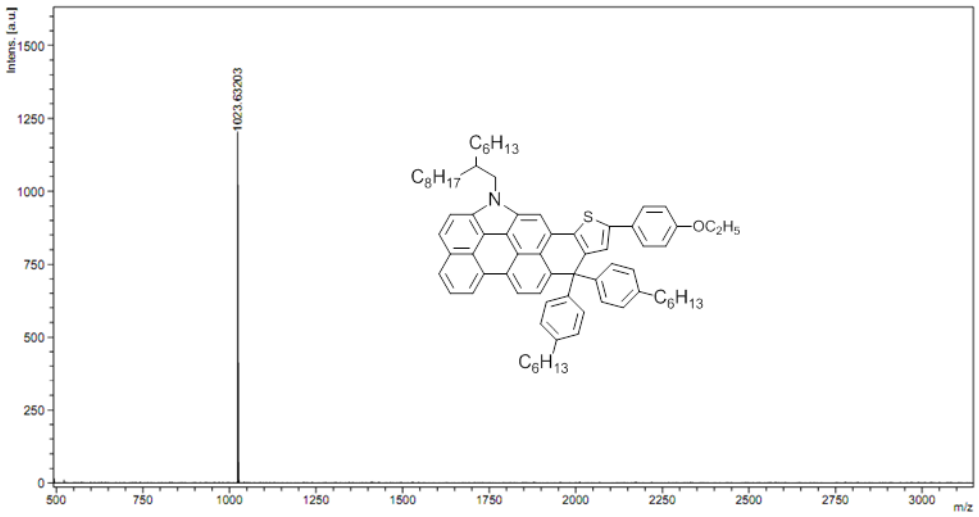


Figure S21. The high resolution mass spectrum (MALDI-TOF) of **4**.

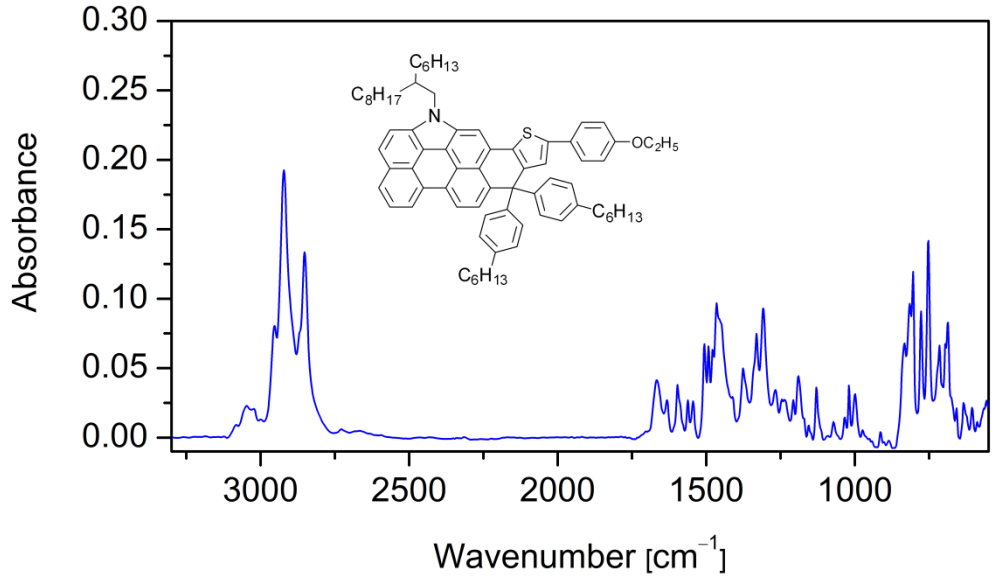


Figure S22. The ATR-IR spectrum of **4**.

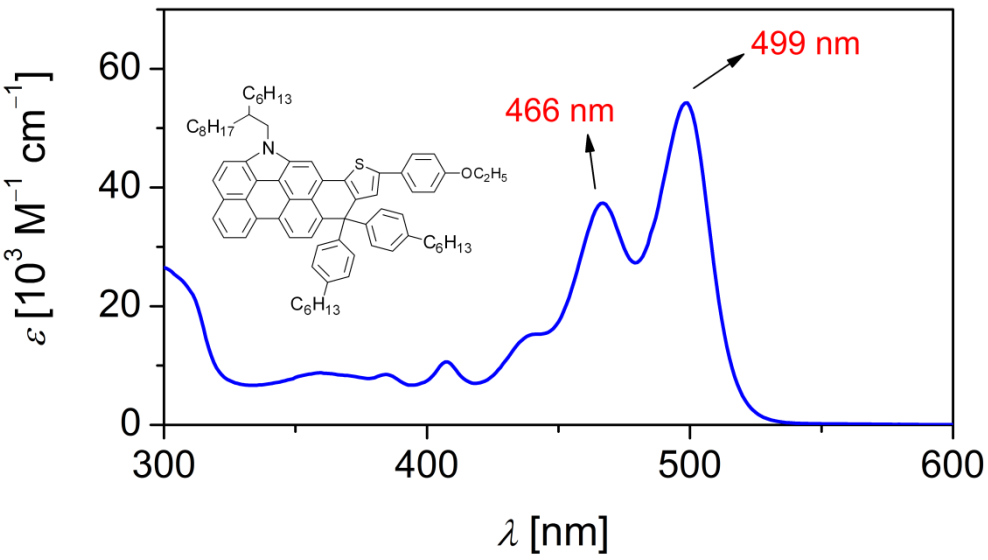


Figure S23. Electronic absorption spectrum of 10 μM **4** dissolved in THF.

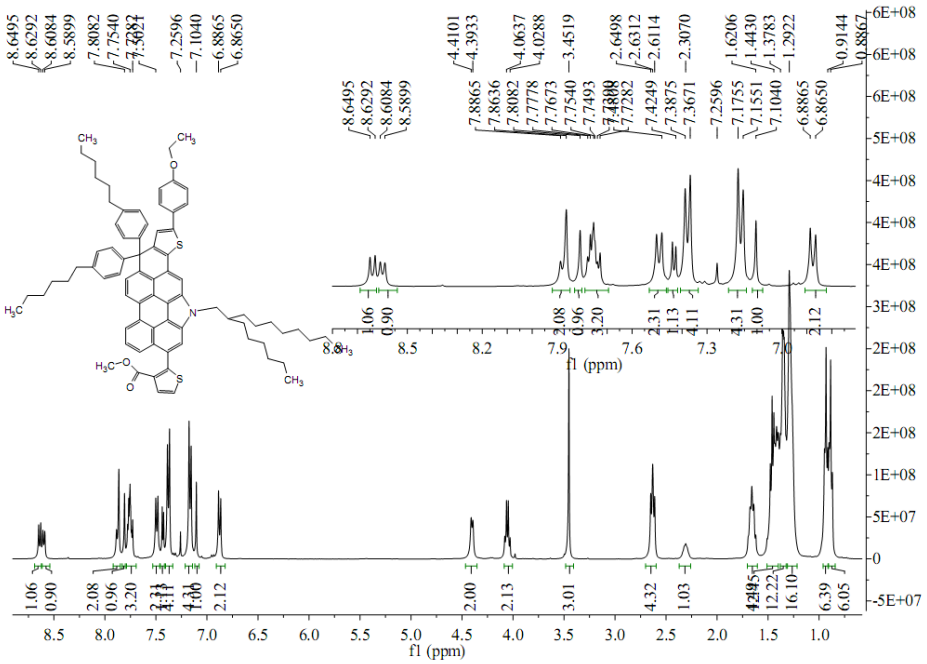


Figure S24. The ^{1}H NMR (400 MHz) spectrum of **5** in $CDCl_3$.

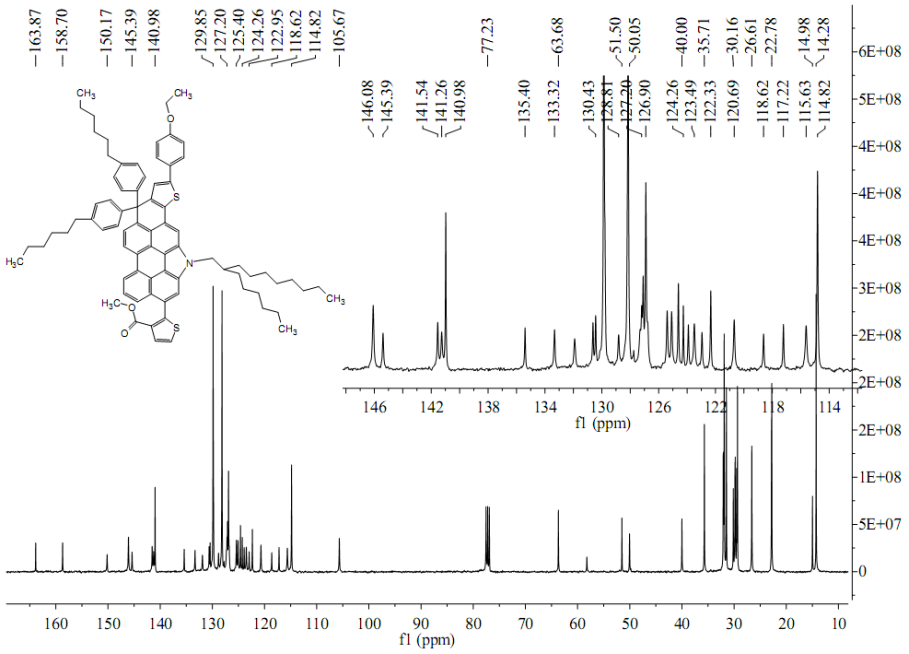


Figure S25. The ^{13}C NMR (100 MHz) spectrum of **5** in $CDCl_3$.

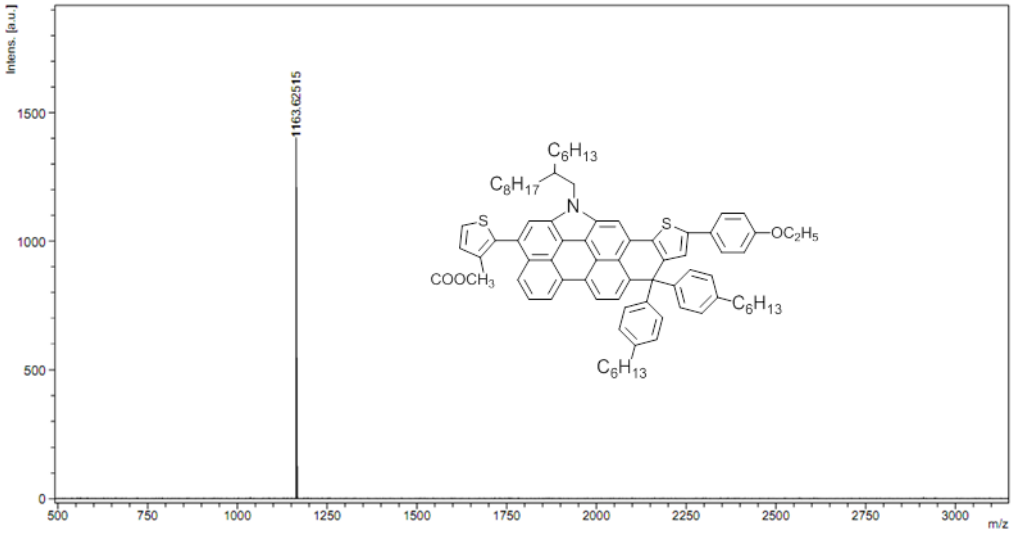


Figure S26. The high resolution mass spectrum (MALDI-TOF) of **5**.

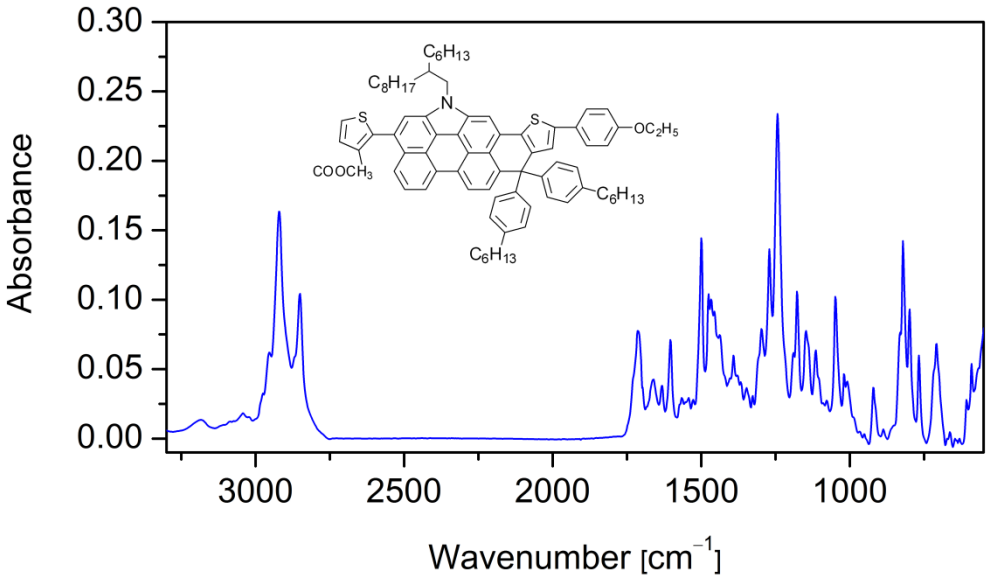


Figure S27. The ATR-IR spectrum of **5**.

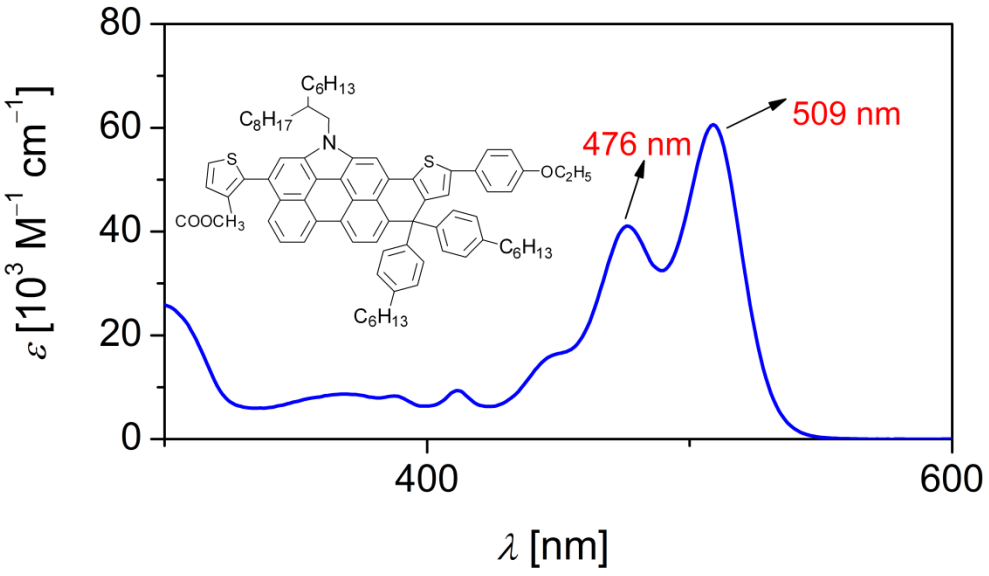


Figure S28. Electronic absorption spectrum of 10 μM **5** dissolved in THF.

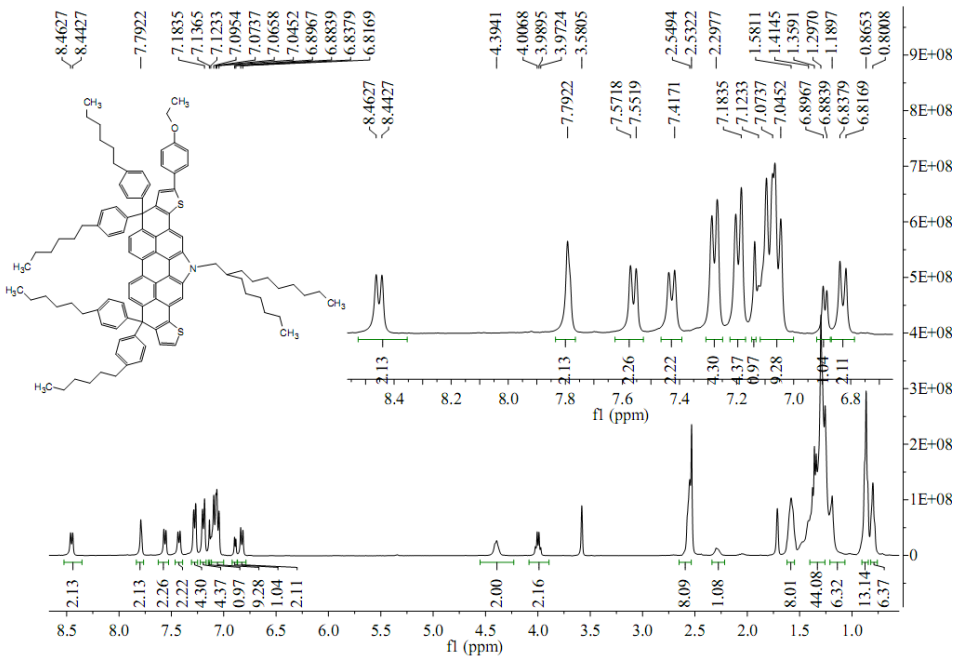


Figure S29. The ^{1}H NMR (400 MHz) spectrum of **6** in THF.

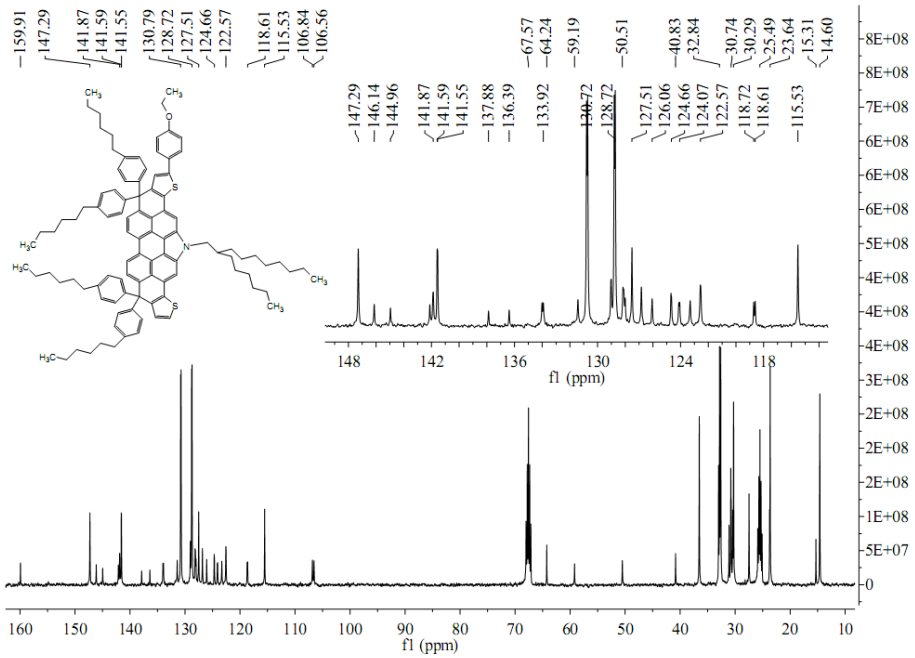


Figure S30. The ^{13}C NMR (100 MHz) spectrum of **6** in THF.

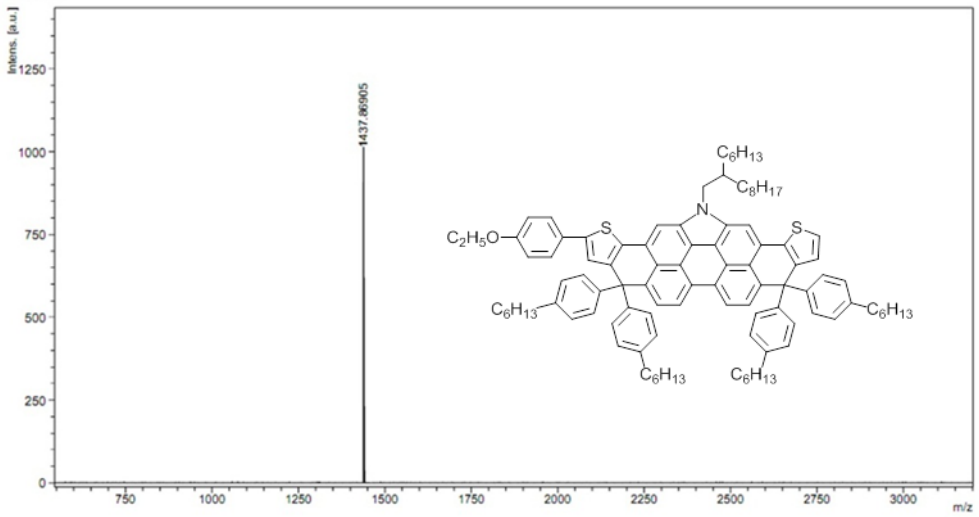


Figure S31. The high resolution mass spectrum (MALDI-TOF) of **6**.

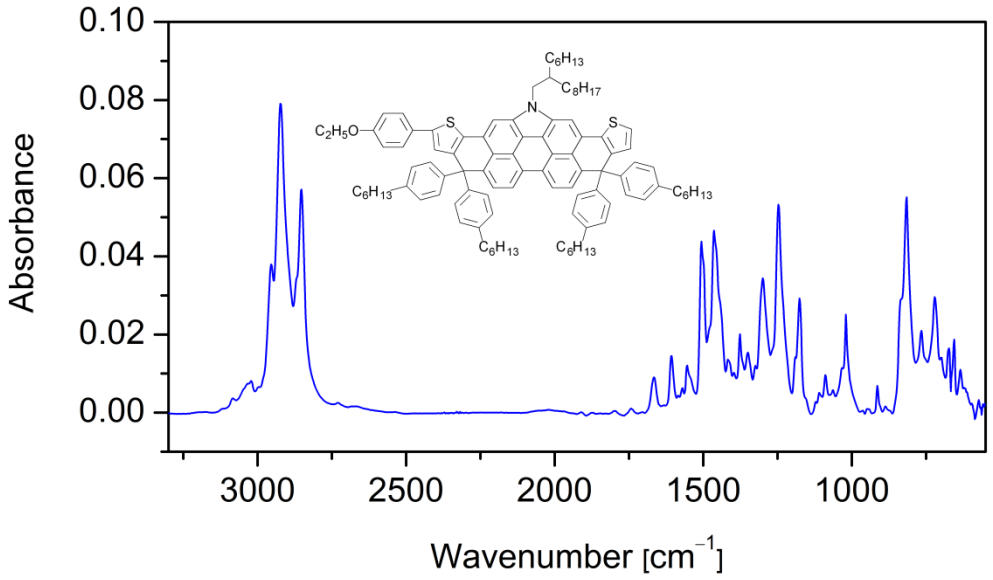


Figure S32. The ATR-IR spectrum of **6**.

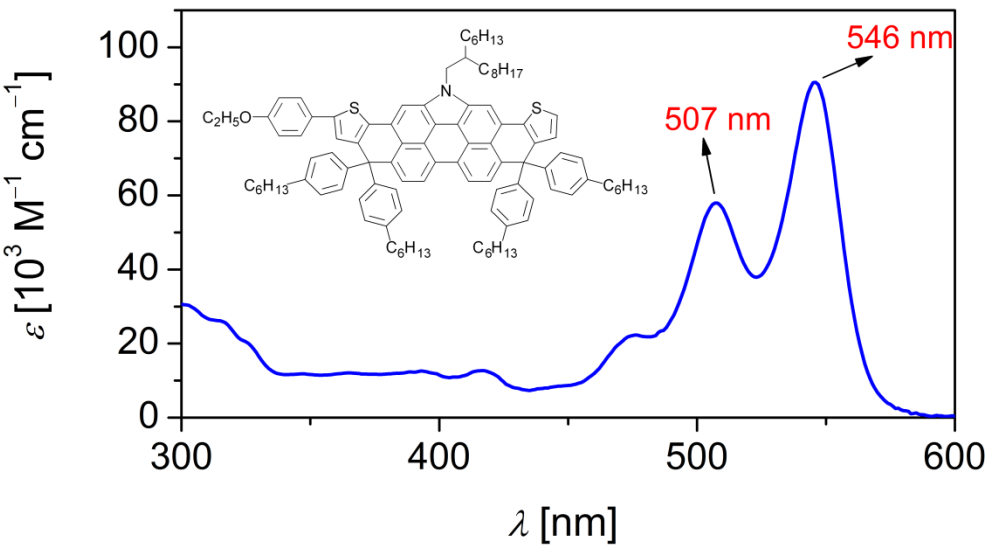


Figure S33. Electronic absorption spectrum of 10 μM **6** dissolved in THF.

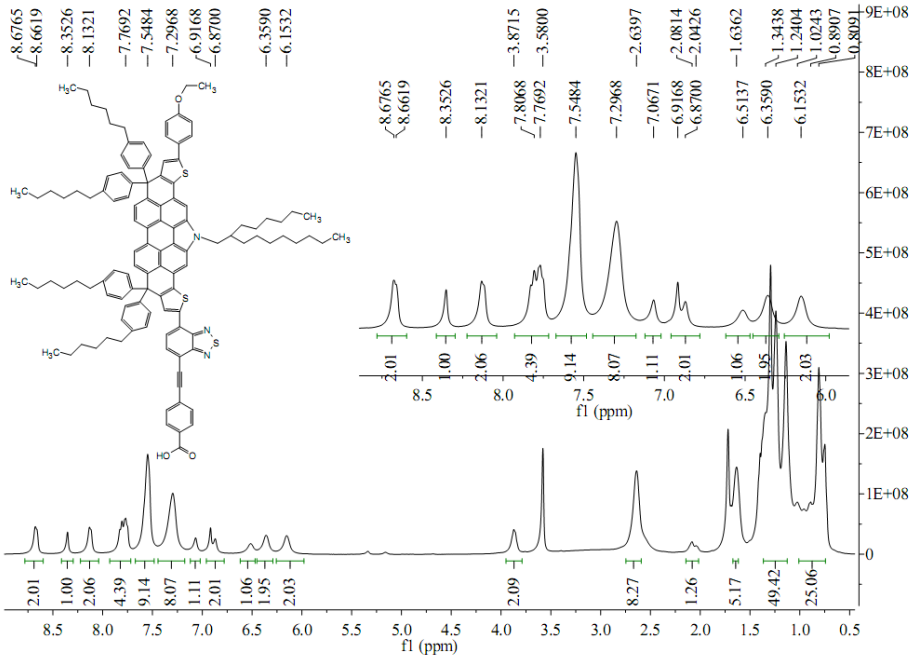


Figure S34. The ^{1}H NMR (400 MHz) spectrum of **C280** in THF.

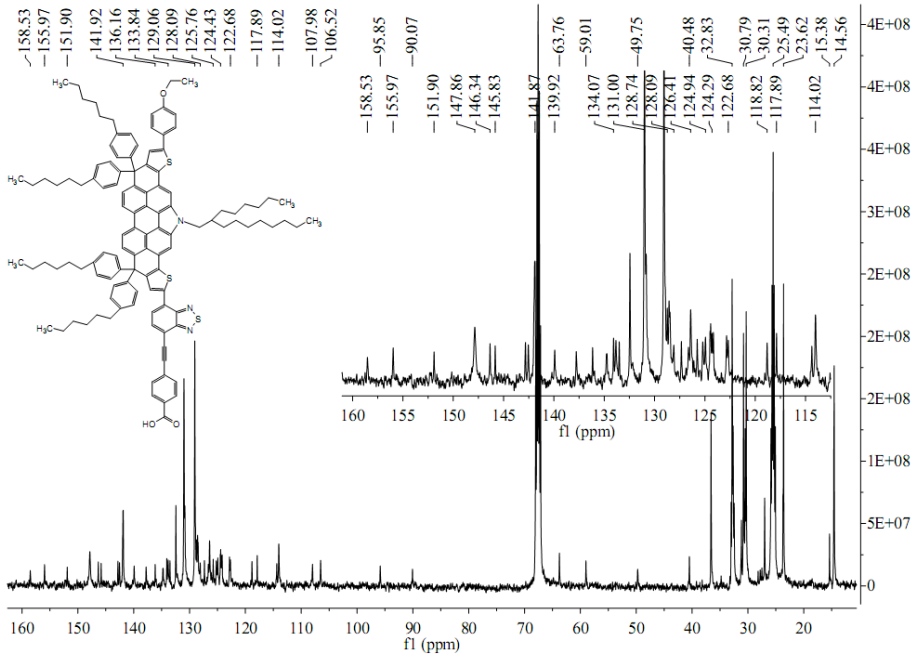


Figure S35. The ^{13}C NMR (100 MHz) spectrum of **C280** in THF.

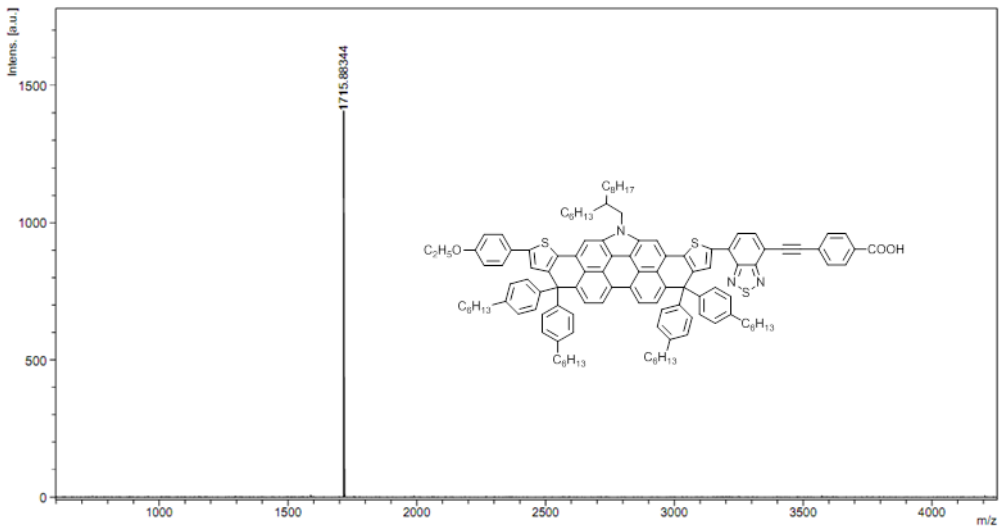


Figure S36. The high resolution mass spectrum (MALDI-TOF) of **C280**.

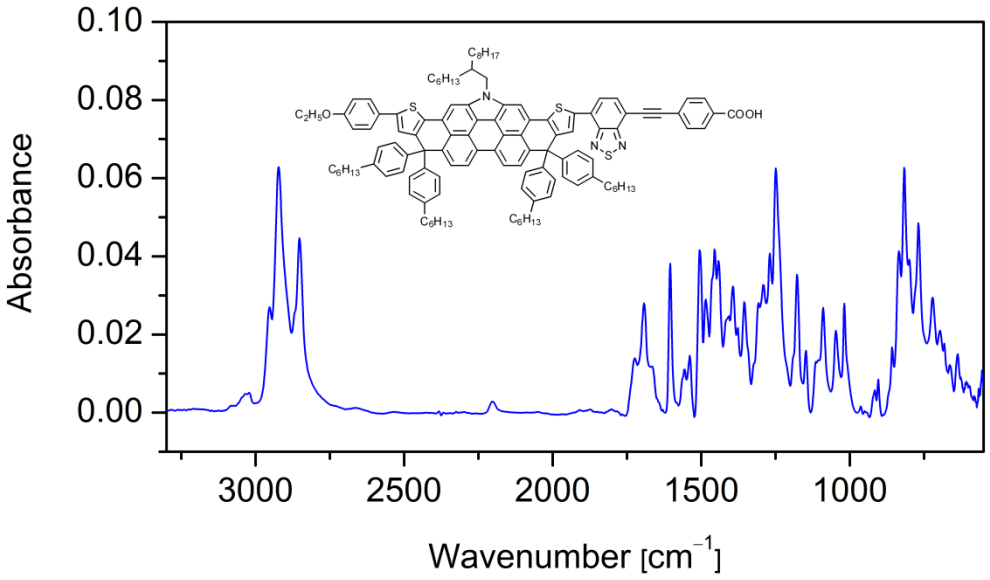


Figure S37. The ATR-IR spectrum of **C280**.

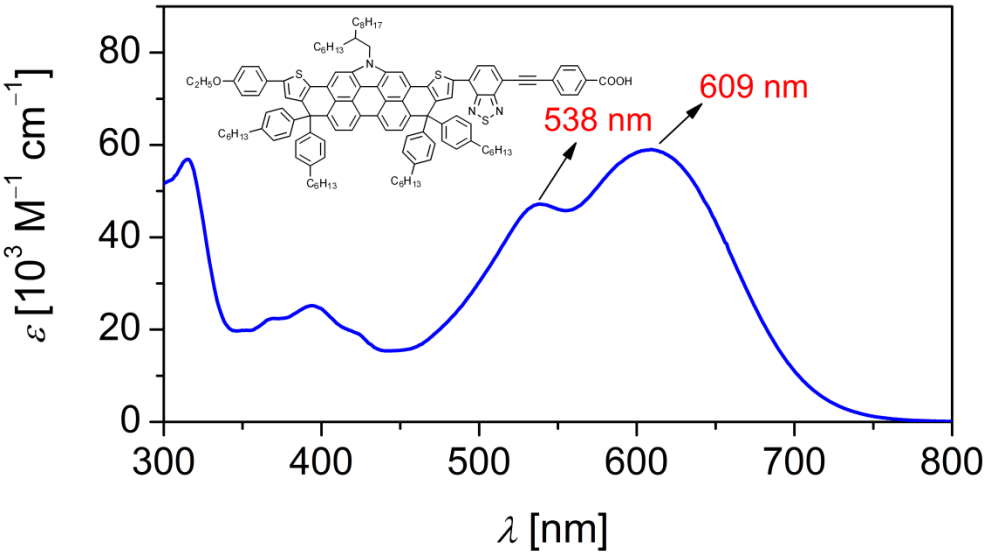


Figure S38. Electronic absorption spectrum of 10 μM **C280** dissolved in THF.

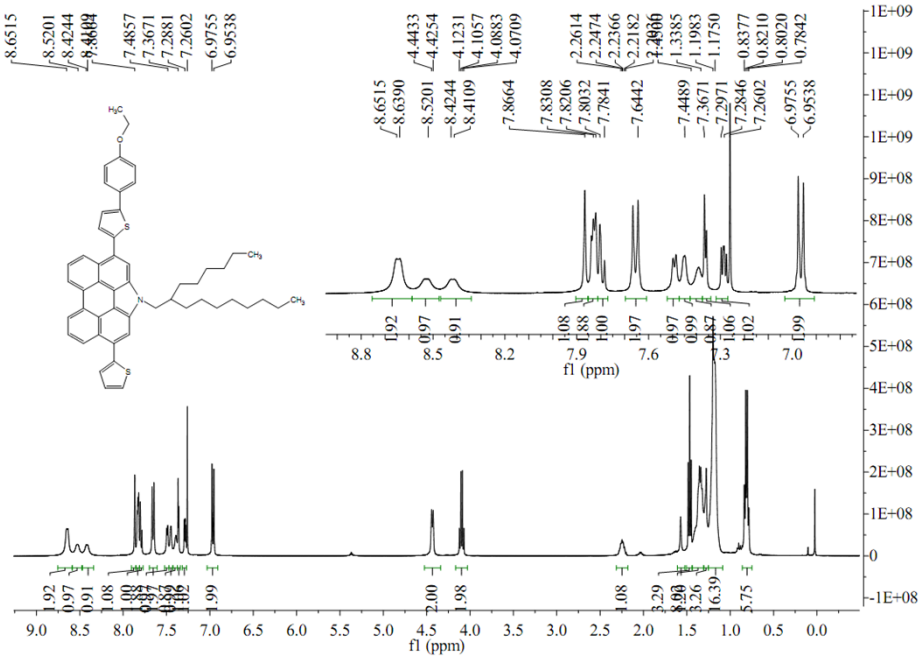


Figure S39. The ^{1}H NMR (400 MHz) spectrum of **8** in $CDCl_3$.

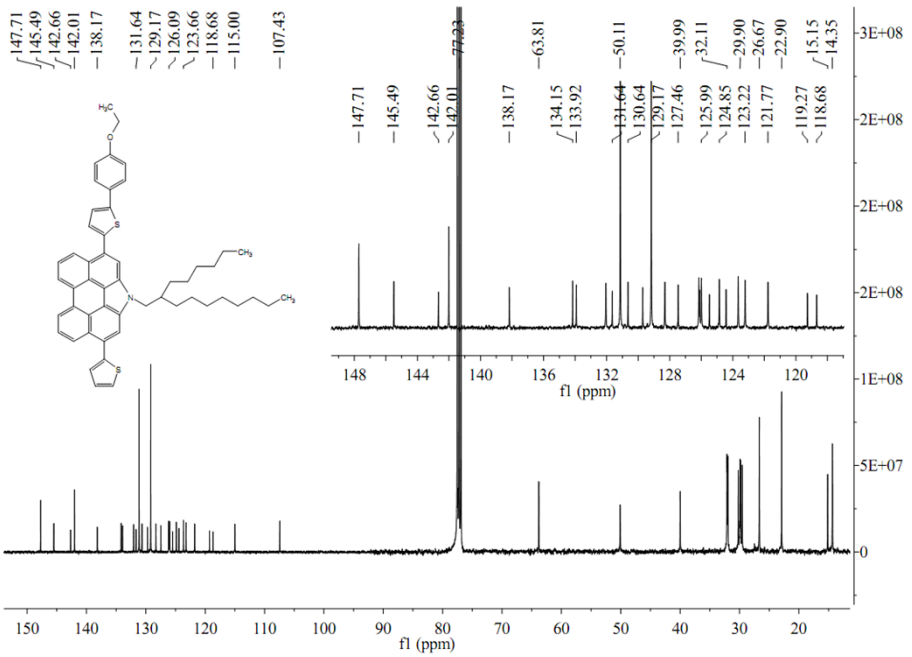


Figure S40. The ^{13}C NMR (100 MHz) spectrum of **8** in $CDCl_3$.

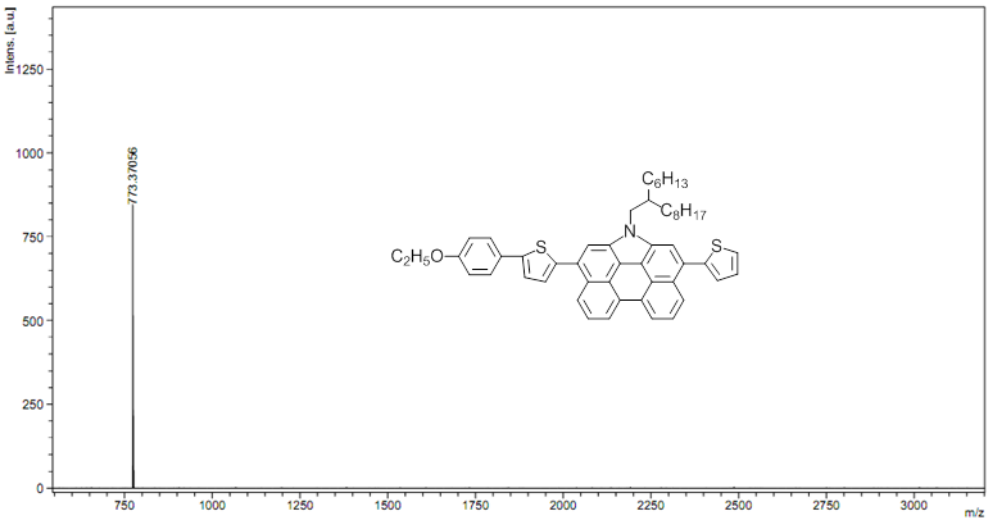


Figure S41. The high resolution mass spectrum (MALDI-TOF) of **8**.

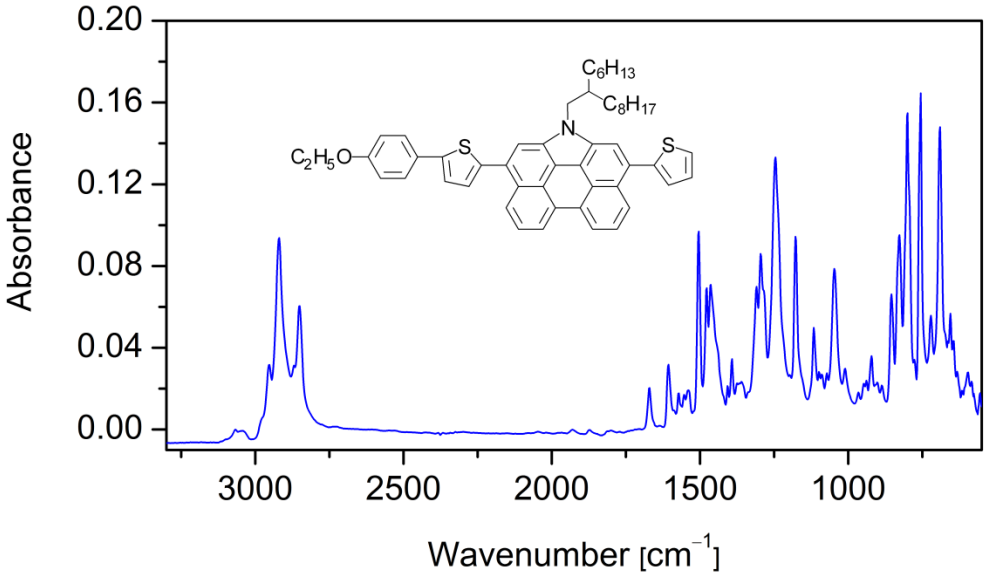


Figure S42. The ATR-IR spectrum of **8**.

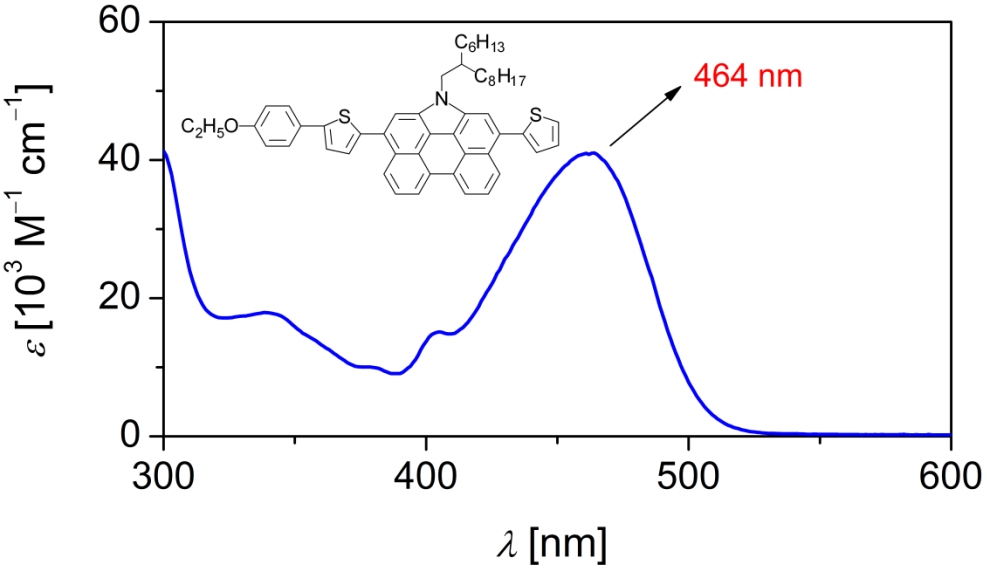


Figure S43. Electronic absorption spectrum of 10 μM **8** dissolved in THF.

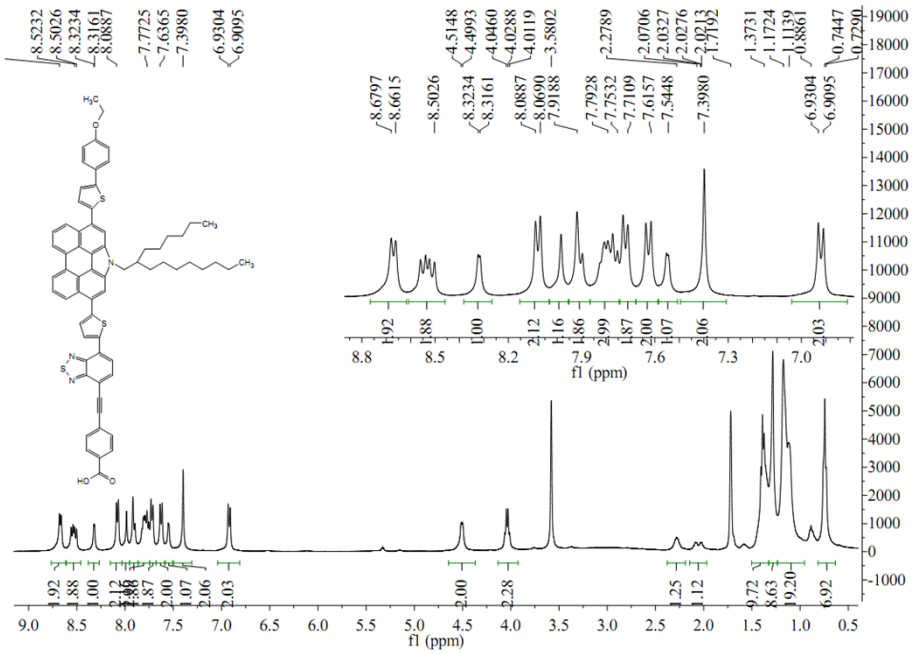


Figure S44. The ^{1}H NMR (400 MHz) spectrum of **C279** in THF.

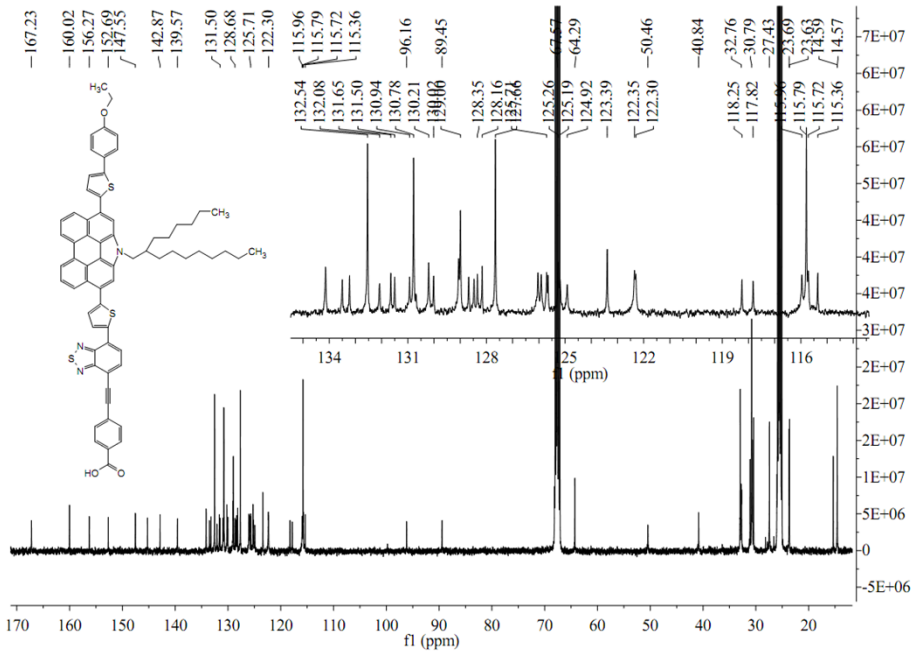


Figure S45. The ^{13}C NMR (100 MHz) spectrum of **C279** in THF.

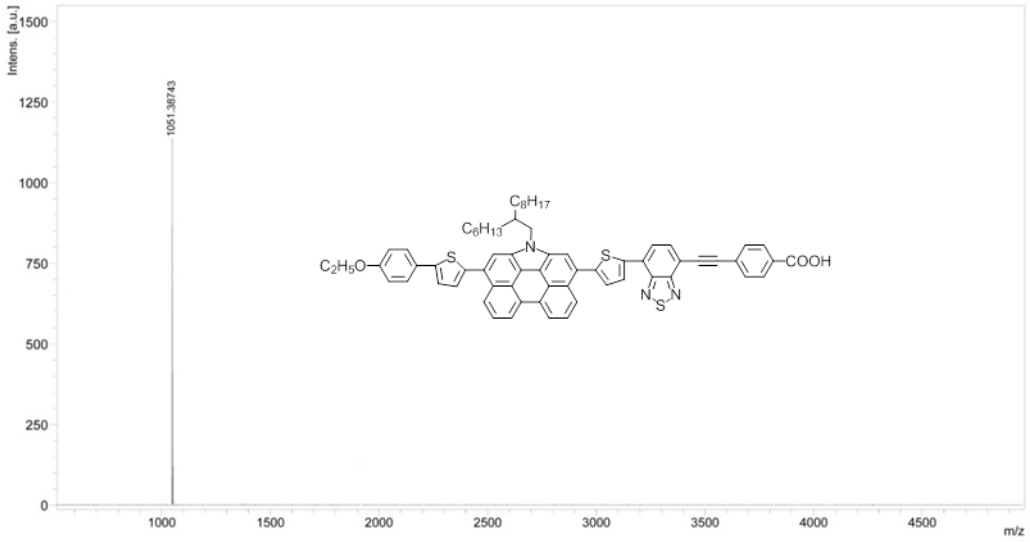


Figure S46. The high resolution mass spectrum (MALDI-TOF) of **C279**.

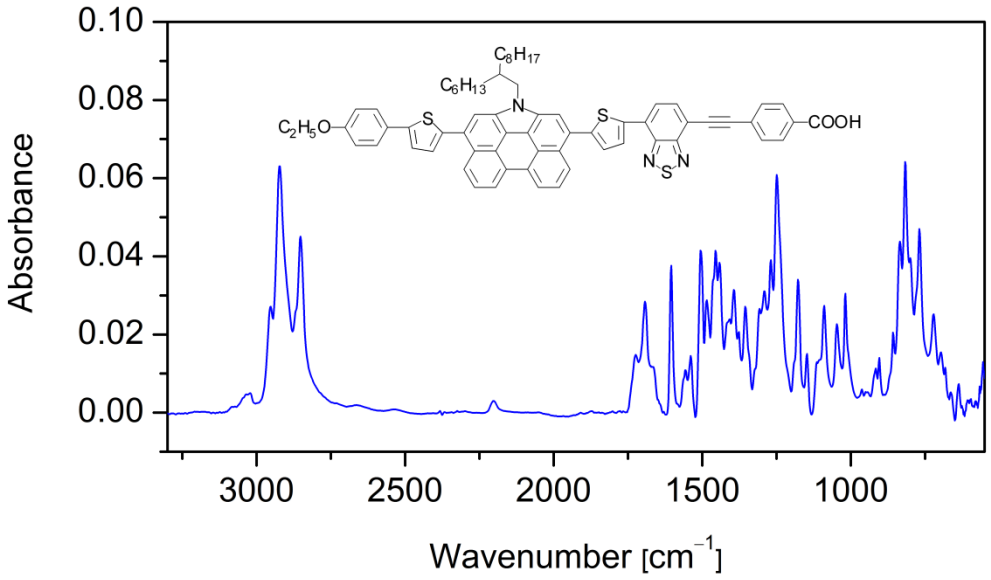


Figure S47. The ATR-IR spectrum of **C279**.

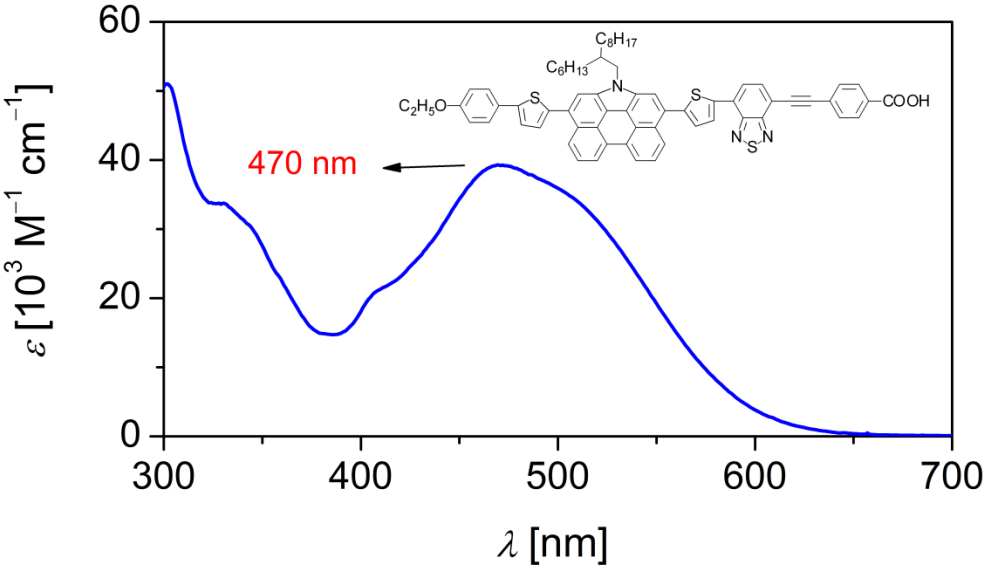


Figure S48. Electronic absorption spectrum of 10 μM **C279** dissolved in THF.

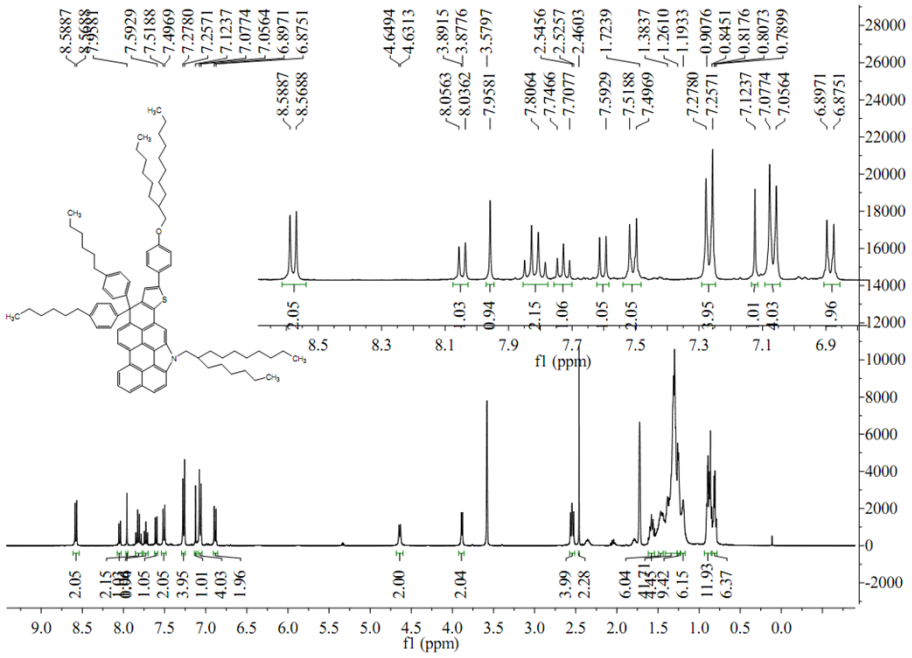


Figure S49. The ^{1}H NMR (400 MHz) spectrum of **9** in THF.

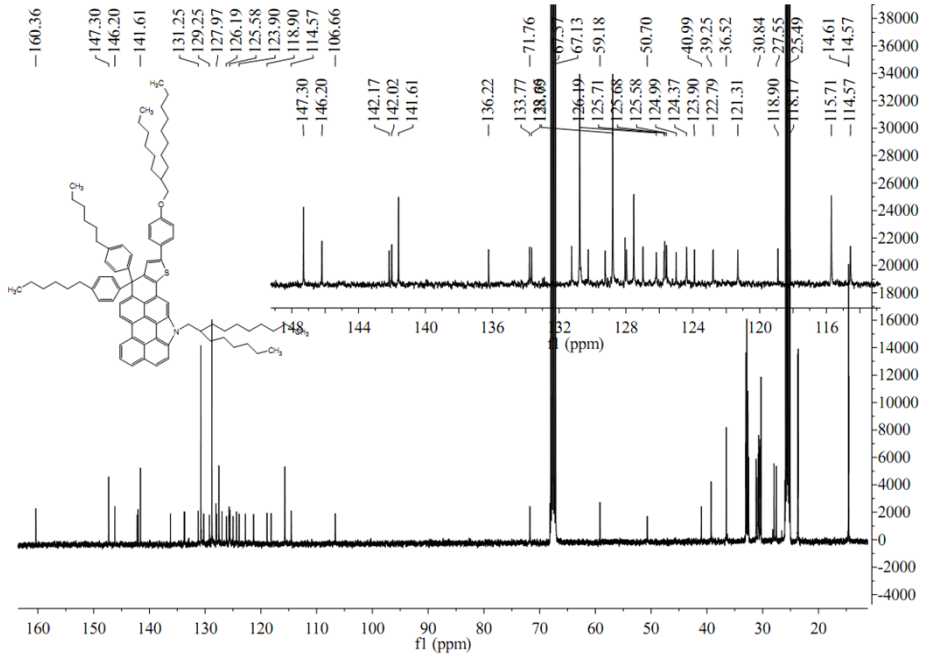


Figure S50. The ^{13}C NMR (100 MHz) spectrum of **9** in THF.

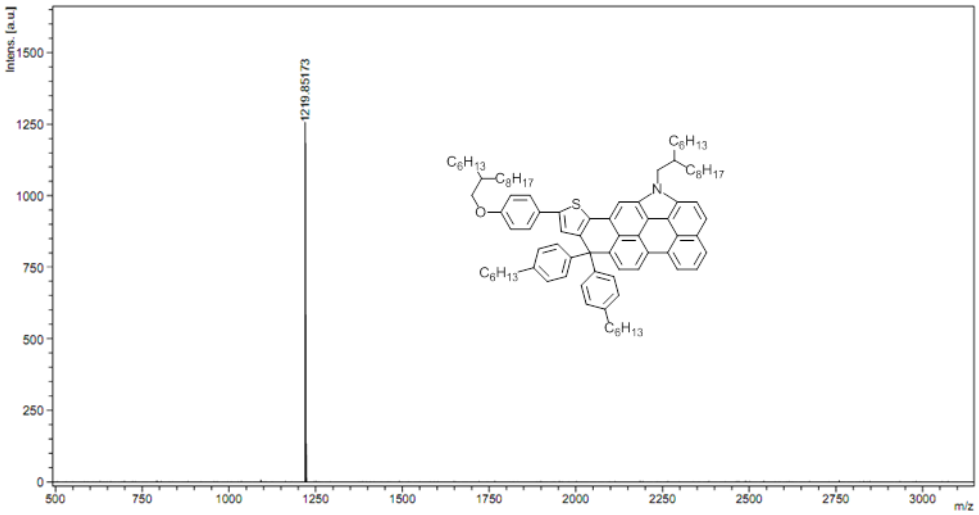


Figure S51. The high resolution mass spectrum (MALDI-TOF) of **9**.

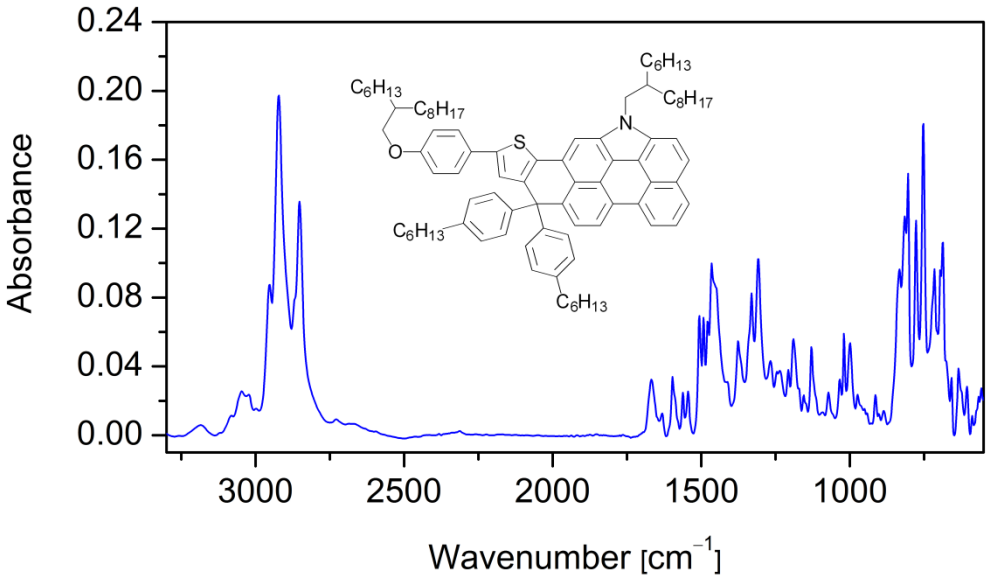


Figure S52. The ATR-IR spectrum of **9**.

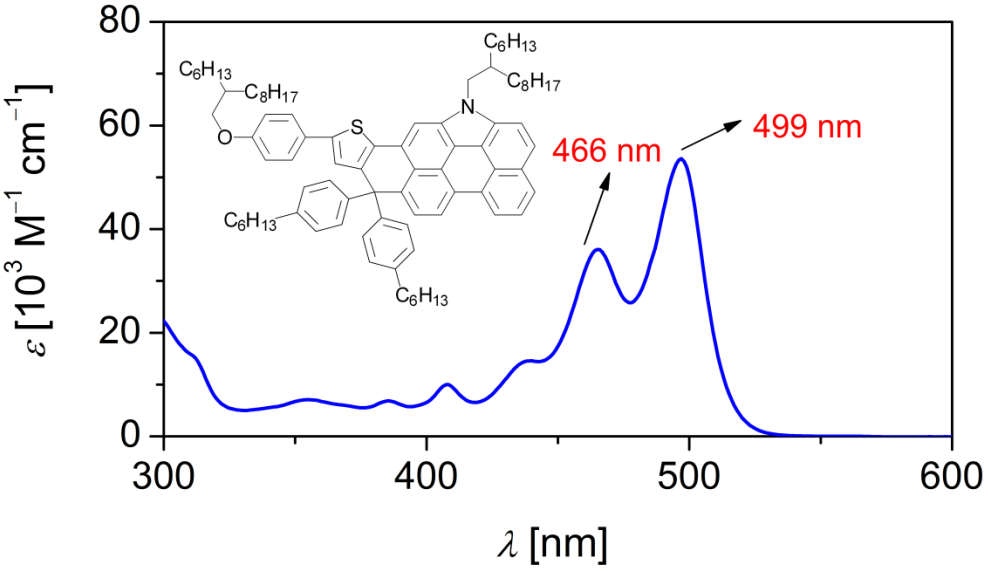


Figure S53. Electronic absorption spectrum of 10 μM **9** dissolved in THF.

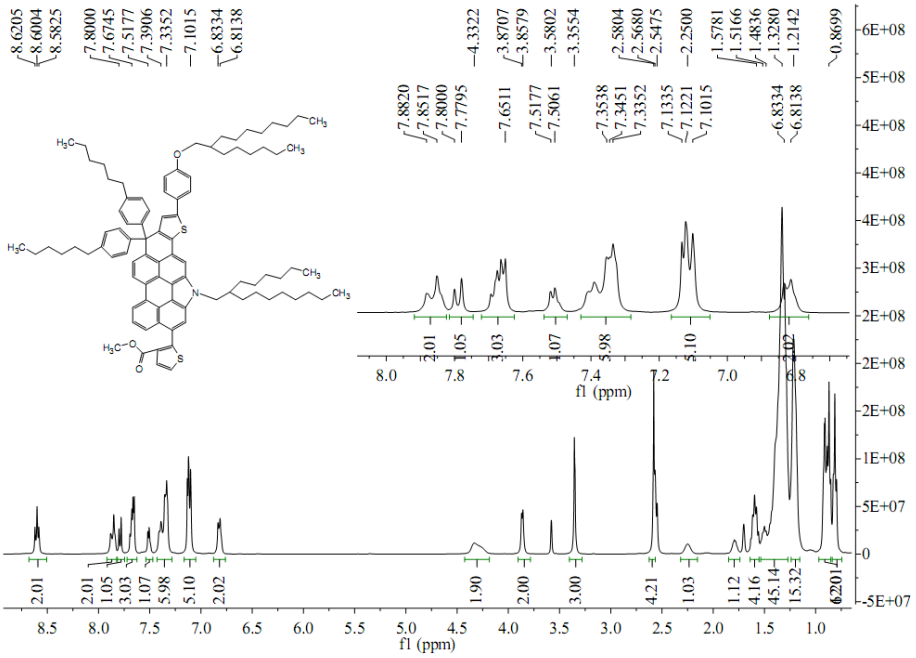


Figure S54. The ^{1}H NMR (400 MHz) spectrum of **10** in THF.

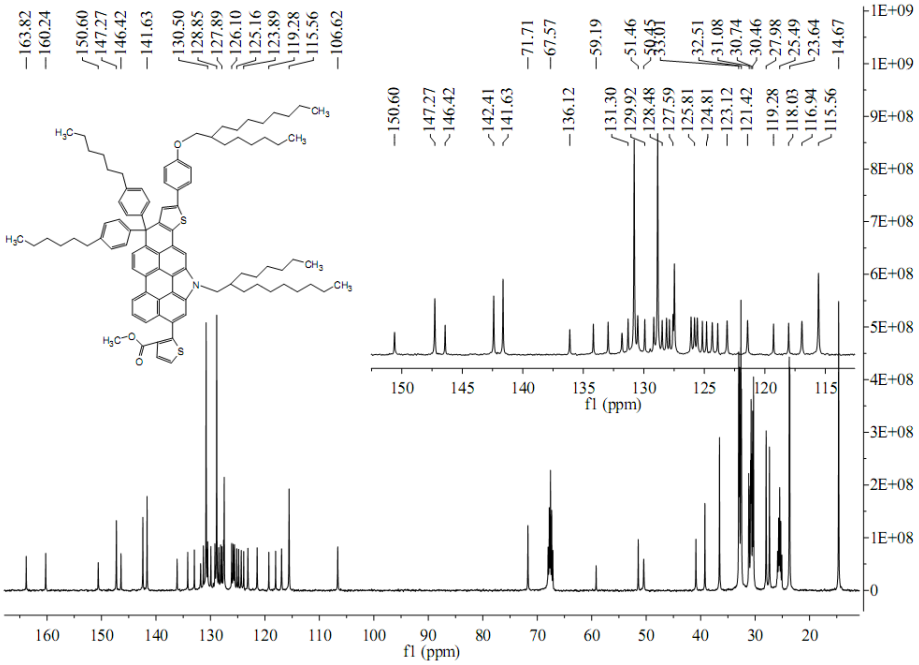


Figure S55. The ^{13}C NMR (100 MHz) spectrum of **10** in THF.

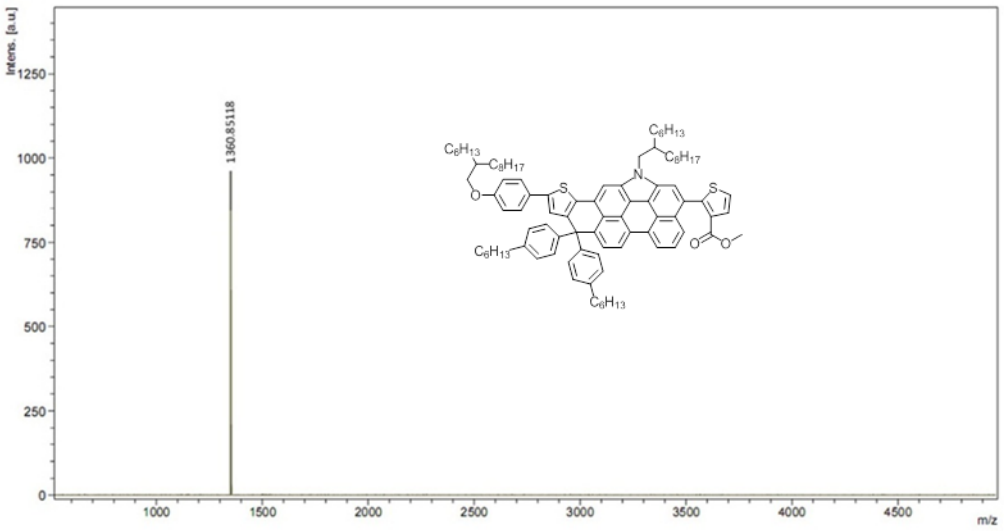


Figure S56. The high resolution mass spectrum (MALDI-TOF) of **10**.

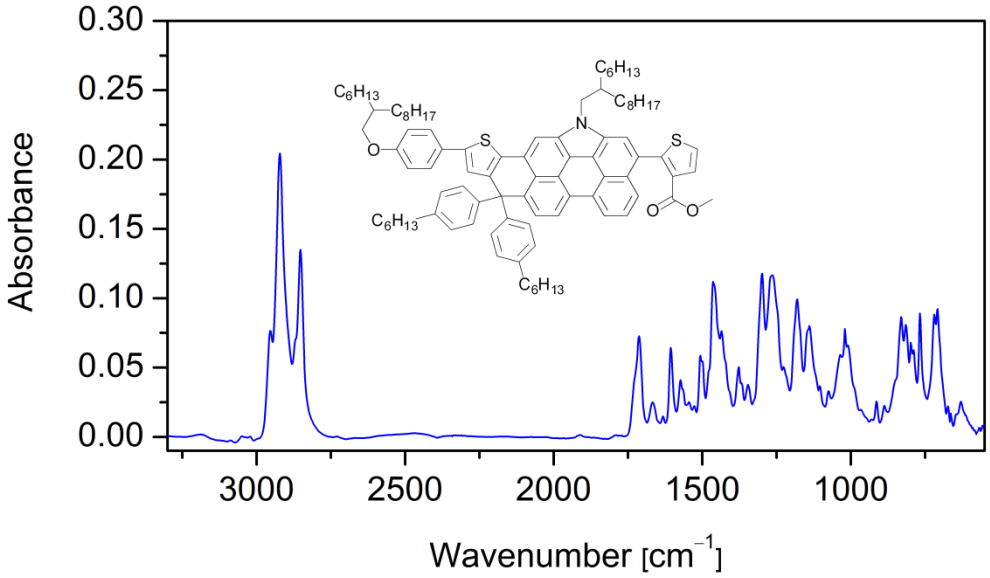


Figure S57. The ATR-IR spectrum of **10**.

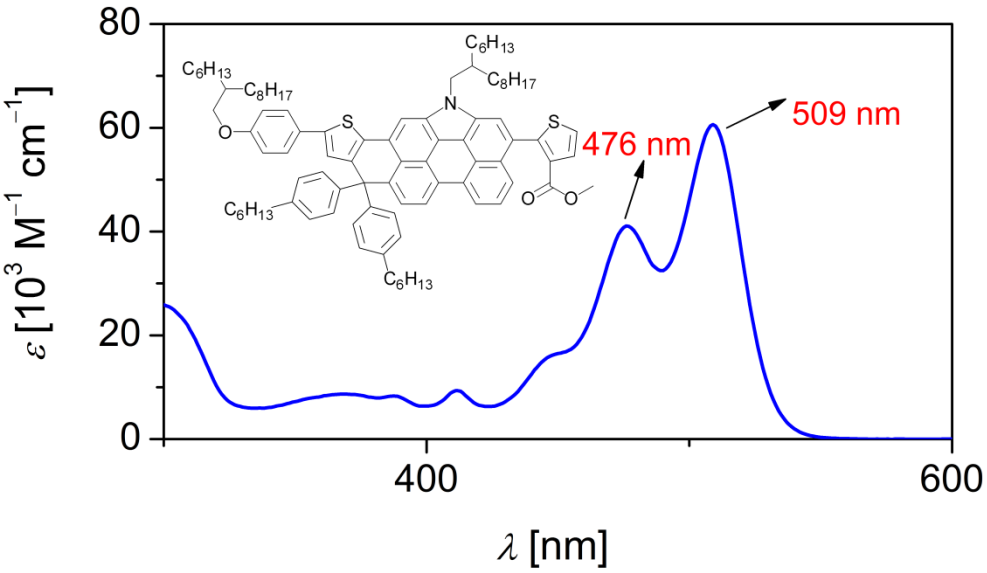


Figure S58. Electronic absorption spectrum of 10 μM **10** dissolved in THF.

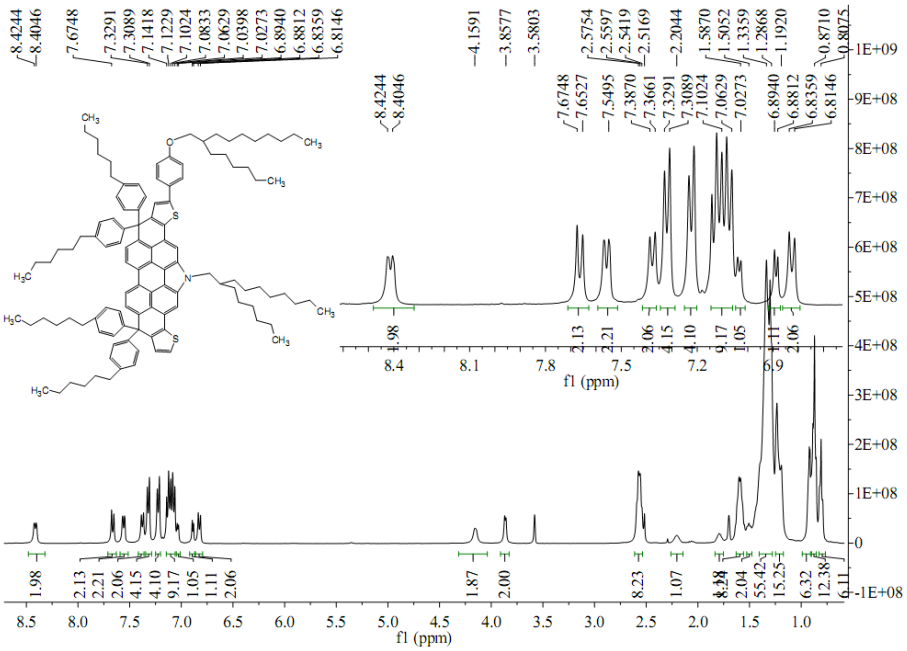


Figure S59. The ^{1}H NMR (400 MHz) spectrum of **11** in THF.

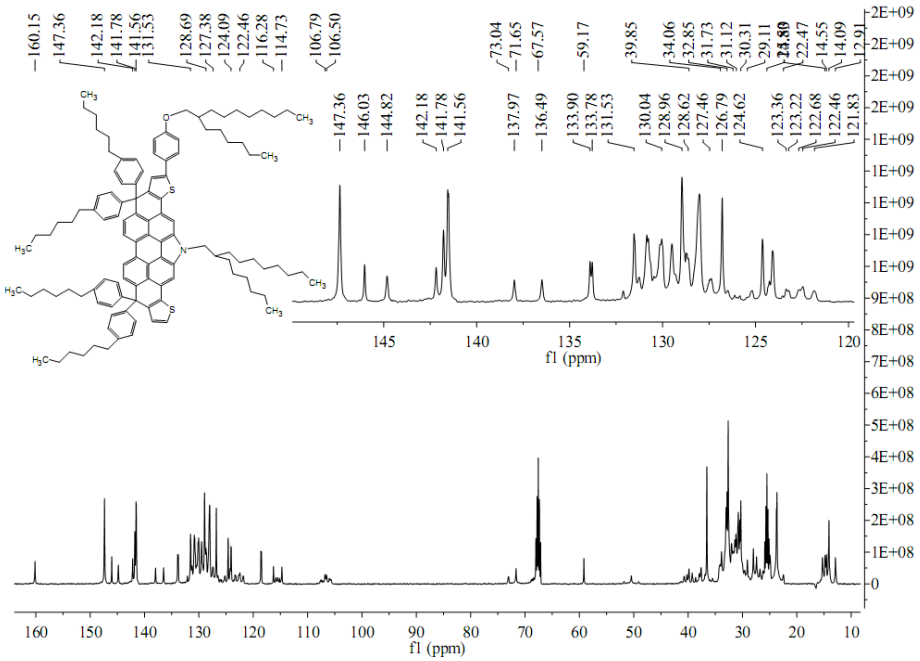


Figure S60. The ^{13}C NMR (100 MHz) spectrum of **11** in THF.

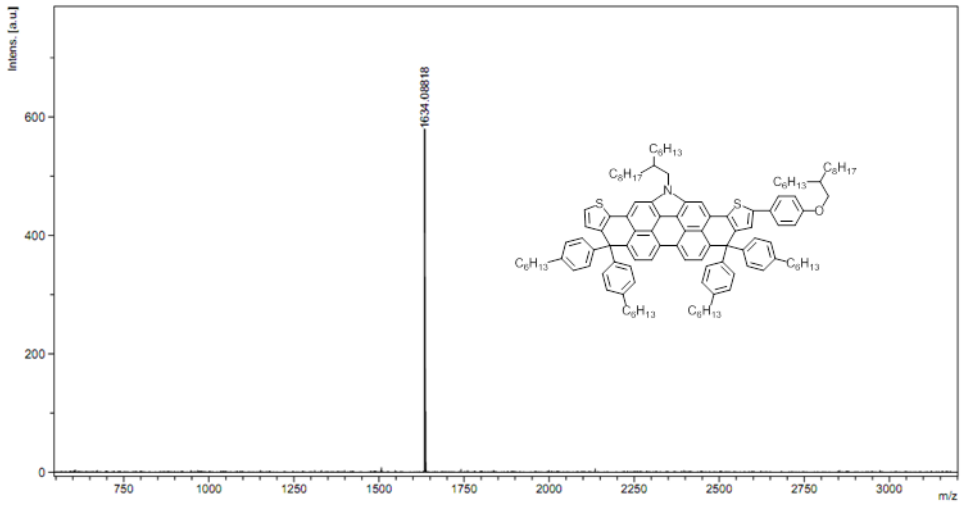


Figure S61. The high resolution mass spectrum (MALDI-TOF) of **11**.

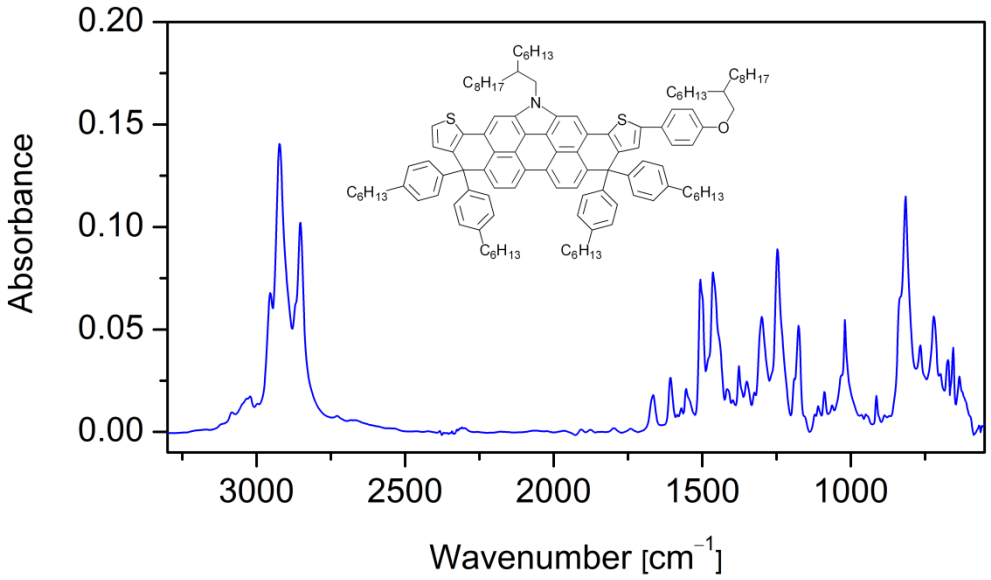


Figure S62. The ATR-IR spectrum of **11**.

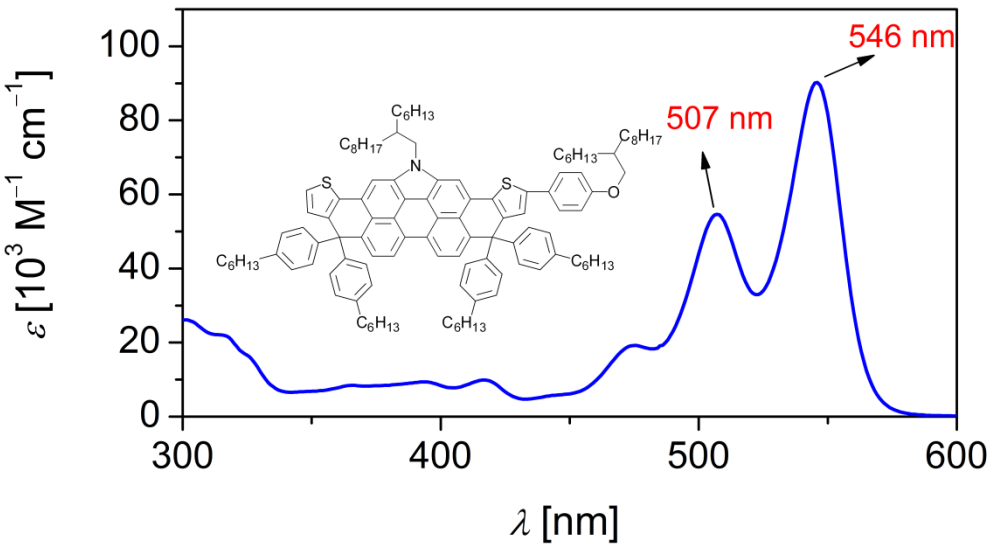


Figure S63. Electronic absorption spectrum of 10 μM **11** dissolved in THF.

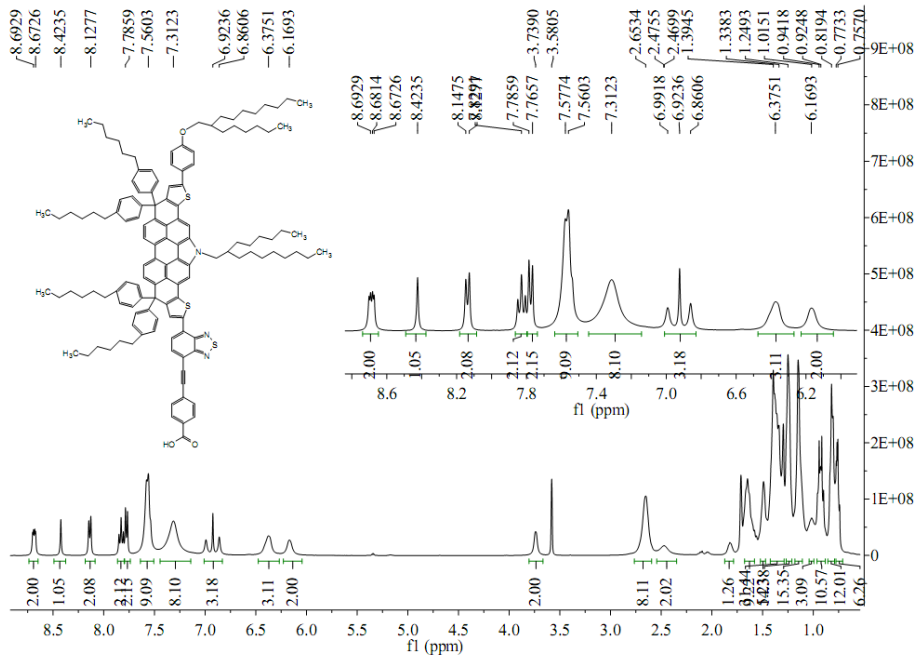


Figure S64. The ^{1}H NMR (400 MHz) spectrum of **C281** in THF.

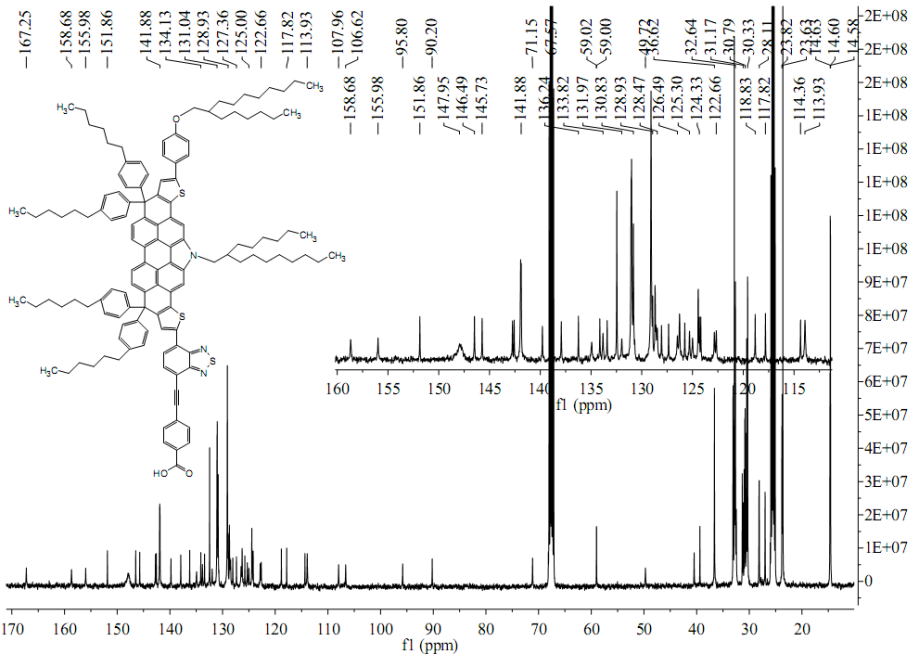


Figure S65. The ^{13}C NMR (100 MHz) spectrum of **C281** in THF.

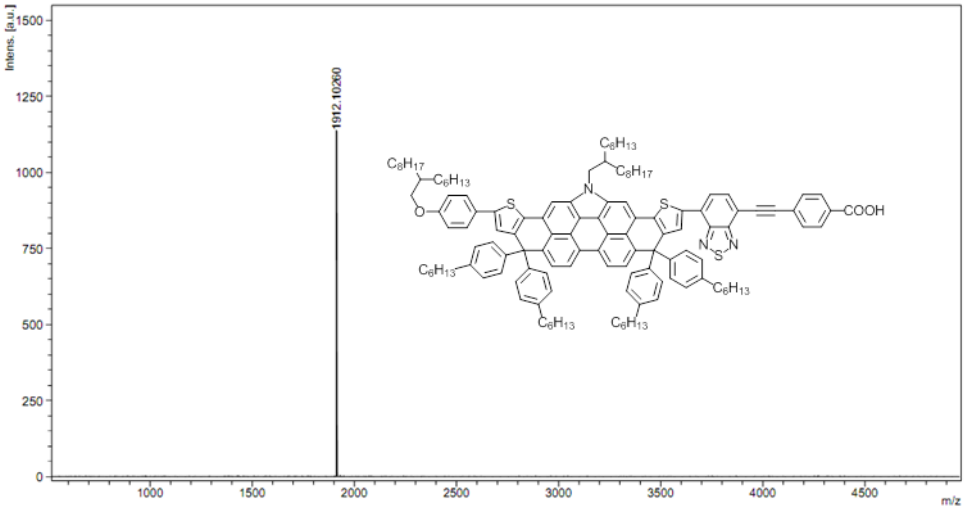


Figure S66. The high resolution mass spectrum (MALDI-TOF) of **C281**.

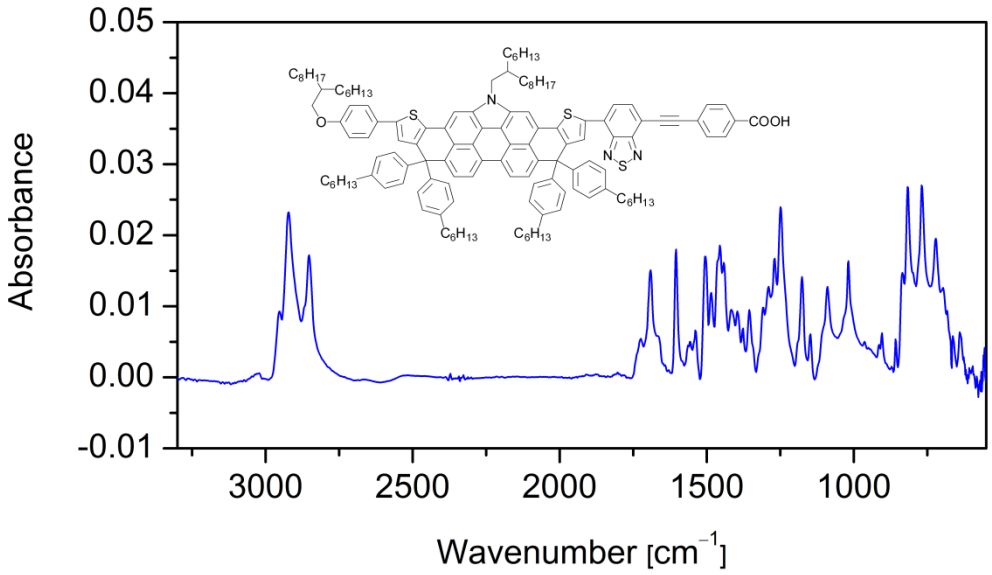


Figure S67. The ATR-IR spectrum of **C281**.

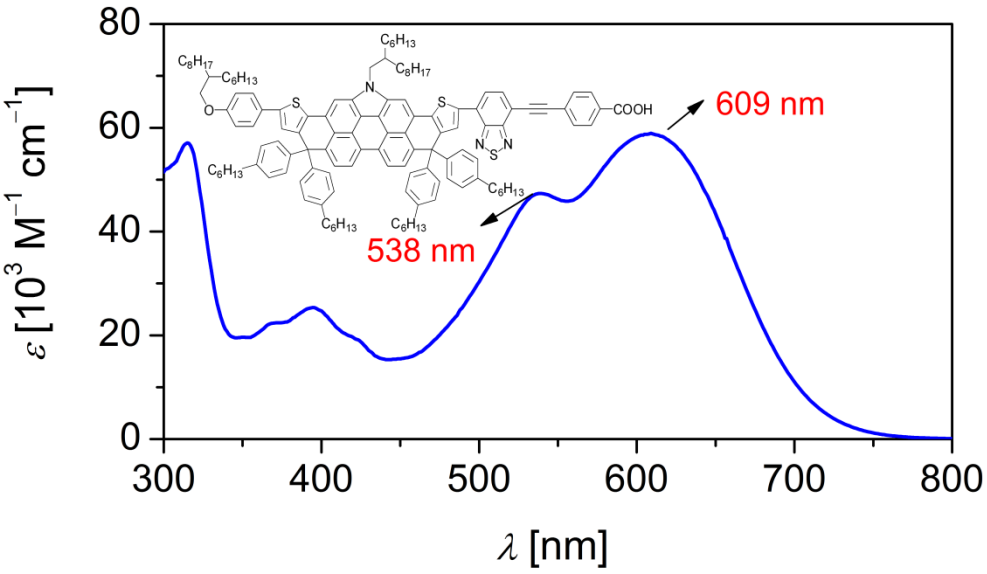


Figure S68. Electronic absorption spectrum of 10 μM **C281** dissolved in THF.

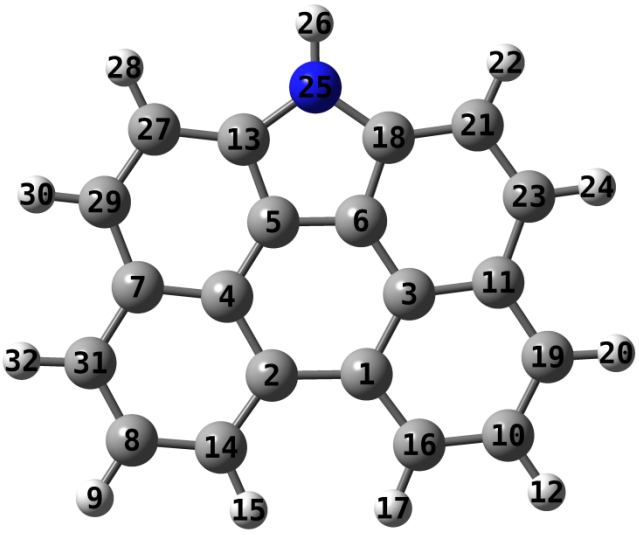


Figure S69. Geometry of the S_0 state of PC in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S2. Geometry parameters and Mulliken atomic charges of the S_0 state of PC in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	0.748375	-1.51474	-0.00013	0.051108
2	6	-0.74832	-1.51477	-5.2E-05	0.051179
3	6	1.440485	-0.25857	-1.2E-05	-0.01516
4	6	-1.44047	-0.25862	-0.00019	-0.01519
5	6	-0.69219	0.907624	-0.00027	-0.17953
6	6	0.692156	0.907628	0.000009	-0.17959
7	6	-2.84992	-0.09292	-5.4E-05	-0.05138
8	6	-2.97447	-2.51114	0.000332	-0.08515
9	1	-3.57333	-3.41528	0.000541	0.106402
10	6	2.974499	-2.51114	-0.00021	-0.08516
11	6	2.849937	-0.09289	0.000075	-0.05135
12	1	3.573409	-3.41524	-0.00031	0.106404
13	6	-1.14699	2.218319	-0.00025	0.238883
14	6	-1.56901	-2.64134	0.000237	-0.10591
15	1	-1.14308	-3.63815	0.000456	0.100088
16	6	1.569048	-2.64132	-0.00027	-0.10588
17	1	1.143065	-3.63812	-0.00045	0.100087
18	6	1.146952	2.218325	0.000187	0.238895
19	6	3.616957	-1.28003	-2.1E-05	-0.0971
20	1	4.700822	-1.23315	0.000063	0.098052
21	6	2.555849	2.39614	0.000329	-0.0643
22	1	3.014858	3.377833	0.000425	0.111946
23	6	3.355962	1.259489	0.000216	-0.06451
24	1	4.43261	1.393075	0.000265	0.099295
25	7	-2.1E-05	3.02877	-0.00013	-0.54673
26	1	-0.00008	4.036673	0.000631	0.261208
27	6	-2.55589	2.396137	-0.00019	-0.0643
28	1	-3.01499	3.377779	-0.00016	0.11195
29	6	-3.35595	1.259439	-6.5E-05	-0.0645
30	1	-4.43261	1.39293	0.000016	0.099291
31	6	-3.61696	-1.28005	0.000193	-0.0971
32	1	-4.70082	-1.23322	0.000264	0.098054

Table S3. The bond lengths of the S_0 state of PC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4967	R20	R(10,19)	1.3887
R2	R(1,3)	1.4342	R21	R(11,19)	1.4134
R3	R(1,16)	1.3938	R22	R(11,23)	1.444
R4	R(2,4)	1.4342	R23	R(13,25)	1.4044
R5	R(2,14)	1.3938	R24	R(13,27)	1.4201
R6	R(3,6)	1.3856	R25	R(14,15)	1.084
R7	R(3,11)	1.4192	R26	R(16,17)	1.084
R8	R(4,5)	1.3856	R27	R(18,21)	1.4201
R9	R(4,7)	1.4192	R28	R(18,25)	1.4044
R10	R(5,6)	1.3843	R29	R(18,26)	2.1499
R11	R(5,13)	1.3874	R30	R(19,20)	1.0849
R12	R(6,18)	1.3874	R31	R(21,22)	1.0837
R13	R(7,29)	1.4439	R32	R(21,23)	1.39
R14	R(7,31)	1.4134	R33	R(23,24)	1.0849
R15	R(8,9)	1.0845	R34	R(25,26)	1.0079
R16	R(8,14)	1.4115	R35	R(27,28)	1.0837
R17	R(8,31)	1.3887	R36	R(27,29)	1.39
R18	R(10,12)	1.0845	R37	R(29,30)	1.0849
R19	R(10,16)	1.4115	R38	R(31,32)	1.0849

Table S4. The bond angles of the S_0 state of PC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	118.8542	A33	A(25,13,27)	137.5615
A2	A(2,1,16)	126.0711	A34	A(2,14,8)	120.7804
A3	A(3,1,16)	115.0747	A35	A(2,14,15)	120.7904
A4	A(1,2,4)	118.8539	A36	A(8,14,15)	118.4292
A5	A(1,2,14)	126.0737	A37	A(1,16,10)	120.7799
A6	A(4,2,14)	115.0724	A38	A(1,16,17)	120.7885
A7	A(1,3,6)	118.4591	A39	A(10,16,17)	118.4316
A8	A(1,3,11)	125.5574	A40	A(6,18,21)	116.3294
A9	A(6,3,11)	115.9835	A41	A(6,18,25)	106.1086
A10	A(2,4,5)	118.4605	A42	A(21,18,25)	137.562
A11	A(2,4,7)	125.5597	A43	A(10,19,11)	119.5751
A12	A(5,4,7)	115.9798	A44	A(10,19,20)	120.0343
A13	A(4,5,6)	122.6849	A45	A(11,19,20)	120.3906
A14	A(4,5,13)	128.1791	A46	A(18,21,22)	122.2525
A15	A(6,5,13)	109.136	A47	A(18,21,23)	117.9493
A16	A(3,6,5)	122.6874	A48	A(22,21,23)	119.7981
A17	A(3,6,18)	128.1762	A49	A(11,23,21)	124.343
A18	A(5,6,18)	109.1364	A50	A(11,23,24)	117.5874
A19	A(4,7,29)	117.2199	A51	A(21,23,24)	118.0697
A20	A(4,7,31)	116.1629	A52	A(13,25,18)	109.51
A21	A(29,7,31)	126.6172	A53	A(13,25,26)	125.2418
A22	A(9,8,14)	118.2266	A54	A(18,25,26)	125.2481
A23	A(9,8,31)	118.9215	A55	A(13,27,28)	122.2583
A24	A(14,8,31)	122.8519	A56	A(13,27,29)	117.9463
A25	A(12,10,16)	118.2299	A57	A(28,27,29)	119.7954
A26	A(12,10,19)	118.9201	A58	A(7,29,27)	124.3454
A27	A(16,10,19)	122.8501	A59	A(7,29,30)	117.5828
A28	A(3,11,19)	116.1628	A60	A(27,29,30)	118.0718
A29	A(3,11,23)	117.2186	A61	A(7,31,8)	119.5727
A30	A(19,11,23)	126.6186	A62	A(7,31,32)	120.3935
A31	A(5,13,25)	106.1089	A63	A(8,31,32)	120.0337
A32	A(5,13,27)	116.3295			

Table S5. The dihedral angles of the S_0 state of PC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	0.015	D53	D(4,7,31,8)	0.0022
D2	D(3,1,2,14)	-179.98	D54	D(4,7,31,32)	-179.997
D3	D(16,1,2,4)	-179.987	D55	D(29,7,31,8)	-179.992
D4	D(16,1,2,14)	0.0173	D56	D(29,7,31,32)	0.0084
D5	D(2,1,3,6)	-0.0076	D57	D(9,8,14,2)	179.9989
D6	D(2,1,3,11)	-180.007	D58	D(9,8,14,15)	-0.0048
D7	D(16,1,3,6)	179.9944	D59	D(31,8,14,2)	-0.0022
D8	D(16,1,3,11)	-0.0049	D60	D(31,8,14,15)	179.9941
D9	D(2,1,16,10)	-179.994	D61	D(9,8,31,7)	179.9988
D10	D(2,1,16,17)	0.0074	D62	D(9,8,31,32)	-0.0018
D11	D(3,1,16,10)	0.0034	D63	D(14,8,31,7)	-0.0001
D12	D(3,1,16,17)	-179.995	D64	D(14,8,31,32)	-180.001
D13	D(1,2,4,5)	-0.0058	D65	D(12,10,16,1)	-180.001
D14	D(1,2,4,7)	-179.996	D66	D(12,10,16,17)	-0.0028
D15	D(14,2,4,5)	179.9901	D67	D(19,10,16,1)	-0.0001
D16	D(14,2,4,7)	0.0002	D68	D(19,10,16,17)	179.9982
D17	D(1,2,14,8)	179.9976	D69	D(12,10,19,11)	179.9986
D18	D(1,2,14,15)	0.0015	D70	D(12,10,19,20)	-0.002
D19	D(4,2,14,8)	0.002	D71	D(16,10,19,11)	-0.0023
D20	D(4,2,14,15)	-179.994	D72	D(16,10,19,20)	-180.003
D21	D(1,3,6,5)	-0.0092	D73	D(3,11,19,10)	0.001
D22	D(1,3,6,18)	-180.004	D74	D(3,11,19,20)	-179.998
D23	D(11,3,6,5)	179.9902	D75	D(23,11,19,10)	-179.997
D24	D(11,3,6,18)	-0.0044	D76	D(23,11,19,20)	0.0033
D25	D(1,3,11,19)	0.0027	D77	D(3,11,23,21)	0.0028
D26	D(1,3,11,23)	180.0012	D78	D(3,11,23,24)	180.0011
D27	D(6,3,11,19)	180.0034	D79	D(19,11,23,21)	180.0011
D28	D(6,3,11,23)	0.0019	D80	D(19,11,23,24)	-0.0006
D29	D(2,4,5,6)	-0.0111	D81	D(5,13,25,18)	-0.0113
D30	D(2,4,5,13)	-179.992	D82	D(5,13,25,26)	-179.95
D31	D(7,4,5,6)	179.9797	D83	D(27,13,25,18)	179.9793
D32	D(7,4,5,13)	-0.0012	D84	D(27,13,25,26)	0.0407
D33	D(2,4,7,29)	179.9926	D85	D(5,13,27,28)	-180.001
D34	D(2,4,7,31)	-0.0023	D86	D(5,13,27,29)	0.0045
D35	D(5,4,7,29)	0.0025	D87	D(25,13,27,28)	0.0092
D36	D(5,4,7,31)	-179.992	D88	D(25,13,27,29)	180.0146
D37	D(4,5,6,3)	0.0195	D89	D(6,18,21,22)	-180.003
D38	D(4,5,6,18)	180.015	D90	D(6,18,21,23)	0.0029
D39	D(13,5,6,3)	-179.996	D91	D(25,18,21,22)	0.0152
D40	D(13,5,6,18)	-0.0009	D92	D(25,18,21,23)	-179.979

D41	D(4,5,13,25)	-180.01	D93	D(6,18,25,13)	0.0107
D42	D(4,5,13,27)	-0.0025	D94	D(6,18,25,26)	179.9493
D43	D(6,5,13,25)	0.0074	D95	D(21,18,25,13)	179.9937
D44	D(6,5,13,27)	-179.986	D96	D(21,18,25,26)	-0.0677
D45	D(3,6,18,21)	0.0019	D97	D(18,21,23,11)	-0.0053
D46	D(3,6,18,25)	179.9891	D98	D(18,21,23,24)	-180.004
D47	D(5,6,18,21)	-179.993	D99	D(22,21,23,11)	-180
D48	D(5,6,18,25)	-0.006	D100	D(22,21,23,24)	0.0022
D49	D(4,7,29,27)	-0.0003	D101	D(13,27,29,7)	-0.0033
D50	D(4,7,29,30)	179.9987	D102	D(13,27,29,30)	-180.002
D51	D(31,7,29,27)	179.994	D103	D(28,27,29,7)	180.0019
D52	D(31,7,29,30)	-0.007	D104	D(28,27,29,30)	0.003

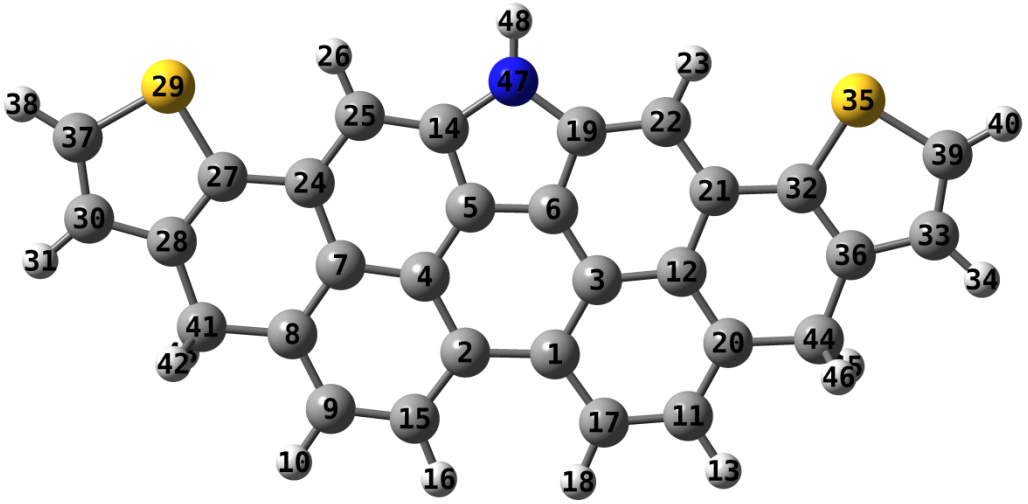


Figure S70. Geometry of the S_0 state of DTPC in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S6. Geometry parameters and Mulliken atomic charges of the S_0 state of DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	0.746774	2.042554	-9.7E-05	0.070945
2	6	-0.74678	2.042557	-2.2E-05	0.070925
3	6	1.437032	0.789329	-0.00014	-0.0258
4	6	-1.43703	0.789334	-5.2E-05	-0.02577
5	6	-0.6896	-0.37826	-0.00015	-0.17902
6	6	0.689613	-0.37828	-1.1E-05	-0.17889
7	6	-2.84106	0.624617	0.000071	-0.00308
8	6	-3.63231	1.79445	0.000272	-0.17724
9	6	-2.97775	3.02816	0.000241	-0.06069
10	1	-3.57879	3.932301	0.000354	0.091114
11	6	2.977733	3.028162	-0.00017	-0.0607
12	6	2.841067	0.624634	-0.00017	-0.0031
13	1	3.57876	3.932312	-0.00017	0.091115
14	6	-1.1484	-1.68834	-0.00012	0.23552
15	6	-1.57827	3.164762	0.000103	-0.10066
16	1	-1.15937	4.164763	0.00013	0.098083
17	6	1.578262	3.16476	-0.00012	-0.10066
18	1	1.159368	4.164763	-7.9E-05	0.098083
19	6	1.148423	-1.68835	-1.4E-05	0.235435
20	6	3.63233	1.794462	-0.00023	-0.17722
21	6	3.372081	-0.73576	-5.5E-05	0.063411
22	6	2.551094	-1.87108	-1E-06	-0.03192
23	1	2.997109	-2.85884	0.000059	0.110854
24	6	-3.37209	-0.73575	0.000015	0.063417
25	6	-2.55106	-1.87108	-5.7E-05	-0.03192
26	1	-2.99708	-2.85884	-0.0001	0.110848
27	6	-4.82537	-0.80862	0.000026	-0.29048
28	6	-5.65951	0.288717	0.000205	-0.08424
29	16	-5.75167	-2.29678	-0.00022	0.251214
30	6	-7.04174	-0.06774	0.000025	-0.06685
31	1	-7.84723	0.655961	0.000088	0.10636
32	6	4.825382	-0.8086	0.000135	-0.29048
33	6	7.041747	-0.06773	0.000005	-0.06684
34	1	7.847233	0.655976	-7.3E-05	0.106362
35	16	5.751673	-2.29681	0.000345	0.251197
36	6	5.659519	0.288712	0.000018	-0.08422
37	6	-7.24878	-1.41525	-0.00024	-0.29109
38	1	-8.1835	-1.95443	-0.00043	0.148303
39	6	7.248781	-1.41524	0.000239	-0.29109

40	1	8.183501	-1.95442	0.000492	0.148302
41	6	-5.14311	1.704184	0.000534	-0.01296
42	1	-5.54411	2.238456	-0.87044	0.148258
43	1	-5.54378	2.237817	0.872063	0.148269
44	6	5.143084	1.704202	-0.00047	-0.01298
45	1	5.544161	2.238582	0.870443	0.148249
46	1	5.543803	2.237742	-0.87206	0.148272
47	7	-7.5E-05	-2.49847	-0.00022	-0.55802
48	1	-1.2E-05	-3.50646	0.000535	0.261383

Table S7. The bond lengths of the S_0 state of DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4936	R31	R(20,44)	1.5134
R2	R(1,3)	1.4307	R32	R(20,46)	2.1472
R3	R(1,17)	1.3967	R33	R(21,22)	1.4011
R4	R(2,4)	1.4307	R34	R(21,32)	1.4551
R5	R(2,15)	1.3967	R35	R(22,23)	1.0838
R6	R(3,6)	1.3863	R36	R(24,25)	1.4011
R7	R(3,12)	1.4137	R37	R(24,27)	1.4551
R8	R(4,5)	1.3863	R38	R(25,26)	1.0838
R9	R(4,7)	1.4137	R39	R(27,28)	1.3784
R10	R(5,6)	1.3792	R40	R(27,29)	1.7529
R11	R(5,14)	1.3881	R41	R(28,30)	1.4274
R12	R(6,19)	1.3881	R42	R(28,41)	1.5067
R13	R(7,8)	1.4123	R43	R(29,37)	1.7374
R14	R(7,24)	1.4603	R44	R(30,31)	1.0828
R15	R(8,9)	1.3966	R45	R(30,37)	1.3633
R16	R(8,41)	1.5135	R46	R(32,35)	1.7529
R17	R(9,10)	1.0857	R47	R(32,36)	1.3784
R18	R(9,15)	1.4061	R48	R(33,34)	1.0828
R19	R(11,13)	1.0857	R49	R(33,36)	1.4274
R20	R(11,17)	1.4061	R50	R(33,39)	1.3633
R21	R(11,20)	1.3966	R51	R(35,39)	1.7374
R22	R(12,20)	1.4123	R52	R(36,44)	1.5068
R23	R(12,21)	1.4604	R53	R(36,45)	2.1384
R24	R(14,25)	1.4145	R54	R(37,38)	1.0791
R25	R(14,47)	1.4053	R55	R(39,40)	1.0791
R26	R(15,16)	1.0842	R56	R(41,42)	1.0977
R27	R(17,18)	1.0842	R57	R(41,43)	1.0977
R28	R(19,22)	1.4145	R58	R(44,45)	1.0977
R29	R(19,47)	1.4055	R59	R(44,46)	1.0977
R30	R(19,48)	2.1505	R60	R(47,48)	1.008

Table S8. The bond angles of the S_0 state of DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	118.8455	A51	A(22,21,32)	123.0023
A2	A(2,1,17)	126.5361	A52	A(19,22,21)	118.4495
A3	A(3,1,17)	114.6184	A53	A(19,22,23)	121.7234
A4	A(1,2,4)	118.8449	A54	A(21,22,23)	119.8271
A5	A(1,2,15)	126.5365	A55	A(7,24,25)	122.8037
A6	A(4,2,15)	114.6186	A56	A(7,24,27)	114.1938
A7	A(1,3,6)	118.5302	A57	A(25,24,27)	123.0025
A8	A(1,3,12)	125.5356	A58	A(14,25,24)	118.4503
A9	A(6,3,12)	115.9341	A59	A(14,25,26)	121.7244
A10	A(2,4,5)	118.5299	A60	A(24,25,26)	119.8253
A11	A(2,4,7)	125.5362	A61	A(24,27,28)	124.37
A12	A(5,4,7)	115.934	A62	A(24,27,29)	124.7704
A13	A(4,5,6)	122.6259	A63	A(28,27,29)	110.8596
A14	A(4,5,14)	128.074	A64	A(27,28,30)	112.7797
A15	A(6,5,14)	109.3001	A65	A(27,28,41)	122.716
A16	A(3,6,5)	122.6237	A66	A(30,28,41)	124.5044
A17	A(3,6,19)	128.0744	A67	A(27,29,37)	91.4095
A18	A(5,6,19)	109.302	A68	A(28,30,31)	123.6007
A19	A(4,7,8)	117.3824	A69	A(28,30,37)	113.1959
A20	A(4,7,24)	118.0145	A70	A(31,30,37)	123.2034
A21	A(8,7,24)	124.6032	A71	A(21,32,35)	124.7686
A22	A(7,8,9)	117.9775	A72	A(21,32,36)	124.3711
A23	A(7,8,41)	120.6543	A73	A(35,32,36)	110.8603
A24	A(9,8,41)	121.3682	A74	A(34,33,36)	123.6008
A25	A(8,9,10)	118.4365	A75	A(34,33,39)	123.2042
A26	A(8,9,15)	123.524	A76	A(36,33,39)	113.195
A27	A(10,9,15)	118.0395	A77	A(32,35,39)	91.4075
A28	A(13,11,17)	118.0388	A78	A(32,36,33)	112.7804
A29	A(13,11,20)	118.4361	A79	A(32,36,44)	122.715
A30	A(17,11,20)	123.5251	A80	A(33,36,44)	124.5045
A31	A(3,12,20)	117.3838	A81	A(29,37,30)	111.7553
A32	A(3,12,21)	118.013	A82	A(29,37,38)	119.532
A33	A(20,12,21)	124.6032	A83	A(30,37,38)	128.7127
A34	A(5,14,25)	116.7236	A84	A(33,39,35)	111.7568
A35	A(5,14,47)	105.9016	A85	A(33,39,40)	128.7125
A36	A(25,14,47)	137.3749	A86	A(35,39,40)	119.5307
A37	A(2,15,9)	120.9615	A87	A(8,41,28)	113.4628
A38	A(2,15,16)	120.7348	A88	A(8,41,42)	109.6037
A39	A(9,15,16)	118.3038	A89	A(8,41,43)	109.6038
A40	A(1,17,11)	120.9614	A90	A(28,41,42)	109.3826

A41	A(1,17,18)	120.7353	A91	A(28,41,43)	109.3766
A42	A(11,17,18)	118.3033	A92	A(42,41,43)	105.0721
A43	A(6,19,22)	116.7236	A93	A(20,44,36)	113.4633
A44	A(6,19,47)	105.8969	A94	A(20,44,45)	109.6078
A45	A(22,19,47)	137.3795	A95	A(20,44,46)	109.6054
A46	A(11,20,12)	117.9756	A96	A(36,44,45)	109.3811
A47	A(11,20,44)	121.3693	A97	A(45,44,46)	105.0686
A48	A(12,20,44)	120.6551	A98	A(14,47,19)	109.5994
A49	A(12,21,22)	122.8055	A99	A(14,47,48)	125.2059
A50	A(12,21,32)	114.1923	A100	A(19,47,48)	125.1946

Table S9. The dihedral angles of the S_0 state of DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	-0.0026	D83	D(3,12,21,22)	0.0038
D2	D(3,1,2,15)	179.9961	D84	D(3,12,21,32)	-179.99
D3	D(17,1,2,4)	-180.002	D85	D(20,12,21,22)	-180
D4	D(17,1,2,15)	-0.003	D86	D(20,12,21,32)	0.0065
D5	D(2,1,3,6)	-0.0047	D87	D(5,14,25,24)	-0.0016
D6	D(2,1,3,12)	-179.998	D88	D(5,14,25,26)	179.9959
D7	D(17,1,3,6)	179.9946	D89	D(47,14,25,24)	-179.999
D8	D(17,1,3,12)	0.0015	D90	D(47,14,25,26)	-0.0014
D9	D(2,1,17,11)	179.9992	D91	D(5,14,47,19)	0.0126
D10	D(2,1,17,18)	-0.0004	D92	D(5,14,47,48)	179.9467
D11	D(3,1,17,11)	0	D93	D(25,14,47,19)	-179.99
D12	D(3,1,17,18)	-180	D94	D(25,14,47,48)	-0.0558
D13	D(1,2,4,5)	0.0001	D95	D(6,19,22,21)	-0.0032
D14	D(1,2,4,7)	179.9969	D96	D(6,19,22,23)	179.9963
D15	D(15,2,4,5)	-179.999	D97	D(47,19,22,21)	179.9852
D16	D(15,2,4,7)	-0.0019	D98	D(47,19,22,23)	-0.0153
D17	D(1,2,15,9)	-179.996	D99	D(6,19,47,14)	-0.0096
D18	D(1,2,15,16)	0.0016	D100	D(6,19,47,48)	-179.944
D19	D(4,2,15,9)	0.0025	D101	D(22,19,47,14)	180.0012
D20	D(4,2,15,16)	-180	D102	D(22,19,47,48)	0.0671
D21	D(1,3,6,5)	0.015	D103	D(11,20,44,36)	179.9784
D22	D(1,3,6,19)	-179.999	D104	D(11,20,44,46)	-57.4391
D23	D(12,3,6,5)	-179.991	D105	D(12,20,44,36)	-0.0258
D24	D(12,3,6,19)	-0.0057	D106	D(12,20,44,46)	122.5567
D25	D(1,3,12,20)	-0.0038	D107	D(12,21,22,19)	-0.002
D26	D(1,3,12,21)	179.9931	D108	D(12,21,22,23)	-180.002
D27	D(6,3,12,20)	-179.997	D109	D(32,21,22,19)	179.9914
D28	D(6,3,12,21)	-0.0002	D110	D(32,21,22,23)	-0.0081
D29	D(2,4,5,6)	0.01	D111	D(12,21,32,35)	179.9983
D30	D(2,4,5,14)	179.9964	D112	D(12,21,32,36)	-0.0095
D31	D(7,4,5,6)	-179.987	D113	D(22,21,32,35)	0.0044
D32	D(7,4,5,14)	-0.0007	D114	D(22,21,32,36)	179.9965
D33	D(2,4,7,8)	-0.0015	D115	D(7,24,25,14)	-0.0023
D34	D(2,4,7,24)	-180	D116	D(7,24,25,26)	180.0002
D35	D(5,4,7,8)	179.9954	D117	D(27,24,25,14)	179.9971
D36	D(5,4,7,24)	-0.0032	D118	D(27,24,25,26)	-0.0004
D37	D(4,5,6,3)	-0.0183	D119	D(7,24,27,28)	-0.0061
D38	D(4,5,6,19)	179.9938	D120	D(7,24,27,29)	179.9927
D39	D(14,5,6,3)	-180.007	D121	D(25,24,27,28)	179.9945
D40	D(14,5,6,19)	0.0051	D122	D(25,24,27,29)	-0.0068

D41	D(4,5,14,25)	0.0032	D123	D(24,27,28,30)	179.9936
D42	D(4,5,14,47)	180.0013	D124	D(24,27,28,41)	-0.0055
D43	D(6,5,14,25)	179.9911	D125	D(29,27,28,30)	-0.0053
D44	D(6,5,14,47)	-0.0108	D126	D(29,27,28,41)	179.9956
D45	D(3,6,19,22)	0.0075	D127	D(24,27,29,37)	180.0066
D46	D(3,6,19,47)	-179.984	D128	D(28,27,29,37)	0.0055
D47	D(5,6,19,22)	179.9946	D129	D(27,28,30,31)	180.0023
D48	D(5,6,19,47)	0.0028	D130	D(27,28,30,37)	0.0021
D49	D(4,7,8,9)	0.0043	D131	D(41,28,30,31)	0.0014
D50	D(4,7,8,41)	-179.995	D132	D(41,28,30,37)	-179.999
D51	D(24,7,8,9)	180.0028	D133	D(27,28,41,8)	0.0154
D52	D(24,7,8,41)	0.0037	D134	D(27,28,41,42)	122.7283
D53	D(4,7,24,25)	0.0048	D135	D(27,28,41,43)	-122.693
D54	D(4,7,24,27)	-179.995	D136	D(30,28,41,8)	-179.984
D55	D(8,7,24,25)	-179.994	D137	D(30,28,41,42)	-57.2707
D56	D(8,7,24,27)	0.0069	D138	D(30,28,41,43)	57.3078
D57	D(7,8,9,10)	-180.003	D139	D(27,29,37,30)	-0.0044
D58	D(7,8,9,15)	-0.004	D140	D(27,29,37,38)	-180.003
D59	D(41,8,9,10)	-0.0034	D141	D(28,30,37,29)	0.0022
D60	D(41,8,9,15)	179.9951	D142	D(28,30,37,38)	180.0008
D61	D(7,8,41,28)	-0.0143	D143	D(31,30,37,29)	180.002
D62	D(7,8,41,42)	-122.605	D144	D(31,30,37,38)	0.0006
D63	D(7,8,41,43)	122.5688	D145	D(21,32,35,39)	-180.008
D64	D(9,8,41,28)	179.9866	D146	D(36,32,35,39)	-0.0011
D65	D(9,8,41,42)	57.3959	D147	D(21,32,36,33)	180.0109
D66	D(9,8,41,43)	-57.4303	D148	D(21,32,36,44)	-0.0063
D67	D(8,9,15,2)	0.0004	D149	D(35,32,36,33)	0.004
D68	D(8,9,15,16)	-179.998	D150	D(35,32,36,44)	179.9868
D69	D(10,9,15,2)	-180.001	D151	D(34,33,36,32)	-180
D70	D(10,9,15,16)	0.001	D152	D(34,33,36,44)	0.0181
D71	D(13,11,17,1)	180.0006	D153	D(39,33,36,32)	-0.0059
D72	D(13,11,17,18)	0.0002	D154	D(39,33,36,44)	-179.988
D73	D(20,11,17,1)	0.0011	D155	D(34,33,39,35)	179.9986
D74	D(20,11,17,18)	180.0007	D156	D(34,33,39,40)	0.0078
D75	D(13,11,20,12)	179.9971	D157	D(36,33,39,35)	0.0049
D76	D(13,11,20,44)	-0.0071	D158	D(36,33,39,40)	-179.986
D77	D(17,11,20,12)	-0.0035	D159	D(32,35,39,33)	-0.0022
D78	D(17,11,20,44)	179.9923	D160	D(32,35,39,40)	179.9895
D79	D(3,12,20,11)	0.0046	D161	D(32,36,44,20)	0.0235
D80	D(3,12,20,44)	-179.991	D162	D(32,36,44,45)	122.741
D81	D(21,12,20,11)	-179.992	D163	D(33,36,44,20)	-179.996
D82	D(21,12,20,44)	0.012	D164	D(33,36,44,45)	-57.2783

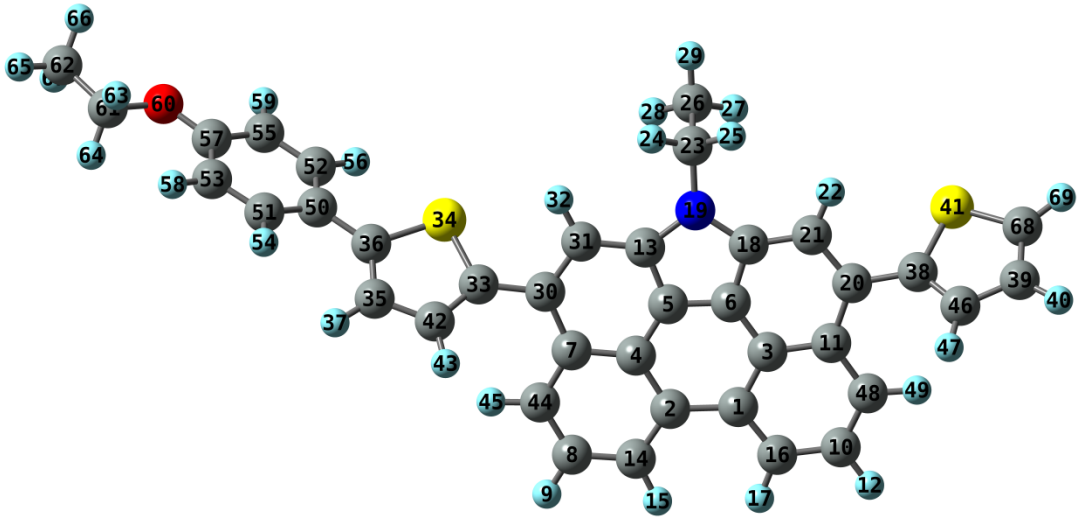


Figure S71. Geometry of the S_0 state of C_2O-P-T-PC-T in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S10. Geometry parameters and Mulliken atomic charges of the S_0 state of C_2O-P-T-PC-T in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	-3.7234	2.483388	-0.347	0.047689
2	6	-2.26967	2.831096	-0.28692	0.045506
3	6	-4.12859	1.127024	-0.11117	-0.02335
4	6	-1.31494	1.800638	0.007383	-0.02307
5	6	-1.79488	0.516926	0.201652	-0.16335
6	6	-3.13739	0.19524	0.144358	-0.16732
7	6	0.093482	1.974139	0.090225	-0.00062
8	6	-0.33751	4.296833	-0.46584	-0.081
9	1	0.046624	5.290255	-0.6693	0.106827
10	6	-6.09013	2.921548	-0.69643	-0.08099
11	6	-5.46485	0.643629	-0.14138	-0.0093
12	1	-6.86515	3.638904	-0.94259	0.106808
13	6	-1.06771	-0.63383	0.468035	0.261607
14	6	-1.73016	4.095248	-0.51407	-0.1029
15	1	-2.36891	4.939883	-0.74456	0.100525
16	6	-4.75714	3.37155	-0.63581	-0.10335
17	1	-4.55393	4.418134	-0.83036	0.100582
18	6	-3.28411	-1.16489	0.37389	0.26251
19	7	-1.9948	-1.68492	0.588109	-0.57737
20	6	-5.66955	-0.78021	0.124202	0.054707
21	6	-4.6066	-1.66242	0.366357	-0.03376
22	1	-4.82875	-2.7029	0.569402	0.124257
23	6	-1.66554	-3.0929	0.804154	-0.09944
24	1	-0.80002	-3.13322	1.469075	0.138568
25	1	-2.49856	-3.54781	1.343856	0.137984
26	6	-1.38395	-3.85631	-0.49175	-0.28178
27	1	-2.25496	-3.84382	-1.15086	0.11819
28	1	-0.53894	-3.41918	-1.02835	0.118392
29	1	-1.14227	-4.89752	-0.26366	0.119923
30	6	0.898684	0.792132	0.401737	0.037493
31	6	0.332178	-0.47976	0.576027	-0.04386
32	1	0.982441	-1.31089	0.819831	0.124503
33	6	2.358231	0.923794	0.543353	-0.32321
34	16	3.437344	-0.21745	-0.24188	0.277894
35	6	4.496487	1.635437	1.184873	-0.04961
36	6	4.86722	0.560015	0.412294	-0.26681
37	1	5.213042	2.27761	1.680111	0.111868
38	6	-7.03902	-1.32569	0.14053	-0.33754
39	6	-9.3091	-1.68297	0.605981	-0.09919

40	1	-10.2697	-1.48199	1.062086	0.116774
41	16	-7.43239	-2.77906	-0.76178	0.260058
42	6	3.093633	1.839125	1.257139	-0.05553
43	1	2.63816	2.628272	1.840379	0.117115
44	6	0.564018	3.27975	-0.17846	-0.0989
45	1	1.624118	3.495036	-0.17634	0.110455
46	6	-8.1537	-0.87349	0.80446	-0.04892
47	1	-8.1389	-0.00011	1.44271	0.118408
48	6	-6.45369	1.601301	-0.46319	-0.0969
49	1	-7.49392	1.31431	-0.54137	0.109316
50	6	6.215084	0.057196	0.125899	-0.02242
51	6	7.272407	0.301079	1.013854	-0.05966
52	6	6.505429	-0.6752	-1.04074	-0.10558
53	6	8.565543	-0.14628	0.755762	-0.15019
54	1	7.085203	0.836437	1.937167	0.109381
55	6	7.784905	-1.1343	-1.30417	-0.11279
56	1	5.720825	-0.87469	-1.76195	0.115349
57	6	8.832626	-0.87133	-0.41084	0.185984
58	1	9.347026	0.064396	1.47274	0.125984
59	1	8.000273	-1.69338	-2.20689	0.110272
60	8	10.05329	-1.35855	-0.76063	-0.36687
61	6	11.17542	-1.11638	0.103833	-0.05218
62	6	12.39022	-1.75656	-0.53769	-0.29685
63	1	10.97787	-1.55023	1.090239	0.123147
64	1	11.31766	-0.03679	0.224517	0.123201
65	1	13.26941	-1.59629	0.090829	0.118099
66	1	12.24228	-2.83208	-0.65698	0.117326
67	1	12.58348	-1.31997	-1.51998	0.11736
68	6	-9.07622	-2.7505	-0.21262	-0.28915
69	1	-9.76293	-3.51995	-0.53053	0.149703

Table S11. The bond lengths of the S_0 state of C_2O-P-T-PC-T in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4959	R40	R(30,33)	1.4723
R2	R(1,3)	1.4351	R41	R(31,32)	1.0831
R3	R(1,16)	1.3931	R42	R(33,34)	1.756
R4	R(2,4)	1.4353	R43	R(33,42)	1.3741
R5	R(2,14)	1.3931	R44	R(34,36)	1.7541
R6	R(3,6)	1.3842	R45	R(35,36)	1.3751
R7	R(3,11)	1.4213	R46	R(35,37)	1.0822
R8	R(4,5)	1.3842	R47	R(35,42)	1.4194
R9	R(4,7)	1.4215	R48	R(36,50)	1.4668
R10	R(5,6)	1.3817	R49	R(38,41)	1.7553
R11	R(5,13)	1.3871	R50	R(38,46)	1.374
R12	R(6,18)	1.3871	R51	R(39,40)	1.0822
R13	R(7,30)	1.4637	R52	R(39,46)	1.4246
R14	R(7,44)	1.4136	R53	R(39,68)	1.3653
R15	R(8,9)	1.0844	R54	R(41,68)	1.7334
R16	R(8,14)	1.408	R55	R(42,43)	1.0818
R17	R(8,44)	1.3892	R56	R(44,45)	1.0817
R18	R(10,12)	1.0844	R57	R(46,47)	1.0818
R19	R(10,16)	1.4082	R58	R(48,49)	1.0819
R20	R(10,48)	1.3891	R59	R(50,51)	1.4021
R21	R(11,20)	1.4628	R60	R(50,52)	1.4077
R22	R(11,48)	1.4137	R61	R(51,53)	1.3925
R23	R(13,19)	1.4067	R62	R(51,54)	1.0836
R24	R(13,31)	1.4125	R63	R(52,55)	1.3846
R25	R(14,15)	1.0838	R64	R(52,56)	1.0842
R26	R(16,17)	1.0837	R65	R(53,57)	1.3993
R27	R(18,19)	1.4066	R66	R(53,58)	1.0813
R28	R(18,21)	1.413	R67	R(55,57)	1.4018
R29	R(19,23)	1.462	R68	R(55,59)	1.0834
R30	R(20,21)	1.4024	R69	R(57,60)	1.3601
R31	R(20,38)	1.4742	R70	R(60,61)	1.437
R32	R(21,22)	1.0831	R71	R(61,62)	1.5156
R33	R(23,24)	1.0922	R72	R(61,63)	1.0956
R34	R(23,25)	1.0919	R73	R(61,64)	1.0956
R35	R(23,26)	1.5302	R74	R(62,65)	1.0926
R36	R(26,27)	1.0924	R75	R(62,66)	1.0922
R37	R(26,28)	1.0923	R76	R(62,67)	1.0922
R38	R(26,29)	1.093	R77	R(68,69)	1.0792
R39	R(30,31)	1.4032			

Table S12. The bond angles of the S_0 state of C_2O-P-T-PC-T in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	119.1735	A67	A(13,31,30)	119.3076
A2	A(2,1,16)	125.5367	A68	A(13,31,32)	121.9067
A3	A(3,1,16)	115.2842	A69	A(30,31,32)	118.7594
A4	A(1,2,4)	119.1949	A70	A(30,33,34)	120.5359
A5	A(1,2,14)	125.5006	A71	A(30,33,42)	129.7985
A6	A(4,2,14)	115.298	A72	A(34,33,42)	109.6532
A7	A(1,3,6)	117.6703	A73	A(33,34,36)	92.6432
A8	A(1,3,11)	125.6894	A74	A(36,35,37)	122.8671
A9	A(6,3,11)	116.6288	A75	A(36,35,42)	114.0353
A10	A(2,4,5)	117.6443	A76	A(37,35,42)	123.0908
A11	A(2,4,7)	125.6901	A77	A(34,36,35)	109.6573
A12	A(5,4,7)	116.6511	A78	A(34,36,50)	121.6207
A13	A(4,5,6)	123.1607	A79	A(35,36,50)	128.7211
A14	A(4,5,13)	127.9218	A80	A(20,38,41)	120.5876
A15	A(6,5,13)	108.9164	A81	A(20,38,46)	129.5846
A16	A(3,6,5)	123.1412	A82	A(41,38,46)	109.8213
A17	A(3,6,18)	127.9414	A83	A(40,39,46)	123.7538
A18	A(5,6,18)	108.9169	A84	A(40,39,68)	123.3212
A19	A(4,7,30)	117.3151	A85	A(46,39,68)	112.9224
A20	A(4,7,44)	115.5606	A86	A(38,41,68)	92.0648
A21	A(30,7,44)	127.0985	A87	A(33,42,35)	114.0109
A22	A(9,8,14)	118.3676	A88	A(33,42,43)	122.7269
A23	A(9,8,44)	118.6637	A89	A(35,42,43)	123.246
A24	A(14,8,44)	122.9673	A90	A(7,44,8)	119.9688
A25	A(12,10,16)	118.3542	A91	A(7,44,45)	120.6408
A26	A(12,10,48)	118.6727	A92	A(8,44,45)	119.3851
A27	A(16,10,48)	122.972	A93	A(38,46,39)	113.8053
A28	A(3,11,20)	117.3063	A94	A(38,46,47)	122.6628
A29	A(3,11,48)	115.5982	A95	A(39,46,47)	123.5042
A30	A(20,11,48)	127.0735	A96	A(10,48,11)	119.934
A31	A(5,13,19)	106.9053	A97	A(10,48,49)	119.4466
A32	A(5,13,31)	116.3442	A98	A(11,48,49)	120.6156
A33	A(19,13,31)	136.734	A99	A(36,50,51)	120.6414
A34	A(2,14,8)	120.4898	A100	A(36,50,52)	121.9831
A35	A(2,14,15)	120.9063	A101	A(51,50,52)	117.3743
A36	A(8,14,15)	118.5986	A102	A(50,51,53)	121.8061
A37	A(1,16,10)	120.5031	A103	A(50,51,54)	119.6889
A38	A(1,16,17)	120.9138	A104	A(53,51,54)	118.4963
A39	A(10,16,17)	118.5788	A105	A(50,52,55)	121.3828
A40	A(6,18,19)	106.9028	A106	A(50,52,56)	119.8501

A41	A(6,18,21)	116.3188	A107	A(55,52,56)	118.7592
A42	A(19,18,21)	136.7618	A108	A(51,53,57)	119.8846
A43	A(13,19,18)	108.3517	A109	A(51,53,58)	119.0577
A44	A(13,19,23)	125.7174	A110	A(57,53,58)	121.053
A45	A(18,19,23)	125.8003	A111	A(52,55,57)	120.4786
A46	A(11,20,21)	122.5204	A112	A(52,55,59)	120.8836
A47	A(11,20,38)	119.4835	A113	A(57,55,59)	118.6345
A48	A(21,20,38)	117.996	A114	A(53,57,55)	119.0692
A49	A(18,21,20)	119.2622	A115	A(53,57,60)	124.8443
A50	A(18,21,22)	121.9512	A116	A(55,57,60)	116.0863
A51	A(20,21,22)	118.7648	A117	A(57,60,61)	119.0615
A52	A(19,23,24)	107.6967	A118	A(60,61,62)	107.4618
A53	A(19,23,25)	107.6056	A119	A(60,61,63)	109.5163
A54	A(19,23,26)	113.3755	A120	A(60,61,64)	109.4936
A55	A(24,23,25)	106.7561	A121	A(62,61,63)	110.9998
A56	A(24,23,26)	110.5695	A122	A(62,61,64)	111.0255
A57	A(25,23,26)	110.5582	A123	A(63,61,64)	108.3281
A58	A(23,26,27)	111.012	A124	A(61,62,65)	109.848
A59	A(23,26,28)	111.0242	A125	A(61,62,66)	110.708
A60	A(23,26,29)	109.8298	A126	A(61,62,67)	110.7121
A61	A(27,26,28)	108.4128	A127	A(65,62,66)	108.4384
A62	A(27,26,29)	108.2483	A128	A(65,62,67)	108.443
A63	A(28,26,29)	108.2227	A129	A(66,62,67)	108.6251
A64	A(7,30,31)	122.4321	A130	A(39,68,41)	111.3832
A65	A(7,30,33)	119.5769	A131	A(39,68,69)	128.7247
A66	A(31,30,33)	117.991	A132	A(41,68,69)	119.8919

Table S13. The dihedral angles of the S_0 state of C_2O-P-T-PC-T in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	-0.107	D102	D(18,19,23,26)	89.3885
D2	D(3,1,2,14)	178.9238	D103	D(11,20,21,18)	0.8531
D3	D(16,1,2,4)	-179.199	D104	D(11,20,21,22)	179.1903
D4	D(16,1,2,14)	-0.1685	D105	D(38,20,21,18)	-179.199
D5	D(2,1,3,6)	-0.9062	D106	D(38,20,21,22)	-0.8619
D6	D(2,1,3,11)	-179.62	D107	D(11,20,38,41)	131.1911
D7	D(16,1,3,6)	178.2769	D108	D(11,20,38,46)	-49.8341
D8	D(16,1,3,11)	-0.4372	D109	D(21,20,38,41)	-48.7583
D9	D(2,1,16,10)	178.439	D110	D(21,20,38,46)	130.2165
D10	D(2,1,16,17)	-0.8007	D111	D(19,23,26,27)	-60.4952
D11	D(3,1,16,10)	-0.6844	D112	D(19,23,26,28)	60.1767
D12	D(3,1,16,17)	-179.924	D113	D(19,23,26,29)	179.8287
D13	D(1,2,4,5)	1.0284	D114	D(24,23,26,27)	178.4464
D14	D(1,2,4,7)	179.5911	D115	D(24,23,26,28)	-60.8817
D15	D(14,2,4,5)	-178.099	D116	D(24,23,26,29)	58.7703
D16	D(14,2,4,7)	0.4638	D117	D(25,23,26,27)	60.437
D17	D(1,2,14,8)	-178.244	D118	D(25,23,26,28)	-178.891
D18	D(1,2,14,15)	0.9046	D119	D(25,23,26,29)	-59.2391
D19	D(4,2,14,8)	0.8201	D120	D(7,30,31,13)	-0.9266
D20	D(4,2,14,15)	179.9688	D121	D(7,30,31,32)	-179.097
D21	D(1,3,6,5)	1.0381	D122	D(33,30,31,13)	178.9724
D22	D(1,3,6,18)	-178.663	D123	D(33,30,31,32)	0.8024
D23	D(11,3,6,5)	179.8698	D124	D(7,30,33,34)	-133.637
D24	D(11,3,6,18)	0.1685	D125	D(7,30,33,42)	47.7919
D25	D(1,3,11,20)	179.8652	D126	D(31,30,33,34)	46.4615
D26	D(1,3,11,48)	1.4508	D127	D(31,30,33,42)	-132.11
D27	D(6,3,11,20)	1.1391	D128	D(30,33,34,36)	-178.686
D28	D(6,3,11,48)	-177.275	D129	D(42,33,34,36)	0.1487
D29	D(2,4,5,6)	-0.9792	D130	D(30,33,42,35)	178.5376
D30	D(2,4,5,13)	178.6041	D131	D(30,33,42,43)	-0.0403
D31	D(7,4,5,6)	-179.673	D132	D(34,33,42,35)	-0.1559
D32	D(7,4,5,13)	-0.0898	D133	D(34,33,42,43)	-178.734
D33	D(2,4,7,30)	-179.931	D134	D(33,34,36,35)	-0.1051
D34	D(2,4,7,44)	-1.6469	D135	D(33,34,36,50)	179.5756
D35	D(5,4,7,30)	-1.3554	D136	D(37,35,36,34)	-179.041
D36	D(5,4,7,44)	176.9285	D137	D(37,35,36,50)	1.3081
D37	D(4,5,6,3)	-0.0792	D138	D(42,35,36,34)	0.0359
D38	D(4,5,6,18)	179.6718	D139	D(42,35,36,50)	-179.616
D39	D(13,5,6,3)	-179.732	D140	D(36,35,42,33)	0.0804
D40	D(13,5,6,18)	0.0193	D141	D(36,35,42,43)	178.6499

D41	D(4,5,13,19)	179.8508	D142	D(37,35,42,33)	179.1546
D42	D(4,5,13,31)	1.081	D143	D(37,35,42,43)	-2.2759
D43	D(6,5,13,19)	-0.518	D144	D(34,36,50,51)	-154.41
D44	D(6,5,13,31)	-179.288	D145	D(34,36,50,52)	25.9905
D45	D(3,6,18,19)	-179.777	D146	D(35,36,50,51)	25.205
D46	D(3,6,18,21)	-1.0082	D147	D(35,36,50,52)	-154.395
D47	D(5,6,18,19)	0.4874	D148	D(20,38,41,68)	178.6395
D48	D(5,6,18,21)	179.2561	D149	D(46,38,41,68)	-0.5206
D49	D(4,7,30,31)	1.9001	D150	D(20,38,46,39)	-178.572
D50	D(4,7,30,33)	-177.997	D151	D(20,38,46,47)	-0.4271
D51	D(44,7,30,31)	-176.159	D152	D(41,38,46,39)	0.4898
D52	D(44,7,30,33)	3.9437	D153	D(41,38,46,47)	178.6348
D53	D(4,7,44,8)	1.5518	D154	D(40,39,46,38)	179.2471
D54	D(4,7,44,45)	-177.605	D155	D(40,39,46,47)	1.1199
D55	D(30,7,44,8)	179.64	D156	D(68,39,46,38)	-0.1777
D56	D(30,7,44,45)	0.4834	D157	D(68,39,46,47)	-178.305
D57	D(9,8,14,2)	178.6866	D158	D(40,39,68,41)	-179.657
D58	D(9,8,14,15)	-0.4815	D159	D(40,39,68,69)	0.5068
D59	D(44,8,14,2)	-0.8789	D160	D(46,39,68,41)	-0.2294
D60	D(44,8,14,15)	179.9529	D161	D(46,39,68,69)	179.9344
D61	D(9,8,44,7)	-179.963	D162	D(38,41,68,39)	0.4297
D62	D(9,8,44,45)	-0.7958	D163	D(38,41,68,69)	-179.718
D63	D(14,8,44,7)	-0.3987	D164	D(36,50,51,53)	-178.955
D64	D(14,8,44,45)	178.7686	D165	D(36,50,51,54)	2.1345
D65	D(12,10,16,1)	-178.854	D166	D(52,50,51,53)	0.6634
D66	D(12,10,16,17)	0.4037	D167	D(52,50,51,54)	-178.248
D67	D(48,10,16,1)	0.7537	D168	D(36,50,52,55)	179.446
D68	D(48,10,16,17)	-179.989	D169	D(36,50,52,56)	0.4825
D69	D(12,10,48,11)	179.946	D170	D(51,50,52,55)	-0.1664
D70	D(12,10,48,49)	0.6406	D171	D(51,50,52,56)	-179.13
D71	D(16,10,48,11)	0.3401	D172	D(50,51,53,57)	-0.6087
D72	D(16,10,48,49)	-178.965	D173	D(50,51,53,58)	-179.832
D73	D(3,11,20,21)	-1.6776	D174	D(54,51,53,57)	178.3148
D74	D(3,11,20,38)	178.3753	D175	D(54,51,53,58)	-0.9082
D75	D(48,11,20,21)	176.53	D176	D(50,52,55,57)	-0.382
D76	D(48,11,20,38)	-3.4171	D177	D(50,52,55,59)	-179.718
D77	D(3,11,48,10)	-1.3467	D178	D(56,52,55,57)	178.5926
D78	D(3,11,48,49)	177.9505	D179	D(56,52,55,59)	-0.7433
D79	D(20,11,48,10)	-179.581	D180	D(51,53,57,55)	0.042
D80	D(20,11,48,49)	-0.2835	D181	D(51,53,57,60)	-179.799
D81	D(5,13,19,18)	0.8182	D182	D(58,53,57,55)	179.2492
D82	D(5,13,19,23)	176.851	D183	D(58,53,57,60)	-0.5914
D83	D(31,13,19,18)	179.2097	D184	D(52,55,57,53)	0.4443

D84	D(31,13,19,23)	-4.7575	D185	D(52,55,57,60)	-179.701
D85	D(5,13,31,30)	-0.521	D186	D(59,55,57,53)	179.795
D86	D(5,13,31,32)	177.5892	D187	D(59,55,57,60)	-0.3507
D87	D(19,13,31,30)	-178.804	D188	D(53,57,60,61)	-0.6678
D88	D(19,13,31,32)	-0.6934	D189	D(55,57,60,61)	179.4874
D89	D(6,18,19,13)	-0.8067	D190	D(57,60,61,62)	-179.482
D90	D(6,18,19,23)	-176.835	D191	D(57,60,61,63)	59.8493
D91	D(21,18,19,13)	-179.196	D192	D(57,60,61,64)	-58.7956
D92	D(21,18,19,23)	4.7758	D193	D(60,61,62,65)	-179.926
D93	D(6,18,21,20)	0.4491	D194	D(60,61,62,66)	-60.1938
D94	D(6,18,21,22)	-177.833	D195	D(60,61,62,67)	60.3343
D95	D(19,18,21,20)	178.7293	D196	D(63,61,62,65)	-60.1979
D96	D(19,18,21,22)	0.4473	D197	D(63,61,62,66)	59.5339
D97	D(13,19,23,24)	36.6949	D198	D(63,61,62,67)	-179.938
D98	D(13,19,23,25)	151.45	D199	D(64,61,62,65)	60.3594
D99	D(13,19,23,26)	-85.9674	D200	D(64,61,62,66)	-179.909
D100	D(18,19,23,24)	-147.949	D201	D(64,61,62,67)	-59.3807
D101	D(18,19,23,25)	-33.194			

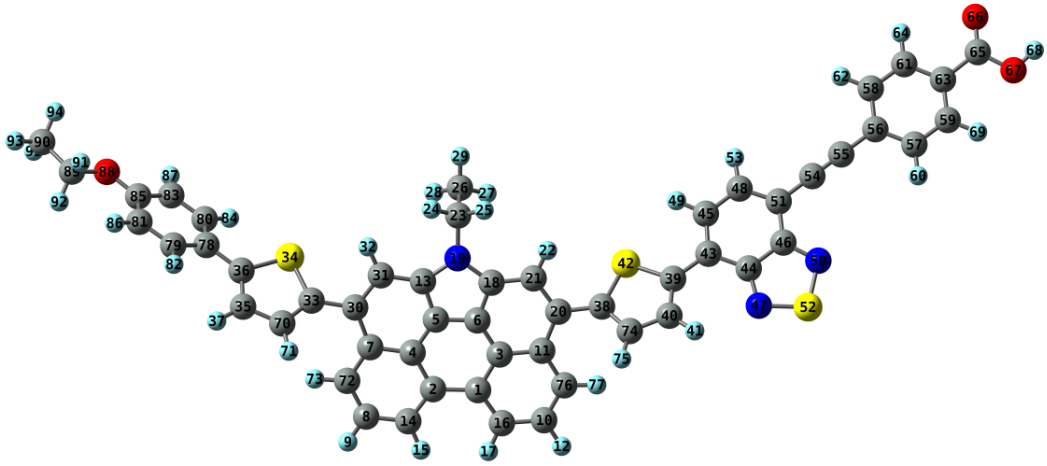


Figure S72. Geometry of the S_0 state of **C279** in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S14. Geometry parameters and Mulliken atomic charges of the S_0 state of **C279** in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	2.569714	-4.18257	0.806112	0.046781
2	6	4.043062	-3.9259	0.819074	0.047178
3	6	1.6839	-3.15548	0.33665	-0.02596
4	6	4.536523	-2.65847	0.36212	-0.02339
5	6	3.607604	-1.7183	-0.04938	-0.16576
6	6	2.247045	-1.95493	-0.06085	-0.16187
7	6	5.902252	-2.26835	0.31477	-0.00086
8	6	6.376502	-4.45626	1.251327	-0.08042
9	1	7.103272	-5.17134	1.620393	0.107599
10	6	0.546797	-5.47194	1.20184	-0.07989
11	6	0.267544	-3.25151	0.263341	0.000384
12	1	0.098509	-6.39101	1.562464	0.108053
13	6	3.844067	-0.4302	-0.50726	0.263909
14	6	5.016726	-4.82055	1.258116	-0.10158
15	1	4.745273	-5.80409	1.623198	0.10129
16	6	1.949201	-5.35494	1.23212	-0.10187
17	1	2.531185	-6.18946	1.605371	0.101411
18	6	1.597525	-0.82007	-0.52651	0.258462
19	7	2.592742	0.130742	-0.81685	-0.57785
20	6	-0.45647	-2.08829	-0.25281	0.032729
21	6	0.192667	-0.89945	-0.6255	-0.03313
22	1	-0.40047	-0.08166	-1.01564	0.128316
23	6	2.36055	1.497961	-1.28046	-0.09975
24	1	3.213476	1.786057	-1.89848	0.138908
25	1	1.487729	1.482058	-1.93666	0.138593
26	6	2.159347	2.499436	-0.14129	-0.28134
27	1	1.292349	2.232154	0.467049	0.118159
28	1	3.037599	2.536631	0.507065	0.118643
29	1	1.994155	3.498916	-0.55143	0.120437
30	6	6.20114	-0.92764	-0.19159	0.038916
31	6	5.196396	-0.02918	-0.58143	-0.04208
32	1	5.484438	0.942991	-0.96203	0.125664
33	6	7.602142	-0.49138	-0.30953	-0.32312
34	16	8.096027	1.093787	0.261665	0.278838
35	6	9.884902	-0.39138	-0.82749	-0.0502
36	6	9.75459	0.851546	-0.25431	-0.26556
37	1	10.82626	-0.7663	-1.20755	0.112401
38	6	-1.91627	-2.14958	-0.40732	-0.31212
39	6	-4.39112	-1.5976	-0.44743	-0.26796

40	6	-4.08276	-2.83844	-0.96859	-0.01466
41	1	-4.83625	-3.49794	-1.37052	0.12615
42	16	-2.91827	-0.80756	0.103731	0.294034
43	6	-5.68012	-0.93631	-0.3315	0.08826
44	6	-6.928	-1.641	-0.50446	0.125434
45	6	-5.79693	0.417056	-0.04538	-0.1113
46	6	-8.19746	-0.94826	-0.38251	0.167031
47	7	-7.07481	-2.94035	-0.77422	-0.50871
48	6	-7.03011	1.091555	0.076822	-0.01277
49	1	-4.89748	1.007291	0.082188	0.123387
50	7	-9.25567	-1.73745	-0.56675	-0.48962
51	6	-8.25026	0.455984	-0.08575	-0.23715
52	16	-8.68174	-3.24183	-0.86755	0.577333
53	1	-7.0179	2.151358	0.299134	0.113206
54	6	-9.48481	1.132738	0.026656	0.140418
55	6	-10.5454	1.712245	0.119586	0.031571
56	6	-11.7932	2.380583	0.223269	-0.17944
57	6	-12.998	1.665478	0.073005	-0.0337
58	6	-11.8485	3.766301	0.475453	-0.037
59	6	-14.2179	2.316381	0.171561	-0.0283
60	1	-12.962	0.600822	-0.12083	0.117359
61	6	-13.0707	4.410095	0.57196	-0.03449
62	1	-10.9274	4.323244	0.592279	0.116503
63	6	-14.2648	3.694143	0.421332	-0.20241
64	1	-13.1183	5.474261	0.764957	0.116464
65	6	-15.5478	4.435	0.534	0.431215
66	8	-15.6401	5.624816	0.745355	-0.36777
67	8	-16.6299	3.643693	0.375807	-0.3401
68	1	-17.4136	4.206984	0.465155	0.277695
69	1	-15.138	1.759578	0.055032	0.120373
70	6	8.681214	-1.14292	-0.85699	-0.05498
71	1	8.608697	-2.1304	-1.29284	0.117816
72	6	6.825952	-3.22125	0.800796	-0.09782
73	1	7.883118	-2.99525	0.838649	0.111375
74	6	-2.7029	-3.14417	-0.94573	-0.05308
75	1	-2.29264	-4.05808	-1.35287	0.122369
76	6	-0.28685	-4.46153	0.738956	-0.09927
77	1	-1.35823	-4.60877	0.760844	0.111814
78	6	10.77608	1.888501	-0.07269	-0.02419
79	6	11.87627	1.964312	-0.93824	-0.05951
80	6	10.70103	2.836606	0.965096	-0.10412
81	6	12.86855	2.928426	-0.78063	-0.15048
82	1	11.95569	1.270185	-1.76657	0.10969

83	6	11.67639	3.806178	1.126908	-0.11285
84	1	9.874632	2.805015	1.666288	0.115528
85	6	12.77461	3.862038	0.257421	0.186226
86	1	13.69598	2.948702	-1.47649	0.12638
87	1	11.61355	4.529766	1.930834	0.110471
88	8	13.67985	4.847509	0.499736	-0.36662
89	6	14.83295	4.960249	-0.35051	-0.0523
90	6	15.65981	6.125328	0.155382	-0.29684
91	1	14.51025	5.127467	-1.38405	0.123233
92	1	15.40622	4.027297	-0.31521	0.123272
93	1	16.54992	6.245466	-0.46667	0.118158
94	1	15.08442	7.052907	0.117932	0.117342
95	1	15.97892	5.954113	1.185776	0.117403

Table S15. The bond lengths of the S_0 state of **C279** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4956	R54	R(40,41)	1.079
R2	R(1,3)	1.4353	R55	R(40,74)	1.4135
R3	R(1,16)	1.3932	R56	R(43,44)	1.4435
R4	R(2,4)	1.4348	R57	R(43,45)	1.3882
R5	R(2,14)	1.3933	R58	R(44,46)	1.4513
R6	R(3,6)	1.3844	R59	R(44,47)	1.3352
R7	R(3,11)	1.4215	R60	R(45,48)	1.4109
R8	R(4,5)	1.3843	R61	R(45,49)	1.0833
R9	R(4,7)	1.4211	R62	R(46,50)	1.3329
R10	R(5,6)	1.381	R63	R(46,51)	1.4362
R11	R(5,13)	1.3874	R64	R(47,52)	1.6376
R12	R(6,18)	1.388	R65	R(48,51)	1.3853
R13	R(7,30)	1.464	R66	R(48,53)	1.0829
R14	R(7,72)	1.4133	R67	R(50,52)	1.638
R15	R(8,9)	1.0843	R68	R(51,54)	1.4123
R16	R(8,14)	1.4077	R69	R(54,55)	1.2122
R17	R(8,72)	1.3893	R70	R(55,56)	1.4193
R18	R(10,12)	1.0843	R71	R(56,57)	1.409
R19	R(10,16)	1.4076	R72	R(56,58)	1.4096
R20	R(10,76)	1.3893	R73	R(57,59)	1.3863
R21	R(11,20)	1.4641	R74	R(57,60)	1.0828
R22	R(11,76)	1.4134	R75	R(58,61)	1.3848
R23	R(13,19)	1.4058	R76	R(58,62)	1.0827
R24	R(13,31)	1.4125	R77	R(59,63)	1.401
R25	R(14,15)	1.0837	R78	R(59,69)	1.0817
R26	R(16,17)	1.0837	R79	R(61,63)	1.4004
R27	R(18,19)	1.4067	R80	R(61,64)	1.0826
R28	R(18,21)	1.4106	R81	R(63,65)	1.4858
R29	R(19,23)	1.4622	R82	R(65,66)	1.212
R30	R(20,21)	1.4049	R83	R(65,67)	1.3499
R31	R(20,38)	1.4692	R84	R(67,68)	0.9692
R32	R(21,22)	1.083	R85	R(70,71)	1.0818
R33	R(23,24)	1.092	R86	R(72,73)	1.0817
R34	R(23,25)	1.0921	R87	R(74,75)	1.0813
R35	R(23,26)	1.5301	R88	R(76,77)	1.0817
R36	R(26,27)	1.0923	R89	R(78,79)	1.4019
R37	R(26,28)	1.0923	R90	R(78,80)	1.4077
R38	R(26,29)	1.0929	R91	R(79,81)	1.3925
R39	R(30,31)	1.4031	R92	R(79,82)	1.0836
R40	R(30,33)	1.4721	R93	R(80,83)	1.3848

R41	R(31,32)	1.083	R94	R(80,84)	1.0843
R42	R(33,34)	1.7558	R95	R(81,85)	1.3993
R43	R(33,70)	1.3743	R96	R(81,86)	1.0813
R44	R(34,36)	1.7538	R97	R(83,85)	1.4019
R45	R(35,36)	1.3749	R98	R(83,87)	1.0834
R46	R(35,37)	1.0822	R99	R(85,88)	1.3599
R47	R(35,70)	1.4193	R100	R(88,89)	1.4371
R48	R(36,78)	1.4669	R101	R(89,90)	1.5156
R49	R(38,42)	1.7511	R102	R(89,91)	1.0956
R50	R(38,74)	1.3776	R103	R(89,92)	1.0956
R51	R(39,40)	1.3807	R104	R(90,93)	1.0926
R52	R(39,42)	1.7599	R105	R(90,94)	1.0922
R53	R(39,43)	1.4534	R106	R(90,95)	1.0922

Table S16. The bond angles of the S_0 state of **C279** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	119.2106	A91	A(39,43,45)	122.3204
A2	A(2,1,16)	125.4881	A92	A(44,43,45)	115.3335
A3	A(3,1,16)	115.2976	A93	A(43,44,46)	120.8692
A4	A(1,2,4)	119.1856	A94	A(43,44,47)	126.4668
A5	A(1,2,14)	125.5191	A95	A(46,44,47)	112.6629
A6	A(4,2,14)	115.2918	A96	A(43,45,48)	123.8805
A7	A(1,3,6)	117.6102	A97	A(43,45,49)	119.0495
A8	A(1,3,11)	125.6952	A98	A(48,45,49)	117.0653
A9	A(6,3,11)	116.6855	A99	A(44,46,50)	113.5923
A10	A(2,4,5)	117.6353	A100	A(44,46,51)	121.0782
A11	A(2,4,7)	125.7047	A101	A(50,46,51)	125.3292
A12	A(5,4,7)	116.6503	A102	A(44,47,52)	107.3718
A13	A(4,5,6)	123.1756	A103	A(45,48,51)	122.7064
A14	A(4,5,13)	127.9035	A104	A(45,48,53)	118.4101
A15	A(6,5,13)	108.9207	A105	A(51,48,53)	118.8817
A16	A(3,6,5)	123.1593	A106	A(46,50,52)	106.9171
A17	A(3,6,18)	127.9535	A107	A(46,51,48)	116.1314
A18	A(5,6,18)	108.8868	A108	A(46,51,54)	121.1366
A19	A(4,7,30)	117.3305	A109	A(48,51,54)	122.7318
A20	A(4,7,72)	115.5653	A110	A(47,52,50)	99.4554
A21	A(30,7,72)	127.083	A111	A(55,56,57)	120.3263
A22	A(9,8,14)	118.3671	A112	A(55,56,58)	120.6949
A23	A(9,8,72)	118.6704	A113	A(57,56,58)	118.9788
A24	A(14,8,72)	122.9615	A114	A(56,57,59)	120.4356
A25	A(12,10,16)	118.3729	A115	A(56,57,60)	119.3225
A26	A(12,10,76)	118.6322	A116	A(59,57,60)	120.2419
A27	A(16,10,76)	122.9938	A117	A(56,58,61)	120.2726
A28	A(3,11,20)	117.2079	A118	A(56,58,62)	119.4473
A29	A(3,11,76)	115.5499	A119	A(61,58,62)	120.2801
A30	A(20,11,76)	127.2161	A120	A(57,59,63)	120.2581
A31	A(5,13,19)	106.944	A121	A(57,59,69)	119.9447
A32	A(5,13,31)	116.3666	A122	A(63,59,69)	119.7972
A33	A(19,13,31)	136.6646	A123	A(58,61,63)	120.4917
A34	A(2,14,8)	120.4868	A124	A(58,61,64)	120.5417
A35	A(2,14,15)	120.9242	A125	A(63,61,64)	118.9666
A36	A(8,14,15)	118.5843	A126	A(59,63,61)	119.5632
A37	A(1,16,10)	120.4719	A127	A(59,63,65)	122.1945
A38	A(1,16,17)	120.9393	A128	A(61,63,65)	118.2423
A39	A(10,16,17)	118.5838	A129	A(63,65,66)	124.6455
A40	A(6,18,19)	106.9067	A130	A(63,65,67)	113.0176

A41	A(6,18,21)	116.3326	A131	A(66,65,67)	122.3369
A42	A(19,18,21)	136.733	A132	A(65,67,68)	107.2573
A43	A(13,19,18)	108.3356	A133	A(33,70,35)	113.9902
A44	A(13,19,23)	125.7501	A134	A(33,70,71)	122.7257
A45	A(18,19,23)	125.8095	A135	A(35,70,71)	123.2668
A46	A(11,20,21)	122.5033	A136	A(7,72,8)	119.9622
A47	A(11,20,38)	119.6864	A137	A(7,72,73)	120.6574
A48	A(21,20,38)	117.8075	A138	A(8,72,73)	119.3757
A49	A(18,21,20)	119.2877	A139	A(38,74,40)	114.0526
A50	A(18,21,22)	121.8883	A140	A(38,74,75)	122.7306
A51	A(20,21,22)	118.7854	A141	A(40,74,75)	123.1662
A52	A(19,23,24)	107.5835	A142	A(10,76,11)	119.9591
A53	A(19,23,25)	107.6861	A143	A(10,76,77)	119.2485
A54	A(19,23,26)	113.3797	A144	A(11,76,77)	120.787
A55	A(24,23,25)	106.7398	A145	A(36,78,79)	120.5498
A56	A(24,23,26)	110.5726	A146	A(36,78,80)	122.0248
A57	A(25,23,26)	110.5969	A147	A(79,78,80)	117.4251
A58	A(23,26,27)	111.0295	A148	A(78,79,81)	121.7894
A59	A(23,26,28)	111.0072	A149	A(78,79,82)	119.6582
A60	A(23,26,29)	109.8188	A150	A(81,79,82)	118.5419
A61	A(27,26,28)	108.4178	A151	A(78,80,83)	121.3446
A62	A(27,26,29)	108.2279	A152	A(78,80,84)	119.8533
A63	A(28,26,29)	108.2488	A153	A(83,80,84)	118.7949
A64	A(7,30,31)	122.4337	A154	A(79,81,85)	119.8731
A65	A(7,30,33)	119.5654	A155	A(79,81,86)	119.0405
A66	A(31,30,33)	118.0001	A156	A(85,81,86)	121.0813
A67	A(13,31,30)	119.2877	A157	A(80,83,85)	120.4782
A68	A(13,31,32)	121.8664	A158	A(80,83,87)	120.8953
A69	A(30,31,32)	118.8151	A159	A(85,83,87)	118.6238
A70	A(30,33,34)	120.6099	A160	A(81,85,83)	119.0865
A71	A(30,33,70)	129.6945	A161	A(81,85,88)	124.8195
A72	A(34,33,70)	109.6788	A162	A(83,85,88)	116.0938
A73	A(33,34,36)	92.6138	A163	A(85,88,89)	119.0481
A74	A(36,35,37)	122.8224	A164	A(88,89,90)	107.4918
A75	A(36,35,70)	114.0135	A165	A(88,89,91)	109.4977
A76	A(37,35,70)	123.1577	A166	A(88,89,92)	109.5104
A77	A(34,36,35)	109.7033	A167	A(90,89,91)	110.993
A78	A(34,36,78)	121.6343	A168	A(90,89,92)	111.0016
A79	A(35,36,78)	128.6581	A169	A(91,89,92)	108.3307
A80	A(20,38,42)	120.3905	A170	A(89,90,93)	109.8135
A81	A(20,38,74)	129.6835	A171	A(89,90,94)	110.7328
A82	A(42,38,74)	109.9156	A172	A(89,90,95)	110.7201
A83	A(40,39,42)	109.5569	A173	A(93,90,94)	108.4389

A84	A(40,39,43)	129.5754	A174	A(93,90,95)	108.4417
A85	A(42,39,43)	120.8647	A175	A(94,90,95)	108.6273
A86	A(39,40,41)	122.2723	A176	L(51,54,55,46,-1)	179.8897
A87	A(39,40,74)	113.9717	A177	L(54,55,56,57,-1)	179.4954
A88	A(41,40,74)	123.7469	A178	L(51,54,55,46,-2)	180.3006
A89	A(38,42,39)	92.4898	A179	L(54,55,56,57,-2)	180.2491
A90	A(39,43,44)	122.346			

Table S17. The dihedral angles of the S_0 state of **C279** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	0.0168	D136	D(37,35,36,34)	179.0917
D2	D(3,1,2,14)	179.3155	D137	D(37,35,36,78)	1.6605
D3	D(16,1,2,4)	179.2522	D138	D(70,35,36,34)	0.0149
D4	D(16,1,2,14)	0.0464	D139	D(70,35,36,78)	179.2329
D5	D(2,1,3,6)	-1.2305	D140	D(36,35,70,33)	0.1184
D6	D(2,1,3,11)	179.91	D141	D(36,35,70,71)	178.6403
D7	D(16,1,3,6)	178.1112	D142	D(37,35,70,33)	179.2216
D8	D(16,1,3,11)	-0.7483	D143	D(37,35,70,71)	-2.2564
D9	D(2,1,16,10)	178.53	D144	D(34,36,78,79)	152.3948
D10	D(2,1,16,17)	-0.6438	D145	D(34,36,78,80)	27.8086
D11	D(3,1,16,10)	-0.7643	D146	D(35,36,78,79)	26.7734
D12	D(3,1,16,17)	179.9381	D147	D(35,36,78,80)	153.0232
D13	D(1,2,4,5)	1.1695	D148	D(20,38,42,39)	177.9048
D14	D(1,2,4,7)	179.9972	D149	D(74,38,42,39)	-1.0301
D15	D(14,2,4,5)	178.1992	D150	D(20,38,74,40)	178.0413
D16	D(14,2,4,7)	0.6286	D151	D(20,38,74,75)	-0.5565
D17	D(1,2,14,8)	178.5685	D152	D(42,38,74,40)	0.7649
D18	D(1,2,14,15)	0.6397	D153	D(42,38,74,75)	178.2497
D19	D(4,2,14,8)	0.7543	D154	D(42,39,40,41)	179.7509
D20	D(4,2,14,15)	179.9625	D155	D(42,39,40,74)	-0.8052
D21	D(1,3,6,5)	1.3129	D156	D(43,39,40,41)	-0.4005
D22	D(1,3,6,18)	178.9302	D157	D(43,39,40,74)	178.5452
D23	D(11,3,6,5)	179.7237	D158	D(40,39,42,38)	1.0438
D24	D(11,3,6,18)	0.0332	D159	D(43,39,42,38)	178.3729
D25	D(1,3,11,20)	179.7424	D160	D(40,39,43,44)	14.034
D26	D(1,3,11,76)	1.9823	D161	D(40,39,43,45)	166.0303
D27	D(6,3,11,20)	1.3887	D162	D(42,39,43,44)	166.6792
D28	D(6,3,11,76)	176.8866	D163	D(42,39,43,45)	13.2566
D29	D(2,4,5,6)	-1.1898	D164	D(39,40,74,38)	0.0307
D30	D(2,4,5,13)	178.9566	D165	D(39,40,74,75)	177.4417
D31	D(7,4,5,6)	179.8752	D166	D(41,40,74,38)	178.9587
D32	D(7,4,5,13)	0.0216	D167	D(41,40,74,75)	1.4863
D33	D(2,4,7,30)	179.7611	D168	D(39,43,44,46)	179.9544
D34	D(2,4,7,72)	-1.7937	D169	D(39,43,44,47)	0.4455
D35	D(5,4,7,30)	-1.4008	D170	D(45,43,44,46)	0.1057
D36	D(5,4,7,72)	177.0444	D171	D(45,43,44,47)	179.4945
D37	D(4,5,6,3)	-0.0808	D172	D(39,43,45,48)	179.8862
D38	D(4,5,6,18)	179.8782	D173	D(39,43,45,49)	0.9256
D39	D(13,5,6,3)	179.7971	D174	D(44,43,45,48)	0.0537
D40	D(13,5,6,18)	-0.0003	D175	D(44,43,45,49)	179.1345

D41	D(4,5,13,19)	179.3957	D176	D(43,44,46,50)	179.8658
D42	D(4,5,13,31)	0.9048	D177	D(43,44,46,51)	-0.0466
D43	D(6,5,13,19)	-0.4748	D178	D(47,44,46,50)	-0.2143
D44	D(6,5,13,31)	178.9656	D179	D(47,44,46,51)	179.605
D45	D(3,6,18,19)	179.31	D180	D(43,44,47,52)	179.8152
D46	D(3,6,18,21)	-0.9014	D181	D(46,44,47,52)	0.1871
D47	D(5,6,18,19)	0.4749	D182	D(43,45,48,51)	-0.2913
D48	D(5,6,18,21)	178.8836	D183	D(43,45,48,53)	179.7912
D49	D(4,7,30,31)	1.9625	D184	D(49,45,48,51)	178.9118
D50	D(4,7,30,33)	177.7117	D185	D(49,45,48,53)	-0.5882
D51	D(72,7,30,31)	176.2793	D186	D(44,46,50,52)	0.1259
D52	D(72,7,30,33)	4.0466	D187	D(51,46,50,52)	179.6844
D53	D(4,7,72,8)	1.581	D188	D(44,46,51,48)	-0.1705
D54	D(4,7,72,73)	177.6187	D189	D(44,46,51,54)	179.6828
D55	D(30,7,72,8)	179.8495	D190	D(50,46,51,48)	179.6264
D56	D(30,7,72,73)	0.6498	D191	D(50,46,51,54)	-0.5202
D57	D(9,8,14,2)	178.7056	D192	D(44,47,52,50)	-0.1047
D58	D(9,8,14,15)	-0.5208	D193	D(45,48,51,46)	0.3342
D59	D(72,8,14,2)	-0.9182	D194	D(45,48,51,54)	179.5166
D60	D(72,8,14,15)	179.8553	D195	D(53,48,51,46)	179.8319
D61	D(9,8,72,7)	179.9622	D196	D(53,48,51,54)	-0.0188
D62	D(9,8,72,73)	-0.7522	D197	D(46,50,52,47)	-0.0153
D63	D(14,8,72,7)	-0.3395	D198	D(46,51,56,57)	1.6314
D64	D(14,8,72,73)	178.8705	D199	D(46,51,56,58)	178.1169
D65	D(12,10,16,1)	178.6272	D200	D(48,51,56,57)	178.6955
D66	D(12,10,16,17)	0.5658	D201	D(48,51,56,58)	1.5562
D67	D(76,10,16,1)	0.9791	D202	D(55,56,57,59)	179.8893
D68	D(76,10,16,17)	179.8279	D203	D(55,56,57,60)	0.0928
D69	D(12,10,76,11)	179.9584	D204	D(58,56,57,59)	0.0197
D70	D(12,10,76,77)	0.7931	D205	D(58,56,57,60)	179.9983
D71	D(16,10,76,11)	0.3531	D206	D(55,56,58,61)	179.8553
D72	D(16,10,76,77)	178.8122	D207	D(55,56,58,62)	-0.096
D73	D(3,11,20,21)	-2.0529	D208	D(57,56,58,61)	-0.0533
D74	D(3,11,20,38)	177.3313	D209	D(57,56,58,62)	179.9954
D75	D(76,11,20,21)	175.9931	D210	D(56,57,59,63)	0.0312
D76	D(76,11,20,38)	-4.6228	D211	D(56,57,59,69)	179.9895
D77	D(3,11,76,10)	-1.7092	D212	D(60,57,59,63)	179.9507
D78	D(3,11,76,77)	177.443	D213	D(60,57,59,69)	0.0286
D79	D(20,11,76,10)	179.7831	D214	D(56,58,61,63)	0.0361
D80	D(20,11,76,77)	-0.6308	D215	D(56,58,61,64)	179.9649
D81	D(5,13,19,18)	0.7673	D216	D(62,58,61,63)	179.9869
D82	D(5,13,19,23)	177.2131	D217	D(62,58,61,64)	-0.014
D83	D(31,13,19,18)	178.7969	D218	D(57,59,63,61)	-0.0489

D84	D(31,13,19,23)	-4.7573	D219	D(57,59,63,65)	179.9452
D85	D(5,13,31,30)	-0.347	D220	D(69,59,63,61)	179.9719
D86	D(5,13,31,32)	177.6101	D221	D(69,59,63,65)	-0.0341
D87	D(19,13,31,30)	178.2432	D222	D(58,61,63,59)	0.0152
D88	D(19,13,31,32)	-0.2861	D223	D(58,61,63,65)	179.9791
D89	D(6,18,19,13)	-0.7673	D224	D(64,61,63,59)	179.9839
D90	D(6,18,19,23)	177.2104	D225	D(64,61,63,65)	0.0218
D91	D(21,18,19,13)	178.6863	D226	D(59,63,65,66)	179.8048
D92	D(21,18,19,23)	4.8706	D227	D(59,63,65,67)	0.197
D93	D(6,18,21,20)	0.2408	D228	D(61,63,65,66)	0.1893
D94	D(6,18,21,22)	177.4725	D229	D(61,63,65,67)	179.8089
D95	D(19,18,21,20)	178.0191	D230	D(63,65,67,68)	179.956
D96	D(19,18,21,22)	0.3058	D231	D(66,65,67,68)	-0.0423
D97	D(13,19,23,24)	33.9405	D232	D(36,78,79,81)	179.2672
D98	D(13,19,23,25)	148.6605	D233	D(36,78,79,82)	1.9271
D99	D(13,19,23,26)	-88.6473	D234	D(80,78,79,81)	0.5386
D100	D(18,19,23,24)	150.2207	D235	D(80,78,79,82)	178.2672
D101	D(18,19,23,25)	-35.5007	D236	D(36,78,80,83)	179.7252
D102	D(18,19,23,26)	87.1915	D237	D(36,78,80,84)	0.7151
D103	D(11,20,21,18)	1.2099	D238	D(79,78,80,83)	-0.0775
D104	D(11,20,21,22)	178.9945	D239	D(79,78,80,84)	179.0876
D105	D(38,20,21,18)	178.1853	D240	D(78,79,81,85)	-0.5767
D106	D(38,20,21,22)	-0.4006	D241	D(78,79,81,86)	179.769
D107	D(11,20,38,42)	135.9302	D242	D(82,79,81,85)	178.2419
D108	D(11,20,38,74)	-45.371	D243	D(82,79,81,86)	-0.9504
D109	D(21,20,38,42)	-44.6569	D244	D(78,80,83,85)	-0.3424
D110	D(21,20,38,74)	134.0419	D245	D(78,80,83,87)	179.7368
D111	D(19,23,26,27)	-60.5125	D246	D(84,80,83,85)	178.678
D112	D(19,23,26,28)	60.1661	D247	D(84,80,83,87)	-0.7165
D113	D(19,23,26,29)	179.8328	D248	D(79,81,85,83)	0.1416
D114	D(24,23,26,27)	178.5703	D249	D(79,81,85,88)	179.682
D115	D(24,23,26,28)	-60.7511	D250	D(86,81,85,83)	179.3171
D116	D(24,23,26,29)	58.9156	D251	D(86,81,85,88)	-0.5065
D117	D(25,23,26,27)	60.555	D252	D(80,83,85,81)	0.3094
D118	D(25,23,26,28)	178.7663	D253	D(80,83,85,88)	179.8519
D119	D(25,23,26,29)	-59.0997	D254	D(87,83,85,81)	179.7174
D120	D(7,30,31,13)	-1.056	D255	D(87,83,85,88)	-0.4439
D121	D(7,30,31,32)	179.0759	D256	D(81,85,88,89)	-0.3772
D122	D(33,30,31,13)	178.623	D257	D(83,85,88,89)	179.7945
D123	D(33,30,31,32)	0.6031	D258	D(85,88,89,90)	179.6202
D124	D(7,30,33,34)	134.0464	D259	D(85,88,89,91)	59.7122
D125	D(7,30,33,70)	47.6072	D260	D(85,88,89,92)	-58.9349
D126	D(31,30,33,34)	46.2651	D261	D(88,89,90,93)	179.9928

D127	D(31,30,33,70)	132.0814	D262	D(88,89,90,94)	-60.2813
D128	D(30,33,34,36)	178.4801	D263	D(88,89,90,95)	60.2713
D129	D(70,33,34,36)	0.1688	D264	D(91,89,90,93)	-60.2875
D130	D(30,33,70,35)	178.297	D265	D(91,89,90,94)	59.4384
D131	D(30,33,70,71)	-0.234	D266	D(91,89,90,95)	179.991
D132	D(34,33,70,35)	-0.1916	D267	D(92,89,90,93)	60.2525
D133	D(34,33,70,71)	178.7226	D268	D(92,89,90,94)	179.9784
D134	D(33,34,36,35)	-0.1045	D269	D(92,89,90,95)	-59.4689
D135	D(33,34,36,78)	179.2056	D136	D(37,35,36,34)	179.0917

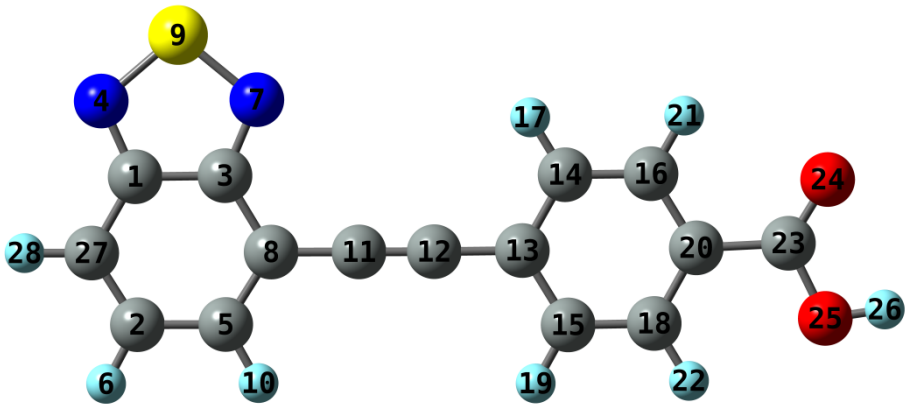


Figure S73. Geometry of the S_0 state of BTEBA in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S18. Geometry parameters and Mulliken atomic charges of the S_0 state of BTEBA in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	-4.59852	0.076706	-1.9E-05	0.12102
2	6	-4.22428	2.439479	0.000151	-0.09712
3	6	-3.16934	-0.15218	0.000015	0.141796
4	7	-5.31315	-1.05475	-4.5E-05	-0.47658
5	6	-2.81719	2.227455	0.000183	-0.01651
6	1	-4.58843	3.459816	0.000224	0.126748
7	7	-2.83511	-1.44331	0.000003	-0.48852
8	6	-2.25862	0.961672	0.000123	-0.22682
9	16	-4.23895	-2.29156	-0.00033	0.569883
10	1	-2.15944	3.087687	0.000278	0.116391
11	6	-0.85831	0.752034	0.000167	0.136204
12	6	0.339175	0.570613	0.000125	0.02915
13	6	1.741638	0.344936	0.000097	-0.17994
14	6	2.250376	-0.96919	0.000406	-0.03245
15	6	2.642815	1.426925	-0.00025	-0.03529
16	6	3.61789	-1.18814	0.000374	-0.03547
17	1	1.562185	-1.80506	0.000668	0.118479
18	6	4.010856	1.200491	-0.00029	-0.02619
19	1	2.258693	2.439224	-0.00049	0.116967
20	6	4.509382	-0.10832	0.000021	-0.20193
21	1	4.013883	-2.19567	0.000617	0.117396
22	1	4.696919	2.036739	-0.00057	0.120668
23	6	5.967089	-0.3992	-7E-06	0.43174
24	8	6.447207	-1.51171	0.000332	-0.36654
25	8	6.727169	0.716053	-0.00053	-0.33971
26	1	7.654069	0.43273	-0.00053	0.278142
27	6	-5.11705	1.400283	0.000058	-0.02767
28	1	-6.18739	1.559878	0.000058	0.126167

Table S19. The bond lengths of the S_0 state of BTEBA in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,3)	1.4474	R16	R(13,14)	1.4092
R2	R(1,4)	1.3382	R17	R(13,15)	1.4081
R3	R(1,27)	1.4215	R18	R(14,16)	1.3849
R4	R(2,5)	1.423	R19	R(14,17)	1.0827
R5	R(2,6)	1.0834	R20	R(15,18)	1.3867
R6	R(2,27)	1.37	R21	R(15,19)	1.0827
R7	R(3,7)	1.3337	R22	R(16,20)	1.4003
R8	R(3,8)	1.4388	R23	R(16,21)	1.0826
R9	R(4,9)	1.6382	R24	R(18,20)	1.4005
R10	R(5,8)	1.3835	R25	R(18,22)	1.0817
R11	R(5,10)	1.0829	R26	R(20,23)	1.4864
R12	R(7,9)	1.6402	R27	R(23,24)	1.2117
R13	R(8,11)	1.4159	R28	R(23,25)	1.3496
R14	R(11,12)	1.2112	R29	R(25,26)	0.9692
R15	R(12,13)	1.4205	R30	R(27,28)	1.0822

Table S20. The bond angles of the S_0 state of BTEBA in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(3,1,4)	113.1781	A25	A(13,15,18)	120.3924
A2	A(3,1,27)	120.4922	A26	A(13,15,19)	119.4299
A3	A(4,1,27)	126.3296	A27	A(18,15,19)	120.1777
A4	A(5,2,6)	118.21	A28	A(14,16,20)	120.4467
A5	A(5,2,27)	122.0968	A29	A(14,16,21)	120.5526
A6	A(6,2,27)	119.6932	A30	A(20,16,21)	119.0007
A7	A(1,3,7)	113.6122	A31	A(15,18,20)	120.25
A8	A(1,3,8)	120.1719	A32	A(15,18,22)	119.9675
A9	A(7,3,8)	126.216	A33	A(20,18,22)	119.7825
A10	A(1,4,9)	106.748	A34	A(16,20,18)	119.6053
A11	A(2,5,8)	122.3802	A35	A(16,20,23)	118.2582
A12	A(2,5,10)	118.8334	A36	A(18,20,23)	122.1365
A13	A(8,5,10)	118.7864	A37	A(20,23,24)	124.6279
A14	A(3,7,9)	106.6283	A38	A(20,23,25)	112.991
A15	A(3,8,5)	116.9183	A39	A(24,23,25)	122.3811
A16	A(3,8,11)	120.7561	A40	A(23,25,26)	107.279
A17	A(5,8,11)	122.3256	A41	A(1,27,2)	117.9406
A18	A(4,9,7)	99.8333	A42	A(1,27,28)	119.8743
A19	A(12,13,14)	120.3043	A43	A(2,27,28)	122.185
A20	A(12,13,15)	120.6492	A44	L(8,11,12,3,-1)	179.8996
A21	A(14,13,15)	119.0465	A45	L(11,12,13,14,-1)	179.4735
A22	A(13,14,16)	120.2591	A46	L(8,11,12,3,-2)	179.9924
A23	A(13,14,17)	119.3715	A47	L(11,12,13,14,-2)	180.0015
A24	A(16,14,17)	120.3693			

Table S21. The dihedral angles of the S_0 state of BTEBA in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(4,1,3,7)	0.0006	D33	D(5,8,13,14)	179.9826
D2	D(4,1,3,8)	180.0036	D34	D(5,8,13,15)	-0.019
D3	D(27,1,3,7)	-180.003	D35	D(12,13,14,16)	179.9998
D4	D(27,1,3,8)	-0.0003	D36	D(12,13,14,17)	-0.0002
D5	D(3,1,4,9)	-0.0112	D37	D(15,13,14,16)	0.0004
D6	D(27,1,4,9)	-180.007	D38	D(15,13,14,17)	-180
D7	D(3,1,27,2)	0.0007	D39	D(12,13,15,18)	-179.999
D8	D(3,1,27,28)	180.0016	D40	D(12,13,15,19)	0.0005
D9	D(4,1,27,2)	-180.004	D41	D(14,13,15,18)	0.0002
D10	D(4,1,27,28)	-0.0028	D42	D(14,13,15,19)	-180
D11	D(6,2,5,8)	-180.001	D43	D(13,14,16,20)	-0.0007
D12	D(6,2,5,10)	-0.0001	D44	D(13,14,16,21)	179.9996
D13	D(27,2,5,8)	0	D45	D(17,14,16,20)	179.9993
D14	D(27,2,5,10)	180.0012	D46	D(17,14,16,21)	-0.0004
D15	D(5,2,27,1)	-0.0005	D47	D(13,15,18,20)	-0.0005
D16	D(5,2,27,28)	-180.002	D48	D(13,15,18,22)	179.9996
D17	D(6,2,27,1)	180.0008	D49	D(19,15,18,20)	179.9998
D18	D(6,2,27,28)	-0.0002	D50	D(19,15,18,22)	-0.0001
D19	D(1,3,7,9)	0.0103	D51	D(14,16,20,18)	0.0004
D20	D(8,3,7,9)	180.0072	D52	D(14,16,20,23)	-180
D21	D(1,3,8,5)	-0.0003	D53	D(21,16,20,18)	-180
D22	D(1,3,8,11)	-180	D54	D(21,16,20,23)	0.0002
D23	D(7,3,8,5)	180.0031	D55	D(15,18,20,16)	0.0002
D24	D(7,3,8,11)	0.0029	D56	D(15,18,20,23)	-180
D25	D(1,4,9,7)	0.0156	D57	D(22,18,20,16)	-180
D26	D(2,5,8,3)	0.0004	D58	D(22,18,20,23)	0
D27	D(2,5,8,11)	180.0006	D59	D(16,20,23,24)	-0.0045
D28	D(10,5,8,3)	-180.001	D60	D(16,20,23,25)	179.9924
D29	D(10,5,8,11)	-0.0007	D61	D(18,20,23,24)	179.9956
D30	D(3,7,9,4)	-0.0152	D62	D(18,20,23,25)	-0.0076
D31	D(3,8,13,14)	-0.0199	D63	D(20,23,25,26)	-179.999
D32	D(3,8,13,15)	179.9785	D64	D(24,23,25,26)	-0.0015

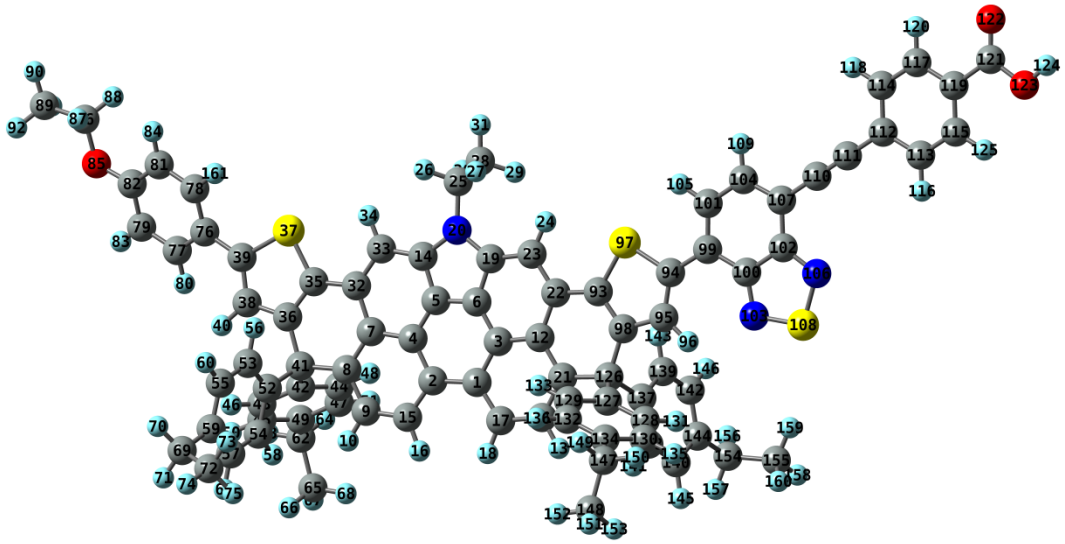


Figure S74. Geometry of the S_0 state of **C280** in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S22. Geometry parameters and Mulliken atomic charges of the S_0 state of **C280** in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	-1.42805	-2.0977	-0.02152	0.07724
2	6	-2.89737	-1.84801	-0.02103	0.074861
3	6	-0.53541	-0.98149	-0.04016	-0.0188
4	6	-3.37135	-0.5004	-0.02947	-0.01364
5	6	-2.43741	0.523249	-0.05085	-0.17176
6	6	-1.07952	0.29288	-0.05531	-0.16281
7	6	-4.73082	-0.10458	-0.01545	0.000351
8	6	-5.70806	-1.12213	0.006341	-0.09266
9	6	-5.259	-2.44746	0.003604	0.006997
10	1	-5.99122	-3.24502	0.012911	0.096128
11	6	0.604272	-3.44088	0.005396	0.007902
12	6	0.878971	-1.0557	-0.03322	0.016424
13	1	1.032139	-4.4352	0.027751	0.096214
14	6	-2.66581	1.894002	-0.04673	0.254553
15	6	-3.90493	-2.81537	-0.00907	-0.09984
16	1	-3.66094	-3.87158	-0.00801	0.098436
17	6	-0.79574	-3.34261	0.005908	-0.10167
18	1	-1.37378	-4.25933	0.029311	0.098313
19	6	-0.41259	1.513319	-0.04963	0.247922
20	7	-1.40325	2.513979	-0.03756	-0.58315
21	6	1.465809	-2.33885	-0.0185	-0.09373
22	6	1.618937	0.200196	-0.02683	0.055511
23	6	0.995992	1.459301	-0.03458	-0.03182
24	1	1.60411	2.35615	-0.02834	0.120426
25	6	-1.15953	3.955	-0.0824	-0.09993
26	1	-1.97168	4.444227	0.459394	0.138344
27	1	-0.24317	4.153188	0.47775	0.138121
28	6	-1.0506	4.509228	-1.50449	-0.28044
29	1	-0.22406	4.042418	-2.04492	0.117938
30	1	-1.97173	4.33473	-2.06501	0.11827
31	1	-0.87059	5.58667	-1.46918	0.120197
32	6	-5.01753	1.324824	-0.02964	0.069989
33	6	-4.01665	2.307461	-0.03972	-0.03419
34	1	-4.29598	3.354384	-0.04422	0.118288
35	6	-6.42879	1.642398	-0.03629	-0.29144
36	6	-7.44823	0.715056	0.002315	0.034289
37	16	-7.06351	3.275592	-0.08976	0.272376
38	6	-8.73684	1.322988	0.008228	0.047866
39	6	-8.72	2.693789	-0.03144	-0.28421

40	1	-9.65798	0.761341	0.069079	0.106552
41	6	-7.219	-0.80166	0.055949	-0.18941
42	6	-7.94391	-1.38984	-1.18455	-0.04915
43	6	-9.30768	-1.70847	-1.16627	-0.08586
44	6	-7.27341	-1.50338	-2.40818	-0.05461
45	6	-9.964	-2.14023	-2.31671	-0.08508
46	1	-9.87276	-1.62629	-0.24642	0.115468
47	6	-7.93232	-1.93325	-3.55727	-0.08819
48	1	-6.22269	-1.24907	-2.47226	0.10858
49	6	-9.29019	-2.26568	-3.53527	-0.09461
50	1	-11.0214	-2.38051	-2.26294	0.097782
51	1	-7.37834	-2.00615	-4.48815	0.097679
52	6	-7.7429	-1.36173	1.407216	-0.04289
53	6	-7.69259	-0.57151	2.561326	-0.04942
54	6	-8.18151	-2.68407	1.550923	-0.08563
55	6	-8.07342	-1.07702	3.802079	-0.0896
56	1	-7.35493	0.455517	2.494242	0.110533
57	6	-8.56377	-3.1863	2.792524	-0.08522
58	1	-8.24252	-3.33463	0.687806	0.11558
59	6	-8.51812	-2.39442	3.944391	-0.09407
60	1	-8.0271	-0.43066	4.673159	0.09686
61	1	-8.90941	-4.21316	2.862428	0.097568
62	6	-9.99409	-2.77443	-4.77349	-0.19934
63	1	-11.048	-2.48154	-4.73742	0.118978
64	1	-9.56387	-2.29438	-5.65802	0.120048
65	6	-9.89916	-4.30217	-4.93218	-0.28236
66	1	-10.3519	-4.81338	-4.07814	0.107929
67	1	-10.4164	-4.63162	-5.83754	0.111654
68	1	-8.85649	-4.6241	-5.00113	0.108502
69	6	-8.9	-2.95454	5.296533	-0.19959
70	1	-9.28617	-2.14813	5.92747	0.118854
71	1	-9.71426	-3.67573	5.174402	0.119889
72	6	-7.72355	-3.63911	6.014799	-0.28251
73	1	-6.90427	-2.93469	6.182697	0.108651
74	1	-8.03703	-4.03251	6.985756	0.111408
75	1	-7.33384	-4.47094	5.421777	0.108371
76	6	-9.85289	3.622232	-0.04112	-0.02207
77	6	-11.1084	3.214416	-0.5347	-0.05612
78	6	-9.74282	4.933709	0.439765	-0.10445
79	6	-12.1931	4.073028	-0.53431	-0.11558
80	1	-11.2279	2.216911	-0.94035	0.109996
81	6	-10.8253	5.810485	0.437582	-0.14974
82	6	-12.0651	5.383034	-0.04852	0.187298

83	1	-13.1545	3.755052	-0.91956	0.111247
84	1	-10.6915	6.811708	0.823179	0.126497
85	8	-13.1876	6.14815	-0.09481	-0.36578
86	6	-13.1286	7.504419	0.377232	-0.05265
87	1	-12.8277	7.511937	1.430551	0.123678
88	1	-12.3806	8.059865	-0.19912	0.123598
89	6	-14.5079	8.107569	0.201771	-0.29685
90	1	-14.5065	9.143107	0.550125	0.118248
91	1	-14.8032	8.096982	-0.84968	0.117499
92	1	-15.2495	7.550137	0.778085	0.117471
93	6	3.053692	0.038797	-0.00616	-0.2787
94	6	5.565115	0.275644	0.004018	-0.30893
95	6	5.122788	-1.02955	-0.01788	0.082831
96	1	5.813192	-1.85699	-0.03337	0.123073
97	16	4.183616	1.373665	0.021284	0.294118
98	6	3.712389	-1.17617	-0.02106	0.014004
99	6	6.919869	0.793036	0.017154	0.107106
100	6	8.08182	-0.06228	-0.06078	0.144815
101	6	7.191708	2.153489	0.103306	-0.13084
102	6	9.421491	0.497574	-0.04625	0.166798
103	7	8.083637	-1.39354	-0.15454	-0.51622
104	6	8.491524	2.698038	0.117098	-0.01364
105	1	6.366457	2.852461	0.167557	0.123643
106	7	10.38431	-0.42045	-0.1274	-0.49054
107	6	9.633036	1.914951	0.045757	-0.23976
108	16	9.646437	-1.88018	-0.21613	0.578175
109	1	8.598985	3.773302	0.18785	0.112219
110	6	10.93497	2.460702	0.060375	0.140968
111	6	12.05355	2.928182	0.07255	0.030778
112	6	13.36654	3.466197	0.087024	-0.17923
113	6	14.48695	2.613348	0.031752	-0.03444
114	6	13.57218	4.859065	0.157403	-0.03717
115	6	15.7702	3.137485	0.047557	-0.02831
116	1	14.33614	1.542551	-0.02259	0.117063
117	6	14.85687	5.375616	0.172006	-0.03491
118	1	12.71679	5.521554	0.199935	0.116245
119	6	15.96646	4.522876	0.117862	-0.20272
120	1	15.01953	6.444566	0.225583	0.116125
121	6	17.32182	5.130692	0.137548	0.430997
122	8	17.54242	6.321252	0.192137	-0.36823
123	8	18.31207	4.214513	0.088484	-0.34025
124	1	19.15206	4.697749	0.105973	0.277585
125	1	16.62439	2.475105	0.005492	0.120192

126	6	2.998321	-2.53508	-0.04718	-0.18161
127	6	3.477459	-3.29558	1.218322	-0.05093
128	6	4.660321	-4.04519	1.229922	-0.08188
129	6	2.797333	-3.14745	2.432886	-0.0536
130	6	5.13074	-4.63368	2.401595	-0.08635
131	1	5.227609	-4.17992	0.317727	0.115486
132	6	3.270947	-3.73534	3.603129	-0.08854
133	1	1.887469	-2.5614	2.472985	0.108645
134	6	4.445182	-4.49412	3.612112	-0.09392
135	1	6.051229	-5.2085	2.370709	0.098032
136	1	2.717216	-3.59527	4.526431	0.097621
137	6	3.325213	-3.27065	-1.37556	-0.04316
138	6	3.292905	-4.66682	-1.48386	-0.08453
139	6	3.556528	-2.53954	-2.54649	-0.04961
140	6	3.496459	-5.30017	-2.70727	-0.08513
141	1	3.113325	-5.277	-0.60794	0.115528
142	6	3.759311	-3.17567	-3.76892	-0.08923
143	1	3.573849	-1.45717	-2.50998	0.110425
144	6	3.736806	-4.56909	-3.87512	-0.09378
145	1	3.464508	-6.3845	-2.75175	0.097746
146	1	3.933386	-2.57418	-4.65577	0.097128
147	6	4.93528	-5.16679	4.875025	-0.19937
148	6	4.362076	-6.5826	5.062097	-0.28229
149	1	4.665466	-4.55307	5.740166	0.119736
150	1	6.02819	-5.22143	4.856286	0.119464
151	1	4.737367	-7.03454	5.984416	0.11164
152	1	3.270249	-6.55887	5.11618	0.108381
153	1	4.6424	-7.23194	4.22816	0.108014
154	6	3.996602	-5.26166	-5.1943	-0.19929
155	6	5.482472	-5.59661	-5.41391	-0.2824
156	1	3.64708	-4.62462	-6.01267	0.119193
157	1	3.410008	-6.1845	-5.24101	0.119866
158	1	5.630154	-6.09575	-6.37559	0.111568
159	1	6.093491	-4.68985	-5.40516	0.108481
160	1	5.854771	-6.25911	-4.62769	0.108058
161	1	-8.79862	5.281374	0.843738	0.115208

Table S23. The bond lengths of the S_0 state of **C280** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4904	R90	R(77,79)	1.3834
R2	R(1,3)	1.4294	R91	R(77,80)	1.0834
R3	R(1,17)	1.3966	R92	R(78,81)	1.393
R4	R(2,4)	1.4286	R93	R(78,161)	1.0842
R5	R(2,15)	1.3968	R94	R(79,82)	1.403
R6	R(3,6)	1.3857	R95	R(79,83)	1.0835
R7	R(3,12)	1.4163	R96	R(81,82)	1.3986
R8	R(4,5)	1.3858	R97	R(81,84)	1.0812
R9	R(4,7)	1.416	R98	R(82,85)	1.3593
R10	R(5,6)	1.3773	R99	R(85,86)	1.4373
R11	R(5,14)	1.3897	R100	R(86,87)	1.0955
R12	R(6,19)	1.3908	R101	R(86,88)	1.0955
R13	R(7,8)	1.411	R102	R(86,89)	1.5156
R14	R(7,32)	1.4579	R103	R(89,90)	1.0926
R15	R(8,9)	1.3993	R104	R(89,91)	1.0922
R16	R(8,41)	1.5453	R105	R(89,92)	1.0922
R17	R(9,10)	1.0827	R106	R(93,97)	1.7491
R18	R(9,15)	1.4032	R107	R(93,98)	1.3821
R19	R(11,13)	1.0827	R108	R(94,95)	1.3783
R20	R(11,17)	1.4035	R109	R(94,97)	1.7648
R21	R(11,21)	1.399	R110	R(94,99)	1.4503
R22	R(12,21)	1.4111	R111	R(95,96)	1.0778
R23	R(12,22)	1.4577	R112	R(95,98)	1.418
R24	R(14,20)	1.4066	R113	R(98,126)	1.5353
R25	R(14,33)	1.4127	R114	R(99,100)	1.4449
R26	R(15,16)	1.084	R115	R(99,101)	1.39
R27	R(17,18)	1.084	R116	R(100,102)	1.452
R28	R(19,20)	1.4081	R117	R(100,103)	1.3346
R29	R(19,23)	1.4097	R118	R(101,104)	1.4093
R30	R(20,25)	1.4622	R119	R(101,105)	1.0834
R31	R(21,126)	1.5453	R120	R(102,106)	1.3328
R32	R(22,23)	1.4048	R121	R(102,107)	1.436
R33	R(22,93)	1.444	R122	R(103,108)	1.638
R34	R(23,24)	1.0836	R123	R(104,107)	1.3861
R35	R(25,26)	1.092	R124	R(104,109)	1.0829
R36	R(25,27)	1.0921	R125	R(106,108)	1.638
R37	R(25,28)	1.5302	R126	R(107,110)	1.4118
R38	R(28,29)	1.0923	R127	R(110,111)	1.2124
R39	R(28,30)	1.0923	R128	R(111,112)	1.419
R40	R(28,31)	1.0929	R129	R(112,113)	1.4092

R41	R(32,33)	1.4027	R130	R(112,114)	1.4097
R42	R(32,35)	1.4466	R131	R(113,115)	1.3862
R43	R(33,34)	1.0836	R132	R(113,116)	1.0827
R44	R(35,36)	1.3787	R133	R(114,117)	1.3847
R45	R(35,37)	1.753	R134	R(114,118)	1.0828
R46	R(36,38)	1.4248	R135	R(115,119)	1.401
R47	R(36,41)	1.5349	R136	R(115,125)	1.0817
R48	R(37,39)	1.7567	R137	R(117,119)	1.4005
R49	R(38,39)	1.3715	R138	R(117,120)	1.0826
R50	R(38,40)	1.0806	R139	R(119,121)	1.4855
R51	R(39,76)	1.4648	R140	R(121,122)	1.2121
R52	R(41,42)	1.5525	R141	R(121,123)	1.35
R53	R(41,52)	1.5537	R142	R(123,124)	0.9692
R54	R(42,43)	1.4006	R143	R(126,127)	1.5522
R55	R(42,44)	1.3999	R144	R(126,137)	1.5532
R56	R(43,45)	1.3931	R145	R(127,128)	1.4004
R57	R(43,46)	1.0827	R146	R(127,129)	1.3999
R58	R(44,47)	1.3926	R147	R(128,130)	1.393
R59	R(44,48)	1.0829	R148	R(128,131)	1.0826
R60	R(45,49)	1.3981	R149	R(129,132)	1.3926
R61	R(45,50)	1.0857	R150	R(129,133)	1.083
R62	R(47,49)	1.3981	R151	R(130,134)	1.3981
R63	R(47,51)	1.0857	R152	R(130,135)	1.0857
R64	R(49,62)	1.5124	R153	R(132,134)	1.3981
R65	R(52,53)	1.3996	R154	R(132,136)	1.0857
R66	R(52,54)	1.4006	R155	R(134,147)	1.5125
R67	R(53,55)	1.3929	R156	R(137,138)	1.4007
R68	R(53,56)	1.0832	R157	R(137,139)	1.3997
R69	R(54,57)	1.3928	R158	R(138,140)	1.3926
R70	R(54,58)	1.0826	R159	R(138,141)	1.0825
R71	R(55,59)	1.3977	R160	R(139,142)	1.3929
R72	R(55,60)	1.0857	R161	R(139,143)	1.0831
R73	R(57,59)	1.3986	R162	R(140,144)	1.3986
R74	R(57,61)	1.0857	R163	R(140,145)	1.0857
R75	R(59,69)	1.5126	R164	R(142,144)	1.3976
R76	R(62,63)	1.0944	R165	R(142,146)	1.0856
R77	R(62,64)	1.0945	R166	R(144,154)	1.5124
R78	R(62,65)	1.5389	R167	R(147,148)	1.5389
R79	R(65,66)	1.0935	R168	R(147,149)	1.0945
R80	R(65,67)	1.0935	R169	R(147,150)	1.0944
R81	R(65,68)	1.0934	R170	R(148,151)	1.0935
R82	R(69,70)	1.0943	R171	R(148,152)	1.0934
R83	R(69,71)	1.0946	R172	R(148,153)	1.0935

R84	R(69,72)	1.539	R173	R(154,155)	1.5389
R85	R(72,73)	1.0934	R174	R(154,156)	1.0944
R86	R(72,74)	1.0935	R175	R(154,157)	1.0945
R87	R(72,75)	1.0934	R176	R(155,158)	1.0935
R88	R(76,77)	1.4093	R177	R(155,159)	1.0934
R89	R(76,78)	1.4012	R178	R(155,160)	1.0935

Table S24. The bond angles of the S_0 state of **C280** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	119.0027	A157	A(77,76,78)	117.4528
A2	A(2,1,17)	126.5623	A158	A(76,77,79)	121.2511
A3	A(3,1,17)	114.4328	A159	A(76,77,80)	119.7238
A4	A(1,2,4)	119.0212	A160	A(79,77,80)	119.0152
A5	A(1,2,15)	126.5206	A161	A(76,78,81)	121.8391
A6	A(4,2,15)	114.4579	A162	A(76,78,161)	119.7621
A7	A(1,3,6)	118.2345	A163	A(81,78,161)	118.3894
A8	A(1,3,12)	125.6376	A164	A(77,79,82)	120.5362
A9	A(6,3,12)	116.1256	A165	A(77,79,83)	120.8988
A10	A(2,4,5)	118.2481	A166	A(82,79,83)	118.5604
A11	A(2,4,7)	125.6039	A167	A(78,81,82)	119.8022
A12	A(5,4,7)	116.148	A168	A(78,81,84)	119.0882
A13	A(4,5,6)	122.7463	A169	A(82,81,84)	121.1069
A14	A(4,5,14)	128.1551	A170	A(79,82,81)	119.1157
A15	A(6,5,14)	109.0889	A171	A(79,82,85)	116.0035
A16	A(3,6,5)	122.7446	A172	A(81,82,85)	124.8807
A17	A(3,6,19)	128.2176	A173	A(82,85,86)	119.0829
A18	A(5,6,19)	109.0255	A174	A(85,86,87)	109.4834
A19	A(4,7,8)	117.6142	A175	A(85,86,88)	109.4917
A20	A(4,7,32)	117.5661	A176	A(85,86,89)	107.4677
A21	A(8,7,32)	124.8193	A177	A(87,86,88)	108.3485
A22	A(7,8,9)	117.4343	A178	A(87,86,89)	111.0132
A23	A(7,8,41)	121.8786	A179	A(88,86,89)	111.0194
A24	A(9,8,41)	120.679	A180	A(86,89,90)	109.8247
A25	A(8,9,10)	118.7257	A181	A(86,89,91)	110.7103
A26	A(8,9,15)	123.9177	A182	A(86,89,92)	110.7161
A27	A(10,9,15)	117.3565	A183	A(90,89,91)	108.4501
A28	A(13,11,17)	117.291	A184	A(90,89,92)	108.4427
A29	A(13,11,21)	118.7117	A185	A(91,89,92)	108.631
A30	A(17,11,21)	123.9971	A186	A(22,93,97)	123.8353
A31	A(3,12,21)	117.5813	A187	A(22,93,98)	124.8656
A32	A(3,12,22)	117.5037	A188	A(97,93,98)	111.2951
A33	A(21,12,22)	124.9113	A189	A(95,94,97)	109.7623
A34	A(5,14,20)	106.6942	A190	A(95,94,99)	129.6264
A35	A(5,14,33)	116.4783	A191	A(97,94,99)	120.611
A36	A(20,14,33)	136.8239	A192	A(94,95,96)	121.4447
A37	A(2,15,9)	120.9684	A193	A(94,95,98)	114.6552
A38	A(2,15,16)	120.8254	A194	A(96,95,98)	123.8999
A39	A(9,15,16)	118.2062	A195	A(93,97,94)	91.7599
A40	A(1,17,11)	120.9345	A196	A(93,98,95)	112.5265

A41	A(1,17,18)	120.8537	A197	A(93,98,126)	123.8198
A42	A(11,17,18)	118.2118	A198	A(95,98,126)	123.6526
A43	A(6,19,20)	106.6336	A199	A(94,99,100)	122.6524
A44	A(6,19,23)	116.46	A200	A(94,99,101)	122.1692
A45	A(20,19,23)	136.8952	A201	A(100,99,101)	115.1783
A46	A(14,20,19)	108.5547	A202	A(99,100,102)	120.8751
A47	A(14,20,25)	125.7185	A203	A(99,100,103)	126.5391
A48	A(19,20,25)	125.6486	A204	A(102,100,103)	112.5855
A49	A(11,21,12)	117.4116	A205	A(99,101,104)	123.9963
A50	A(11,21,126)	120.7309	A206	A(99,101,105)	119.0884
A51	A(12,21,126)	121.8521	A207	A(104,101,105)	116.915
A52	A(12,22,23)	123.1671	A208	A(100,102,106)	113.5981
A53	A(12,22,93)	114.0891	A209	A(100,102,107)	121.139
A54	A(23,22,93)	122.7434	A210	A(106,102,107)	125.2628
A55	A(19,23,22)	118.5218	A211	A(100,103,108)	107.476
A56	A(19,23,24)	121.945	A212	A(101,104,107)	122.7336
A57	A(22,23,24)	119.5332	A213	A(101,104,109)	118.4119
A58	A(20,25,26)	107.5987	A214	A(107,104,109)	118.8544
A59	A(20,25,27)	107.6362	A215	A(102,106,108)	106.9599
A60	A(20,25,28)	113.4111	A216	A(102,107,104)	116.0776
A61	A(26,25,27)	106.754	A217	A(102,107,110)	121.2027
A62	A(26,25,28)	110.5963	A218	A(104,107,110)	122.7196
A63	A(27,25,28)	110.5611	A219	A(103,108,106)	99.3805
A64	A(25,28,29)	111.0322	A220	A(111,112,113)	120.3857
A65	A(25,28,30)	111.0399	A221	A(111,112,114)	120.6702
A66	A(25,28,31)	109.8013	A222	A(113,112,114)	118.9441
A67	A(29,28,30)	108.4184	A223	A(112,113,115)	120.4467
A68	A(29,28,31)	108.2194	A224	A(112,113,116)	119.3251
A69	A(30,28,31)	108.2378	A225	A(115,113,116)	120.2282
A70	A(7,32,33)	123.1331	A226	A(112,114,117)	120.2939
A71	A(7,32,35)	114.0253	A227	A(112,114,118)	119.4228
A72	A(33,32,35)	122.8414	A228	A(117,114,118)	120.2833
A73	A(14,33,32)	118.51	A229	A(113,115,119)	120.2745
A74	A(14,33,34)	121.9551	A230	A(113,115,125)	119.9344
A75	A(32,33,34)	119.5348	A231	A(119,115,125)	119.7911
A76	A(32,35,36)	125.0015	A232	A(114,117,119)	120.4988
A77	A(32,35,37)	123.9113	A233	A(114,117,120)	120.548
A78	A(36,35,37)	111.0869	A234	A(119,117,120)	118.9532
A79	A(35,36,38)	112.4495	A235	A(115,119,117)	119.542
A80	A(35,36,41)	123.7258	A236	A(115,119,121)	122.2139
A81	A(38,36,41)	123.8177	A237	A(117,119,121)	118.2441
A82	A(35,37,39)	91.8254	A238	A(119,121,122)	124.6494
A83	A(36,38,39)	114.5343	A239	A(119,121,123)	113.0225

A84	A(36,38,40)	123.3272	A240	A(122,121,123)	122.3281
A85	A(39,38,40)	122.1137	A241	A(121,123,124)	107.2596
A86	A(37,39,38)	110.0947	A242	A(21,126,98)	110.3978
A87	A(37,39,76)	121.2769	A243	A(21,126,127)	110.6839
A88	A(38,39,76)	128.6258	A244	A(21,126,137)	106.5425
A89	A(8,41,36)	110.4766	A245	A(98,126,127)	106.0342
A90	A(8,41,42)	110.629	A246	A(98,126,137)	109.6227
A91	A(8,41,52)	106.4304	A247	A(127,126,137)	113.5951
A92	A(36,41,42)	106.0642	A248	A(126,127,128)	121.9868
A93	A(36,41,52)	109.6475	A249	A(126,127,129)	120.3671
A94	A(42,41,52)	113.6345	A250	A(128,127,129)	117.3752
A95	A(41,42,43)	122.0326	A251	A(127,128,130)	121.2209
A96	A(41,42,44)	120.3647	A252	A(127,128,131)	120.1471
A97	A(43,42,44)	117.3432	A253	A(130,128,131)	118.6318
A98	A(42,43,45)	121.2292	A254	A(127,129,132)	121.277
A99	A(42,43,46)	120.1333	A255	A(127,129,133)	119.8381
A100	A(45,43,46)	118.6369	A256	A(132,129,133)	118.884
A101	A(42,44,47)	121.3085	A257	A(128,130,134)	121.3646
A102	A(42,44,48)	119.8269	A258	A(128,130,135)	119.0829
A103	A(47,44,48)	118.8639	A259	A(134,130,135)	119.552
A104	A(43,45,49)	121.3676	A260	A(129,132,134)	121.3419
A105	A(43,45,50)	119.1141	A261	A(129,132,136)	119.1246
A106	A(49,45,50)	119.5181	A262	A(134,132,136)	119.5328
A107	A(44,47,49)	121.3278	A263	A(130,134,132)	117.4152
A108	A(44,47,51)	119.1285	A264	A(130,134,147)	121.3092
A109	A(49,47,51)	119.543	A265	A(132,134,147)	121.2577
A110	A(45,49,47)	117.4161	A266	A(126,137,138)	122.2289
A111	A(45,49,62)	121.2946	A267	A(126,137,139)	120.1908
A112	A(47,49,62)	121.2718	A268	A(138,137,139)	117.3719
A113	A(41,52,53)	120.0991	A269	A(137,138,140)	121.1895
A114	A(41,52,54)	122.355	A270	A(137,138,141)	120.2051
A115	A(53,52,54)	117.3681	A271	A(140,138,141)	118.6044
A116	A(52,53,55)	121.3193	A272	A(137,139,142)	121.3123
A117	A(52,53,56)	119.6999	A273	A(137,139,143)	119.7635
A118	A(55,53,56)	118.9804	A274	A(142,139,143)	118.9232
A119	A(52,54,57)	121.1888	A275	A(138,140,144)	121.3964
A120	A(52,54,58)	120.2133	A276	A(138,140,145)	119.0717
A121	A(57,54,58)	118.5925	A277	A(144,140,145)	119.5317
A122	A(53,55,59)	121.3168	A278	A(139,142,144)	121.3098
A123	A(53,55,60)	119.1431	A279	A(139,142,146)	119.1593
A124	A(59,55,60)	119.5394	A280	A(144,142,146)	119.5303
A125	A(54,57,59)	121.4038	A281	A(140,144,142)	117.4166
A126	A(54,57,61)	119.0652	A282	A(140,144,154)	121.2302

A127	A(59,57,61)	119.5301	A283	A(142,144,154)	121.3358
A128	A(55,59,57)	117.4008	A284	A(134,147,148)	112.9536
A129	A(55,59,69)	121.3583	A285	A(134,147,149)	109.3146
A130	A(57,59,69)	121.221	A286	A(134,147,150)	109.3592
A131	A(49,62,63)	109.3398	A287	A(148,147,149)	109.1463
A132	A(49,62,64)	109.3387	A288	A(148,147,150)	109.1545
A133	A(49,62,65)	112.9325	A289	A(149,147,150)	106.7206
A134	A(63,62,64)	106.7246	A290	A(147,148,151)	110.79
A135	A(63,62,65)	109.1766	A291	A(147,148,152)	110.9768
A136	A(64,62,65)	109.1379	A292	A(147,148,153)	110.9867
A137	A(62,65,66)	110.9806	A293	A(151,148,152)	108.0561
A138	A(62,65,67)	110.8113	A294	A(151,148,153)	108.0499
A139	A(62,65,68)	110.9539	A295	A(152,148,153)	107.8543
A140	A(66,65,67)	108.0582	A296	A(144,154,155)	112.9545
A141	A(66,65,68)	107.8427	A297	A(144,154,156)	109.3191
A142	A(67,65,68)	108.0674	A298	A(144,154,157)	109.3457
A143	A(59,69,70)	109.3668	A299	A(155,154,156)	109.1685
A144	A(59,69,71)	109.3942	A300	A(155,154,157)	109.1397
A145	A(59,69,72)	112.8883	A301	A(156,154,157)	106.7214
A146	A(70,69,71)	106.6996	A302	A(154,155,158)	110.8087
A147	A(70,69,72)	109.1751	A303	A(154,155,159)	110.9718
A148	A(71,69,72)	109.1269	A304	A(154,155,160)	110.9778
A149	A(69,72,73)	110.969	A305	A(158,155,159)	108.065
A150	A(69,72,74)	110.8112	A306	A(158,155,160)	108.0466
A151	A(69,72,75)	110.9611	A307	A(159,155,160)	107.8435
A152	A(73,72,74)	108.072	A308	L(107,110,111,102,-1)	179.9374
A153	A(73,72,75)	107.8383	A309	L(110,111,112,113,-1)	179.6019
A154	A(74,72,75)	108.0627	A310	L(107,110,111,102,-2)	179.9724
A155	A(39,76,77)	120.5243	A311	L(110,111,112,113,-2)	180.059
A156	A(39,76,78)	122.0218			

Table S25. The dihedral angles of the S_0 state of **C280** in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	-0.4466	D238	D(49,62,65,66)	60.0736
D2	D(3,1,2,15)	179.7525	D239	D(49,62,65,67)	-179.866
D3	D(17,1,2,4)	178.9828	D240	D(49,62,65,68)	-59.8106
D4	D(17,1,2,15)	-0.8181	D241	D(63,62,65,66)	-61.7872
D5	D(2,1,3,6)	0.0829	D242	D(63,62,65,67)	58.2738
D6	D(2,1,3,12)	179.512	D243	D(63,62,65,68)	178.3287
D7	D(17,1,3,6)	-179.414	D244	D(64,62,65,66)	-178.095
D8	D(17,1,3,12)	0.0154	D245	D(64,62,65,67)	-58.0338
D9	D(2,1,17,11)	-179.841	D246	D(64,62,65,68)	62.0211
D10	D(2,1,17,18)	0.0888	D247	D(59,69,72,73)	60.0366
D11	D(3,1,17,11)	-0.3891	D248	D(59,69,72,74)	-179.893
D12	D(3,1,17,18)	179.5407	D249	D(59,69,72,75)	-59.8391
D13	D(1,2,4,5)	0.6122	D250	D(70,69,72,73)	-61.8278
D14	D(1,2,4,7)	-179.269	D251	D(70,69,72,74)	58.2428
D15	D(15,2,4,5)	-179.564	D252	D(70,69,72,75)	178.2965
D16	D(15,2,4,7)	0.5554	D253	D(71,69,72,73)	-178.098
D17	D(1,2,15,9)	179.3508	D254	D(71,69,72,74)	-58.0278
D18	D(1,2,15,16)	-0.5676	D255	D(71,69,72,75)	62.0259
D19	D(4,2,15,9)	-0.4579	D256	D(39,76,77,79)	179.1199
D20	D(4,2,15,16)	179.6237	D257	D(39,76,77,80)	-2.0332
D21	D(1,3,6,5)	0.1123	D258	D(78,76,77,79)	-0.5058
D22	D(1,3,6,19)	178.6966	D259	D(78,76,77,80)	178.3412
D23	D(12,3,6,5)	-179.371	D260	D(39,76,78,81)	-179.532
D24	D(12,3,6,19)	-0.7867	D261	D(39,76,78,161)	-0.6614
D25	D(1,3,12,21)	0.5927	D262	D(77,76,78,81)	0.088
D26	D(1,3,12,22)	-178.742	D263	D(77,76,78,161)	178.9582
D27	D(6,3,12,21)	-179.968	D264	D(76,77,79,82)	0.502
D28	D(6,3,12,22)	0.6979	D265	D(76,77,79,83)	179.7034
D29	D(2,4,5,6)	-0.438	D266	D(80,77,79,82)	-178.353
D30	D(2,4,5,14)	-179.18	D267	D(80,77,79,83)	0.8485
D31	D(7,4,5,6)	179.4543	D268	D(76,78,81,82)	0.3331
D32	D(7,4,5,14)	0.7119	D269	D(76,78,81,84)	179.7478
D33	D(2,4,7,8)	-0.1211	D270	D(161,78,81,82)	-178.552
D34	D(2,4,7,32)	-179.897	D271	D(161,78,81,84)	0.8627
D35	D(5,4,7,8)	179.9957	D272	D(77,79,82,81)	-0.0673
D36	D(5,4,7,32)	0.2196	D273	D(77,79,82,85)	179.82
D37	D(4,5,6,3)	0.0666	D274	D(83,79,82,81)	-179.287
D38	D(4,5,6,19)	-178.757	D275	D(83,79,82,85)	0.6003
D39	D(14,5,6,3)	179.0202	D276	D(78,81,82,79)	-0.343
D40	D(14,5,6,19)	0.1968	D277	D(78,81,82,85)	179.7804

D41	D(4,5,14,20)	178.4037	D278	D(84,81,82,79)	-179.746
D42	D(4,5,14,33)	-1.024	D279	D(84,81,82,85)	0.3777
D43	D(6,5,14,20)	-0.4771	D280	D(79,82,85,86)	-179.556
D44	D(6,5,14,33)	-179.905	D281	D(81,82,85,86)	0.3239
D45	D(3,6,19,20)	-178.576	D282	D(82,85,86,87)	-59.5228
D46	D(3,6,19,23)	0.4157	D283	D(82,85,86,88)	59.1263
D47	D(5,6,19,20)	0.1649	D284	D(82,85,86,89)	179.8079
D48	D(5,6,19,23)	179.1562	D285	D(85,86,89,90)	-179.996
D49	D(4,7,8,9)	-0.408	D286	D(85,86,89,91)	-60.2628
D50	D(4,7,8,41)	178.5614	D287	D(85,86,89,92)	60.277
D51	D(32,7,8,9)	179.3502	D288	D(87,86,89,90)	60.3053
D52	D(32,7,8,41)	-1.6804	D289	D(87,86,89,91)	-179.962
D53	D(4,7,32,33)	-0.8039	D290	D(87,86,89,92)	-59.4221
D54	D(4,7,32,35)	179.0291	D291	D(88,86,89,90)	-60.2828
D55	D(8,7,32,33)	179.4378	D292	D(88,86,89,91)	59.45
D56	D(8,7,32,35)	-0.7292	D293	D(88,86,89,92)	179.9898
D57	D(7,8,9,10)	-179.568	D294	D(22,93,97,94)	-179.027
D58	D(7,8,9,15)	0.5068	D295	D(98,93,97,94)	0.276
D59	D(41,8,9,10)	1.4495	D296	D(22,93,98,95)	178.9655
D60	D(41,8,9,15)	-178.476	D297	D(22,93,98,126)	-0.6705
D61	D(7,8,41,36)	2.9287	D298	D(97,93,98,95)	-0.3288
D62	D(7,8,41,42)	120.0702	D299	D(97,93,98,126)	-179.965
D63	D(7,8,41,52)	-116.039	D300	D(97,94,95,96)	179.86
D64	D(9,8,41,36)	-178.135	D301	D(97,94,95,98)	-0.0076
D65	D(9,8,41,42)	-60.9933	D302	D(99,94,95,96)	-0.3288
D66	D(9,8,41,52)	62.8979	D303	D(99,94,95,98)	179.8035
D67	D(8,9,15,2)	-0.0486	D304	D(95,94,97,93)	-0.1509
D68	D(8,9,15,16)	179.8718	D305	D(99,94,97,93)	-179.982
D69	D(10,9,15,2)	-179.975	D306	D(95,94,99,100)	3.2546
D70	D(10,9,15,16)	-0.0543	D307	D(95,94,99,101)	-176.88
D71	D(13,11,17,1)	179.9821	D308	D(97,94,99,100)	-176.952
D72	D(13,11,17,18)	0.0506	D309	D(97,94,99,101)	2.9134
D73	D(21,11,17,1)	0.1578	D310	D(94,95,98,93)	0.2205
D74	D(21,11,17,18)	-179.774	D311	D(94,95,98,126)	179.8572
D75	D(13,11,21,12)	-179.353	D312	D(96,95,98,93)	-179.644
D76	D(13,11,21,126)	1.4681	D313	D(96,95,98,126)	-0.0067
D77	D(17,11,21,12)	0.4692	D314	D(93,98,126,21)	-1.4066
D78	D(17,11,21,126)	-178.71	D315	D(93,98,126,127)	-121.338
D79	D(3,12,21,11)	-0.7967	D316	D(93,98,126,137)	115.6636
D80	D(3,12,21,126)	178.3725	D317	D(95,98,126,21)	178.9973
D81	D(22,12,21,11)	178.4835	D318	D(95,98,126,127)	59.0659
D82	D(22,12,21,126)	-2.3472	D319	D(95,98,126,137)	-63.9325
D83	D(3,12,22,23)	-0.357	D320	D(94,99,100,102)	179.919

D84	D(3,12,22,93)	179.3995	D321	D(94,99,100,103)	0.1233
D85	D(21,12,22,23)	-179.638	D322	D(101,99,100,102)	0.0451
D86	D(21,12,22,93)	0.1187	D323	D(101,99,100,103)	-179.751
D87	D(5,14,20,19)	0.5781	D324	D(94,99,101,104)	-179.902
D88	D(5,14,20,25)	177.5018	D325	D(94,99,101,105)	0.293
D89	D(33,14,20,19)	179.8294	D326	D(100,99,101,104)	-0.027
D90	D(33,14,20,25)	-3.2469	D327	D(100,99,101,105)	-179.832
D91	D(5,14,33,32)	0.3618	D328	D(99,100,102,106)	-179.886
D92	D(5,14,33,34)	-179.494	D329	D(99,100,102,107)	-0.0015
D93	D(20,14,33,32)	-178.837	D330	D(103,100,102,106)	-0.0637
D94	D(20,14,33,34)	1.3068	D331	D(103,100,102,107)	179.8207
D95	D(6,19,20,14)	-0.4609	D332	D(99,100,103,108)	179.872
D96	D(6,19,20,25)	-177.387	D333	D(102,100,103,108)	0.062
D97	D(23,19,20,14)	-179.139	D334	D(99,101,104,107)	-0.0391
D98	D(23,19,20,25)	3.9344	D335	D(99,101,104,109)	-179.952
D99	D(6,19,23,22)	0.0149	D336	D(105,101,104,107)	179.7701
D100	D(6,19,23,24)	-179.95	D337	D(105,101,104,109)	-0.1431
D101	D(20,19,23,22)	178.6004	D338	D(100,102,106,108)	0.0312
D102	D(20,19,23,24)	-1.3644	D339	D(107,102,106,108)	-179.848
D103	D(14,20,25,26)	33.7623	D340	D(100,102,107,104)	-0.0612
D104	D(14,20,25,27)	148.4815	D341	D(100,102,107,110)	179.982
D105	D(14,20,25,28)	-88.887	D342	D(106,102,107,104)	179.8091
D106	D(19,20,25,26)	-149.827	D343	D(106,102,107,110)	-0.1476
D107	D(19,20,25,27)	-35.1081	D344	D(100,103,108,106)	-0.0401
D108	D(19,20,25,28)	87.5234	D345	D(101,104,107,102)	0.0817
D109	D(11,21,126,98)	-178.058	D346	D(101,104,107,110)	-179.962
D110	D(11,21,126,127)	-60.9681	D347	D(109,104,107,102)	179.9946
D111	D(11,21,126,137)	62.9815	D348	D(109,104,107,110)	-0.0494
D112	D(12,21,126,98)	2.8002	D349	D(102,106,108,103)	0.0043
D113	D(12,21,126,127)	119.8899	D350	D(102,107,112,113)	-0.9969
D114	D(12,21,126,137)	-116.161	D351	D(102,107,112,114)	179.051
D115	D(12,22,23,19)	-0.0169	D352	D(104,107,112,113)	179.0445
D116	D(12,22,23,24)	179.9488	D353	D(104,107,112,114)	-0.9076
D117	D(93,22,23,19)	-179.753	D354	D(111,112,113,115)	-179.917
D118	D(93,22,23,24)	0.2131	D355	D(111,112,113,116)	0.0404
D119	D(12,22,93,97)	-179.376	D356	D(114,112,113,115)	0.0528
D120	D(12,22,93,98)	1.4155	D357	D(114,112,113,116)	-179.99
D121	D(23,22,93,97)	0.3815	D358	D(111,112,114,117)	179.9544
D122	D(23,22,93,98)	-178.827	D359	D(111,112,114,118)	-0.0464
D123	D(20,25,28,29)	-60.4464	D360	D(113,112,114,117)	-0.0149
D124	D(20,25,28,30)	60.2569	D361	D(113,112,114,118)	179.9844
D125	D(20,25,28,31)	179.9192	D362	D(112,113,115,119)	-0.0428
D126	D(26,25,28,29)	178.5777	D363	D(112,113,115,125)	179.9563

D127	D(26,25,28,30)	-60.719	D364	D(116,113,115,119)	-179.999
D128	D(26,25,28,31)	58.9432	D365	D(116,113,115,125)	-0.0001
D129	D(27,25,28,29)	60.5524	D366	D(112,114,117,119)	-0.0332
D130	D(27,25,28,30)	-178.744	D367	D(112,114,117,120)	179.9761
D131	D(27,25,28,31)	-59.0821	D368	D(118,114,117,119)	179.9676
D132	D(7,32,33,14)	0.4975	D369	D(118,114,117,120)	-0.0231
D133	D(7,32,33,34)	-179.643	D370	D(113,115,119,117)	-0.0055
D134	D(35,32,33,14)	-179.321	D371	D(113,115,119,121)	179.9921
D135	D(35,32,33,34)	0.5388	D372	D(125,115,119,117)	179.9954
D136	D(7,32,35,36)	1.6498	D373	D(125,115,119,121)	-0.007
D137	D(7,32,35,37)	-178.564	D374	D(114,117,119,115)	0.0436
D138	D(33,32,35,36)	-178.517	D375	D(114,117,119,121)	-179.954
D139	D(33,32,35,37)	1.2695	D376	D(120,117,119,115)	-179.966
D140	D(32,35,36,38)	178.9603	D377	D(120,117,119,121)	0.0368
D141	D(32,35,36,41)	-0.1084	D378	D(115,119,121,122)	179.6917
D142	D(37,35,36,38)	-0.8495	D379	D(115,119,121,123)	-0.3352
D143	D(37,35,36,41)	-179.918	D380	D(117,119,121,122)	-0.3106
D144	D(32,35,37,39)	-178.898	D381	D(117,119,121,123)	179.6625
D145	D(36,35,37,39)	0.914	D382	D(119,121,123,124)	-179.98
D146	D(35,36,38,39)	0.293	D383	D(122,121,123,124)	-0.0064
D147	D(35,36,38,40)	-177.93	D384	D(21,126,127,128)	154.866
D148	D(41,36,38,39)	179.3608	D385	D(21,126,127,129)	-31.2706
D149	D(41,36,38,40)	1.1378	D386	D(98,126,127,128)	-85.3895
D150	D(35,36,41,8)	-2.121	D387	D(98,126,127,129)	88.4739
D151	D(35,36,41,42)	-122.048	D388	D(137,126,127,128)	35.0631
D152	D(35,36,41,52)	114.8739	D389	D(137,126,127,129)	-151.074
D153	D(38,36,41,8)	178.915	D390	D(21,126,137,138)	-86.6976
D154	D(38,36,41,42)	58.9884	D391	D(21,126,137,139)	87.9185
D155	D(38,36,41,52)	-64.0902	D392	D(98,126,137,138)	153.8369
D156	D(35,37,39,38)	-0.741	D393	D(98,126,137,139)	-31.547
D157	D(35,37,39,76)	179.7889	D394	D(127,126,137,138)	35.4305
D158	D(36,38,39,37)	0.4014	D395	D(127,126,137,139)	-149.953
D159	D(36,38,39,76)	179.8217	D396	D(126,127,128,130)	174.838
D160	D(40,38,39,37)	178.6484	D397	D(126,127,128,131)	-5.343
D161	D(40,38,39,76)	-1.9313	D398	D(129,127,128,130)	0.7997
D162	D(37,39,76,77)	153.7979	D399	D(129,127,128,131)	-179.381
D163	D(37,39,76,78)	-26.5939	D400	D(126,127,129,132)	-174.849
D164	D(38,39,76,77)	-25.5651	D401	D(126,127,129,133)	4.8075
D165	D(38,39,76,78)	154.043	D402	D(128,127,129,132)	-0.7088
D166	D(8,41,42,43)	154.8858	D403	D(128,127,129,133)	178.9473
D167	D(8,41,42,44)	-31.1225	D404	D(127,128,130,134)	-0.3165
D168	D(36,41,42,43)	-85.2871	D405	D(127,128,130,135)	179.9297
D169	D(36,41,42,44)	88.7046	D406	D(131,128,130,134)	179.8617

D170	D(52,41,42,43)	35.2398	D407	D(131,128,130,135)	0.108
D171	D(52,41,42,44)	-150.769	D408	D(127,129,132,134)	0.1308
D172	D(8,41,52,53)	87.6905	D409	D(127,129,132,136)	179.815
D173	D(8,41,52,54)	-87.3348	D410	D(133,129,132,134)	-179.528
D174	D(36,41,52,53)	-31.8177	D411	D(133,129,132,136)	0.1558
D175	D(36,41,52,54)	153.157	D412	D(128,130,134,132)	-0.2782
D176	D(42,41,52,53)	-150.305	D413	D(128,130,134,147)	178.2007
D177	D(42,41,52,54)	34.6702	D414	D(135,130,134,132)	179.4744
D178	D(41,42,43,45)	175.1042	D415	D(135,130,134,147)	-2.0467
D179	D(41,42,43,46)	-5.1797	D416	D(129,132,134,130)	0.3697
D180	D(44,42,43,45)	0.9398	D417	D(129,132,134,147)	-178.11
D181	D(44,42,43,46)	-179.344	D418	D(136,132,134,130)	-179.313
D182	D(41,42,44,47)	-175.107	D419	D(136,132,134,147)	2.2071
D183	D(41,42,44,48)	4.577	D420	D(130,134,147,148)	-89.5192
D184	D(43,42,44,47)	-0.8404	D421	D(130,134,147,149)	148.7545
D185	D(43,42,44,48)	178.8437	D422	D(130,134,147,150)	32.2494
D186	D(42,43,45,49)	-0.346	D423	D(132,134,147,148)	88.9013
D187	D(42,43,45,50)	179.8431	D424	D(132,134,147,149)	-32.825
D188	D(46,43,45,49)	179.9338	D425	D(132,134,147,150)	-149.33
D189	D(46,43,45,50)	0.1229	D426	D(126,137,138,140)	175.3819
D190	D(42,44,47,49)	0.1429	D427	D(126,137,138,141)	-4.9854
D191	D(42,44,47,51)	179.8588	D428	D(139,137,138,140)	0.6218
D192	D(48,44,47,49)	-179.544	D429	D(139,137,138,141)	-179.746
D193	D(48,44,47,51)	0.1717	D430	D(126,137,139,142)	-175.471
D194	D(43,45,49,47)	-0.3703	D431	D(126,137,139,143)	4.1672
D195	D(43,45,49,62)	178.1249	D432	D(138,137,139,142)	-0.599
D196	D(50,45,49,47)	179.4398	D433	D(138,137,139,143)	179.0393
D197	D(50,45,49,62)	-2.065	D434	D(137,138,140,144)	-0.1944
D198	D(44,47,49,45)	0.4705	D435	D(137,138,140,145)	179.9699
D199	D(44,47,49,62)	-178.025	D436	D(141,138,140,144)	-179.833
D200	D(51,47,49,45)	-179.244	D437	D(141,138,140,145)	0.3315
D201	D(51,47,49,62)	2.26	D438	D(137,139,142,144)	0.1469
D202	D(45,49,62,63)	31.3109	D439	D(137,139,142,146)	179.8549
D203	D(45,49,62,64)	147.8235	D440	D(143,139,142,144)	-179.494
D204	D(45,49,62,65)	-90.4579	D441	D(143,139,142,146)	0.2136
D205	D(47,49,62,63)	-150.252	D442	D(138,140,144,142)	-0.2705
D206	D(47,49,62,64)	-33.7394	D443	D(138,140,144,154)	178.23
D207	D(47,49,62,65)	87.9792	D444	D(145,140,144,142)	179.5645
D208	D(41,52,53,55)	-175.75	D445	D(145,140,144,154)	-1.935
D209	D(41,52,53,56)	4.4671	D446	D(139,142,144,140)	0.294
D210	D(54,52,53,55)	-0.4812	D447	D(139,142,144,154)	-178.205
D211	D(54,52,53,56)	179.7357	D448	D(146,142,144,140)	-179.413
D212	D(41,52,54,57)	175.7392	D449	D(146,142,144,154)	2.0882

D213	D(41,52,54,58)	-5.119	D450	D(140,144,154,155)	-87.7514
D214	D(53,52,54,57)	0.5852	D451	D(140,144,154,156)	150.4901
D215	D(53,52,54,58)	179.7271	D452	D(140,144,154,157)	33.9892
D216	D(52,53,55,59)	0.1442	D453	D(142,144,154,155)	90.6902
D217	D(52,53,55,60)	-179.565	D454	D(142,144,154,156)	-31.0683
D218	D(56,53,55,59)	179.9289	D455	D(142,144,154,157)	-147.569
D219	D(56,53,55,60)	0.2202	D456	D(134,147,148,151)	-179.916
D220	D(52,54,57,59)	-0.3572	D457	D(134,147,148,152)	-59.8748
D221	D(52,54,57,61)	179.2839	D458	D(134,147,148,153)	60.0431
D222	D(58,54,57,59)	-179.513	D459	D(149,147,148,151)	-58.0953
D223	D(58,54,57,61)	0.1285	D460	D(149,147,148,152)	61.9463
D224	D(53,55,59,57)	0.1034	D461	D(149,147,148,153)	-178.136
D225	D(53,55,59,69)	178.4959	D462	D(150,147,148,151)	58.1997
D226	D(60,55,59,57)	179.8109	D463	D(150,147,148,152)	178.2414
D227	D(60,55,59,69)	-1.7966	D464	D(150,147,148,153)	-61.8407
D228	D(54,57,59,55)	0.0016	D465	D(144,154,155,158)	179.9694
D229	D(54,57,59,69)	-178.393	D466	D(144,154,155,159)	-59.9686
D230	D(61,57,59,55)	-179.638	D467	D(144,154,155,160)	59.9267
D231	D(61,57,59,69)	1.9674	D468	D(156,154,155,158)	-58.1873
D232	D(55,59,69,70)	30.2147	D469	D(156,154,155,159)	61.8747
D233	D(55,59,69,71)	146.7441	D470	D(156,154,155,160)	-178.23
D234	D(55,59,69,72)	-91.5416	D471	D(157,154,155,158)	58.1129
D235	D(57,59,69,70)	-151.454	D472	D(157,154,155,159)	178.1749
D236	D(57,59,69,71)	-34.9248	D473	D(157,154,155,160)	-61.9299
D237	D(57,59,69,72)	86.7895			

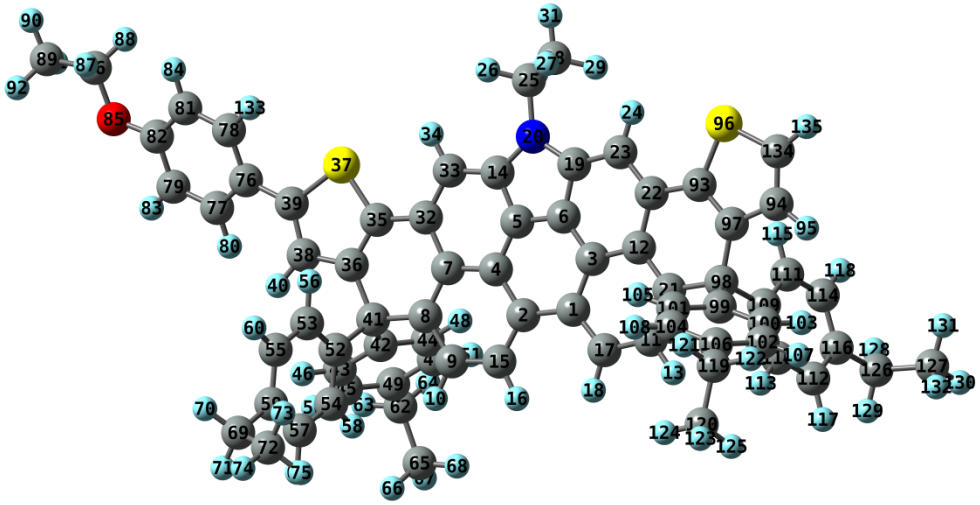


Figure S75. Geometry of the S_0 state of C_2O-P-DTPC in THF optimized at the B3LYP/6-311G(d,p) level of theory.

Table S26. Geometry parameters and Mulliken atomic charges of the S_0 state of C_2O-P-DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Center number	Atom	Coordinate [Å]			Mulliken atomic charge
		x	y	z	
1	6	0	-2.20393	-0.74144	0.030457
2	6	0	-0.74422	-1.04115	0.066346
3	6	0	-2.63042	0.620434	-0.0477
4	6	0	0.187412	0.041034	0.006638
5	6	0	-0.31108	1.331775	-0.06767
6	6	0	-1.66109	1.609437	-0.09221
7	6	0	1.59817	-0.08345	0.020105
8	6	0	2.138372	-1.38469	0.105391
9	6	0	1.238116	-2.45333	0.173304
10	1	0	1.630243	-3.46006	0.243844
11	6	0	-4.58457	-1.25887	0.017351
12	6	0	-3.97552	1.062278	-0.09404
13	1	0	-5.34387	-2.03039	0.04066
14	6	0	0.398858	2.523003	-0.14302
15	6	0	-0.15747	-2.30518	0.15458
16	1	0	-0.76864	-3.19875	0.211073
17	6	0	-3.24394	-1.67279	0.056769
18	1	0	-3.0371	-2.73574	0.107039
19	6	0	-1.84057	2.983264	-0.18788
20	7	0	-0.55457	3.555737	-0.2268
21	6	0	-4.98757	0.078818	-0.05158
22	6	0	-4.2113	2.496077	-0.19682
23	6	0	-3.17681	3.440969	-0.24203
24	1	0	-3.4187	4.494566	-0.31858
25	6	0	-0.25913	4.986983	-0.26175
26	1	0	0.67466	5.119123	-0.81243
27	1	0	-1.042	5.472698	-0.84812
28	6	0	-0.15745	5.619928	1.127871
29	1	0	-1.09513	5.510682	1.677334
30	1	0	0.640592	5.156129	1.711968
31	1	0	0.062338	6.68653	1.034775
32	6	0	2.384353	1.141812	-0.05126
33	6	0	1.80802	2.418069	-0.13261
34	1	0	2.44802	3.290976	-0.18484
35	6	0	3.815255	0.924083	-0.03806
36	6	0	4.427259	-0.30955	0.023213
37	16	0	5.001766	2.212478	-0.11817
38	6	0	5.848541	-0.21478	-0.01422
39	6	0	6.33329	1.065452	-0.09442

40	1	0	6.499276	-1.07727	-0.01122
41	6	0	3.662996	-1.63717	0.12008
42	6	0	4.095212	-2.27985	1.466813
43	6	0	5.268648	-3.03663	1.583479
44	6	0	3.38176	-2.01591	2.641802
45	6	0	5.696154	-3.52163	2.817085
46	1	0	5.860919	-3.26035	0.705287
47	6	0	3.812247	-2.5009	3.874574
48	1	0	2.479711	-1.41846	2.601293
49	6	0	4.975284	-3.26789	3.988266
50	1	0	6.609422	-4.10657	2.867202
51	1	0	3.232584	-2.27323	4.763887
52	6	0	3.979232	-2.5191	-1.11782
53	6	0	4.218751	-1.92109	-2.36075
54	6	0	3.936265	-3.91801	-1.07375
55	6	0	4.41509	-2.68741	-3.50671
56	1	0	4.255402	-0.84114	-2.43797
57	6	0	4.133523	-4.68237	-2.22182
58	1	0	3.759444	-4.42779	-0.13518
59	6	0	4.376987	-4.08446	-3.46187
60	1	0	4.605665	-2.18726	-4.4513
61	1	0	4.102873	-5.76503	-2.14671
62	6	0	5.416586	-3.8327	5.320089
63	1	0	6.508529	-3.90409	5.339968
64	1	0	5.13149	-3.14165	6.119507
65	6	0	4.814278	-5.21832	5.612217
66	1	0	5.1077	-5.94186	4.846674
67	1	0	5.154314	-5.59363	6.581432
68	1	0	3.721888	-5.17398	5.630221
69	6	0	4.555384	-4.91576	-4.71298
70	1	0	5.2402	-4.40239	-5.3951
71	1	0	5.026749	-5.86831	-4.45164
72	6	0	3.228859	-5.19191	-5.4425
73	1	0	2.747622	-4.25823	-5.74608
74	1	0	3.396877	-5.79418	-6.33964
75	1	0	2.532123	-5.73303	-4.79642
76	6	0	7.726434	1.514928	-0.14454
77	6	0	8.758723	0.708263	0.375353
78	6	0	8.091253	2.744887	-0.70841
79	6	0	10.08122	1.110376	0.32075
80	1	0	8.517249	-0.23785	0.8448
81	6	0	9.418319	3.165439	-0.76058
82	6	0	10.42815	2.345393	-0.24739

83	1	0	10.86925	0.487089	0.726327
84	1	0	9.64944	4.121888	-1.2087
85	8	0	11.75314	2.650143	-0.24838
86	6	0	12.18036	3.904991	-0.80357
87	1	0	11.87634	3.962376	-1.8545
88	1	0	11.70065	4.72689	-0.26079
89	6	0	13.68852	3.971736	-0.66957
90	1	0	14.05608	4.91472	-1.08115
91	1	0	13.98606	3.913506	0.37969
92	1	0	14.1613	3.150278	-1.21229
93	6	0	-5.61392	2.860381	-0.25549
94	6	0	-7.93547	2.620716	-0.26021
95	1	0	-8.88209	2.100445	-0.22478
96	16	0	-6.19302	4.509225	-0.40234
97	6	0	-6.66301	1.96879	-0.1939
98	6	0	-6.4876	0.450471	-0.05952
99	6	0	-7.1994	-0.17493	-1.28917
100	6	0	-8.5694	-0.46474	-1.28965
101	6	0	-6.50374	-0.3533	-2.49114
102	6	0	-9.20817	-0.93259	-2.43621
103	1	0	-9.15329	-0.33084	-0.3878
104	6	0	-7.14488	-0.81851	-3.63616
105	1	0	-5.44688	-0.12206	-2.54023
106	6	0	-8.50973	-1.12316	-3.63198
107	1	0	-10.2714	-1.14891	-2.39776
108	1	0	-6.57165	-0.94125	-4.55004
109	6	0	-7.06646	-0.02348	1.302436
110	6	0	-7.54045	-1.32623	1.50237
111	6	0	-7.02548	0.823716	2.415939
112	6	0	-7.96638	-1.75455	2.757502
113	1	0	-7.58679	-2.02217	0.674405
114	6	0	-7.45036	0.392351	3.670167
115	1	0	-6.65149	1.834421	2.3071
116	6	0	-7.93301	-0.90467	3.867413
117	1	0	-8.32793	-2.77171	2.873253
118	1	0	-7.39976	1.078261	4.510292
119	6	0	-9.19564	-1.66899	-4.86448
120	6	0	-9.11005	-3.20193	-4.96964
121	1	0	-8.74609	-1.22271	-5.75712
122	1	0	-10.2476	-1.36721	-4.85722
123	1	0	-9.61367	-3.5582	-5.87253
124	1	0	-8.06895	-3.53377	-5.0089
125	1	0	-9.5819	-3.68049	-4.10707

126	6	0	-8.43106	-1.36019	5.220835
127	6	0	-9.92878	-1.07926	5.435824
128	1	0	-7.85582	-0.85935	6.00581
129	1	0	-8.24753	-2.43338	5.332345
130	1	0	-10.2505	-1.42157	6.423331
131	1	0	-10.1409	-0.00904	5.362698
132	1	0	-10.5354	-1.59307	4.685031
133	1	0	7.329995	3.389084	-1.13401
134	6	0	-7.84497	3.973796	-0.3721
135	1	0	-8.642	4.697925	-0.44158

Table S27. The bond lengths of the S_0 state of C_2O-P-DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Length [Å]	Number	Name	Length [Å]
R1	R(1,2)	1.4906	R76	R(62,63)	1.0945
R2	R(1,3)	1.4292	R77	R(62,64)	1.0945
R3	R(1,17)	1.3963	R78	R(62,65)	1.5388
R4	R(2,4)	1.4292	R79	R(65,66)	1.0935
R5	R(2,15)	1.3964	R80	R(65,67)	1.0936
R6	R(3,6)	1.3855	R81	R(65,68)	1.0934
R7	R(3,12)	1.4166	R82	R(69,70)	1.0944
R8	R(4,5)	1.3856	R83	R(69,71)	1.0945
R9	R(4,7)	1.4163	R84	R(69,72)	1.5389
R10	R(5,6)	1.3785	R85	R(72,73)	1.0934
R11	R(5,14)	1.3888	R86	R(72,74)	1.0935
R12	R(6,19)	1.3888	R87	R(72,75)	1.0935
R13	R(7,8)	1.4115	R88	R(76,77)	1.4095
R14	R(7,32)	1.4575	R89	R(76,78)	1.4014
R15	R(8,9)	1.399	R90	R(77,79)	1.3834
R16	R(8,41)	1.5455	R91	R(77,80)	1.0834
R17	R(9,10)	1.0827	R92	R(78,81)	1.3931
R18	R(9,15)	1.4036	R93	R(78,133)	1.0843
R19	R(11,13)	1.0827	R94	R(79,82)	1.403
R20	R(11,17)	1.4036	R95	R(79,83)	1.0835
R21	R(11,21)	1.3988	R96	R(81,82)	1.3984
R22	R(12,21)	1.4118	R97	R(81,84)	1.0812
R23	R(12,22)	1.4567	R98	R(82,85)	1.3596
R24	R(14,20)	1.408	R99	R(85,86)	1.4371
R25	R(14,33)	1.4131	R100	R(86,87)	1.0955
R26	R(15,16)	1.0841	R101	R(86,88)	1.0956
R27	R(17,18)	1.0841	R102	R(86,89)	1.5156
R28	R(19,20)	1.4082	R103	R(89,90)	1.0926
R29	R(19,23)	1.4135	R104	R(89,91)	1.0922
R30	R(20,25)	1.4618	R105	R(89,92)	1.0922
R31	R(21,98)	1.5454	R106	R(93,96)	1.7537
R32	R(22,23)	1.4018	R107	R(93,97)	1.3782
R33	R(22,93)	1.4503	R108	R(94,95)	1.0808
R34	R(23,24)	1.0837	R109	R(94,97)	1.4313
R35	R(25,26)	1.0921	R110	R(94,134)	1.3607
R36	R(25,27)	1.0921	R111	R(96,134)	1.7368
R37	R(25,28)	1.5304	R112	R(97,98)	1.5343
R38	R(28,29)	1.0923	R113	R(98,99)	1.5524
R39	R(28,30)	1.0923	R114	R(98,109)	1.5539
R40	R(28,31)	1.093	R115	R(99,100)	1.4003

R41	R(32,33)	1.4027	R116	R(99,101)	1.4002
R42	R(32,35)	1.4474	R117	R(100,102)	1.3934
R43	R(33,34)	1.0836	R118	R(100,103)	1.0827
R44	R(35,36)	1.3785	R119	R(101,104)	1.3923
R45	R(35,37)	1.7533	R120	R(101,105)	1.083
R46	R(36,38)	1.4249	R121	R(102,106)	1.3979
R47	R(36,41)	1.5349	R122	R(102,107)	1.0857
R48	R(37,39)	1.7576	R123	R(104,106)	1.3984
R49	R(38,39)	1.3713	R124	R(104,108)	1.0857
R50	R(38,40)	1.0804	R125	R(106,119)	1.5124
R51	R(39,76)	1.4647	R126	R(109,110)	1.4006
R52	R(41,42)	1.5536	R127	R(109,111)	1.3998
R53	R(41,52)	1.5525	R128	R(110,112)	1.3929
R54	R(42,43)	1.4012	R129	R(110,113)	1.0826
R55	R(42,44)	1.3997	R130	R(111,114)	1.3927
R56	R(43,45)	1.3928	R131	R(111,115)	1.0832
R57	R(43,46)	1.0826	R132	R(112,116)	1.3983
R58	R(44,47)	1.3929	R133	R(112,117)	1.0857
R59	R(44,48)	1.0827	R134	R(114,116)	1.3979
R60	R(45,49)	1.3985	R135	R(114,118)	1.0857
R61	R(45,50)	1.0857	R136	R(116,126)	1.5124
R62	R(47,49)	1.3978	R137	R(119,120)	1.5389
R63	R(47,51)	1.0857	R138	R(119,121)	1.0946
R64	R(49,62)	1.5125	R139	R(119,122)	1.0944
R65	R(52,53)	1.4	R140	R(120,123)	1.0935
R66	R(52,54)	1.4003	R141	R(120,124)	1.0934
R67	R(53,55)	1.3925	R142	R(120,125)	1.0935
R68	R(53,56)	1.0833	R143	R(126,127)	1.5389
R69	R(54,57)	1.3933	R144	R(126,128)	1.0945
R70	R(54,58)	1.0826	R145	R(126,129)	1.0945
R71	R(55,59)	1.3983	R146	R(127,130)	1.0936
R72	R(55,60)	1.0857	R147	R(127,131)	1.0935
R73	R(57,59)	1.398	R148	R(127,132)	1.0935
R74	R(57,61)	1.0857	R149	R(134,135)	1.0791
R75	R(59,69)	1.5127			

Table S28. The bond angles of the S_0 state of C_2O-P-DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Angle [°]	Number	Name	Angle [°]
A1	A(2,1,3)	119.021	A133	A(49,62,65)	112.9057
A2	A(2,1,17)	126.4997	A134	A(63,62,64)	106.7268
A3	A(3,1,17)	114.4779	A135	A(63,62,65)	109.1666
A4	A(1,2,4)	119.0189	A136	A(64,62,65)	109.142
A5	A(1,2,15)	126.5144	A137	A(62,65,66)	110.9696
A6	A(4,2,15)	114.4667	A138	A(62,65,67)	110.8289
A7	A(1,3,6)	118.2393	A139	A(62,65,68)	110.9556
A8	A(1,3,12)	125.616	A140	A(66,65,67)	108.0572
A9	A(6,3,12)	116.1432	A141	A(66,65,68)	107.8449
A10	A(2,4,5)	118.2334	A142	A(67,65,68)	108.0574
A11	A(2,4,7)	125.6161	A143	A(59,69,70)	109.3599
A12	A(5,4,7)	116.1502	A144	A(59,69,71)	109.3661
A13	A(4,5,6)	122.745	A145	A(59,69,72)	112.8953
A14	A(4,5,14)	128.171	A146	A(70,69,71)	106.7135
A15	A(6,5,14)	109.0803	A147	A(70,69,72)	109.1527
A16	A(3,6,5)	122.7384	A148	A(71,69,72)	109.1639
A17	A(3,6,19)	128.1636	A149	A(69,72,73)	110.9642
A18	A(5,6,19)	109.0896	A150	A(69,72,74)	110.8124
A19	A(4,7,8)	117.5695	A151	A(69,72,75)	110.9747
A20	A(4,7,32)	117.5758	A152	A(73,72,74)	108.0681
A21	A(8,7,32)	124.8545	A153	A(73,72,75)	107.8296
A22	A(7,8,9)	117.4429	A154	A(74,72,75)	108.0648
A23	A(7,8,41)	121.9206	A155	A(39,76,77)	120.5546
A24	A(9,8,41)	120.6363	A156	A(39,76,78)	122.0535
A25	A(8,9,10)	118.7104	A157	A(77,76,78)	117.3912
A26	A(8,9,15)	123.9583	A158	A(76,77,79)	121.2822
A27	A(10,9,15)	117.3313	A159	A(76,77,80)	119.7599
A28	A(13,11,17)	117.327	A160	A(79,77,80)	118.948
A29	A(13,11,21)	118.7155	A161	A(76,78,81)	121.8718
A30	A(17,11,21)	123.9574	A162	A(76,78,133)	119.7767
A31	A(3,12,21)	117.5431	A163	A(81,78,133)	118.3438
A32	A(3,12,22)	117.5815	A164	A(77,79,82)	120.5479
A33	A(21,12,22)	124.8717	A165	A(77,79,83)	120.885
A34	A(5,14,20)	106.6309	A166	A(82,79,83)	118.562
A35	A(5,14,33)	116.4663	A167	A(78,81,82)	119.81
A36	A(20,14,33)	136.8986	A168	A(78,81,84)	119.0911
A37	A(2,15,9)	120.9445	A169	A(82,81,84)	121.0963
A38	A(2,15,16)	120.8344	A170	A(79,82,81)	119.0936
A39	A(9,15,16)	118.2211	A171	A(79,82,85)	116.0142
A40	A(1,17,11)	120.9416	A172	A(81,82,85)	124.8921

A41	A(1,17,18)	120.8492	A173	A(82,85,86)	119.0588
A42	A(11,17,18)	118.2092	A174	A(85,86,87)	109.5013
A43	A(6,19,20)	106.6204	A175	A(85,86,88)	109.4803
A44	A(6,19,23)	116.4318	A176	A(85,86,89)	107.4646
A45	A(20,19,23)	136.9376	A177	A(87,86,88)	108.3282
A46	A(14,20,19)	108.5756	A178	A(87,86,89)	111.018
A47	A(14,20,25)	125.6388	A179	A(88,86,89)	111.0319
A48	A(19,20,25)	125.6793	A180	A(86,89,90)	109.845
A49	A(11,21,12)	117.4595	A181	A(86,89,91)	110.7129
A50	A(11,21,98)	120.6565	A182	A(86,89,92)	110.7139
A51	A(12,21,98)	121.8782	A183	A(90,89,91)	108.4376
A52	A(12,22,23)	123.1133	A184	A(90,89,92)	108.4405
A53	A(12,22,93)	113.9928	A185	A(91,89,92)	108.6244
A54	A(23,22,93)	122.8931	A186	A(22,93,96)	123.9791
A55	A(19,23,22)	118.5638	A187	A(22,93,97)	124.8807
A56	A(19,23,24)	121.9059	A188	A(96,93,97)	111.1385
A57	A(22,23,24)	119.5302	A189	A(95,94,97)	123.9115
A58	A(20,25,26)	107.6574	A190	A(95,94,134)	122.6594
A59	A(20,25,27)	107.6621	A191	A(97,94,134)	113.4291
A60	A(20,25,28)	113.3697	A192	A(93,96,134)	91.305
A61	A(26,25,27)	106.7614	A193	A(93,97,94)	112.3346
A62	A(26,25,28)	110.5495	A194	A(93,97,98)	123.8544
A63	A(27,25,28)	110.5629	A195	A(94,97,98)	123.8097
A64	A(25,28,29)	111.0001	A196	A(21,98,97)	110.4508
A65	A(25,28,30)	111.0074	A197	A(21,98,99)	110.6251
A66	A(25,28,31)	109.8542	A198	A(21,98,109)	106.4827
A67	A(29,28,30)	108.4048	A199	A(97,98,99)	106.0736
A68	A(29,28,31)	108.2444	A200	A(97,98,109)	109.6334
A69	A(30,28,31)	108.2395	A201	A(99,98,109)	113.6142
A70	A(7,32,33)	123.0978	A202	A(98,99,100)	122.1577
A71	A(7,32,35)	113.9744	A203	A(98,99,101)	120.2313
A72	A(33,32,35)	122.927	A204	A(100,99,101)	117.3498
A73	A(14,33,32)	118.5363	A205	A(99,100,102)	121.2168
A74	A(14,33,34)	121.923	A206	A(99,100,103)	120.1158
A75	A(32,33,34)	119.5407	A207	A(102,100,103)	118.6669
A76	A(32,35,36)	125.0248	A208	A(99,101,104)	121.3156
A77	A(32,35,37)	123.9201	A209	A(99,101,105)	119.7736
A78	A(36,35,37)	111.0514	A210	A(104,101,105)	118.91
A79	A(35,36,38)	112.4667	A211	A(100,102,106)	121.3742
A80	A(35,36,41)	123.766	A212	A(100,102,107)	119.1244
A81	A(38,36,41)	123.7673	A213	A(106,102,107)	119.5009
A82	A(35,37,39)	91.8622	A214	A(101,104,106)	121.3154
A83	A(36,38,39)	114.5969	A215	A(101,104,108)	119.1347

A84	A(36,38,40)	123.2008	A216	A(106,104,108)	119.5491
A85	A(39,38,40)	122.1762	A217	A(102,106,104)	117.4195
A86	A(37,39,38)	110.0146	A218	A(102,106,119)	121.3128
A87	A(37,39,76)	121.321	A219	A(104,106,119)	121.2519
A88	A(38,39,76)	128.662	A220	A(98,109,110)	122.3346
A89	A(8,41,36)	110.444	A221	A(98,109,111)	120.114
A90	A(8,41,42)	110.5046	A222	A(110,109,111)	117.342
A91	A(8,41,52)	106.6294	A223	A(109,110,112)	121.2055
A92	A(36,41,42)	105.9017	A224	A(109,110,113)	120.2141
A93	A(36,41,52)	109.8529	A225	A(112,110,113)	118.5797
A94	A(42,41,52)	113.5494	A226	A(109,111,114)	121.3322
A95	A(41,42,43)	121.9111	A227	A(109,111,115)	119.6654
A96	A(41,42,44)	120.5222	A228	A(114,111,115)	119.0015
A97	A(43,42,44)	117.3103	A229	A(110,112,116)	121.4018
A98	A(42,43,45)	121.2578	A230	A(110,112,117)	119.0769
A99	A(42,43,46)	120.1475	A231	A(116,112,117)	119.5209
A100	A(45,43,46)	118.594	A232	A(111,114,116)	121.3173
A101	A(42,44,47)	121.3148	A233	A(111,114,118)	119.1399
A102	A(42,44,48)	119.821	A234	A(116,114,118)	119.5421
A103	A(47,44,48)	118.8631	A235	A(112,116,114)	117.3977
A104	A(43,45,49)	121.3572	A236	A(112,116,126)	121.2917
A105	A(43,45,50)	119.1242	A237	A(114,116,126)	121.2942
A106	A(49,45,50)	119.5185	A238	A(106,119,120)	112.9521
A107	A(44,47,49)	121.3441	A239	A(106,119,121)	109.34
A108	A(44,47,51)	119.1385	A240	A(106,119,122)	109.3293
A109	A(49,47,51)	119.5169	A241	A(120,119,121)	109.1212
A110	A(45,49,47)	117.409	A242	A(120,119,122)	109.1828
A111	A(45,49,62)	121.2851	A243	A(121,119,122)	106.7236
A112	A(47,49,62)	121.2857	A244	A(119,120,123)	110.8149
A113	A(41,52,53)	120.008	A245	A(119,120,124)	110.9601
A114	A(41,52,54)	122.4245	A246	A(119,120,125)	110.9805
A115	A(53,52,54)	117.3833	A247	A(123,120,124)	108.0586
A116	A(52,53,55)	121.3122	A248	A(123,120,125)	108.0594
A117	A(52,53,56)	119.664	A249	A(124,120,125)	107.8401
A118	A(55,53,56)	119.0236	A250	A(116,126,127)	112.9874
A119	A(52,54,57)	121.1847	A251	A(116,126,128)	109.3241
A120	A(52,54,58)	120.1795	A252	A(116,126,129)	109.3473
A121	A(57,54,58)	118.6316	A253	A(127,126,128)	109.1333
A122	A(53,55,59)	121.3054	A254	A(127,126,129)	109.1456
A123	A(53,55,60)	119.159	A255	A(128,126,129)	106.7085
A124	A(59,55,60)	119.535	A256	A(126,127,130)	110.8147
A125	A(54,57,59)	121.394	A257	A(126,127,131)	110.9866
A126	A(54,57,61)	119.0821	A258	A(126,127,132)	110.9916

A127	A(59,57,61)	119.5228	A259	A(130,127,131)	108.0391
A128	A(55,59,57)	117.4191	A260	A(130,127,132)	108.0417
A129	A(55,59,69)	121.2877	A261	A(131,127,132)	107.838
A130	A(57,59,69)	121.2735	A262	A(94,134,96)	111.7922
A131	A(49,62,63)	109.3577	A263	A(94,134,135)	128.5694
A132	A(49,62,64)	109.3528	A264	A(96,134,135)	119.6382

Table S29. The dihedral angles of the S_0 state of C_2O-P-DTPC in THF computed at the B3LYP/6-311G(d,p) level of theory

Number	Name	Dihedral angle [°]	Number	Name	Dihedral angle [°]
D1	D(3,1,2,4)	-0.6862	D204	D(45,49,62,65)	-89.6541
D2	D(3,1,2,15)	179.3331	D205	D(47,49,62,63)	-149.579
D3	D(17,1,2,4)	178.8595	D206	D(47,49,62,64)	-33.0459
D4	D(17,1,2,15)	-1.1213	D207	D(47,49,62,65)	88.6699
D5	D(2,1,3,6)	0.2464	D208	D(41,52,53,55)	-175.589
D6	D(2,1,3,12)	179.7775	D209	D(41,52,53,56)	4.5541
D7	D(17,1,3,6)	-179.352	D210	D(54,52,53,55)	-0.4018
D8	D(17,1,3,12)	0.1788	D211	D(54,52,53,56)	179.741
D9	D(2,1,17,11)	-179.992	D212	D(41,52,54,57)	175.4862
D10	D(2,1,17,18)	-0.0652	D213	D(41,52,54,58)	-5.2695
D11	D(3,1,17,11)	-0.4283	D214	D(53,52,54,57)	0.4242
D12	D(3,1,17,18)	179.4983	D215	D(53,52,54,58)	179.6685
D13	D(1,2,4,5)	0.7046	D216	D(52,53,55,59)	0.1836
D14	D(1,2,4,7)	-179.479	D217	D(52,53,55,60)	-179.543
D15	D(15,2,4,5)	-179.312	D218	D(56,53,55,59)	-179.958
D16	D(15,2,4,7)	0.5045	D219	D(56,53,55,60)	0.3156
D17	D(1,2,15,9)	179.6839	D220	D(52,54,57,59)	-0.23
D18	D(1,2,15,16)	-0.353	D221	D(52,54,57,61)	179.3873
D19	D(4,2,15,9)	-0.2976	D222	D(58,54,57,59)	-179.486
D20	D(4,2,15,16)	179.6655	D223	D(58,54,57,61)	0.1316
D21	D(1,3,6,5)	0.1719	D224	D(53,55,59,57)	0.0265
D22	D(1,3,6,19)	178.9926	D225	D(53,55,59,69)	178.4282
D23	D(12,3,6,5)	-179.404	D226	D(60,55,59,57)	179.7516
D24	D(12,3,6,19)	-0.5827	D227	D(60,55,59,69)	-1.8466
D25	D(1,3,12,21)	0.411	D228	D(54,57,59,55)	-0.0035
D26	D(1,3,12,22)	-178.927	D229	D(54,57,59,69)	-178.406
D27	D(6,3,12,21)	179.9508	D230	D(61,57,59,55)	-179.619
D28	D(6,3,12,22)	0.6125	D231	D(61,57,59,69)	1.9788
D29	D(2,4,5,6)	-0.3044	D232	D(55,59,69,70)	32.7807
D30	D(2,4,5,14)	-179.527	D233	D(55,59,69,71)	149.3069
D31	D(7,4,5,6)	179.8614	D234	D(55,59,69,72)	-88.9468
D32	D(7,4,5,14)	0.6386	D235	D(57,59,69,70)	-148.879
D33	D(2,4,7,8)	-0.2867	D236	D(57,59,69,71)	-32.3529
D34	D(2,4,7,32)	179.8853	D237	D(57,59,69,72)	89.3933
D35	D(5,4,7,8)	179.5336	D238	D(49,62,65,66)	59.9757
D36	D(5,4,7,32)	-0.2944	D239	D(49,62,65,67)	-179.96
D37	D(4,5,6,3)	-0.1531	D240	D(49,62,65,68)	-59.9051
D38	D(4,5,6,19)	-179.172	D241	D(63,62,65,66)	-61.8827
D39	D(14,5,6,3)	179.2003	D242	D(63,62,65,67)	58.1813
D40	D(14,5,6,19)	0.1814	D243	D(63,62,65,68)	178.2364

D41	D(4,5,14,20)	178.8324	D244	D(64,62,65,66)	-178.19
D42	D(4,5,14,33)	-0.5561	D245	D(64,62,65,67)	-58.1256
D43	D(6,5,14,20)	-0.4758	D246	D(64,62,65,68)	61.9295
D44	D(6,5,14,33)	-179.864	D247	D(59,69,72,73)	59.9516
D45	D(3,6,19,20)	-178.762	D248	D(59,69,72,74)	-179.985
D46	D(3,6,19,23)	0.2718	D249	D(59,69,72,75)	-59.919
D47	D(5,6,19,20)	0.1887	D250	D(70,69,72,73)	-61.8928
D48	D(5,6,19,23)	179.2221	D251	D(70,69,72,74)	58.1706
D49	D(4,7,8,9)	-0.1438	D252	D(70,69,72,75)	178.2366
D50	D(4,7,8,41)	179.6772	D253	D(71,69,72,73)	-178.188
D51	D(32,7,8,9)	179.6704	D254	D(71,69,72,74)	-58.1249
D52	D(32,7,8,41)	-0.5086	D255	D(71,69,72,75)	61.9412
D53	D(4,7,32,33)	-0.0586	D256	D(39,76,77,79)	179.176
D54	D(4,7,32,35)	-179.739	D257	D(39,76,77,80)	-1.9827
D55	D(8,7,32,33)	-179.873	D258	D(78,76,77,79)	-0.5301
D56	D(8,7,32,35)	0.4467	D259	D(78,76,77,80)	178.3112
D57	D(7,8,9,10)	-179.723	D260	D(39,76,78,81)	-179.647
D58	D(7,8,9,15)	0.339	D261	D(39,76,78,133)	-0.6719
D59	D(41,8,9,10)	0.4534	D262	D(77,76,78,81)	0.0549
D60	D(41,8,9,15)	-179.484	D263	D(77,76,78,133)	179.0295
D61	D(7,8,41,36)	-0.3232	D264	D(76,77,79,82)	0.5572
D62	D(7,8,41,42)	116.5227	D265	D(76,77,79,83)	179.7293
D63	D(7,8,41,52)	-119.637	D266	D(80,77,79,82)	-178.293
D64	D(9,8,41,36)	179.4922	D267	D(80,77,79,83)	0.8787
D65	D(9,8,41,42)	-63.6619	D268	D(76,78,81,82)	0.3929
D66	D(9,8,41,52)	60.1785	D269	D(76,78,81,84)	179.8109
D67	D(8,9,15,2)	-0.1054	D270	D(133,78,81,82)	-178.596
D68	D(8,9,15,16)	179.9305	D271	D(133,78,81,84)	0.8221
D69	D(10,9,15,2)	179.956	D272	D(77,79,82,81)	-0.095
D70	D(10,9,15,16)	-0.0081	D273	D(77,79,82,85)	179.7651
D71	D(13,11,17,1)	179.9964	D274	D(83,79,82,81)	-179.286
D72	D(13,11,17,18)	0.068	D275	D(83,79,82,85)	0.5741
D73	D(21,11,17,1)	0.097	D276	D(78,81,82,79)	-0.3715
D74	D(21,11,17,18)	-179.832	D277	D(78,81,82,85)	179.7817
D75	D(13,11,21,12)	-179.384	D278	D(84,81,82,79)	-179.778
D76	D(13,11,21,98)	1.4733	D279	D(84,81,82,85)	0.3756
D77	D(17,11,21,12)	0.5143	D280	D(79,82,85,86)	-179.443
D78	D(17,11,21,98)	-178.629	D281	D(81,82,85,86)	0.408
D79	D(3,12,21,11)	-0.728	D282	D(82,85,86,87)	-59.3426
D80	D(3,12,21,98)	178.4037	D283	D(82,85,86,88)	59.2856
D81	D(22,12,21,11)	178.5571	D284	D(82,85,86,89)	179.9738
D82	D(22,12,21,98)	-2.3112	D285	D(85,86,89,90)	-179.975
D83	D(3,12,22,23)	-0.4285	D286	D(85,86,89,91)	-60.2429

D84	D(3,12,22,93)	179.2637	D287	D(85,86,89,92)	60.2888
D85	D(21,12,22,23)	-179.713	D288	D(87,86,89,90)	60.3034
D86	D(21,12,22,93)	-0.0212	D289	D(87,86,89,91)	-179.965
D87	D(5,14,20,19)	0.5919	D290	D(87,86,89,92)	-59.4329
D88	D(5,14,20,25)	177.0087	D291	D(88,86,89,90)	-60.2707
D89	D(33,14,20,19)	179.7908	D292	D(88,86,89,91)	59.4613
D90	D(33,14,20,25)	-3.7925	D293	D(88,86,89,92)	179.993
D91	D(5,14,33,32)	0.1302	D294	D(22,93,96,134)	-179.329
D92	D(5,14,33,34)	-179.833	D295	D(97,93,96,134)	0.2178
D93	D(20,14,33,32)	-179.012	D296	D(22,93,97,94)	179.3087
D94	D(20,14,33,34)	1.0242	D297	D(22,93,97,98)	-0.2864
D95	D(6,19,20,14)	-0.484	D298	D(96,93,97,94)	-0.2329
D96	D(6,19,20,25)	-176.899	D299	D(96,93,97,98)	-179.828
D97	D(23,19,20,14)	-179.216	D300	D(95,94,97,93)	-179.811
D98	D(23,19,20,25)	4.3688	D301	D(95,94,97,98)	-0.2151
D99	D(6,19,23,22)	-0.0174	D302	D(134,94,97,93)	0.126
D100	D(6,19,23,24)	-179.916	D303	D(134,94,97,98)	179.7213
D101	D(20,19,23,22)	178.626	D304	D(95,94,134,96)	179.9798
D102	D(20,19,23,24)	-1.2721	D305	D(95,94,134,135)	-0.1735
D103	D(14,20,25,26)	34.663	D306	D(97,94,134,96)	0.0424
D104	D(14,20,25,27)	149.4329	D307	D(97,94,134,135)	179.8892
D105	D(14,20,25,28)	-87.9419	D308	D(93,96,134,94)	-0.1473
D106	D(19,20,25,26)	-149.519	D309	D(93,96,134,135)	179.9906
D107	D(19,20,25,27)	-34.7495	D310	D(93,97,98,21)	-1.8472
D108	D(19,20,25,28)	87.8757	D311	D(93,97,98,99)	-121.761
D109	D(11,21,98,97)	-177.856	D312	D(93,97,98,109)	115.1877
D110	D(11,21,98,99)	-60.7208	D313	D(94,97,98,21)	178.6035
D111	D(11,21,98,109)	63.1772	D314	D(94,97,98,99)	58.6902
D112	D(12,21,98,97)	3.04	D315	D(94,97,98,109)	-64.3616
D113	D(12,21,98,99)	120.1748	D316	D(21,98,99,100)	154.0382
D114	D(12,21,98,109)	-115.927	D317	D(21,98,99,101)	-31.9897
D115	D(12,22,23,19)	0.1163	D318	D(97,98,99,100)	-86.1622
D116	D(12,22,23,24)	-179.983	D319	D(97,98,99,101)	87.8099
D117	D(93,22,23,19)	-179.549	D320	D(109,98,99,100)	34.3417
D118	D(93,22,23,24)	0.3517	D321	D(109,98,99,101)	-151.686
D119	D(12,22,93,96)	-179.167	D322	D(21,98,109,110)	-86.6251
D120	D(12,22,93,97)	1.3482	D323	D(21,98,109,111)	87.9754
D121	D(23,22,93,96)	0.5256	D324	D(97,98,109,110)	153.8749
D122	D(23,22,93,97)	-178.959	D325	D(97,98,109,111)	-31.5246
D123	D(20,25,28,29)	-60.2236	D326	D(99,98,109,110)	35.3989
D124	D(20,25,28,30)	60.4188	D327	D(99,98,109,111)	-150.001
D125	D(20,25,28,31)	-179.903	D328	D(98,99,100,102)	175.1531
D126	D(26,25,28,29)	178.7874	D329	D(98,99,100,103)	-5.1015

D127	D(26,25,28,30)	-60.5701	D330	D(101,99,100,102)	1.0161
D128	D(26,25,28,31)	59.1079	D331	D(101,99,100,103)	-179.239
D129	D(27,25,28,29)	60.7811	D332	D(98,99,101,104)	-175.149
D130	D(27,25,28,30)	-178.577	D333	D(98,99,101,105)	4.5301
D131	D(27,25,28,31)	-58.8985	D334	D(100,99,101,104)	-0.8934
D132	D(7,32,33,14)	0.1444	D335	D(100,99,101,105)	178.7857
D133	D(7,32,33,34)	-179.891	D336	D(99,100,102,106)	-0.3998
D134	D(35,32,33,14)	179.7965	D337	D(99,100,102,107)	179.8485
D135	D(35,32,33,34)	-0.2391	D338	D(103,100,102,106)	179.8512
D136	D(7,32,35,36)	0.5595	D339	D(103,100,102,107)	0.0995
D137	D(7,32,35,37)	179.796	D340	D(99,101,104,106)	0.1487
D138	D(33,32,35,36)	-179.122	D341	D(99,101,104,108)	179.8386
D139	D(33,32,35,37)	0.1149	D342	D(105,101,104,106)	-179.533
D140	D(32,35,36,38)	178.4627	D343	D(105,101,104,108)	0.1568
D141	D(32,35,36,41)	-1.5023	D344	D(100,102,106,104)	-0.3657
D142	D(37,35,36,38)	-0.8584	D345	D(100,102,106,119)	178.203
D143	D(37,35,36,41)	179.1766	D346	D(107,102,106,104)	179.385
D144	D(32,35,37,39)	-178.467	D347	D(107,102,106,119)	-2.0462
D145	D(36,35,37,39)	0.8627	D348	D(101,104,106,102)	0.4894
D146	D(35,36,38,39)	0.3824	D349	D(101,104,106,119)	-178.08
D147	D(35,36,38,40)	-177.794	D350	D(108,104,106,102)	-179.199
D148	D(41,36,38,39)	-179.653	D351	D(108,104,106,119)	2.2311
D149	D(41,36,38,40)	2.1712	D352	D(102,106,119,120)	-91.4112
D150	D(35,36,41,8)	1.2859	D353	D(102,106,119,121)	146.8775
D151	D(35,36,41,42)	-118.377	D354	D(102,106,119,122)	30.3712
D152	D(35,36,41,52)	118.6286	D355	D(104,106,119,120)	87.1027
D153	D(38,36,41,8)	-178.675	D356	D(104,106,119,121)	-34.6086
D154	D(38,36,41,42)	61.6615	D357	D(104,106,119,122)	-151.115
D155	D(38,36,41,52)	-61.3325	D358	D(98,109,110,112)	175.3893
D156	D(35,37,39,38)	-0.6411	D359	D(98,109,110,113)	-4.9175
D157	D(35,37,39,76)	179.8783	D360	D(111,109,110,112)	0.6471
D158	D(36,38,39,37)	0.2761	D361	D(111,109,110,113)	-179.66
D159	D(36,38,39,76)	179.7079	D362	D(98,109,111,114)	-175.429
D160	D(40,38,39,37)	178.4731	D363	D(98,109,111,115)	4.2181
D161	D(40,38,39,76)	-2.0952	D364	D(110,109,111,114)	-0.5646
D162	D(37,39,76,77)	155.4347	D365	D(110,109,111,115)	179.0828
D163	D(37,39,76,78)	-24.8731	D366	D(109,110,112,116)	-0.259
D164	D(38,39,76,77)	-23.9403	D367	D(109,110,112,117)	179.965
D165	D(38,39,76,78)	155.7519	D368	D(113,110,112,116)	-179.957
D166	D(8,41,42,43)	156.6639	D369	D(113,110,112,117)	0.2669
D167	D(8,41,42,44)	-29.311	D370	D(109,111,114,116)	0.0901
D168	D(36,41,42,43)	-83.7126	D371	D(109,111,114,118)	179.7873
D169	D(36,41,42,44)	90.3125	D372	D(115,111,114,116)	-179.56

D170	D(52,41,42,43)	36.909	D373	D(115,111,114,118)	0.1376
D171	D(52,41,42,44)	-149.066	D374	D(110,112,116,114)	-0.2287
D172	D(8,41,52,53)	86.3677	D375	D(110,112,116,126)	178.3186
D173	D(8,41,52,54)	-88.5685	D376	D(117,112,116,114)	179.5463
D174	D(36,41,52,53)	-33.3292	D377	D(117,112,116,126)	-1.9064
D175	D(36,41,52,54)	151.7345	D378	D(111,114,116,112)	0.3119
D176	D(42,41,52,53)	-151.697	D379	D(111,114,116,126)	-178.235
D177	D(42,41,52,54)	33.3666	D380	D(118,114,116,112)	-179.384
D178	D(41,42,43,45)	175.0854	D381	D(118,114,116,126)	2.0687
D179	D(41,42,43,46)	-5.2429	D382	D(112,116,126,127)	-89.6921
D180	D(44,42,43,45)	0.8774	D383	D(112,116,126,128)	148.5686
D181	D(44,42,43,46)	-179.451	D384	D(112,116,126,129)	32.0794
D182	D(41,42,44,47)	-175.1	D385	D(114,116,126,127)	88.7985
D183	D(41,42,44,48)	4.5076	D386	D(114,116,126,128)	-32.9407
D184	D(43,42,44,47)	-0.8068	D387	D(114,116,126,129)	-149.43
D185	D(43,42,44,48)	178.8003	D388	D(106,119,120,123)	-179.852
D186	D(42,43,45,49)	-0.2899	D389	D(106,119,120,124)	-59.8021
D187	D(42,43,45,50)	179.8428	D390	D(106,119,120,125)	60.0829
D188	D(46,43,45,49)	-179.967	D391	D(121,119,120,123)	-58.0178
D189	D(46,43,45,50)	0.1661	D392	D(121,119,120,124)	62.0325
D190	D(42,44,47,49)	0.1456	D393	D(121,119,120,125)	-178.083
D191	D(42,44,47,51)	179.8861	D394	D(122,119,120,123)	58.2827
D192	D(48,44,47,49)	-179.465	D395	D(122,119,120,124)	178.333
D193	D(48,44,47,51)	0.2753	D396	D(122,119,120,125)	-61.7821
D194	D(43,45,49,47)	-0.3885	D397	D(116,126,127,130)	-179.978
D195	D(43,45,49,62)	177.9982	D398	D(116,126,127,131)	-59.9352
D196	D(50,45,49,47)	179.4783	D399	D(116,126,127,132)	59.9719
D197	D(50,45,49,62)	-2.1351	D400	D(128,126,127,130)	-58.1318
D198	D(44,47,49,45)	0.4597	D401	D(128,126,127,131)	61.9113
D199	D(44,47,49,62)	-177.927	D402	D(128,126,127,132)	-178.182
D200	D(51,47,49,45)	-179.28	D403	D(129,126,127,130)	58.1366
D201	D(51,47,49,62)	2.3336	D404	D(129,126,127,131)	178.1797
D202	D(45,49,62,63)	32.0967	D405	D(129,126,127,132)	-61.9131
D203	D(45,49,62,64)	148.6301			