**Supporting Information**

**General:** All experiments with moisture- or air-sensitive compounds were performed in anhydrous solvents under nitrogen atmosphere in well-dried glassware. Dried solvents were prepared by distillation under nitrogen. THF was dried and distilled over sodium/benzophenone. Dichloromethane and toluene were dried and distilled over calcium hydride. Column chromatography was performed with silica gel [Silica gel 60 (MERCK)]. Infrared spectra were recorded on a JASCO FT/IR-660M spectrometer. $^{1}$H NMR spectra were obtained on Bruker Mercury-300 or JEOL JNM-GSX-400. $^{13}$C NMR spectra were obtained on Bruker Mercury-300, JEOL JNM-GSX-400 or JEOL lambda-500 spectrometer. Positive EI mass spectra were taken by using Shimadzu QP-5050. High resolution mass spectra were analyzed by using Applied Biosystems Japan Ltd. Analyst QS 2.0. Data collection for X-ray crystal analysis was performed on Rigaku/Varimax diffractometer (Mo-Kα, λ = 0.71069 Å). The structure was solved with direct methods and refined with full-matrix least squares. Cyclic voltammetric measurement was conducted with a BAS Model 612D electrochemical analyzer. The cyclic voltammogram of 2,3,10,11,20,21-hexamethoxyfluorantheno-[3.3.3]propellane **6** ($1.0 \times 10^{-3}$ M) was recorded with a glassy carbon working electrode and a Pt counter electrode in dichloromethane containing 0.1 M $^{n}Bu_4NPF_6$ as a supporting electrolyte. The experiment employed an $Ag/AgNO_3$ reference electrode, and was done under argon atmosphere at room temperature.

**Computational Methods.** All DFT calculations were performed with the Gaussian 03 program.[S1] The molecular geometries were optimized with a $C_{2v}$ (for fluoranthene) or $D_{3h}$ symmetry (for **5**) constraint at the B3LYP/6-31G** level of calculation. TD calculations of fluoranthene and **5** were performed with a $C_{2v}$ (for fluoranthene) or $D_{3h}$ symmetry (for **5**) constraint by a B3LYP/6-31G method.

**1,2-Di-(1-naphthyl)acenaphthene-1,2-diol (1)** [S2] Magnesium turnings (0.61 g, 25 mmol) were treated with 1-bromonaphthalene (3.5 mL, 25 mmol) in THF at 50 °C for 30 min, and after the formation of the Grignard reagent, 1-naphthylmagnesium bromide was added to a suspension of acenaphthenequinone (1.8 g, 10 mmol) in THF (25 mL), and then the reaction mixture was heated at 50 °C for 3 h under nitrogen atmosphere. After cooling to 0 °C, the reaction mixture was poured into water, and the aqueous layer was extracted with diethyl ether three times. The combined organic layer was washed with a saturated aqueous solution of $NH_4Cl$ and brine and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (dichloromethane/hexane = 1 : 1, *v*/*v*) to give **1** as a colorless powder (4.2 g, 95%) that was used without further purification for the next step. Recrystallization of the crude compound from ethanol gave a colorless platelet crystal and the structure of **1** was confirmed by X-ray crystallographic analyses. *Crystal data* for **1**: orthorhombic, space group *P*bca (no. 61), $a$ = 10.2267(9), $b$ = 35.341(3), $c$ = 12.1236(11) Å, $V$ = 4381.7(7) Å$^3$, $T$ = 200 K, $Z$ = 8, $R1$ (w$R2$) = 0.0752 (0.2055) for 309 parameters and 4995 unique reflections. GOF = 1.026. CCDC-1037539.

**Trinaphtho[3.3.3]propellane (TNP)**

To a solution of 1,2-di(1-naphthyl)acenaphthene-1,2-diol (**1**) (10 g, 23 mmol) in toluene (400 mL) was added trifluoromethanesulfonic acid (4.0 mL, 46 mmol) at 90 °C under nitrogen. The solution was heated to reflux for 24 h and then concentrated to 150 mL. The precipitate was collected by filtration and washed with hot toluene and water, and then dried *in vacuo* to give trinaphtho[3.3.3]propellane (**TNP**) as a colorless solid (5.2 g, 57%). mp > 300 °C; $R_f$ = 0.66 (dichloromethane/hexane = 1 : 1, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ 8.02 (dd, $J$ = 6.9 Hz, 0.9 Hz, 6H), 7.60 (dd, $J$ = 8.1 Hz, 0.9 Hz, 6H), 7.53 (dd, $J$ = 8.2 Hz, 6.8 Hz, 6H); $^{13}$C NMR (126 MHz, $CDCl_3$) $\delta$ 146.6, 137.2, 132.4, 128.4, 124.2, 119.1, 79.9; EI-MS *m/z* 402 ($M^{+\bullet}$); Anal. Calcd for $C_{32}H_{18}$: C, 95.49; H, 4.51. Found: C, 95.22; H, 4.51.

**3,10,15-/-3,10,16-Tribromotrinaphtho[3.3.3]propellane (2) (mixture of isomers)**

To a solution of trinaphtho[3.3.3]propellane (0.84 g, 2.1 mmol) in dichloromethane (50 mL) was added elemental bromine (1.0 g, 6.5 mmol) and the solution was stirred at room temperature for 72 h. After quenching with saturated aqueous solution of sodium sulfite, the aqueous layer was extracted with dichloromethane. The combined organic layer was washed with and brine and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated to give **2** as a brown powder, mixture of isomers (1.3 g, quant.). mp > 300 °C; $R_f$ = 0.66 (dichloromethane/hexane = 1 : 1, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ 8.02 (m, 3H), 7.82–7.73 (m, 9H), 7.46–7.59 (m, 3H); MALDI-TOF-MS *m/z* 637.8 ($M^{+\bullet}$); $^{13}$C NMR showed complicated peaks due to the mixture of isomers; HRMS (ESI, positive): *m/z* Calcd for $C_{32}H_{15}{}^{79}Br_3$: 635.8718 [$M^{+\bullet}$]; Found: 635.8732.

**3,10,15-/-3,10,16-Tris(2-chlorophenyl)trinaphtho[3.3.3]propellane (3) (mixture of isomers)**

A mixture of 3,10,15-/-3,10,16-tribromo-trinaphtho[3.3.3]propellane (**2**) (0.83 g, 1.3 mmol), 2-chlorophenylboronic acid (0.60 g, 3.9 mmol), $Na_2CO_3$ (1.1 g, 10 mmol), and $Pd(PPh_3)_4$ (0.30 mg, 0.26 mmol) in toluene (30 mL), EtOH (30 mL) and $H_2O$ (8 mL) was stirred at 100 °C for 24 h under nitrogen. After cooling to room

temperature, the mixture was diluted with dichloromethane and washed with 1 M HCl aq. and brine, and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (dichloromethane) to give **3** as a colorless powder, mixture of isomers (0.96 g, quant.). mp > 300 °C; $R_f$ = 0.51 (dichloromethane/hexane = 2 : 3, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ 8.18–8.05 (m, 6H), 7.54–7.48 (m, 9H), 7.36–7.26 (m, 12H); $^{13}$C NMR showed complicated peaks due to the mixture of isomers; EI-MS *m/z* 733 ($M^{+\bullet}$); HRMS (ESI, positive): *m/z* Calcd for $C_{50}H_{27}{}^{35}Cl_3Na$: 755.1071 $[M+Na]^+$; Found: 755.1081.

**3,10,15-/-3,10,16-Tris(2-chloro-4,5-dimethoxyphenyl)trinaphtho[3.3.3]propellane (4) (mixture of isomers)**

A mixture of 3,10,15-/-3,10,16-tribromo-trinaphtho[3.3.3]propellane (**2**) (0.54 g, 0.84 mmol), 2-chloro-4,5-dimethoxyphenylboronic acid (0.91 g, 4.2 mmol), $Na_2CO_3$ (0.72 g, 6.8 mmol), and $Pd(PPh_3)_4$ (0.38 g, 0.33 mmol) in toluene (20 mL), EtOH (20 mL) and $H_2O$ (7 mL) was stirred at 100 °C for 24 h under nitrogen. After cooling to room temperature, the mixture was diluted with dichloromethane and washed with 1 M HCl aq. and brine, and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (dichloromethane) to give **4** as a colorless powder, mixture of isomers (0.60 g, 78%). mp > 300 °C; $R_f$ = 0.54 (dichloromethane/hexane = 2 : 3, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ 8.14–8.09 (m, 6H), 7.53–7.49 (m, 6H), 7.36 (m, 3H), 6.99 (d, *J* = 4.2 Hz, 3H), 6.75 (m, 3H), 3.93 (m, 9H) , 3.75 (m, 9H); $^{13}$C NMR showed complicated peaks due to the mixture of isomers; MALDI-TOF-MS *m/z* 912.2 ($M^{+\bullet}$); Anal. Calcd for $C_{56}H_{39}Cl_3O_6$: C, 73.57; H, 4.30. Found: C, 73.19; H, 4.41.

**Trifluorantheno[3.3.3]propellane (5)**

A mixture of 3,10,15-/-3,10,16-tris(2-chlorophenyl)trinaphtho[3.3.3]propellane (**3**) (0.87 g, 1.2 mmol), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU, 3.8 mL, 25 mmol), and $Pd(PCy_3)_2Cl_2$ (0.27 g, 0.37 mmol) in *N*-methylpyrrolidone (NMP, 30 mL) was stirred at 180 °C for 24 h under nitrogen. After cooling to room temperature, the reaction was quenched with $H_2O$ and filtered through Celite. The aqueous layer was extracted with dichloromethane and hexane several times. The combined organic layer was washed with $H_2O$ and brine and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (dichloromethane) to give **5** as a yellow powder (0.36 g, 48%). mp > 300°C; $R_f$ = 0.36 (dichloromethane/hexane = 2 : 3, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ 8.09 (d, *J* = 6.9 Hz, 6H), 7.92 (d, *J* = 6.9 Hz, 6H), 7.81 (dd, *J* = 5.4 Hz, 3.3 Hz, 6H), 7.29 (dd, *J* = 5.4 Hz, 3.3 Hz, 6H); $^{13}$C NMR (75 MHz, $CDCl_3$) $\delta$ 143.7, 140.2, 135.2, 134.5, 132.3, 127.3, 122.5, 122.2, 120.7, 93.0; MALDI-TOF-MS *m/z* 624.2 ($M^{+\bullet}$); Anal. Calcd for $C_{50}H_{24}$: C, 96.13; H, 3.87. Found: C, 95.80; H, 3.81.

**2,3,10,11,20,21-Hexamethoxyfluorantheno[3.3.3]propellane (6)**

Into a 10 mL vial were added 3,10,15-/-3,10,16-tris(2-chloro-4,5-dimethoxyphenyl)trinaphtho[3.3.3]propellane (**4**) (0.10 g, 0.11 mmol), DBU (0.30 mL, 2.0 mmol), and $Pd(PCy_3)_2Cl_2$ (42 mg, 0.057 mmol) in NMP (6 mL) and then bubbled with nitrogen. The vial was sealed with a silicon septum in an aluminum cap and then irradiated with microwaves in a CEM Discover Microwave Unit, at 150 °C for 1 h with a 300 W power max. After cooling to room

temperature, the reaction was quenched with 1 M HCl aq. and the aqueous layer was extracted with chloroform. The combined organic layer was washed with brine and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (ethyl acetate/hexane = 4 :1, *v*/*v*) to give **6** as a yellow powder (55 mg, 60%). mp > 300 °C; $R_f$ = 0.34 (ethylacetate/hexane = 4 : 1, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$8.05 (d, *J* = 3.6 Hz, 6H), 7.83 (d, *J* = 3.6 Hz, 6H), 7.37 (s, 6H), 3.98 (s, 18H); $^{13}$C NMR (75 MHz, $CDCl_3$) $\delta$148.9, 143.1, 135.4, 134.2, 133.4, 132.3 121.5, 120.5, 106.1, 92.8, 56.2; MALDI-TOF-MS *m/z* 804.4 ($M^{+\bullet}$); HRMS (ESI, positive): *m/z* Calcd for $C_{56}H_{36}O_6$: 804.2506 [$M^{+\bullet}$]; Found: 804.2518.

**1-(2-Chloro-4,5-dimethoxyphenyl)naphthalene (7)**

A mixture of naphthalen-1-ylboronic acid (0.49 g, 2.6 mmol), 1-bromo-2-chloro-4,5-dimethoxybenzene (0.57 g, 2.6 mmol), $Na_2CO_3$ (1.6 g, 15 mmol), and $Pd(PPh_3)_4$ (0.62 mg, 0.53 mmol) in toluene (20 mL), EtOH (20 mL) and $H_2O$ (10 mL) was stirred at 100 °C for 24 h under nitrogen. After cooling to room temperature, the mixture was diluted with dichloromethane and washed with 1 M HCl aq. and brine, and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (dichloromethane) to give **7** as a colorless powder (0.66 mg, 85%). mp 104-105 °C; $R_f$ = 0.36 (dichloromethane/hexane = 2 : 3, *v*/*v*); $^1$H NMR (400 MHz, $CDCl_3$) $\delta$7.99 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.55-7.38 (m, 5H), 7.03 (s, 1H), 6.85 (d, 1H), 3.95 (s, 3H), 3.82 (s, 3H); $^{13}$C NMR (101 MHz, $CDCl_3$) $\delta$150.3, 148.9, 138.6, 134.8, 133.1, 132.3, 129.5, 129.4, 128.7, 127.4, 127.2, 127.1, 126.5, 126.4, 115.7, 113.7, 57.5, 57.4; EI-MS *m/z* 732.8 ($M^{+\bullet}$); HRMS (ESI, positive): m/z Calcd for $C_{18}H_{15}O_2{}^{35}Cl$: 298.0755 [$M^{+\bullet}$]; Found: 298.0760.

**8,9-dimethoxyfluoranthene (8)**

Into a 10 mL glass reaction vial were added 1-(2-chloro-4,5-dimethoxyphenyl)naphthalene (67 mg, 0.21 mmol), DBU (0.60 mL, 4.0 mmol), and $Pd(PCy_3)_2Cl_2$ (46 mg, 0.063 mmol) in NMP (5 mL) and then bubbled with nitrogen. The vial was sealed with a silicon septum in an aluminum cap and then irradiated with microwaves at 180 °C and the vial was then irradiated with microwaves in a CEM Discover Microwave Unit, at 150 °C for 30 min with a 300 W power max. After cooling to room temperature, the reaction was quenched with 1 M HCl aq. and the aqueous layer was extracted with chloroform. The combined organic layer was washed with brine and then dried over anhydrous sodium sulfate. After filtration, the filtrate was evaporated and the residue was purified by column chromatography on silica gel (ethylacetate/hexane = 1 : 4, *v*/*v*) to give **8** as a yellow powder (31 mg, 57%). mp > 300 °C; $R_f$ = 0.40 (ethylacetate/hexane = 1 : 4, *v*/*v*); $^1$H NMR (300 MHz, $CDCl_3$) $\delta$7.82 (d, *J* = 7.5 Hz, 2H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.58 (dd, *J* = 7.8 Hz, 7.2 Hz, 2H), 7.45 (s, 2H), 4.03 (s, 6H); $^{13}$C NMR (75 MHz, $CDCl_3$) $\delta$149.4, 137.3, 132.7, 132.5, 130.0, 129.8, 126.0, 119.3, 105.4, 56.4; EI-MS *m/z* 262 ($M^{+\bullet}$); Anal. Calcd for $C_{18}H_{14}O_2$: C, 82.42; H, 5.38. Found: C, 82.26; H, 5.43.

**References**


S1. Frisch, M. J.; et al. Gaussian 03, revision D.01; Gaussian, Inc.:Wallingford, CT, 2004.

S2. E. J. Moriconi, W. F. O'Connor, L. P. Kuhn, E. A. Keneally, and F. T. Wallenberger, *J. Am. Chem. Soc.*, 1959, **81**, 6472–6477.

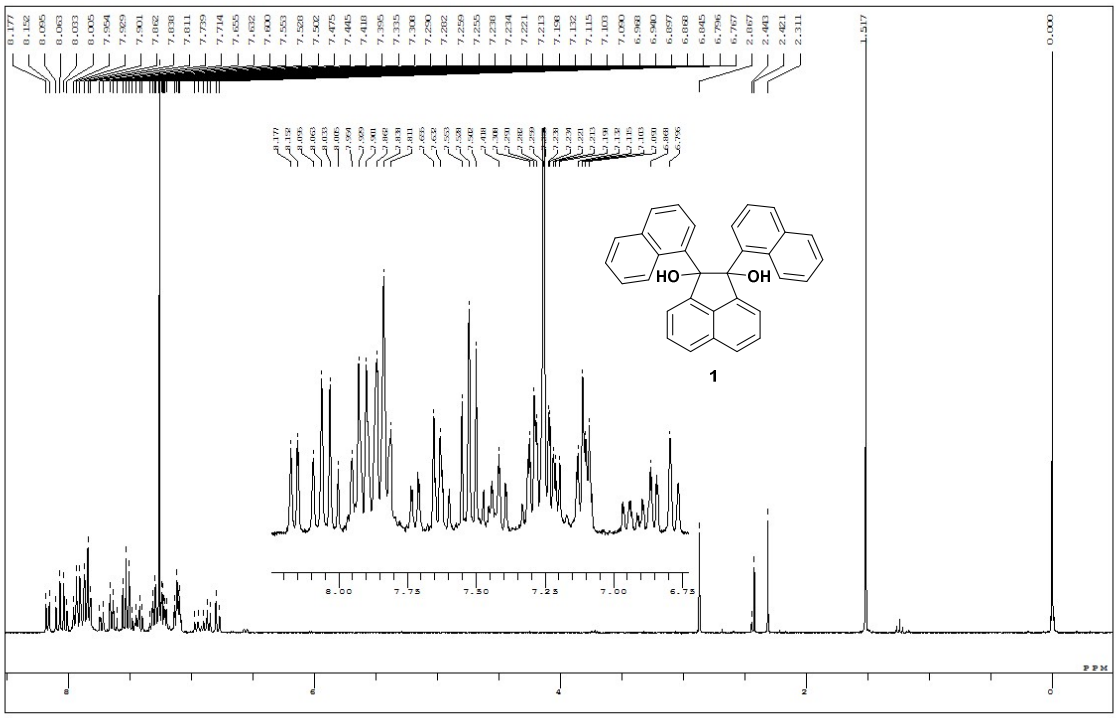


**Figure S1** $^{1}$H NMR spectrum of **1**

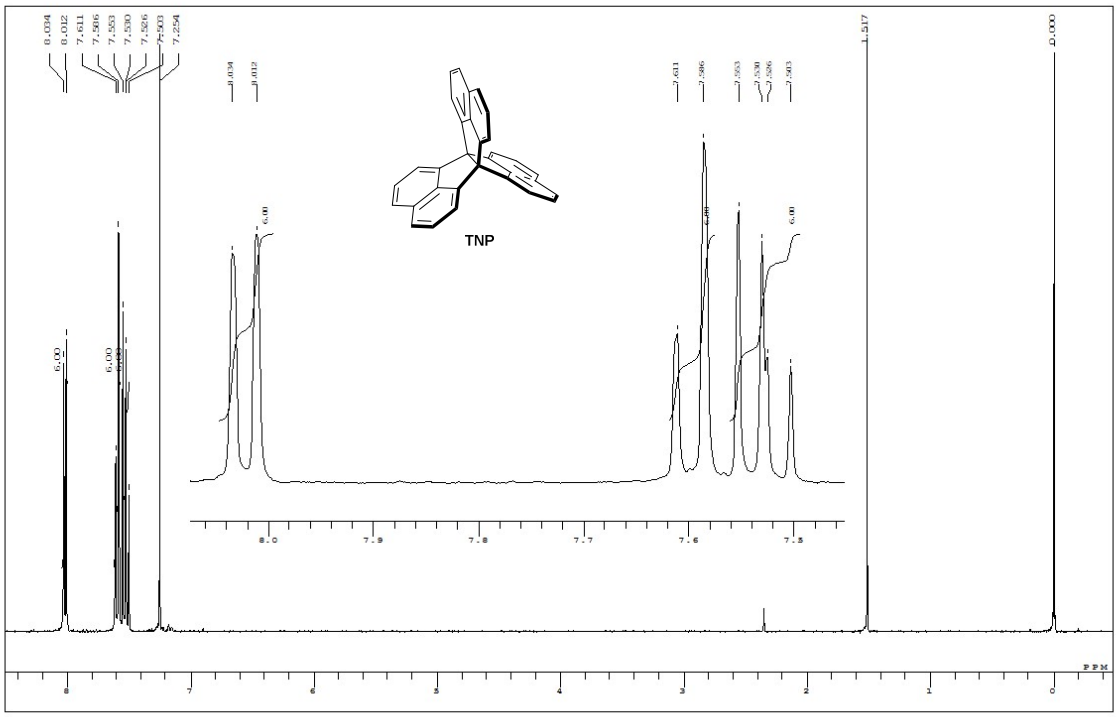


**Figure S2** $^{1}$H NMR spectrum of Trinaphtho[3.3.3]propellane

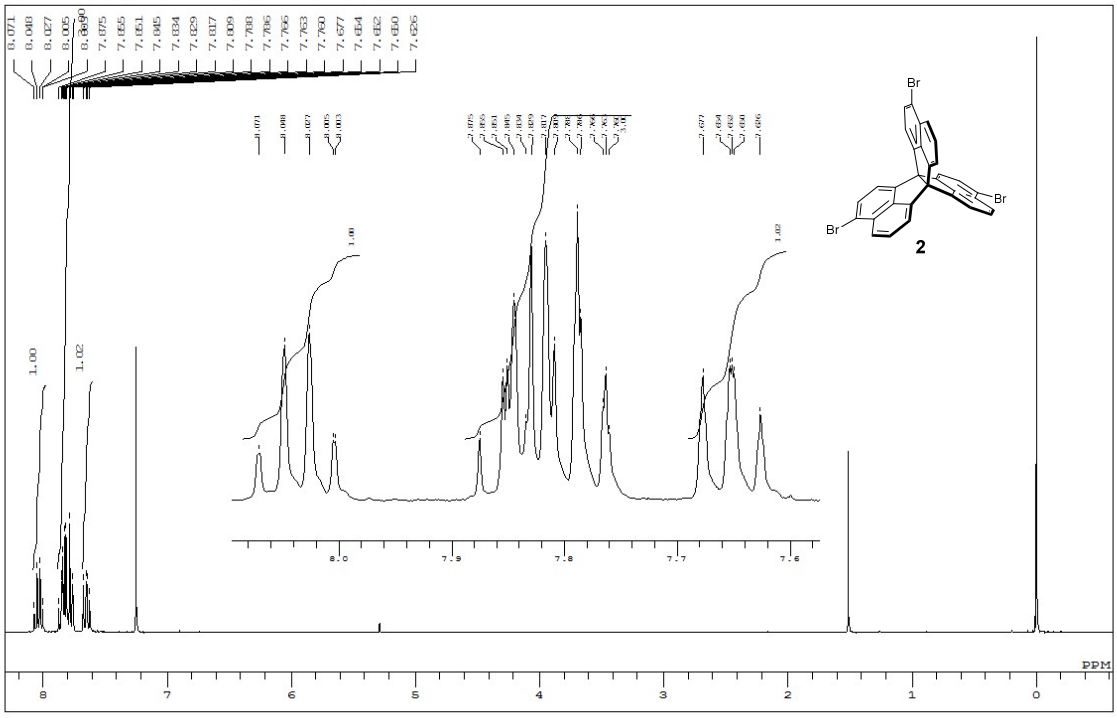


**Figure S3** $^{1}$H NMR spectrum of **2**

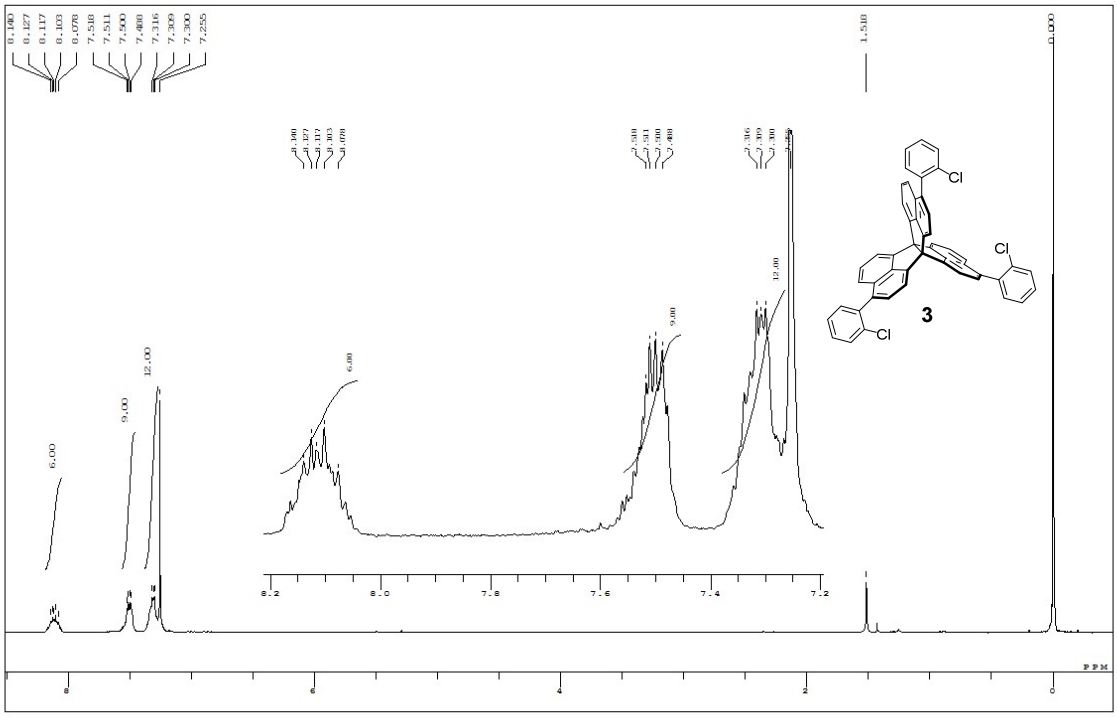


**Figure S4** $^{1}$H NMR spectrum of **3**

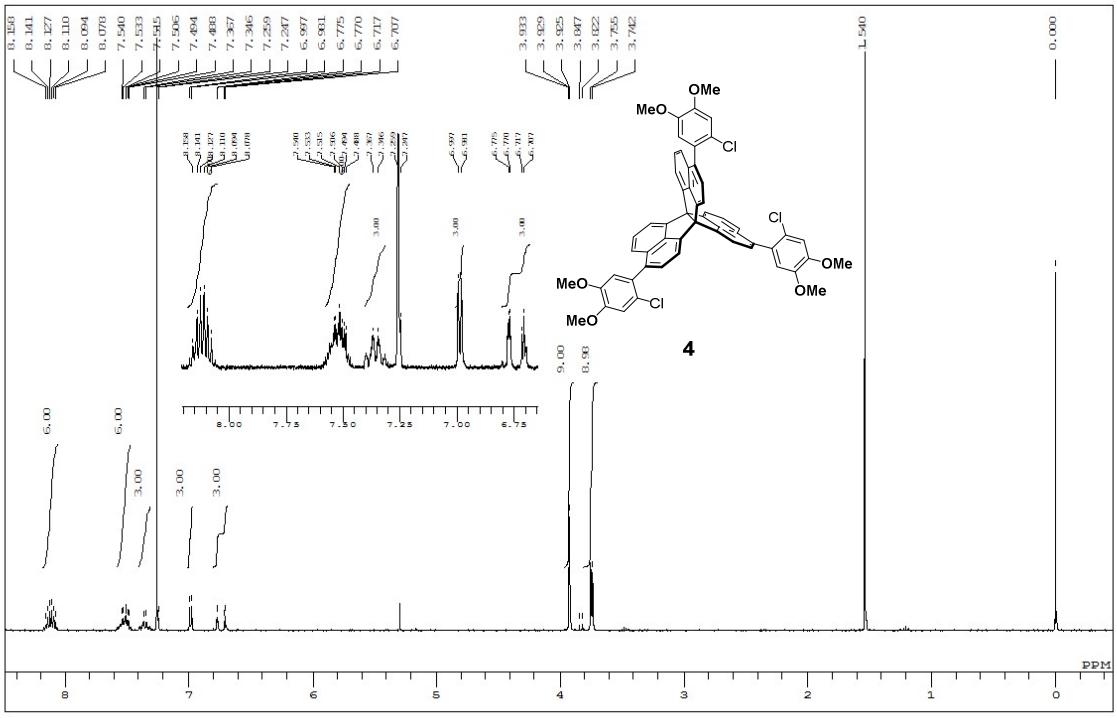


**Figure S5** $^{1}$H NMR spectrum of **4**

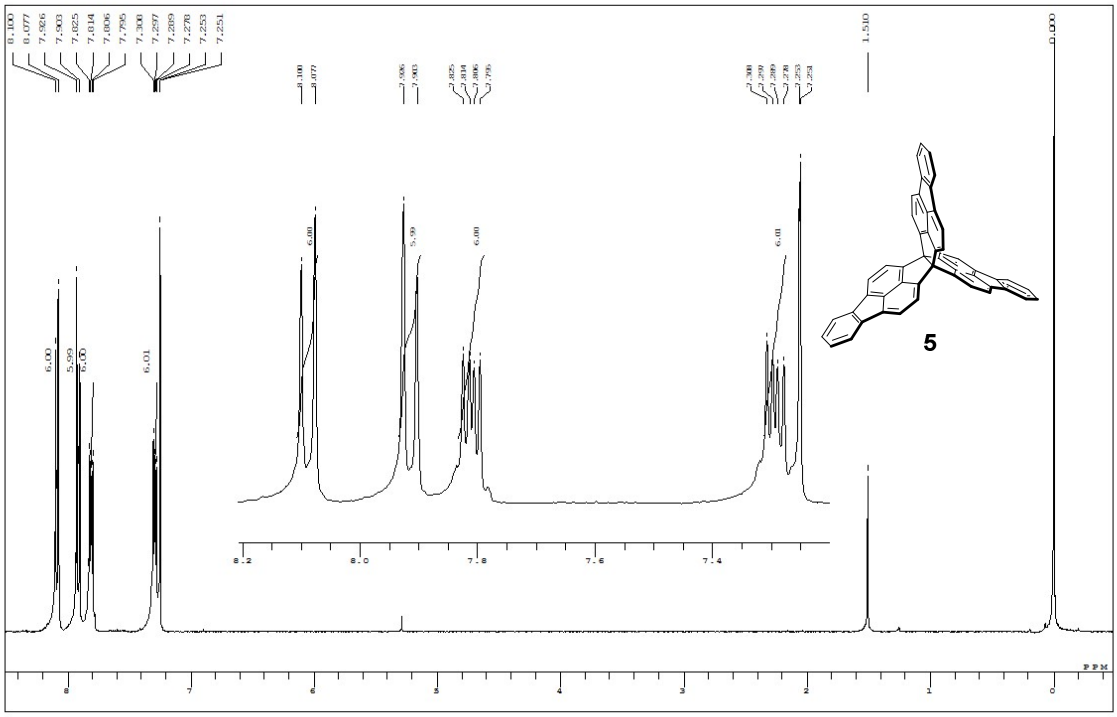


**Figure S6** $^{1}$H NMR spectrum of **5**

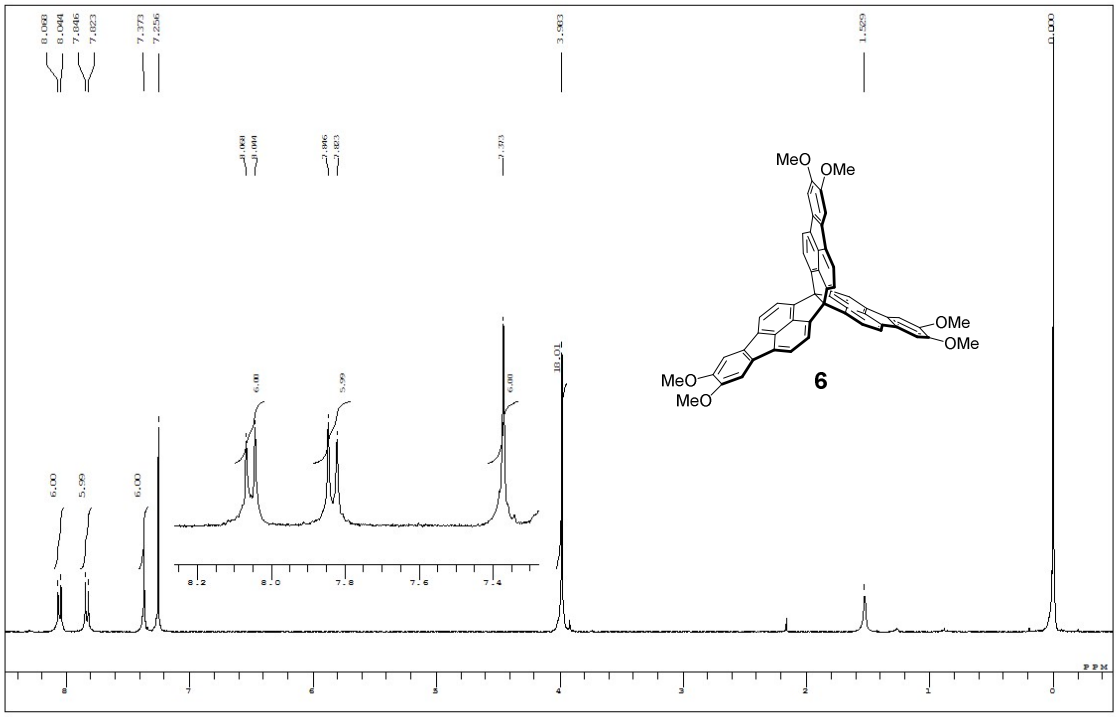


**Figure S7** $^{1}$H NMR spectrum of **6**

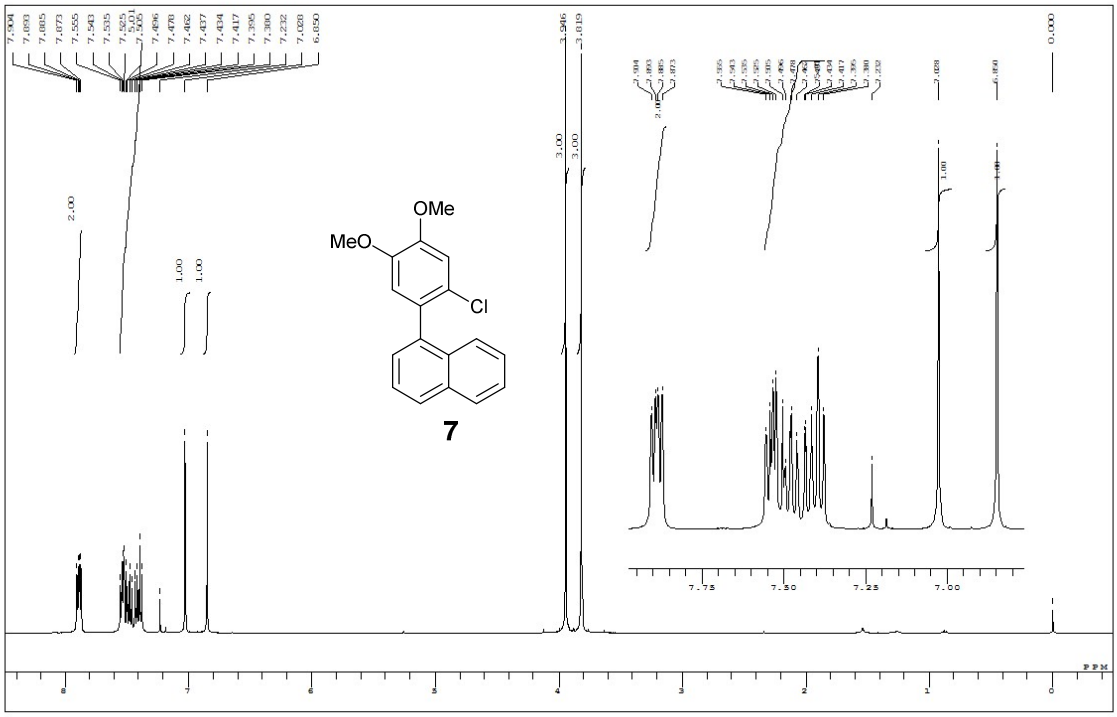


**Figure S8** $^{1}$H NMR spectrum of **7**

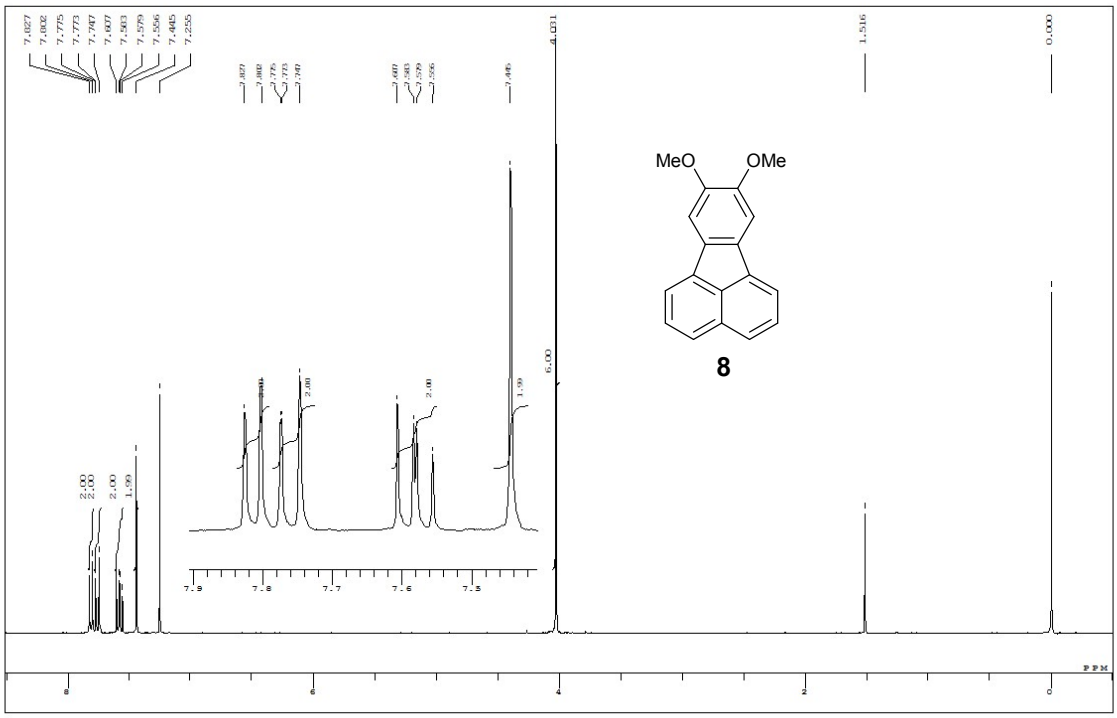


**Figure S9** $^{1}$H NMR spectrum of **8**

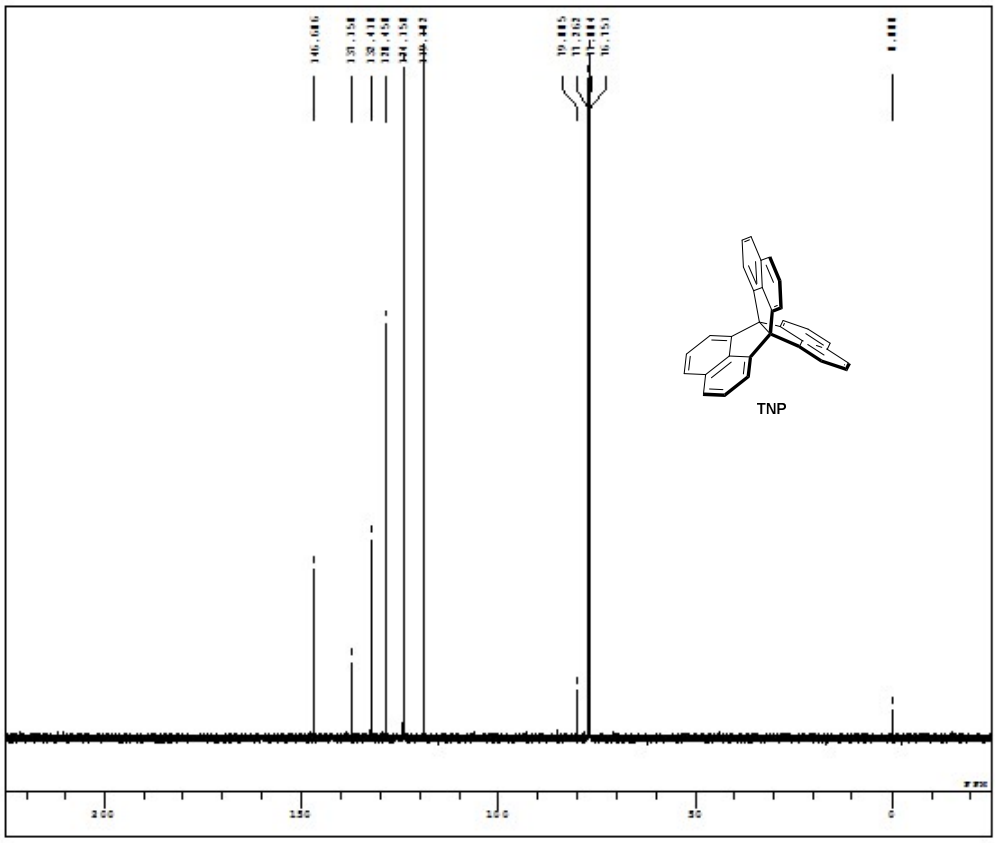


**Figure S10** $^{13}$C NMR spectrum of Trinaphtho[3.3.3]propellane

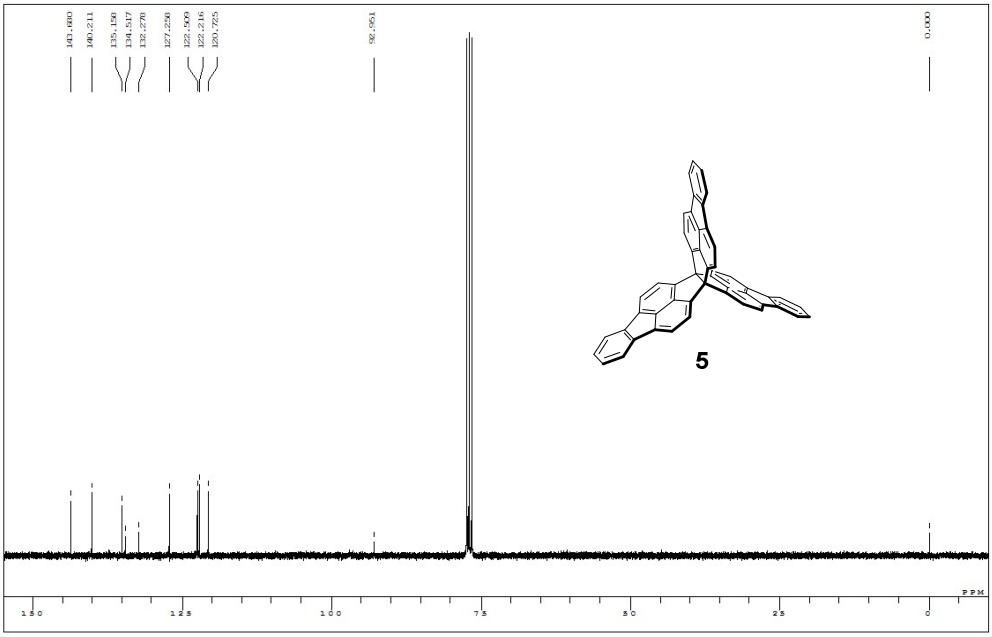


**Figure S11** $^{13}$C NMR spectrum of **5**

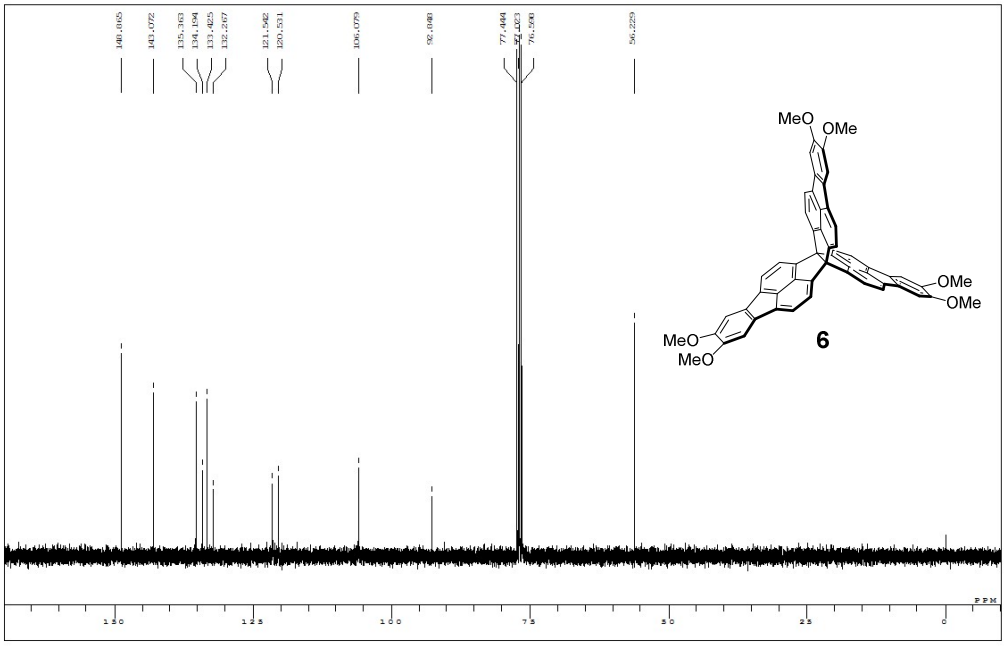


**Figure S12** $^{13}$C NMR spectrum of **6**

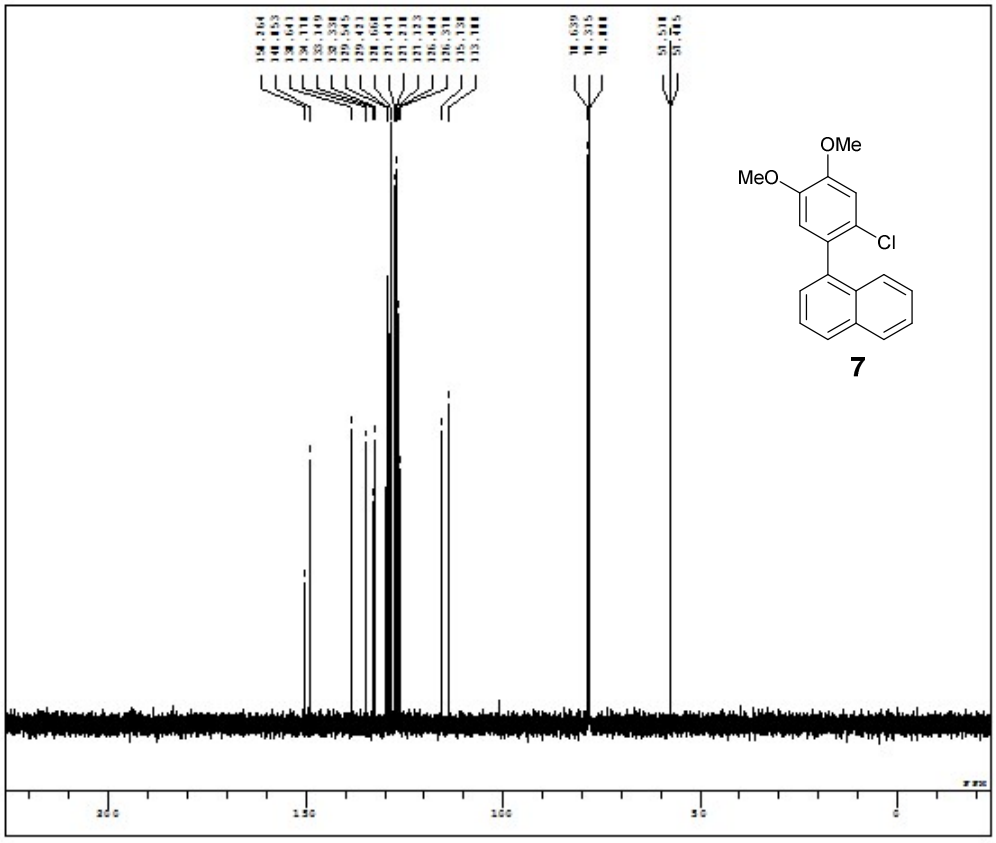


**Figure S13** $^{13}$C NMR spectrum of **7**

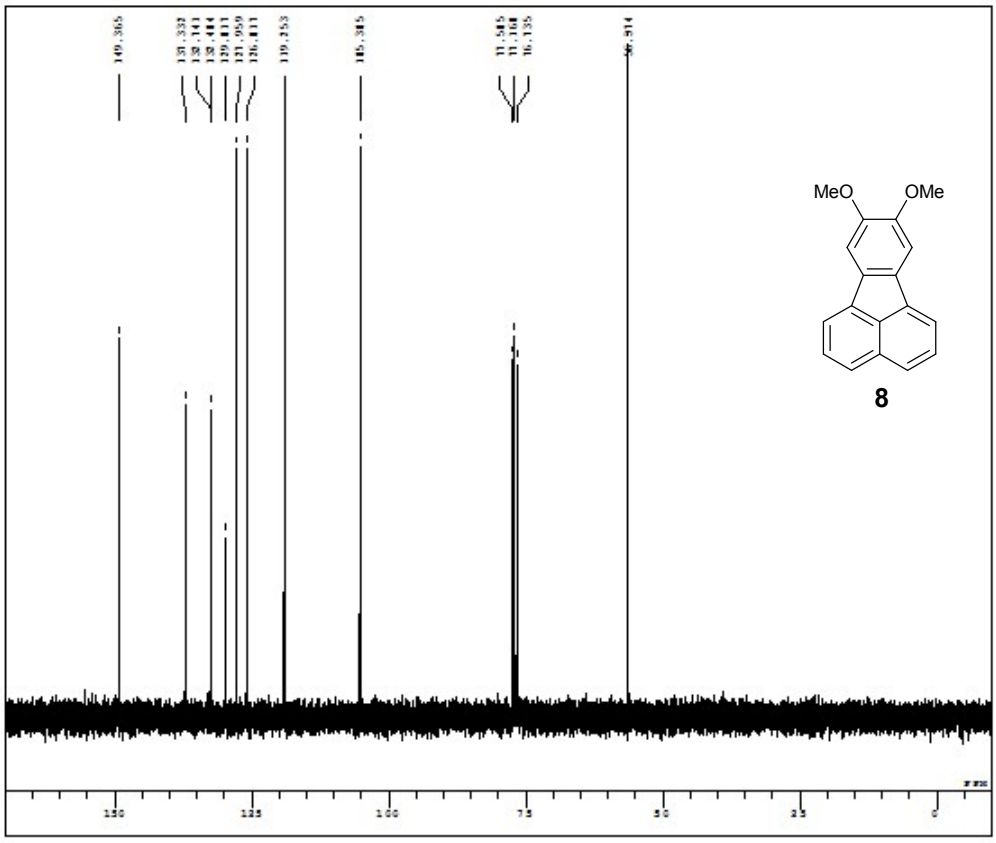


**Figure S14** $^{13}$C NMR spectrum of **8**

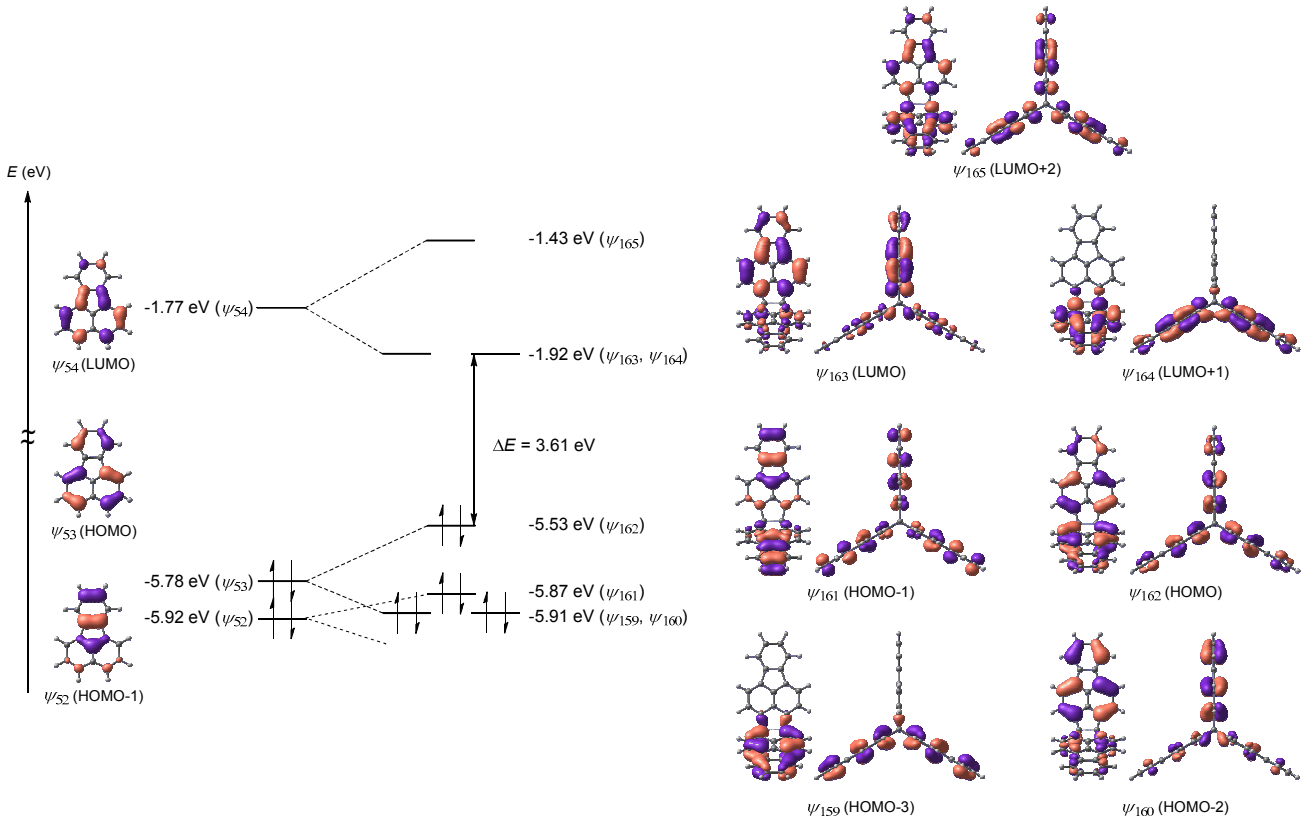


**Figure S15** MO correlation diagram between fluoranthene and **5** estimated at the B3LYP/6-31G** level of calculation.

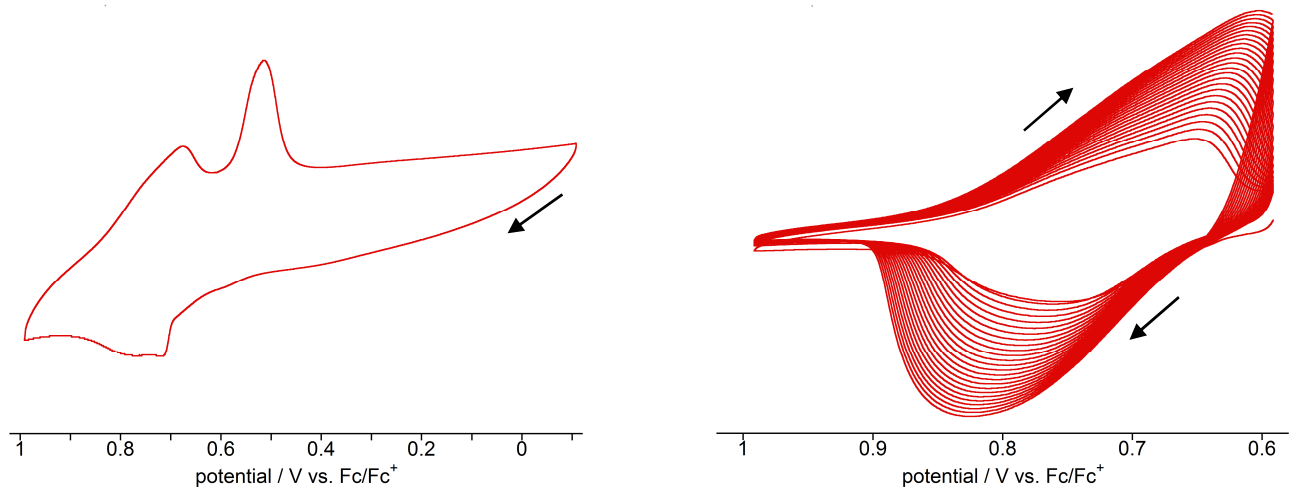


**Figure S16** Cyclic voltammograms of **6** ($1.0 \times 10^{-3}$ M) in $CH_2Cl_2$ at room temperature. Scan rate = 0.1 V $s^{-1}$. (left) Single scan in the range of –0.1 to +1.0 V. (right) Repeated scans in the range of +0.6 to +1.0 V.

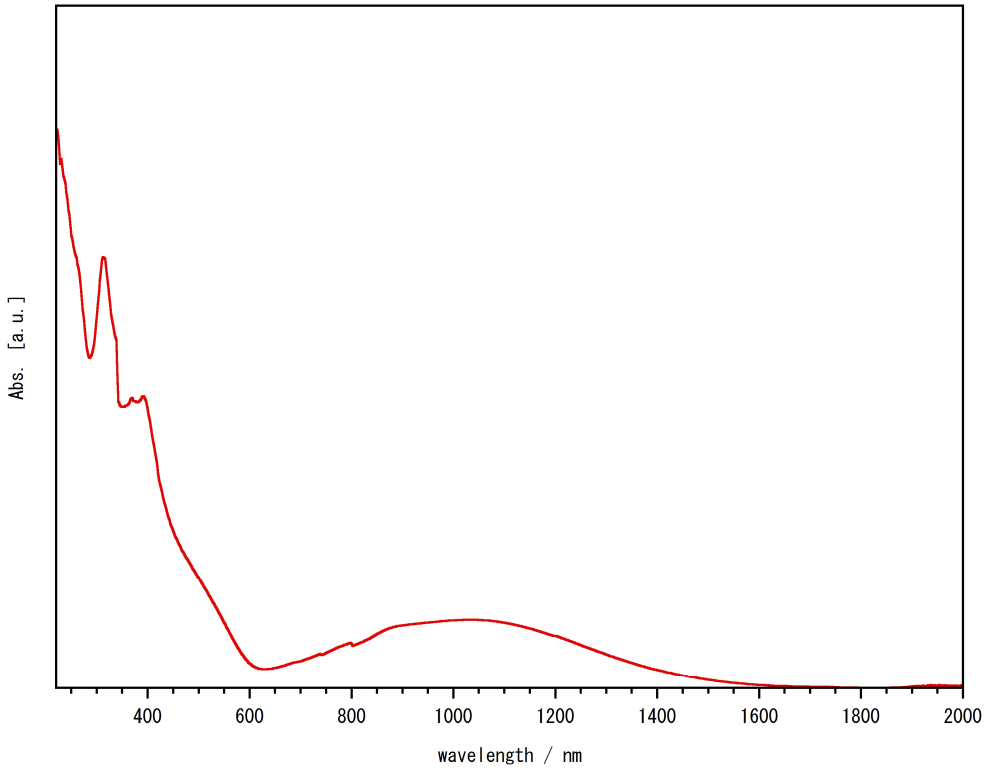


**Figure S17** Solid state electronic absorption spectrum of $\mathbf{6}_2(F_4\text{-TCNQ})_3$ in a KBr pellet.

# GAUSSIAN INPUT DATA

**Geometry optimization of fluoranthene**

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fluoranthene

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6       0.000000000     0.000000000    -2.293934018
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1      -2.524455945     0.000000000     2.478448690
1      -1.242494323     0.000000000     4.637426348
1       1.242494323     0.000000000     4.637426348
1       2.524455945     0.000000000     2.478448690
```

**TD calculation of fluoranthene**

```
#P B3LYP/6-31G TD FormCheck=All Pop=(Reg) SCF=(MaxCycle=200)

fluoranthene

   0   1
6       2.401863831     0.000000000    -0.715767469
6       2.434015325     0.000000000    -2.141841488
6       1.285331115     0.000000000    -2.913858494
6       0.000000000     0.000000000    -2.293934018
6       0.000000000     0.000000000    -0.901599004
6       1.170627011     0.000000000    -0.101084945
6      -1.285331115     0.000000000    -2.913858494
6      -2.434015325     0.000000000    -2.141841488
6      -2.401863831     0.000000000    -0.715767469
6      -1.170627011     0.000000000    -0.101084945
6       0.706220183     0.000000000     1.285077986
6      -0.706220183     0.000000000     1.285077986
6      -1.423918346     0.000000000     2.479708586
6      -0.700404067     0.000000000     3.677544304
6       0.700404067     0.000000000     3.677544304
6       1.423918346     0.000000000     2.479708586
1       3.329191695     0.000000000    -0.123474231
1       3.414932441     0.000000000    -2.646094030
```

```
1       1.360225744     0.000000000    -4.013058087
1      -1.360225744     0.000000000    -4.013058087
1      -3.414932441     0.000000000    -2.646094030
1      -3.329191695     0.000000000    -0.123474231
1      -2.524455945     0.000000000     2.478448690
1      -1.242494323     0.000000000     4.637426348
1       1.242494323     0.000000000     4.637426348
1       2.524455945     0.000000000     2.478448690
```

**Geometry optimization of 5**

```
#P B3LYP/6-31G** opt FormCheck=All Pop=(Reg) SCF=(MaxCycle=200)

fluoranthene propellane

   0   1
6       3.133651474    -1.809214522    -2.388902045
6       1.890761797    -1.091631832    -2.395548777
6       1.264542959    -0.730084218    -1.227650308
6       1.880263759    -1.085570788     0.000000000
6       3.062847560    -1.768335863     0.000000000
6       3.727637593    -2.152152568    -1.200026431
6       1.264542959    -0.730084218     1.227650308
6       1.890761797    -1.091631832     2.395548777
6       3.133651474    -1.809214522     2.388902045
6       3.727637593    -2.152152568     1.200026431
6       4.934436712    -2.848898364    -0.720224617
6       4.934436712    -2.848898364     0.720224617
6       5.964562711    -3.443641887     1.416927152
6       7.003863492    -4.043682472     0.692824020
6       7.003863492    -4.043682472    -0.692824020
6       5.964562711    -3.443641887    -1.416927152
6      -3.133651474    -1.809214522    -2.388902045
6      -1.890761797    -1.091631832    -2.395548777
6      -1.264542959    -0.730084218    -1.227650308
6      -1.880263759    -1.085570788     0.000000000
6      -3.062847560    -1.768335863     0.000000000
6      -3.727637593    -2.152152568    -1.200026431
6      -1.264542959    -0.730084218     1.227650308
6      -1.890761797    -1.091631832     2.395548777
6      -3.133651474    -1.809214522     2.388902045
6      -3.727637593    -2.152152568     1.200026431
6      -4.934436712    -2.848898364    -0.720224617
6      -4.934436712    -2.848898364     0.720224617
6      -5.964562711    -3.443641887     1.416927152
6      -7.003863492    -4.043682472     0.692824020
6      -7.003863492    -4.043682472    -0.692824020
6      -5.964562711    -3.443641887    -1.416927152
6       0.000000000     3.618429044    -2.388902045
6       0.000000000     2.183263664    -2.395548777
6       0.000000000     1.460168436    -1.227650308
6       0.000000000     2.171141575     0.000000000
6       0.000000000     3.536671726     0.000000000
6       0.000000000     4.304305136    -1.200026431
6       0.000000000     1.460168436     1.227650308
6       0.000000000     2.183263664     2.395548777
6       0.000000000     3.618429044     2.388902045
6       0.000000000     4.304305136     1.200026431
6       0.000000000     5.697796728    -0.720224617
6       0.000000000     5.697796728     0.720224617
6       0.000000000     6.887283774     1.416927152
```

```
6       0.000000000     8.087364945     0.692824020
6       0.000000000     8.087364945    -0.692824020
6       0.000000000     6.887283774    -1.416927152
6       0.000000000     0.000000000    -0.894103708
6       0.000000000     0.000000000     0.894103708
1       3.593375732    -2.074636446    -3.346076921
1       1.440441255    -0.831639146    -3.359745521
1       1.440441255    -0.831639146     3.359745521
1       3.593375732    -2.074636446     3.346076921
1       5.972297375    -3.448107497     2.511424017
1       7.827148535    -4.519006314     1.235916631
1       7.827148535    -4.519006314    -1.235916631
1       5.972297375    -3.448107497    -2.511424017
1      -3.593375732    -2.074636446    -3.346076921
1      -1.440441255    -0.831639146    -3.359745521
1      -1.440441255    -0.831639146     3.359745521
1      -3.593375732    -2.074636446     3.346076921
1      -5.972297375    -3.448107497     2.511424017
1      -7.827148535    -4.519006314     1.235916631
1      -7.827148535    -4.519006314    -1.235916631
1      -5.972297375    -3.448107497    -2.511424017
1       0.000000000     4.149272892    -3.346076921
1       0.000000000     1.663278293    -3.359745521
1       0.000000000     1.663278293     3.359745521
1       0.000000000     4.149272892     3.346076921
1       0.000000000     6.896214994     2.511424017
1       0.000000000     9.038012628     1.235916631
1       0.000000000     9.038012628    -1.235916631
1       0.000000000     6.896214994    -2.511424017
```

**TD calculation of 5**

```
#P B3LYP/6-31G TD(nstate=10) FormCheck=All Pop=(Reg) SCF=(MaxCycle=200)

fluoranthene propellane

   0   1
6       0.000000000     3.646896000     2.382248000
6       0.000000000     2.211768000     2.388103000
6       0.000000000     1.487749000     1.204170000
6       0.000000000     2.213707000     0.000000000
6       0.000000000     3.589380000     0.000000000
6       0.000000000     4.351472000     1.184796000
6       0.000000000     1.487749000    -1.204170000
6       0.000000000     2.211768000    -2.388103000
6       0.000000000     3.646896000    -2.382248000
6       0.000000000     4.351472000    -1.184796000
6       0.000000000     5.756871000     0.719018000
6       0.000000000     5.756871000    -0.719018000
6       0.000000000     6.961488000    -1.414310000
6       0.000000000     8.164959000    -0.698516000
6       0.000000000     8.164959000     0.698516000
6       0.000000000     6.961488000     1.414310000
6      -3.158304000    -1.823448000     2.382248000
6      -1.915448000    -1.105884000     2.388103000
6      -1.288429000    -0.743875000     1.204170000
6      -1.917126000    -1.106853000     0.000000000
6      -3.108494000    -1.794690000     0.000000000
6      -3.768485000    -2.175736000     1.184796000
6      -1.288429000    -0.743875000    -1.204170000
6      -1.915448000    -1.105884000    -2.388103000
6      -3.158304000    -1.823448000    -2.382248000
```

| | | | |
|---|---|---|---|
| 6 | -3.768485000 | -2.175736000 | -1.184796000 |
| 6 | -4.985596000 | -2.878435000 | 0.719018000 |
| 6 | -4.985596000 | -2.878435000 | -0.719018000 |
| 6 | -6.028825000 | -3.480744000 | -1.414310000 |
| 6 | -7.071062000 | -4.082479000 | -0.698516000 |
| 6 | -7.071062000 | -4.082479000 | 0.698516000 |
| 6 | -6.028825000 | -3.480744000 | 1.414310000 |
| 6 | 3.158304000 | -1.823448000 | 2.382248000 |
| 6 | 1.915448000 | -1.105884000 | 2.388103000 |
| 6 | 1.288429000 | -0.743875000 | 1.204170000 |
| 6 | 1.917126000 | -1.106853000 | 0.000000000 |
| 6 | 3.108494000 | -1.794690000 | 0.000000000 |
| 6 | 3.768485000 | -2.175736000 | 1.184796000 |
| 6 | 1.288429000 | -0.743875000 | -1.204170000 |
| 6 | 1.915448000 | -1.105884000 | -2.388103000 |
| 6 | 3.158304000 | -1.823448000 | -2.382248000 |
| 6 | 3.768485000 | -2.175736000 | -1.184796000 |
| 6 | 4.985596000 | -2.878435000 | 0.719018000 |
| 6 | 4.985596000 | -2.878435000 | -0.719018000 |
| 6 | 6.028825000 | -3.480744000 | -1.414310000 |
| 6 | 7.071062000 | -4.082479000 | -0.698516000 |
| 6 | 7.071062000 | -4.082479000 | 0.698516000 |
| 6 | 6.028825000 | -3.480744000 | 1.414310000 |
| 6 | 0.000000000 | 0.000000000 | 0.854601000 |
| 6 | 0.000000000 | 0.000000000 | -0.854601000 |
| 1 | 0.000000000 | 4.161039000 | 3.339757000 |
| 1 | 0.000000000 | 1.707855000 | 3.350598000 |
| 1 | 0.000000000 | 1.707855000 | -3.350598000 |
| 1 | 0.000000000 | 4.161039000 | -3.339757000 |
| 1 | 0.000000000 | 6.973095000 | -2.500778000 |
| 1 | 0.000000000 | 9.108514000 | -1.236237000 |
| 1 | 0.000000000 | 9.108514000 | 1.236237000 |
| 1 | 0.000000000 | 6.973095000 | 2.500778000 |
| 1 | -3.603566000 | -2.080520000 | 3.339757000 |
| 1 | -1.479046000 | -0.853928000 | 3.350598000 |
| 1 | -1.479046000 | -0.853928000 | -3.350598000 |
| 1 | -3.603566000 | -2.080520000 | -3.339757000 |
| 1 | -6.038877000 | -3.486548000 | -2.500778000 |
| 1 | -7.888204000 | -4.554257000 | -1.236237000 |
| 1 | -7.888204000 | -4.554257000 | 1.236237000 |
| 1 | -6.038877000 | -3.486548000 | 2.500778000 |
| 1 | 3.603566000 | -2.080520000 | 3.339757000 |
| 1 | 1.479046000 | -0.853928000 | 3.350598000 |
| 1 | 1.479046000 | -0.853928000 | -3.350598000 |
| 1 | 3.603566000 | -2.080520000 | -3.339757000 |
| 1 | 6.038877000 | -3.486548000 | -2.500778000 |
| 1 | 7.888204000 | -4.554257000 | -1.236237000 |
| 1 | 7.888204000 | -4.554257000 | 1.236237000 |
| 1 | 6.038877000 | -3.486548000 | 2.500778000 |