Electronic Supplementary Information

for

Boron-Doped Double [6]Carbohelicenes: A Combination of Helicene and Boron-Doped π-System

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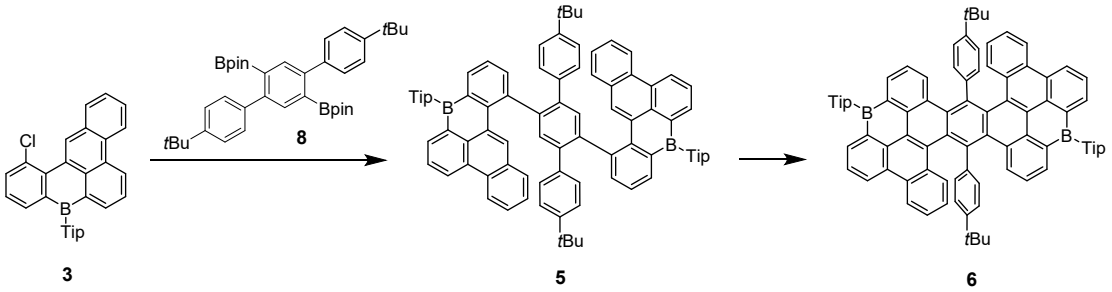
Contents

1. Experimental details

General. ^{1}H and ^{13}C NMR spectra were obtained using Zhongke Niujin AS400 or Bruker AV III HD-500 spectrometer (400 MHz for ^{1}H NMR, and 101 MHz for ^{13}C NMR) spectrometer in $CDCl_3$. Chemical shifts are reported in δ ppm using $CDCl_3$ (7.26 ppm) for ^{1}H NMR and $CDCl_3$ (77.16 ppm) for ^{13}C NMR as internal standard. High resolution mass spectra were measured with a Brucker Autoflex speed TOF spectrometer. UV-vis-NIR absorption and fluorescence spectra were measured using Hitachi U-2900 spectrometer and Hitachi F-7000 spectrometer, respectively. The absolute fluorescence quantum yields and fluorescence lifetimes were measured using Edinburgh FLS920 steady state fluorimeter equipping with an integrating sphere. Femtosecond transient absorption spectra were measured with Ultrafast Systems LLC Helios Fire spectrometer. Cyclic voltammetry (CV) was performed on a CHI660e electrochemical workstation using nBu$_4$NPF$_6$ (0.1 M) as electrolyte at a scan rate of 100 mV s^{-1}. The CV cell has the glassy carbon electrode, Pt wire counter electrode and Ag/Ag^{+} reference electrode. The measurement was carried out under an argon atmosphere in $C_2H_4Cl_2$ (1.0 mM). The redox potentials were internally calibrated using the ferrocene/ferrocenium couple. The blend film was spin-coated on the quartz substrate and then irradiated with the third harmonic (355 nm) of a Nd:YAG (yttrium-aluminum-garnet) laser at a repetition rate of 10 Hz and pulse duration of about 10 ns in the laser test. The energy of the pumping laser was adjusted by using the calibrated neutral density filters. A cylindrical lens and a slit were used to focus the beam into a stripe whose shape is adjusted to 3.3 × 0.6 mm. The edge emission of the film was detected by using a Maya2000 Pro CCD spectrometer.

Materials and reagents. All reactions were performed under an argon atmosphere, unless stated otherwise. Commercially available solvents and reagents were used without further purification unless otherwise mentioned. Compounds **3**, **4** and **8** were prepared according to the literature methods.[1,2]

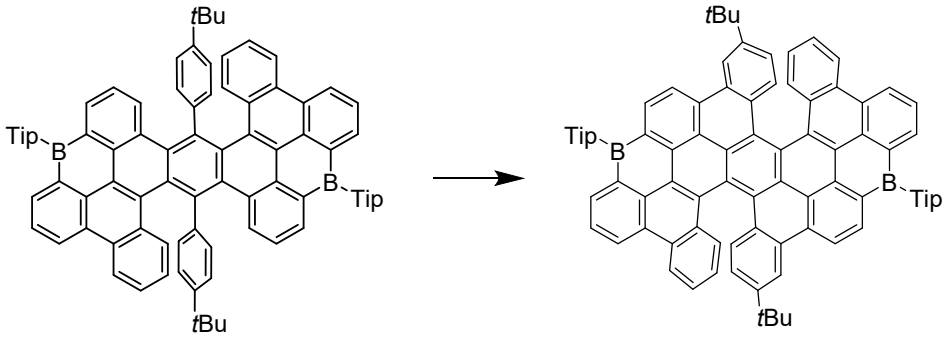
2. Syntheses and characterizations



Compound 5: In a Schlenk tube, a mixture of **3** (199.8 mg, 0.40 mmol), **8** (108 mg, 0.18 mmol), $Pd(PPh_3)_4$ (8.4 mg, 0.0073 mmol), 2-dicyclohexylphosphino-2′,6′-dimethoxybiphenyl (6.1 mg, 0.015 mmol) and K_3PO_4 (152.6 mg, 0.72 mmol) was dispersed in toluene (8 mL), ethanol (1.5 mL) and water (1.5 mL) under argon. The reaction mixture was stirred at 100 °C for 24 h. After cooling down to room temperature, the mixture was poured into water and extracted with ethyl acetate for three times. The combined organic layer was washed with water and dried over anhydrous Na_2SO_4. The solvents were removed under reduced pressure and the residue was purified on silica gel column chromatography with CH_2Cl_2/hexane (1/6) as eluent to give compound **5** (143.6 mg, 62%) as a yellow-green solid. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 8.91 (d, J = 8.0 Hz, 2H), 8.71 (d, J = 8.0 Hz, 2H), 8.22 (s, 2H), 7.99 (d, J = 8.0 Hz, 2H), 7.90 (d, J = 8.0 Hz, 2H), 7.83 (d, J = 8.0 Hz, 2H), 7.73 (t, J = 16.0 Hz, 2H), 7.67 (s, 2H), 7.63 (t, J = 16.0 Hz, 4H), 7.56 (t, J = 12.0 Hz, 2H), 7.41 (d, J = 8.0 Hz, 2H), 7.17 (s, 2H), 7.05 (s, 2H), 6.54 (d, J = 8.0 Hz, 4H), 6.37 (d, J = 8.0 Hz, 4H), 3.06−2.99 (m, 2H), 2.54 −2.48 (m, 2H), 2.18−2.13 (m, 2H), 1.39 (d, J = 8.0 Hz, 12H), 1.26−1.20 (m, 12H), 0.98 (d, J = 8.0 Hz, 6H), 0.88 (s, 18H), 0.76 (d, J = 8.0 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ (ppm) 150.32, 150.05, 149.00, 148.27, 142.92, 142.21, 140.59, 140.02, 139.52, 138.37, 137.49, 137.23, 133.47, 132.57, 132.30, 131.64, 130.86, 130.77, 129.35, 129.10, 128.78, 128.28, 127.63, 126.76, 126.68, 125.61, 123.62, 122.38, 120.13, 120.02, 35.36, 34.43, 31.11, 24.99, 24.37, 24.09. HR-MALDI-TOF MS (m/z): [M] calcd. for $C_{96}H_{96}B_2$, 1270.7742; found: 1270.7791.

Compound 6: 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (57.2 mg, 0.25 mmol)

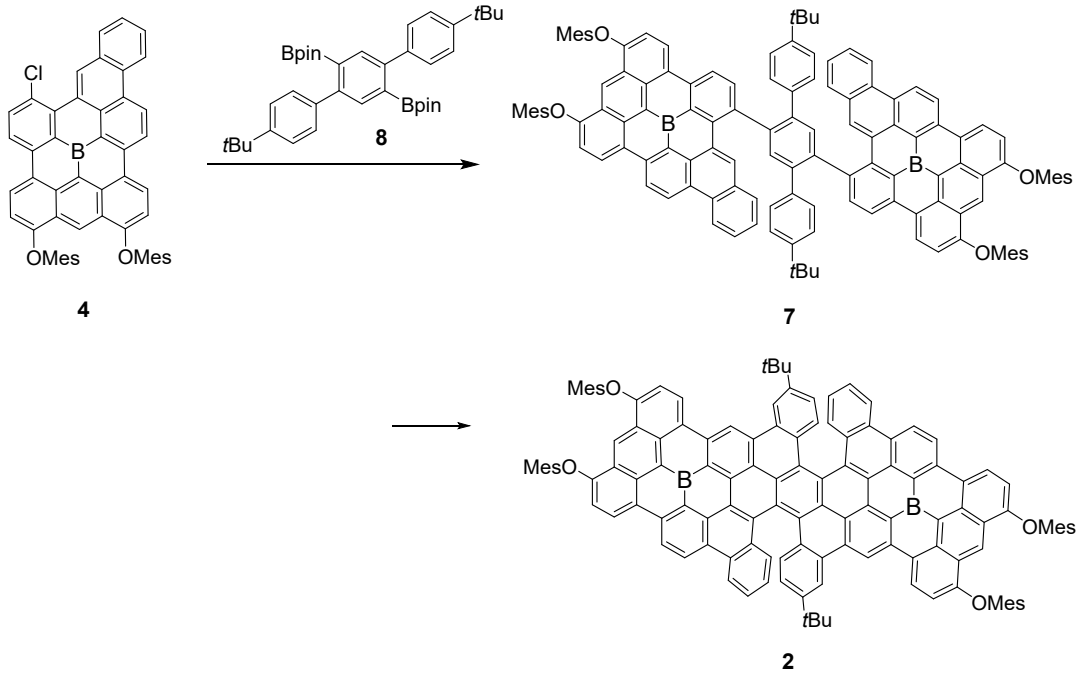
and **5** (40.0 mg, 0.031 mmol) were dissolved in dry CH_2Cl_2 (20 mL) in a two-necked flask under argon, and the methanesulfonic acid (0.1 mL) was added dropwise at 0 °C. The mixture was stirred at 0 °C for 40 minutes before quenching the reaction with methanol (2 mL). All volatiles were removed under reduced pressure. After addition of methanol (10 mL), some yellow precipitates were collected by filtration. The obtained solids were purified on silica gel column chromatography with CH_2Cl_2/hexane (1/6) as eluent to give compound **6** (16.0 mg, 40%) as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 9.09 (d, J = 8.0 Hz, 2H), 8.49 (d, J = 8.0 Hz, 2H), 8.36 (d, J = 8.0 Hz, 2H), 8.05 (d, J = 8.0 Hz, 2H), 7.93−7.87 (m, 4H), 7.69 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8.0 Hz, 2H), 7.29 (t, J = 16.0 Hz, 2H), 7.15−7.08 (m, 8H), 7.00 (t, J = 16.0 Hz, 2H), 6.83−6.80 (m, 2H), 6.77−6.74 (m, 2H), 3.08−3.01 (m, 2H), 2.64−2.58 (m, 2H), 2.54−2.47 (m, 2H), 1.40 (d, J = 8.0 Hz, 12H), 1.16−1.14 (m, 24H), 1.07−1.01 (m, 18H),. ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ (ppm) 150.68, 150.56, 150.51, 148.30, 140.49, 139.81, 138.75, 135.64, 135.16, 134.95, 133.62, 132.94, 132.39, 131.89, 130.86, 130.44, 130.24, 129.65, 129.56, 129.40, 128.80, 128.50, 126.68, 126.36, 126.11, 126.06, 125.85, 125.45, 124.70, 121.84, 120.08, 120.02, 35.54, 34.44, 31.27, 24.58, 24.46, 24.22. HR-MALDI-TOF MS (m/z): [M] calcd. for $C_{96}H_{92}B_2$, 1266.7411; found: 1266.7472.



6 **1**

Compound 1: $FeCl_3$ (30.7 mg, 0.19 mmol) was dissolved in CH_3NO_2 (0.8 mL) in a two-necked flask under argon. This solution was slowly added to a solution of **6** (20.0 mg, 0.016 mmol) in dry CH_2Cl_2 (10 mL) at 0 °C. The mixture was warmed to 25 °C and stirred for 20 minutes before quenching the reaction with methanol (1 mL). All volatiles were removed under reduced pressure. After addition of methanol (20 mL),

some purple precipitates were collected by filtration. The obtained solids were purified on silica gel column chromatography with CH_2Cl_2/hexane (1/6) as eluent to yield the target compound **1** (3.0 mg, 15%) as a purple solid. ^{1}H NMR (400 MHz, $CDCl_3$, 25 °C): δ (ppm) 9.28 (d, J = 8.0 Hz, 4H), 8.84−8.81 (m, 4H), 8.74 (d, J = 8.0 Hz, 2H), 8.55 (d, J = 8.0 Hz, 2H), 8.02 (s, 2H), 7.93 (d, J = 8.0 Hz, 2H), 7.83 (s, 2H), 7.38 (t, J = 12.0 Hz, 2H), 7.25 (s, 4H), 6.98 (d, J = 12.0 Hz, 2H), 6.82 (t, J = 16.0 Hz, 2H), 3.16−3.09 (m, 2H), 2.82−2.78 (m, 2H), 2.66−2.63 (m, 2H), 1.47 (d, J = 4.0 Hz, 12H), 1.36 (s, 18H), 1.23−1.18 (m 12H), 1.07−1.05 (m, 12H). ^{13}C NMR (101 MHz, $CDCl_3$, 25 °C): δ (ppm) 150.85, 148.57, 140.59, 140.52, 138.79, 134.84, 131.37, 130.92, 130.72, 130.58, 130.07, 127.02, 125.88, 123.82, 122.65, 120.19, 35.95, 34.61, 31.89, 24.51, 24.46, 21.57. HR-MALDI-TOF MS (m/z): [M] calcd. for $C_{96}H_{88}B_2$, 1262.7098; found: 1262.7056.



Compound 7: The synthesis of **7** is similar to that of **5**. In a Schlenk tube, a mixture of **4** (136.7 mg, 0.18 mmol), **8** (50.0 mg, 0.084 mmol), $Pd(PPh_3)_4$ (3.9 mg, 0.0033 mmol), 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (2.8 mg, 0.0067 mmol) and K_3PO_4 (71.4 mg, 0.34 mmol) was dissolved in toluene (8 mL), ethanol (1.5 mL) and water (1.5 mL) under argon. The reaction mixture was stirred at 100 °C for 5 h. After cooling down to room temperature, the mixture was poured into water

and extracted with ethyl acetate for three times. The combined organic layer was washed with water and dried over anhydrous Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified with column chromatography on silica gel with CH_2Cl_2/hexane (1/3) to give compound **7** (14.7 mg, 10%) as a deep purple solid. In this step, the main product is the mono-coupling product, which can be used to further perform the Suzuki–Miyaura cross-coupling reaction to obtain compound **7**. The chemical structure of **7** was determined by high-resolution mass spectrometry (Fig. S1), and the ^{1}H NMR and ^{13}C NMR spectra were not obtained due to the presence of stereoisomers. HR-MALDI-TOF MS (m/z): [M] calcd. for $C_{130}H_{100}B_2O_4$, 1747.7863; found: 1747.7843.

Compound 2: The precursor **7** (40.0 mg, 0.023 mmol) was dissolved in dry CH_2Cl_2 (20 mL) in a Schlenk tube under argon. After cooling to 0 ^{o}C, a solution of $FeCl_3$ (44.7 mg, 0.28 mmol) in CH_3NO_2 (1.0 mL) was added dropwise. The mixture was warmed to 25 °C and stirred for 30 minutes. After quenching the reaction with methanol (1 mL), all volatiles were removed under reduced pressure. After addition of methanol (8 mL), some black precipitates were collected by filtration. The obtained solids were purified with silica gel column chromatography with CH_2Cl_2/hexane (1/5) as eluent to yield the target compound **2** as a black-blue solid (6.0 mg, 15%). Due to its insufficient solubility, the ^{1}H NMR and ^{13}C NMR spectra were not obtained. HR-MALDI-TOF MS (m/z): [M] calcd. for $C_{130}H_{96}B_2O_4$, 1739.7237; found: 1739.7271.

3. HRMS spectra and NMR analysis

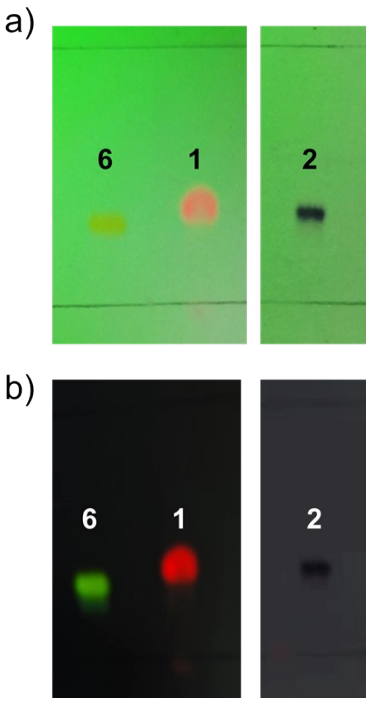


Fig. S1. Thin layer chromatography (TLC) analysis of **6**, **1** and **2** excited at a) 254 nm and b) 365 nm (eluent for **6** and **1**: *n*-hexane:CH_2Cl_2 = 1:8; eluent for **2**: *n*-hexane:CH_2Cl_2 = 1:3). All of them show only one point without any decomposition and impurity, indicative of their successful synthesis and high purity.

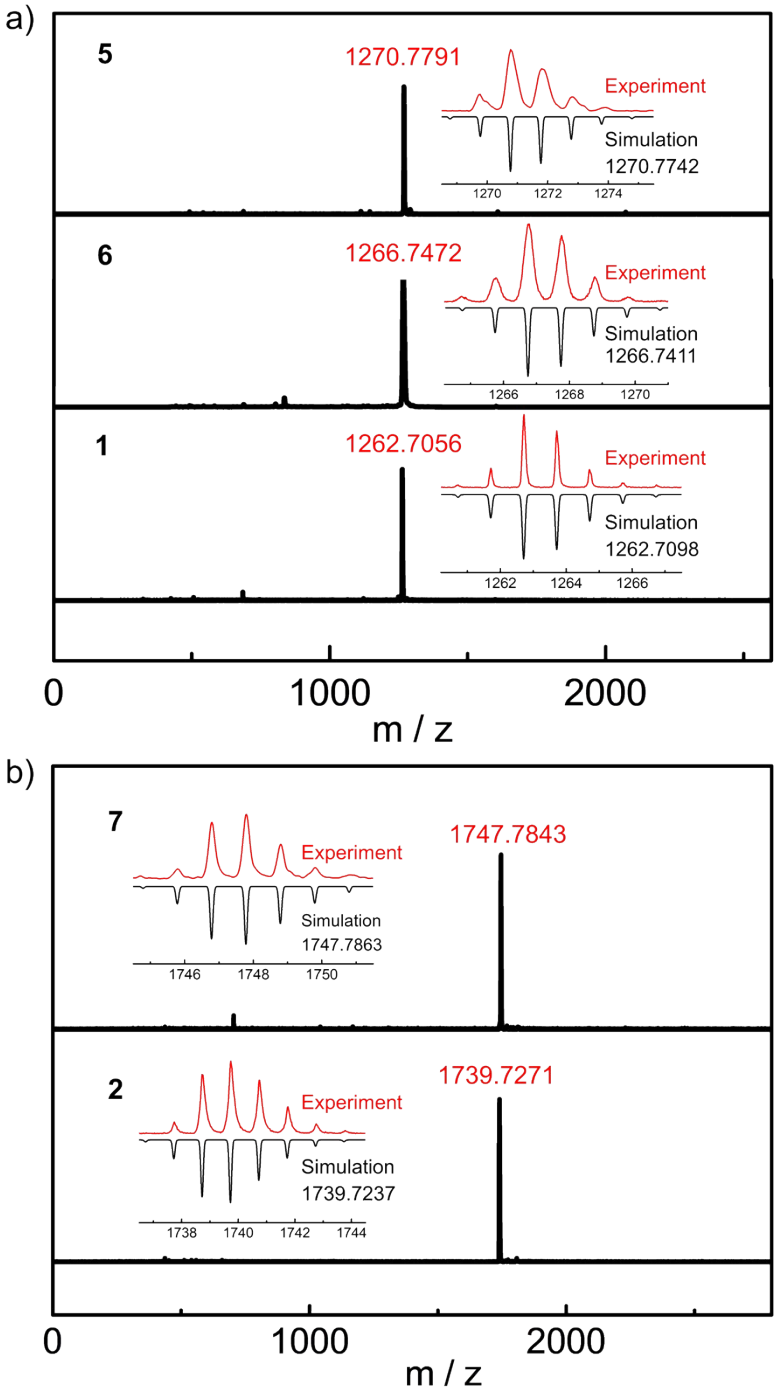


Fig. S2. HRMS spectra with the corresponding experimental and simulated isotopic distributions of a) **5**, **6** and **1** and b) **7** and **2**.

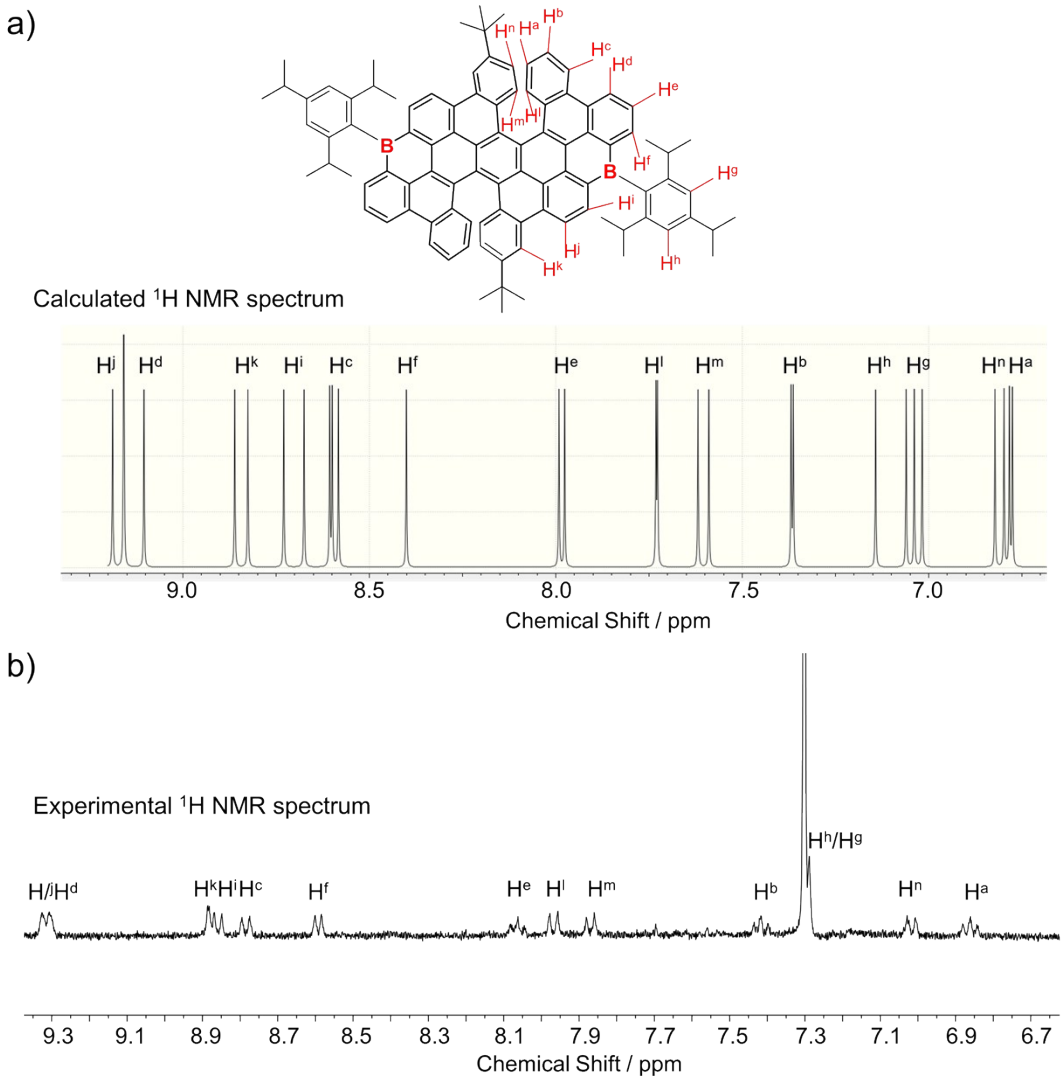


Fig. S3. a) Chemical structure with the aromatic protons and the simulated ^{1}H NMR spectrum of **1** (calculated at the B3LYP/6-311G(d) level). b) The aromatic region for the experimental ^{1}H NMR spectrum of **1** in $CDCl_3$ at 25 ^{o}C.

4. Geometry optimizations and aromaticity calculations

All calculations were carried out using the Gaussian 09 program.[3] Density functional theory (DFT) calculations were performed on **6**, **1**, **2** and **1C** at the B3LYP/6-311G(d) level of theory to obtain the optimized structures and molecular orbitals. Nucleus-independent chemical shift (NICS) and anisotropy of the induced current density (ACID) were used to investigate the aromaticity. The $NICS(1)_{ZZ}$ calculations were conducted with the nmr=GIAO key word based on the B3LYP/6-311+G(d) level of theory. All of the calculated points are set on top the molecules. The ACID calculations (contribution from π electrons only) were performed with the nmr=CSGT iop(10/93=2) key word based on the B3LYP/6-311G(d) level of theory.

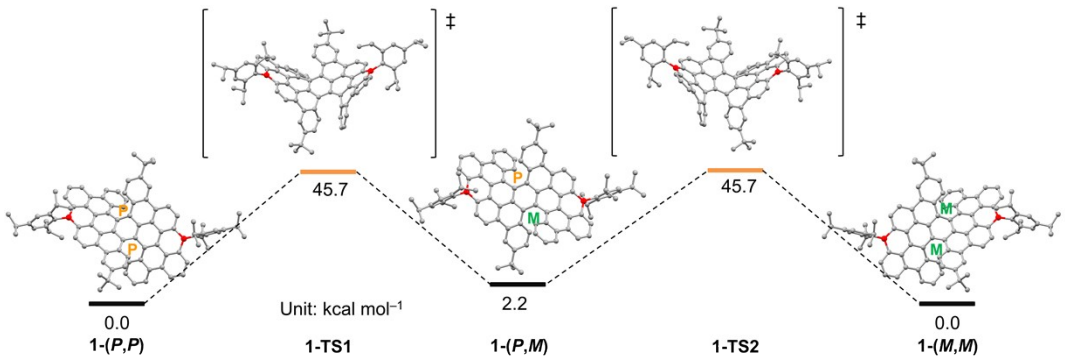


Fig. S4. Energy diagram for the racemization of **1**. The relative Gibbs free energy was calculated at the B3LYP/6-311G(d) level of theory.

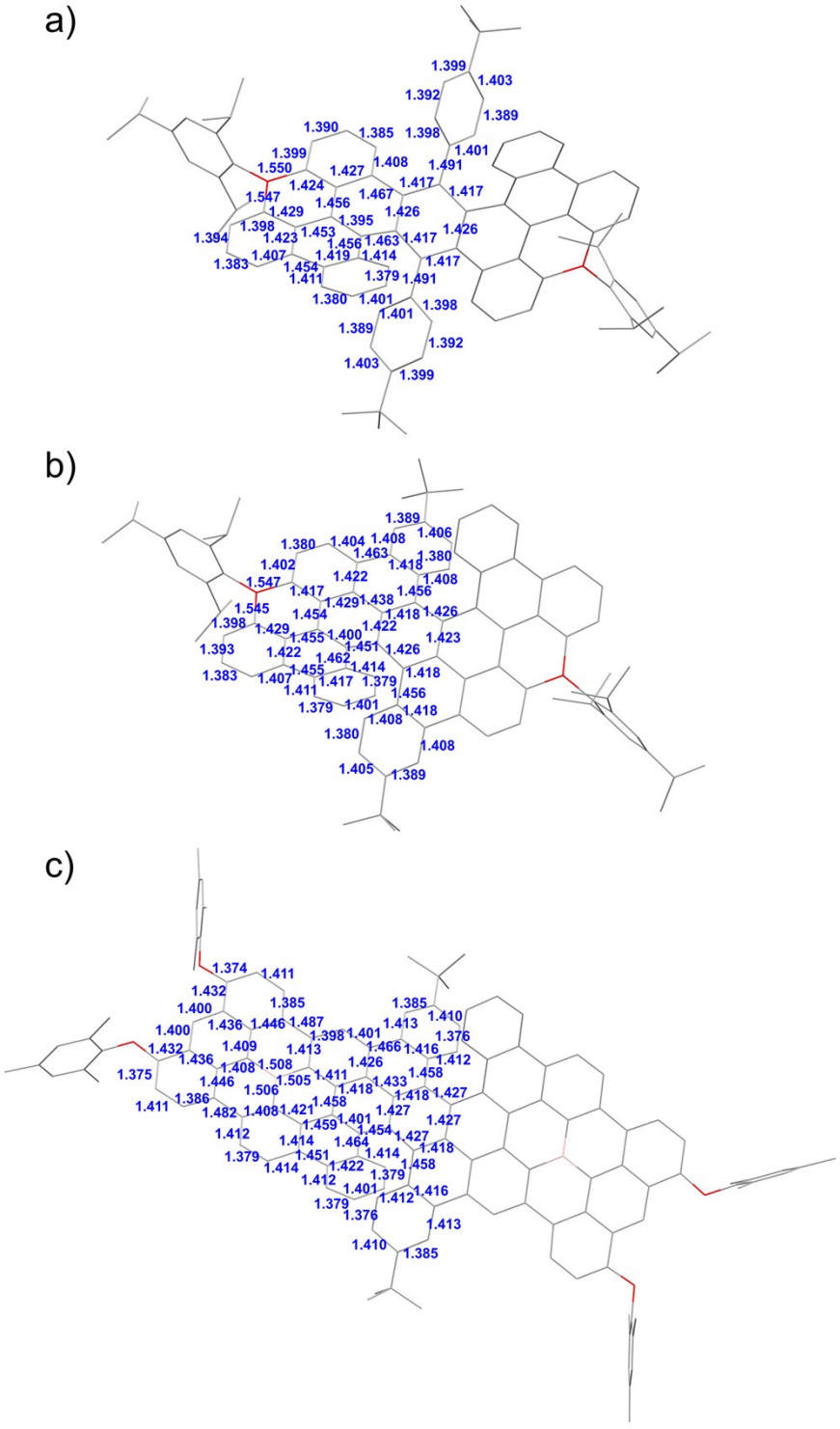


Fig. S5. Optimized geometries with the lowest total energies and their bond lengths of a) **6**, b) **1-(*P, P*)** and c) **2-(*P, P*)**, calculated at the B3LYP/6-311G(d) level of theory.

Table S1. Coordinates of the optimized structure for **6** at the B3LYP/6-311G(d) level.

Atom	x	y	z
C	4.79995900	2.69282400	2.08494800
C	4.82368500	1.60412400	1.17022700
C	3.60975000	0.84653600	0.92142500
C	5.94456500	3.50377700	2.20350900
C	7.09739500	3.24330300	1.48509800
C	7.13654800	2.14269100	0.63028600
C	6.02512600	1.31277900	0.45419300
C	3.60875200	-0.33424800	0.07048900
C	4.78492100	-0.72473900	-0.63507400
C	4.74803800	-1.87207000	-1.43621200
C	3.58558400	-2.62399600	-1.56450100
C	2.44999000	-2.25687600	-0.86177800
C	2.43007700	-1.13248900	-0.01266700
B	6.08122500	0.10512000	-0.50778700
C	2.40507000	1.28722300	1.46930100
C	1.18600400	-0.66989800	0.61244500
C	1.14940800	0.70416900	0.99395200
C	-0.06388700	1.41704400	0.83009900
C	-1.25145200	0.67401000	0.61608000
C	-1.21857600	-0.70870500	0.96390400
C	-0.00372800	-1.41764600	0.79497000
C	-0.00664300	-2.90833500	0.75652500
C	-0.06194300	2.90828000	0.82921700
C	0.88365300	-3.66008100	1.52864100
C	0.89026500	-5.05079000	1.47653200
C	0.01054000	-5.75769200	0.64883800
C	-0.87812000	-4.99715100	-0.12598500
C	-0.89232400	-3.60910300	-0.07312100
C	-0.96175200	3.63959600	1.60982100
C	-0.96972100	5.03113300	1.59213200
C	-0.08199400	5.75935500	0.79188900
C	0.81667500	5.01930900	0.00884900
C	0.83218100	3.63041000	0.02744100
C	-4.87821100	-2.71997600	1.97630400

C	-4.89477900	-1.61051800	1.08551900
C	-3.67843400	-0.84763700	0.86500500
C	-6.02221100	-3.53489200	2.06685100
C	-7.16937300	-3.25864700	1.34558500
C	-7.20163700	-2.13853100	0.51644100
C	-6.09068700	-1.30365200	0.36602600
C	-3.66992700	0.35326700	0.04159600
C	-4.83709700	0.76034700	-0.66577400
C	-4.78830800	1.92272400	-1.44217000
C	-3.62398600	2.67542000	-1.54284300
C	-2.49629500	2.29401000	-0.83516900
C	-2.48854000	1.15178700	-0.01114400
B	-6.14036300	-0.07346000	-0.57047500
C	-7.44078200	0.34304300	-1.38272100
C	-2.47884800	-1.30224600	1.41297700
C	-0.01456500	-7.29310600	0.56798400
C	1.02775700	-7.94557300	1.49292500
C	-1.41277200	-7.80539500	0.98260700
C	0.28431500	-7.73834300	-0.88164200
C	-0.05918900	7.29634300	0.74811800
C	-1.11272600	7.92454800	1.67712800
C	1.33334000	7.80149100	1.18964500
C	-0.34369800	7.77527800	-0.69365500
C	-7.65497300	-0.11642900	-2.71492200
C	-8.75066000	0.35511100	-3.44664900
C	-9.67216600	1.26012000	-2.92771400
C	-9.47421300	1.67522000	-1.61686500
C	-8.39791100	1.23990400	-0.83176300
C	-8.43849100	1.75698100	0.61834600
C	-9.20717000	0.78145700	1.53306300
C	-7.11770400	2.17553600	1.27667500
C	-6.82655600	-1.18403900	-3.45384900
C	-5.29961000	-1.14127500	-3.31484400
C	-7.35120200	-2.60208200	-3.14897100
C	-10.84413300	1.77848600	-3.74808200
C	-10.37686700	2.58544500	-4.97198700
C	-11.80278700	0.64936500	-4.16434000

C	7.39949200	-0.26996500	-1.30546300
C	7.62548800	0.24421800	-2.60244900
C	8.79112800	-0.09473800	-3.29278600
C	9.75736900	-0.93823400	-2.74005800
C	9.52395700	-1.43963200	-1.46062900
C	8.36967100	-1.12237600	-0.73733000
C	6.60711800	1.17353300	-3.26322300
C	8.17781300	-1.71026400	0.66043900
C	11.02474600	-1.30528700	-3.49968400
C	10.71845300	-2.08355800	-4.79117000
C	11.90051100	-0.07438400	-3.79158200
C	7.18879600	2.57189400	-3.53409400
C	6.01169400	0.56512600	-4.54467200
C	8.08450500	-3.24587700	0.63525700
C	9.26539900	-1.23978900	1.64171000
H	5.92535100	4.36435300	2.86129400
H	7.96212600	3.89057200	1.59178700
H	8.04314100	1.92511600	0.07542200
H	5.64372900	-2.16317800	-1.97477400
H	3.55512900	-3.49002400	-2.21807000
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H	-8.10478200	-1.90960900	-0.03849100
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H	1.27167400	-7.39481900	-1.20238500
H	0.26623900	-8.82995000	-0.95817000

H	-0.44916800	-7.34625600	-1.58984100
H	-1.05953300	9.01465700	1.61264300
H	-2.12967500	7.63148200	1.40232100
H	-0.95104000	7.65189700	2.72355900
H	1.36738000	8.89529100	1.16958100
H	2.12784900	7.43457700	0.53597000
H	1.56494000	7.47402400	2.20667400
H	-1.32652100	7.43685700	-1.03320100
H	-0.32793000	8.86844600	-0.74404700
H	0.39851900	7.40202400	-1.40292900
H	-8.87894800	-0.00484100	-4.46431700
H	-10.18595800	2.37207400	-1.17945900
H	-9.04345800	2.66989400	0.57232200
H	-9.37822700	1.23298400	2.51584200
H	-10.18061800	0.52264800	1.10843500
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H	-7.33423100	2.68256500	2.22255400
H	-6.54571600	2.86392600	0.65243500
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H	-4.85475400	-1.83407600	-4.03652000
H	-4.89449000	-0.14768800	-3.51261000
H	-4.95330700	-1.45334300	-2.32726700
H	-6.87155900	-3.33655400	-3.80438100
H	-8.43115800	-2.66820400	-3.30417400
H	-7.14152700	-2.89372900	-2.11773900
H	-11.40759500	2.46273400	-3.10195100
H	-11.23168700	3.00515300	-5.51150300
H	-9.72541000	3.41182600	-4.67629000
H	-9.81853200	1.95938000	-5.67426900
H	-12.67221400	1.05228300	-4.69313700
H	-12.16396100	0.09521300	-3.29414800
H	-11.31368500	-0.06576100	-4.83236200
H	8.95015200	0.30922200	-4.28877800
H	10.26727400	-2.09804800	-1.01783600
H	5.77551900	1.30744700	-2.56131900
H	7.22089000	-1.34136600	1.04774500

H	11.60542300	-1.97054600	-2.84905000
H	11.64317600	-2.39691900	-5.28584000
H	10.12660200	-2.97865800	-4.58320500
H	10.15488200	-1.47282400	-5.50272900
H	12.83659400	-0.36860400	-4.27651600
H	12.15029600	0.46103300	-2.87197200
H	11.39244800	0.63022500	-4.45665600
H	6.42472200	3.23559400	-3.95085200
H	7.56615600	3.02915900	-2.61605200
H	8.01580800	2.53164100	-4.24910000
H	5.24272200	1.22124200	-4.96429900
H	5.55181200	-0.40596000	-4.34576500
H	6.77610700	0.41955100	-5.31365800
H	7.88771700	-3.63847800	1.63779500
H	7.27886800	-3.58350900	-0.02135700
H	9.01459300	-3.69944100	0.28018700
H	9.07290000	-1.62565600	2.64764600
H	9.30009200	-0.14922500	1.70196800
H	10.25753200	-1.58765100	1.33918100
H	-1.67018700	3.11376200	2.24138700
C	3.62050600	2.91000600	2.90790500
C	2.42835000	2.20481400	2.59942100
C	3.64266900	3.74121200	4.04802900
H	4.54957000	4.27152600	4.31059900
C	2.54780900	3.85343900	4.88067800
H	2.59899300	4.48698300	5.76040000
C	1.38987700	3.11254000	4.60970600
H	0.54096900	3.15791000	5.28404400
C	1.33660600	2.30727300	3.49171400
H	0.45175500	1.71205300	3.31254100
H	1.58536600	-3.15109600	2.18119500
C	-2.51171900	-2.24444300	2.52226500
C	-1.42778100	-2.36703300	3.42163400
C	-3.70642400	-2.95562200	2.80481200
C	-3.73911300	-3.81148600	3.92639500
C	-2.65167000	-3.94258100	4.76588300
C	-1.49110200	-3.19665500	4.52110200

H	-0.54126300	-1.76837000	3.26343300
H	-0.64813400	-3.25719100	5.20167800
H	-2.71083700	-4.59501600	5.63116300
H	-4.64856100	-4.34659700	4.16968900
H	-1.59421800	2.87397400	-0.95303300
H	1.53750600	3.09734600	-0.60098500
H	-1.58983400	-3.05965100	-0.69609200
H	1.55002300	-2.83517900	-1.00209100

Table S2. Coordinates of the optimized structure for **1** at the B3LYP/6-311G(d) level.

Atom	x	y	z
C	4.20909200	3.52567400	1.64280700
C	4.51124200	2.25900900	1.07258400
C	3.43616900	1.32176300	0.78579500
C	5.23194300	4.48783700	1.74066900
C	6.52998400	4.21103400	1.35092500
C	6.84230000	2.93961400	0.87315100
C	5.86271400	1.95262400	0.72632000
C	3.71497300	-0.00955900	0.27356100
C	5.05095900	-0.44193700	0.06716000
C	5.26927700	-1.78387900	-0.28168200
C	4.23130200	-2.67813200	-0.44743500
C	2.89543400	-2.27029200	-0.30445000
C	2.63525600	-0.92147600	0.06706600
B	6.22894800	0.53958600	0.22464400
C	2.10891000	1.71740400	0.99239800
C	1.27720700	-0.46531000	0.19420300
C	1.03246500	0.91410200	0.44192100
C	-0.26272500	1.40081800	0.09488300
C	-1.34762600	0.49265200	0.19665700
C	-1.10298300	-0.88942000	0.42835900
C	0.19289600	-1.37217400	0.07936000
C	0.44654300	-2.70606100	-0.44782100
C	-0.51472400	2.74043800	-0.41785200
C	-0.59054200	-3.53625200	-0.91569700

C	-0.34684000	-4.79087800	-1.43714300
C	0.96094600	-5.29678800	-1.53410800
C	1.99067700	-4.45551400	-1.13098900
C	1.77875600	-3.16453000	-0.60942300
C	0.52376600	3.57645300	-0.87228000
C	0.28149700	4.83741200	-1.37871400
C	-1.02622900	5.34412700	-1.47311300
C	-2.05710000	4.49748700	-1.08438200
C	-1.84659500	3.19996700	-0.57869200
C	-4.27762800	-3.51910300	1.58721800
C	-4.58162900	-2.24596700	1.03065800
C	-3.50735700	-1.30267200	0.76026100
C	-5.29644500	-4.48663500	1.66804800
C	-6.59391300	-4.20931600	1.27730800
C	-6.90808600	-2.93255900	0.81582500
C	-5.93307400	-1.93957000	0.68291900
C	-3.78688800	0.03498700	0.26354300
C	-5.12078200	0.46789200	0.05765000
C	-5.33692200	1.81146200	-0.28178200
C	-4.29938700	2.70790100	-0.43563600
C	-2.96365300	2.30145100	-0.28845700
C	-2.70551700	0.94961700	0.07063900
B	-6.30353400	-0.51952000	0.19871800
C	-7.79364100	-0.07275100	-0.12327500
C	-2.18036300	-1.69946400	0.96643700
C	1.27729600	-6.69826300	-2.08563900
C	0.00475700	-7.47166700	-2.47463200
C	2.16682500	-6.57509600	-3.34352800
C	2.02422300	-7.51645800	-1.00784300
C	-1.34117700	6.75257700	-2.00744600
C	-0.06740300	7.53285000	-2.37825100
C	-2.22303600	6.64516600	-3.27216800
C	-2.09567500	7.55531600	-0.92331400
C	-8.32102000	-0.15913900	-1.44481100
C	-9.60050000	0.33765400	-1.71778200
C	-10.41034500	0.91481200	-0.74390400
C	-9.90021500	0.96564200	0.54720300

C	-8.62799400	0.48475000	0.88559100
C	-8.31645500	0.55973700	2.39204200
C	-8.74089400	-0.73630800	3.11252500
C	-6.90114300	0.96884500	2.81960500
C	-7.64722000	-0.83924200	-2.65120100
C	-6.14693800	-0.60587100	-2.86878600
C	-7.96386700	-2.34825800	-2.68799800
C	-11.79007400	1.46929700	-1.06656700
C	-11.71882300	2.65164900	-2.04864900
C	-12.74503300	0.37916200	-1.58305200
C	7.72347800	0.11841900	-0.09592700
C	8.24111000	0.24713900	-1.40488900
C	9.55874600	-0.12978300	-1.67304200
C	10.39753700	-0.63890100	-0.67914200
C	9.87646000	-0.76199200	0.60777500
C	8.56268500	-0.39428200	0.91595900
C	7.37486000	0.79931800	-2.53706600
C	8.05682700	-0.55863500	2.34892700
C	11.83310800	-1.04798900	-0.97888600
C	11.90472500	-2.20664900	-1.98869500
C	12.68767500	0.14371600	-1.44465500
C	7.93317300	2.11566800	-3.10511700
C	7.15214900	-0.23421500	-3.65464100
C	8.05435900	-2.03043400	2.79775900
C	8.83638300	0.31926700	3.34322100
H	5.00299900	5.47621500	2.12024200
H	7.29652200	4.97521400	1.43140200
H	7.86506300	2.70392300	0.59832300
H	6.28947900	-2.12366300	-0.42646900
H	4.46754600	-3.70025700	-0.71231600
H	-1.19064800	-5.37497400	-1.78184000
H	3.00688200	-4.80608400	-1.24649100
H	1.12623600	5.42608900	-1.71316100
H	-3.07302700	4.84951000	-1.19809600
H	-5.06493300	-5.47897500	2.03540100
H	-7.35883600	-4.97621600	1.34526100
H	-7.93141900	-2.69742700	0.54489900

H	-6.35584600	2.15323700	-0.43001800
H	-4.53608000	3.73141000	-0.69504200
H	0.27474900	-8.46359500	-2.84657800
H	-0.66514500	-7.61377600	-1.62230200
H	-0.55547400	-6.96914700	-3.26777300
H	2.39530200	-7.56579900	-3.74859200
H	3.11694100	-6.08098800	-3.12784600
H	1.66469400	-5.99897700	-4.12539700
H	1.41781300	-7.62191100	-0.10423600
H	2.25379600	-8.51977000	-1.37990000
H	2.96806800	-7.04800700	-0.71940300
H	-0.33642300	8.52978100	-2.73732500
H	0.59765000	7.66320800	-1.52027000
H	0.49773600	7.04245000	-3.17547500
H	-2.45057900	7.64091200	-3.66526200
H	-3.17359300	6.14675600	-3.06863500
H	-1.71540500	6.08031300	-4.05869900
H	-1.49492000	7.64922000	-0.01467500
H	-2.32409100	8.56331500	-1.28323400
H	-3.04075400	7.08207900	-0.64700800
H	-9.96932000	0.26722600	-2.73789000
H	-10.51560500	1.39981100	1.33223400
H	-8.97518600	1.34815900	2.77400600
H	-8.67446900	-0.60943300	4.19807000
H	-9.77155400	-1.00668100	2.86852100
H	-8.09936300	-1.57620600	2.83859600
H	-6.89172900	1.15238300	3.89881300
H	-6.56897500	1.88265800	2.32399000
H	-6.15618800	0.19403600	2.62839900
H	-8.14027500	-0.40427100	-3.52810500
H	-5.86475800	-0.98283000	-3.85708600
H	-5.88347500	0.45230800	-2.82789700
H	-5.52463100	-1.13438600	-2.14382900
H	-7.62662600	-2.78675900	-3.63294100
H	-9.03758300	-2.53173700	-2.59691600
H	-7.46156300	-2.88300900	-1.87915500
H	-12.20825000	1.85043300	-0.12688000

H	-12.71246600	3.07836300	-2.21749200
H	-11.07103800	3.44502000	-1.66693000
H	-11.32356300	2.34095900	-3.02031800
H	-13.74875300	0.78510300	-1.74301900
H	-12.82449600	-0.44723200	-0.87206000
H	-12.40220600	-0.03563200	-2.53555300
H	9.94184500	-0.02371400	-2.68418100
H	10.51791600	-1.15728000	1.39158000
H	6.38791800	1.02912300	-2.11831700
H	7.01523000	-0.21770400	2.37486100
H	12.26495400	-1.40968500	-0.03774000
H	12.93969300	-2.53011200	-2.13762500
H	11.32783800	-3.06869800	-1.64397000
H	11.50795400	-1.91245900	-2.96486600
H	13.73020100	-0.15707400	-1.58829000
H	12.66811400	0.95519800	-0.71263900
H	12.32742200	0.54755000	-2.39545400
H	7.26393300	2.52266600	-3.86952200
H	8.04601500	2.86957900	-2.32198300
H	8.91325600	1.96990700	-3.56883800
H	6.47977400	0.16285300	-4.42144700
H	6.70838400	-1.15251600	-3.26232200
H	8.09155800	-0.50288800	-4.14678500
H	7.63213800	-2.12819100	3.80272900
H	7.45943100	-2.65055300	2.12256500
H	9.06660400	-2.44455700	2.82350100
H	8.41792300	0.22907100	4.35046000
H	8.79692500	1.37308500	3.05686900
H	9.88970300	0.02843000	3.39618600
H	1.54387600	3.21891300	-0.84931400
C	2.87359900	3.77545000	2.16488500
C	1.83388400	2.86057200	1.86178200
C	2.59838200	4.85958300	3.02566300
H	3.38636100	5.55573600	3.28422200
C	1.35495900	5.02805300	3.59913100
H	1.17513000	5.86348400	4.26811000
C	0.34404400	4.09131400	3.34944200

H	-0.62245100	4.18561800	3.83331400
C	0.58420800	3.03183100	2.49995800
H	-0.19749700	2.30238400	2.34376700
H	-1.61064900	-3.17876300	-0.89160600
C	-1.90571100	-2.85125900	1.82416700
C	-0.65818200	-3.02659700	2.46549700
C	-2.94430200	-3.77148900	2.11306000
C	-2.67068700	-4.86395800	2.96384300
C	-1.42935200	-5.03579000	3.54071800
C	-0.41936000	-4.09443100	3.30480500
H	0.12256300	-2.29389100	2.32015000
H	0.54531600	-4.19182400	3.79168300
H	-1.25056900	-5.87761400	4.20189600
H	-3.45831700	-5.56418600	3.21224800

Table S3. Coordinates of the optimized structure for **2** at the B3LYP/6-311G(d) level.

Atom	x	y	z
C	-4.03207200	3.79248900	-1.79953400
C	-4.39547000	2.53760600	-1.25897200
C	-3.37659200	1.54070200	-0.94866100
C	-5.05157600	4.76121600	-1.94676900
C	-6.37339900	4.50710200	-1.64517200
C	-6.77544800	3.23551000	-1.18038700
C	-5.76475600	2.27460800	-0.98436800
C	-3.72868200	0.21885700	-0.44458500
C	-5.08145900	-0.13627800	-0.25547000
C	-5.46132000	-1.44007600	0.13559900
C	-4.44712700	-2.38347200	0.32504700
C	-3.09038900	-2.06974300	0.17221700
C	-2.71723300	-0.74958000	-0.21847300
B	-6.14459700	0.90194300	-0.49384300
C	-2.02543600	1.86622200	-1.12932200
C	-2.66862800	4.00627600	-2.24938100
C	-1.68141200	3.02625900	-1.95362500
C	-0.40989100	3.16358500	-2.55675500

C	-0.09243400	4.24740800	-3.34796300
C	-1.04456400	5.25038300	-3.57356800
C	-2.31065500	5.11796900	-3.04376000
C	-7.59537800	0.55847200	-0.26435800
C	-7.92603600	-0.74919300	0.14416200
C	-9.31063600	-1.06431700	0.36045900
C	-10.27884200	-0.07030300	0.16996600
C	-9.94451100	1.22740800	-0.23499800
C	-8.56667600	1.55718600	-0.46855300
C	-6.90130100	-1.75116100	0.33797500
C	-7.33242500	-3.00732700	0.73079200
C	-8.68730600	-3.33794500	0.94417500
C	-9.66674900	-2.39033000	0.76682000
C	-10.94242300	2.23713200	-0.42483700
C	-10.57322000	3.49835500	-0.82903500
C	-9.21521800	3.79984200	-1.06336300
C	-8.18829000	2.88328500	-0.90401400
O	-12.23112800	1.85299200	-0.17971200
C	-13.27561200	2.77033800	-0.33512800
C	-13.68086100	3.51583300	0.77505400
C	-14.77106500	4.37338900	0.61304700
C	-15.44700000	4.48940100	-0.60337600
C	-15.00974000	3.71429500	-1.67930700
C	-13.92488500	2.84145100	-1.57021200
C	-13.46985400	1.99592100	-2.73215300
C	-12.96747900	3.38387300	2.09633200
C	-16.64421300	5.39939800	-0.73991400
O	-11.00241900	-2.61707900	0.95282600
C	2.33175300	4.30351300	1.03693700
C	2.03390800	3.03432500	0.49098500
C	0.67594200	2.67211100	0.31419500
C	-0.30739300	3.56738500	0.79022000
C	0.01886400	4.78865100	1.33280300
C	1.36163900	5.20317200	1.44660700
C	-1.33728500	-0.38401600	-0.34805700
C	-1.00443600	0.98213300	-0.59072100
C	1.69037300	6.58582300	2.03178100

C	1.02578600	7.67711000	1.16154600
C	3.20264200	6.86555200	2.07513900
C	1.14360100	6.67951900	3.47464900
H	-4.79776200	5.75031700	-2.30924400
H	-7.08958400	5.30781900	-1.79120100
H	-4.70938400	-3.39043500	0.61412300
H	0.89038800	4.31175000	-3.80330400
H	-0.80116500	6.10921400	-4.19109600
H	-3.05424500	5.86826600	-3.28251900
H	-11.31857900	-0.31410600	0.33991600
H	-6.61266900	-3.80071000	0.89347000
H	-8.94960300	-4.34299500	1.25101200
H	-11.32342000	4.26613300	-0.97312400
H	-8.99312400	4.81024200	-1.38575400
H	-15.10105200	4.96313800	1.46436100
H	-15.52752000	3.78520900	-2.63232900
H	-14.13839500	2.11584000	-3.58633200
H	-13.44391900	0.93622000	-2.46551500
H	-12.46010100	2.26394200	-3.05704900
H	-11.92990500	3.72488600	2.03224300
H	-12.93672500	2.34291200	2.42830900
H	-13.46558800	3.97288800	2.86828100
H	-17.57083200	4.87727000	-0.47705200
H	-16.75794200	5.76388700	-1.76359100
H	-16.56591100	6.26873000	-0.08263200
H	3.36789200	4.57802500	1.16153600
H	-0.78313500	5.42860000	1.68441900
H	1.24199800	8.67192200	1.56378300
H	-0.05996400	7.56479000	1.12350000
H	1.39713500	7.63945700	0.13388900
H	3.38249600	7.86341500	2.48427500
H	3.73395700	6.15336500	2.71268900
H	3.65296200	6.83601600	1.07898100
H	0.06094400	6.54027200	3.51248000
H	1.36500800	7.66141500	3.90474600
H	1.59751900	5.91962600	4.11654300
C	4.03210800	-3.79247300	-1.79955600

C	4.39549200	-2.53758500	-1.25899700
C	3.37660400	-1.54069000	-0.94868700
C	5.05161900	-4.76119500	-1.94677300
C	6.37343800	-4.50707000	-1.64516600
C	6.77547400	-3.23547000	-1.18039300
C	5.76477400	-2.27457300	-0.98439300
C	3.72867900	-0.21884800	-0.44460200
C	5.08145900	0.13632900	-0.25556700
C	5.46130500	1.44013900	0.13547300
C	4.44708900	2.38348300	0.32506700
C	3.09035300	2.06969700	0.17236200
C	2.71721400	0.74955000	-0.21840300
B	6.14460600	-0.90188300	-0.49393300
C	2.02545000	-1.86622200	-1.12936000
C	2.66867500	-4.00625900	-2.24943700
C	1.68145500	-3.02623900	-1.95370400
C	0.40996000	-3.16353800	-2.55689300
C	0.09252300	-4.24734700	-3.34813000
C	1.04464800	-5.25033400	-3.57369800
C	2.31071900	-5.11794300	-3.04383500
C	7.59538700	-0.55838300	-0.26449200
C	7.92603900	0.74931500	0.14392600
C	9.31064300	1.06447800	0.36013500
C	10.27885500	0.07045700	0.16971200
C	9.94452800	-1.22729100	-0.23513600
C	8.56669200	-1.55709600	-0.46865200
C	6.90129500	1.75128300	0.33770000
C	7.33242200	3.00751000	0.73031300
C	8.68731000	3.33817300	0.94358800
C	9.66675700	2.39054300	0.76632700
C	10.94244300	-2.23702600	-0.42490100
C	10.57324400	-3.49828300	-0.82899200
C	9.21524300	-3.79979300	-1.06329900
C	8.18831300	-2.88322500	-0.90402800
O	12.23115300	-1.85284900	-0.17985100
C	13.27560200	-2.77030200	-0.33486600
C	13.92521500	-2.84156200	-1.56979500

C	15.01000000	-3.71449100	-1.67854400
C	15.44690600	-4.48957900	-0.60242400
C	14.77066900	-4.37342300	0.61378800
C	13.68048100	-3.51573600	0.77545700
C	12.96676500	-3.38366600	2.09654300
C	13.47052700	-1.99607900	-2.73190400
C	16.64408400	-5.39965900	-0.73872000
O	11.00243300	2.61733100	0.95223300
C	-2.33182100	-4.30376100	1.03631700
C	-2.03396100	-3.03444900	0.49066000
C	-0.67598600	-2.67220500	0.31399000
C	0.30732700	-3.56752800	0.78996800
C	-0.01894900	-4.78888900	1.33232300
C	-1.36172300	-5.20347700	1.44589700
C	-0.32182000	-1.36740000	-0.23219600
C	0.32180000	1.36734700	-0.23211300
C	1.33727200	0.38396900	-0.34799300
C	1.00443400	-0.98216600	-0.59073700
C	-1.69047700	-6.58627300	2.03071700
C	-1.14382900	-6.68030600	3.47360900
C	-3.20274400	-6.86604500	2.07387800
C	-1.02579000	-7.67733400	1.16027500
H	4.79781400	-5.75029800	-2.30924800
H	7.08963100	-5.30778100	-1.79119200
H	4.70932500	3.39044900	0.61415300
H	-0.89027700	-4.31166700	-3.80352100
H	0.80126400	-6.10915900	-4.19124000
H	3.05430800	-5.86824900	-3.28256700
H	11.31859300	0.31429000	0.33961300
H	6.61266800	3.80091600	0.89288400
H	8.94961100	4.34327000	1.25027100
H	11.32344500	-4.26607400	-0.97300400
H	8.99315100	-4.81022200	-1.38560400
H	15.52803900	-3.78551800	-2.63142200
H	15.10037300	-4.96313000	1.46523400
H	13.46498400	-3.97219900	2.86879000
H	12.93545100	-2.34261300	2.42816800

H	11.92936400	-3.72519300	2.03234800
H	12.46088600	-2.26415300	-3.05710800
H	13.44445700	-0.93637300	-2.46530400
H	14.13934200	-2.11599800	-3.58586800
H	17.57125100	-4.87610600	-0.48066900
H	16.56799000	-6.26635500	-0.07773400
H	16.75504600	-5.76822800	-1.76125500
H	-3.36796400	-4.57835100	1.16071400
H	0.78303200	-5.42887300	1.68391500
H	-1.36524600	-7.66231400	3.90344500
H	-0.06117900	-6.54104100	3.51157100
H	-1.59782400	-5.92058400	4.11565100
H	-3.38260900	-7.86402300	2.48273000
H	-3.65298600	-6.83624900	1.07769200
H	-3.73412400	-6.15404100	2.71157900
H	0.05996200	-7.56498700	1.12236700
H	-1.24202800	-8.67225000	1.56224200
H	-1.39703600	-7.63942800	0.13259000
H	-0.32933000	-2.38795700	-2.41809400
H	1.34891000	-3.28053700	0.75097800
H	-1.34898000	3.28042700	0.75109700
H	0.32940500	2.38801300	-2.41793900
C	-11.44726800	-3.88283300	1.34788800
C	-11.59399900	-4.14397200	2.71266900
C	-11.80618700	-4.80375200	0.36024700
C	-12.10578500	-5.39050600	3.07964900
C	-12.31314500	-6.03543100	0.78025300
C	-12.46861500	-6.34962100	2.13188400
H	-12.22620700	-5.61361300	4.13659800
H	-12.59685600	-6.76615800	0.02728600
C	11.44727800	3.88306400	1.34737400
C	11.59390300	4.14418300	2.71217600
C	11.80633400	4.80396500	0.35977700
C	12.10574300	5.39067500	3.07920400
C	12.31335400	6.03560700	0.77983200
C	12.46873100	6.34977400	2.13147000
H	12.22607500	5.61377500	4.13616500

H	12.59715900	6.76632600	0.02689500
C	-11.22007000	-3.10813200	3.74189800
H	-10.14750500	-2.89265100	3.72831300
H	-11.73370700	-2.16127300	3.55659100
H	-11.48014800	-3.44582700	4.74653300
C	-11.65721600	-4.46646700	-1.10131400
H	-12.17704100	-3.53741200	-1.34900800
H	-10.60861300	-4.32450900	-1.37932100
H	-12.06409600	-5.26193900	-1.72793100
C	-13.05127400	-7.67635000	2.55660000
H	-12.66717400	-7.99144800	3.52973500
H	-14.14219400	-7.62116900	2.64146000
H	-12.82285900	-8.46528500	1.83604700
C	11.21992600	3.10831700	3.74136100
H	10.14756800	2.89190600	3.72690800
H	11.73454800	2.16184400	3.55676500
H	11.47886300	3.44650000	4.74612700
C	11.65750600	4.46667000	-1.10179700
H	12.17818800	3.53812300	-1.34962600
H	10.60901600	4.32374200	-1.37971300
H	12.06358700	5.26256800	-1.72839100
C	13.05143100	7.67645000	2.55629500
H	12.66599800	7.99231600	3.52865800
H	14.14218900	7.62074300	2.64288200
H	12.82453800	8.46508200	1.83493500

Table S4. Coordinates of the optimized structure for **1C** at the B3LYP/6-311G(d) level.

Atom	x	y	z
C	-4.66311900	3.14897000	0.98645500
C	-3.51073500	3.70927600	0.37277500
C	-2.24100000	2.98728500	0.42119700
C	-5.90097600	3.80761900	0.84803400
C	-6.02343700	4.97064700	0.11255500
C	-4.90217000	5.49658200	-0.53966400

C	-3.67522300	4.87372200	-0.41410600
C	-0.94876000	3.62980000	0.22576000
C	-0.77649300	5.01143600	0.43209700
C	0.47650900	5.59748800	0.35196400
C	1.58987200	4.83560200	0.02323400
C	1.48337600	3.45321500	-0.16135200
C	0.21491100	2.83164400	0.01782300
C	-2.27661900	1.61632000	0.67597000
C	0.10730000	1.39547100	0.02846700
C	-1.16485500	0.78846100	0.23319000
C	-1.27433000	-0.59512800	-0.08582600
C	-0.10727900	-1.39548300	0.02845300
C	1.16487900	-0.78847700	0.23316600
C	1.27435300	0.59511700	-0.08583500
C	2.49661600	1.22152600	-0.58210400
C	-2.49660300	-1.22152700	-0.58208000
C	3.54108700	0.47482500	-1.15845600
C	4.68127200	1.07424700	-1.65762700
C	4.84570400	2.46922400	-1.62093200
C	3.79207300	3.21286700	-1.10085300
C	2.61560700	2.63262500	-0.59321900
C	-3.54109100	-0.47480800	-1.15837600
C	-4.68129400	-1.07421800	-1.65752300
C	-4.84571800	-2.46919700	-1.62087100
C	-3.79208200	-3.21285200	-1.10081900
C	-2.61560000	-2.63262500	-0.59320600
C	4.66313300	-3.14899800	0.98643700
C	3.51074800	-3.70930200	0.37275600
C	2.24101700	-2.98730600	0.42117200
C	5.90098800	-3.80765300	0.84802400
C	6.02344700	-4.97068400	0.11255100
C	4.90218100	-5.49661700	-0.53967000
C	3.67523500	-4.87375200	-0.41411900
C	0.94877300	-3.62981600	0.22574200
C	0.77649900	-5.01145000	0.43208600
C	-0.47650500	-5.59749800	0.35195100
C	-1.58986500	-4.83560900	0.02322200

C	-1.48336500	-3.45322200	-0.16136200
C	-0.21489600	-2.83165700	0.01780500
C	2.27664300	-1.61634000	0.67593800
C	6.10234900	3.17766500	-2.15721900
C	7.15421600	2.18245800	-2.67873200
C	5.71407000	4.11806600	-3.32060200
C	6.74853000	4.00562300	-1.02333500
C	-6.10240500	-3.17761700	-2.15708600
C	-7.15437700	-2.18237800	-2.67832600
C	-5.71426200	-4.11785700	-3.32064500
C	-6.74840000	-4.00573900	-1.02321600
H	-6.78882100	3.37498600	1.29326800
H	-6.99134900	5.45116300	0.01298200
H	-4.99701600	6.37715500	-1.16686500
H	0.58651600	6.65922600	0.54815600
H	2.55228000	5.32474700	-0.05833100
H	5.44358800	0.44076300	-2.09307300
H	3.86476700	4.29242800	-1.12399300
H	-5.44363100	-0.44072300	-2.09291600
H	-3.86479200	-4.29241200	-1.12395000
H	6.78883300	-3.37502000	1.29325900
H	6.99135800	-5.45120500	0.01298300
H	4.99702400	-6.37719400	-1.16686600
H	-0.58651500	-6.65923500	0.54814700
H	-2.55227400	-5.32475100	-0.05834000
H	8.03393100	2.72640600	-3.03321200
H	7.48831600	1.49335400	-1.89840900
H	6.77893400	1.59005800	-3.51753400
H	6.60025700	4.62522700	-3.71499600
H	5.00619100	4.88854600	-3.00639800
H	5.25269700	3.55978300	-4.13966700
H	7.03506200	3.36581300	-0.18436600
H	7.64846600	4.51326000	-1.38449400
H	6.07037800	4.77081800	-0.63845900
H	-8.03412300	-2.72630900	-3.03275300
H	-7.48839100	-1.49338500	-1.89786800
H	-6.77922900	-1.58985900	-3.51710400

H	-6.60049500	-4.62496300	-3.71500400
H	-5.00634700	-4.88838200	-3.00663700
H	-5.25298800	-3.55945900	-4.13968800
H	-7.03484800	-3.36604300	-0.18413100
H	-7.64836100	-4.51337400	-1.38431500
H	-6.07015800	-4.77094800	-0.63852200
H	-3.44528400	0.59965600	-1.23918200
C	-4.52866000	1.89561100	1.71561000
C	-3.37083100	1.10244800	1.50328000
C	-5.50902300	1.44988100	2.62464100
H	-6.37966800	2.06541900	2.81696000
C	-5.36561900	0.26229500	3.31420900
H	-6.12954500	-0.05377600	4.01730000
C	-4.21453800	-0.51200500	3.12430600
H	-4.07400700	-1.43035400	3.68498700
C	-3.24015900	-0.09614000	2.23938700
H	-2.34086500	-0.68722600	2.13718100
H	3.44527700	-0.59963600	-1.23929600
C	3.37085700	-1.10246600	1.50324200
C	3.24019400	0.09613900	2.23932200
C	4.52868000	-1.89563300	1.71558400
C	5.50904400	-1.44989600	2.62460900
C	5.36564700	-0.26229700	3.31415600
C	4.21457500	0.51201200	3.12423600
H	2.34090700	0.68723400	2.13709500
H	4.07405200	1.43037400	3.68489800
H	6.12957500	0.05378000	4.01724300
H	6.37968500	-2.06543600	2.81694000
H	2.83628500	-5.25567900	-0.97981700
H	1.62026000	-5.61997200	0.72456000
H	-1.62025900	5.61995600	0.72456000
H	-2.83627100	5.25564900	-0.97980200

5. Electrochemical properties

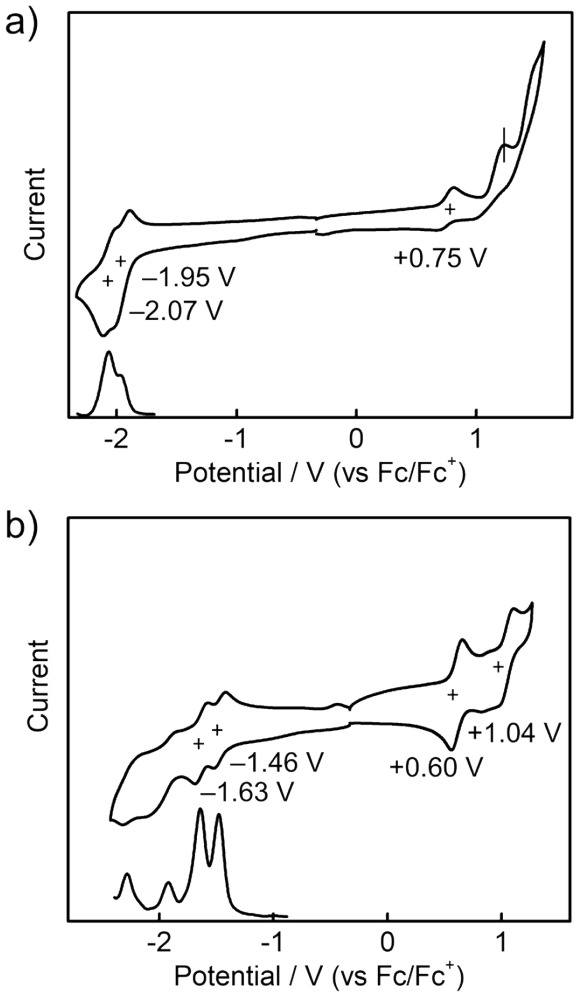

Fig. S6. Cyclic voltammograms of a) **6** and b) **1** in $C_2H_4Cl_2$ (1.0 mM). Fc = ferrocene.

6. Photophysical properties

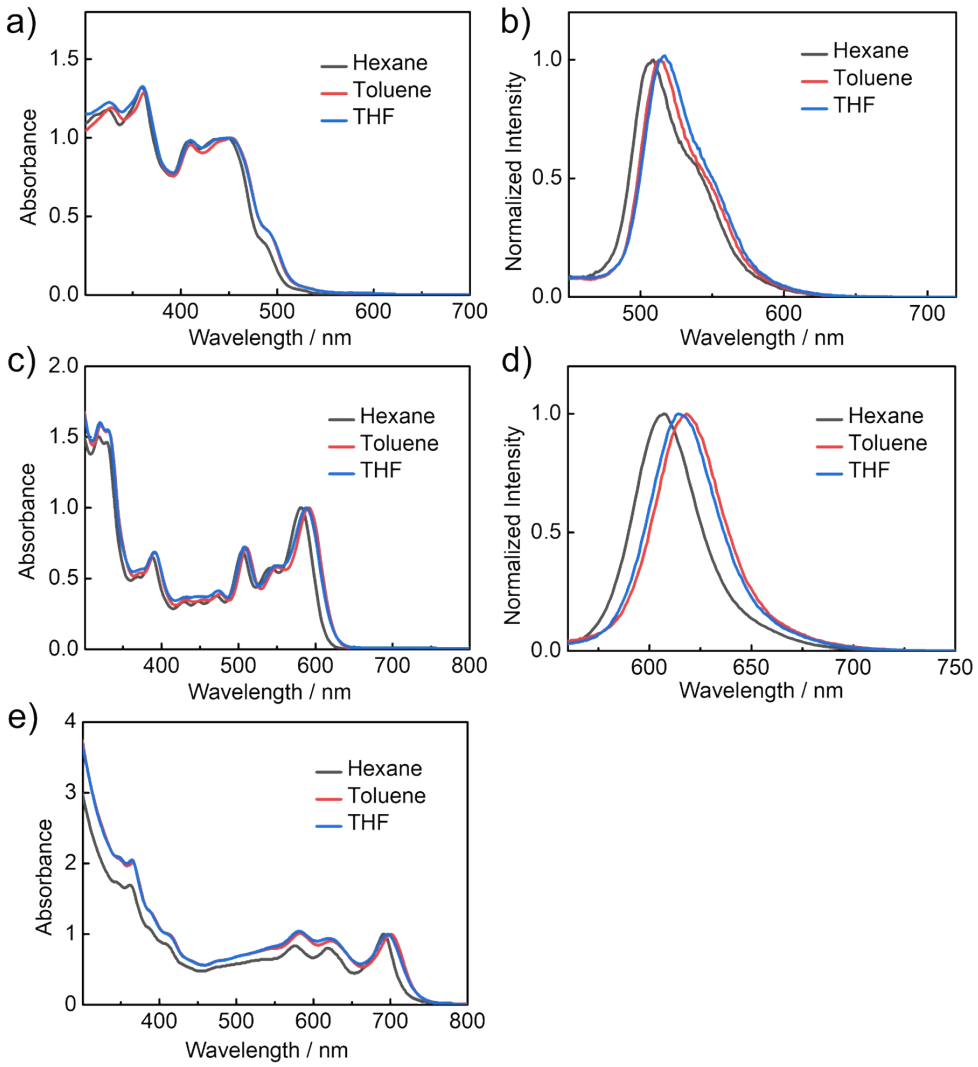

Fig. S7. Absorption and fluorescence spectra of a,b) **6** c,d) **1** and e) **2** in various solvents, respectively.

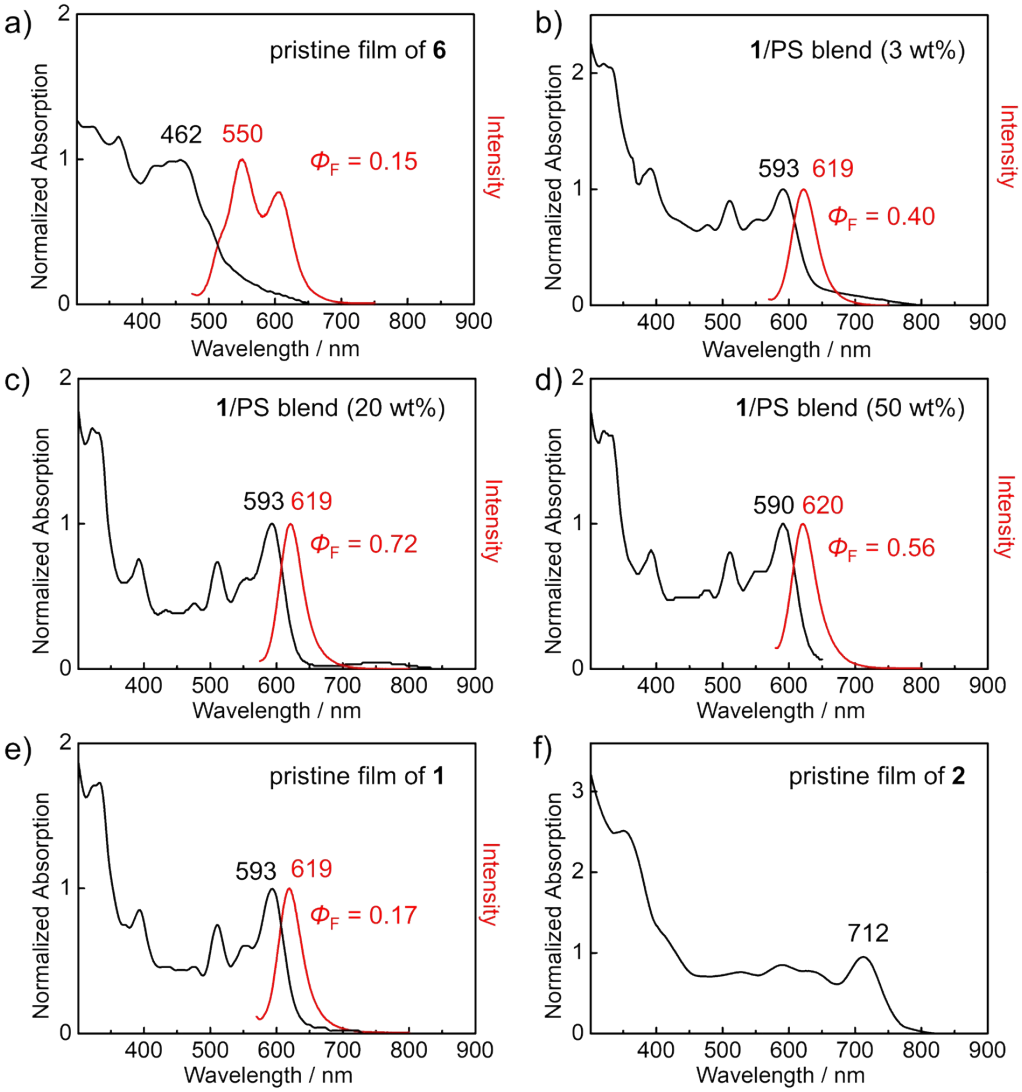

Fig. S8. Absorption and fluorescence spectra for a) the pristine film of **6**, the **1**/PS blend film with the ratio of b) 3 wt%, c) 20 wt%, d) 50 wt%, and the pristine films of e) **1** and f) **2**, respectively.

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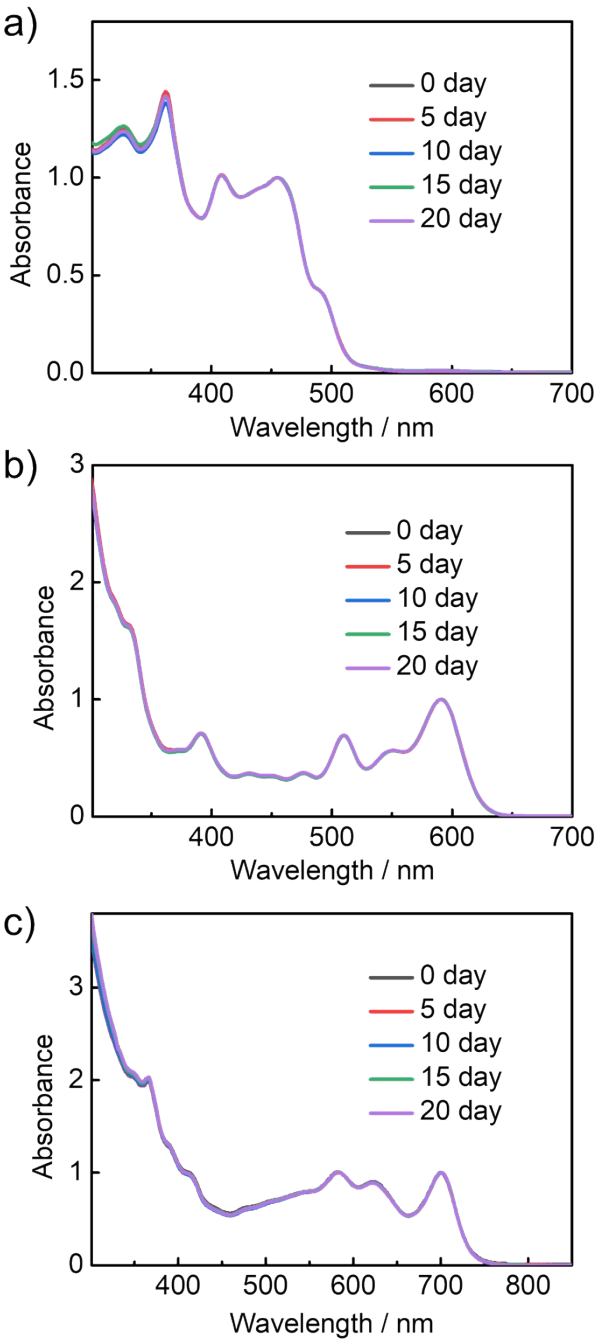

Fig. S9. Absorption spectra of a) **6**, b) **1** and c) **2** in toluene with the solution left at ambient conditions for 20 days. The unchanged spectra indicate that they are very stable toward air, moisture and light.

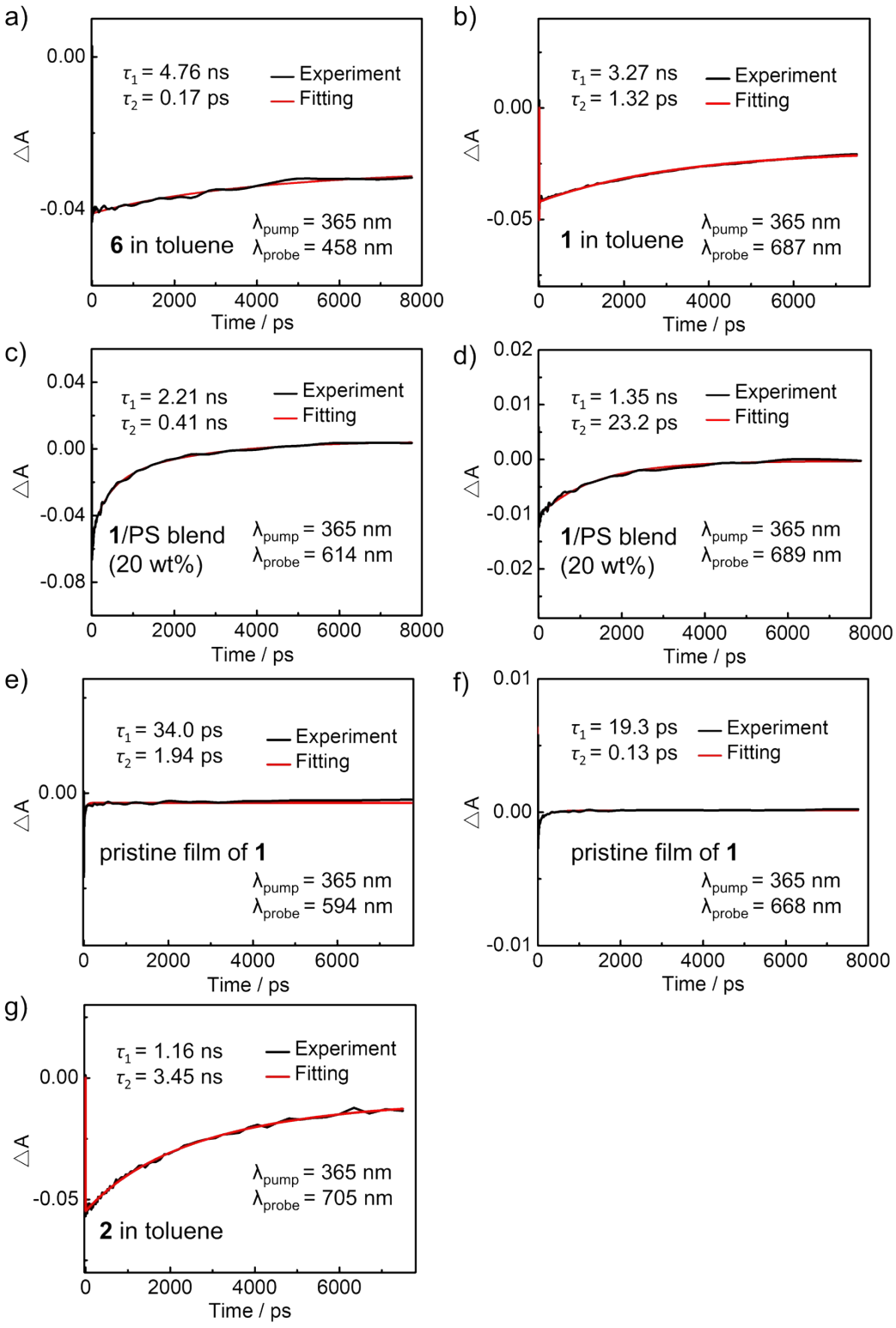

Fig. S10. Exponential fitting of the fs-TA signals for a) **6** and b) **1** in toluene, c,d) the **1**/PS blend film (20 wt%), e,f) the pristine film of **1** and g) **2** in toluene, respectively.

7. Amplified spontaneous emission properties

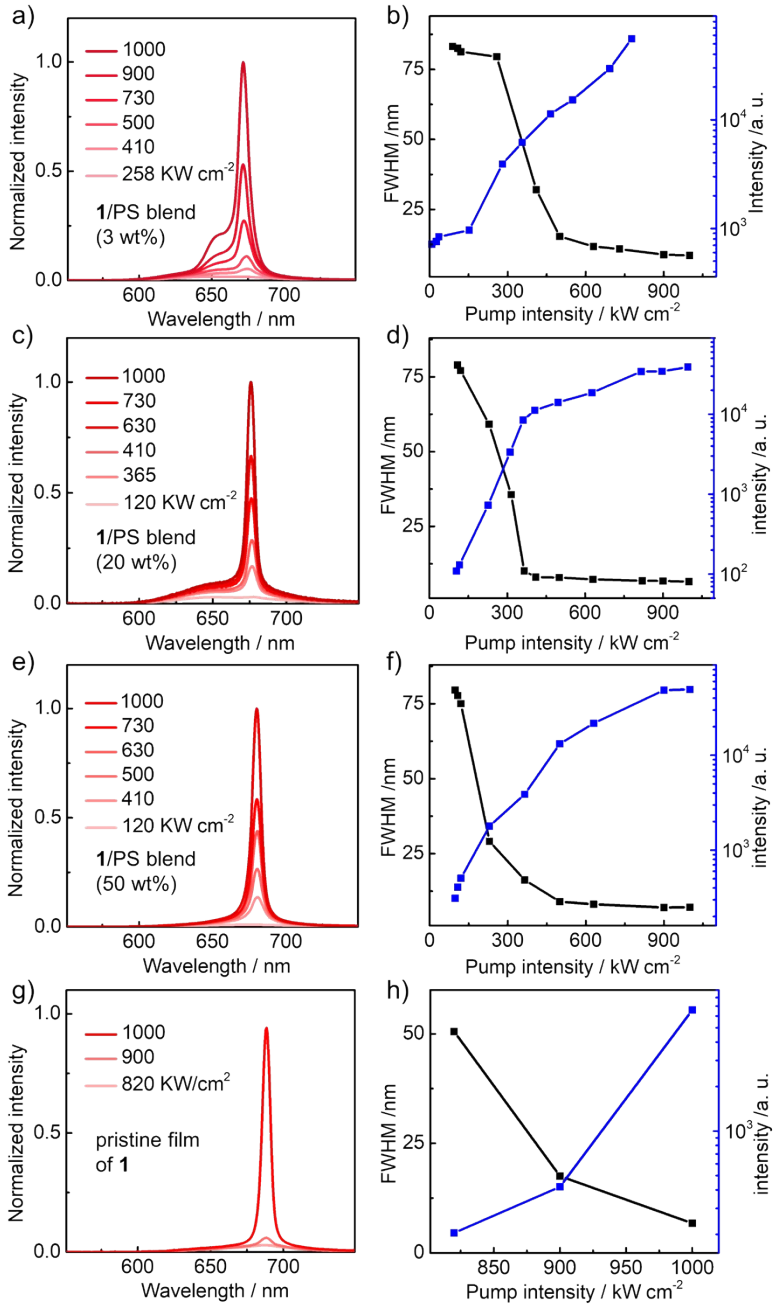

Fig. S11. Photoluminescence spectra taken at the different laser power fluences for the **1**/PS blend film with the ratio of a) 3 wt% and c) 20 wt%, e) 50 wt% and g) the pristine film of **1**. Dependences of FWHM and emission peak intensity on the laser energies of the **1**/PS blend film with the ratio of b) 3 wt%, d) 20 wt%, f) 50 wt% and h) the pristine film of **1**. As the pump energy increases exceeding a certain threshold, the FWHM is narrowed dramatically. Therefore, the threshold value is determined to be 258 kW cm^{-2} for the 3 wt% film and 120 kW cm^{-2} for the 20 wt% and 50 wt% films.

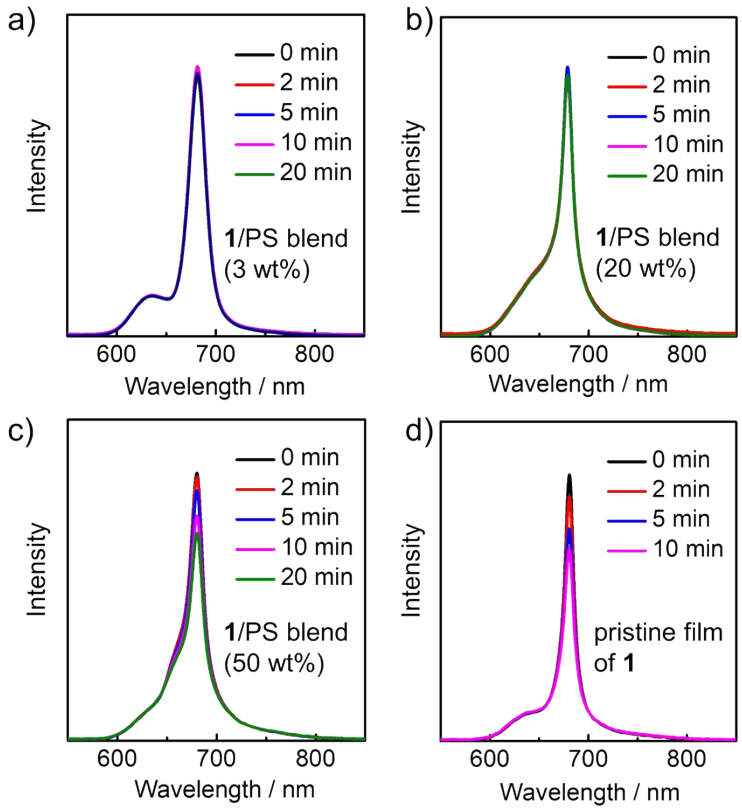

Fig. S12. a–d) Evolution of the ASE signal over time taken at a laser fluence of 500 kW cm^{-2} for the blend and pristine films of **1**. The ASE spectra for the 3 wt% and 20 wt% **1**/PS blend films exhibit excellent environmental and operational stability after the sample being irradiated for 20 min, whereas higher concentration may decrease the stability to a certain extent.

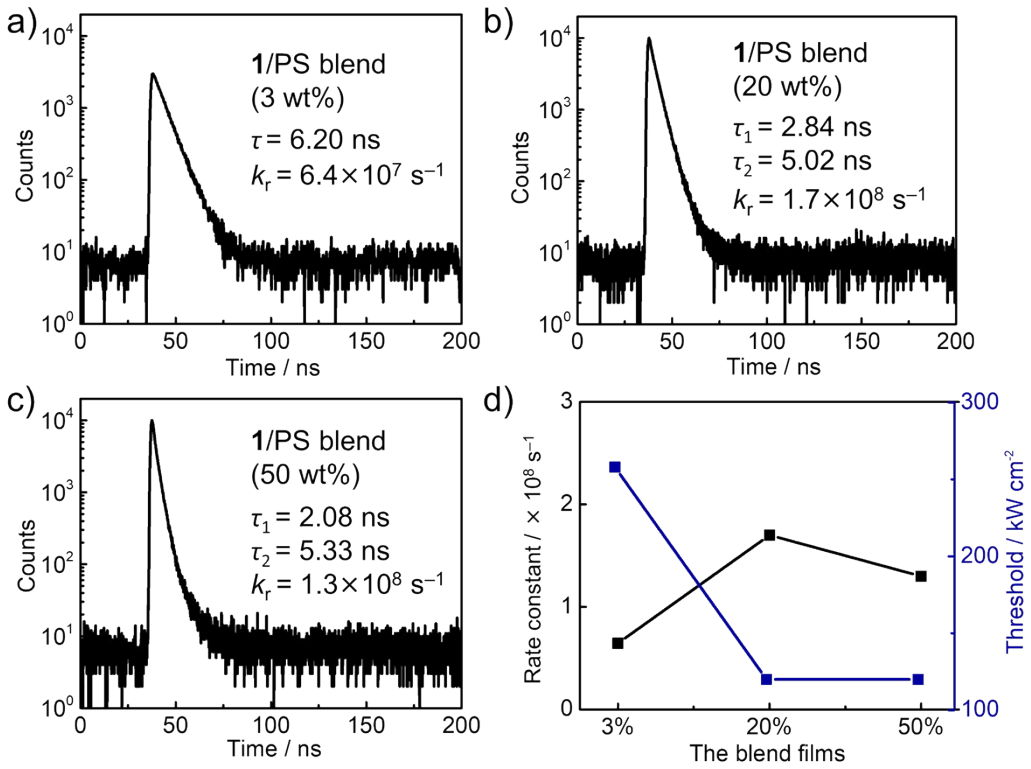

Fig. S13. Fluorescence decay curves and lifetimes of the **1**/PS blend film with the ratio of a) 3 wt%, b) 20 wt%, c) 50 wt%. d) The relationship between k_r and the threshold for the **1**/PS blend films.

Table S5. The ASE performance of **1** and several reported PAHs.

Compound	λ_{ASE} [nm]	$FWHM_{ASE}$ [nm]	E_{th}^{ASE} [μJ cm^{-2}]
1 (3 wt%)	672	8.7	2580
1 (20 wt%)	676	6.5	1200
1 (50 wt%)	680	7.2	1200
1 (100 wt%)	688	6.7	–
DBO 1 (1 wt%)[4]	695	–	60
ZY-02 (1 wt%)[5]	570	4	700
HBPO (1.24 wt%)[6]	613	–	2400
DBDNC1 (1 wt%)[7]	655	5	13000
	700	8	5300
BMC2 (3 wt%)[1]	669	6.4	1200

8. Time-dependent DFT calculations

To assign the absorption properties of **6**, **1**, **2** and **1C**, time-dependent (TD) DFT calculations were performed at the B3LYP/6-311G(d) level.

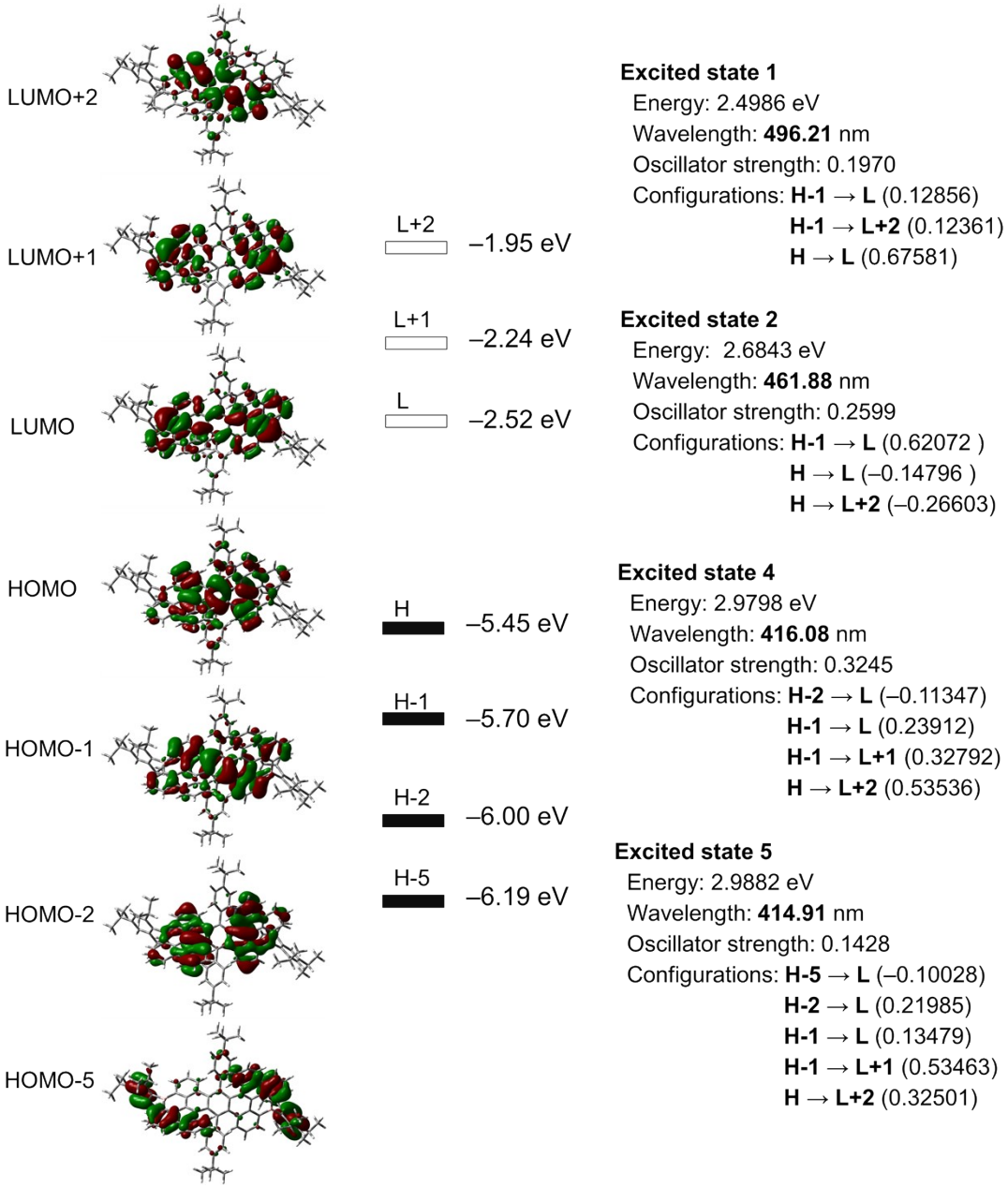

Fig. S14. The molecular orbitals, energy levels, excitation energies and oscillator strengths of **6**.

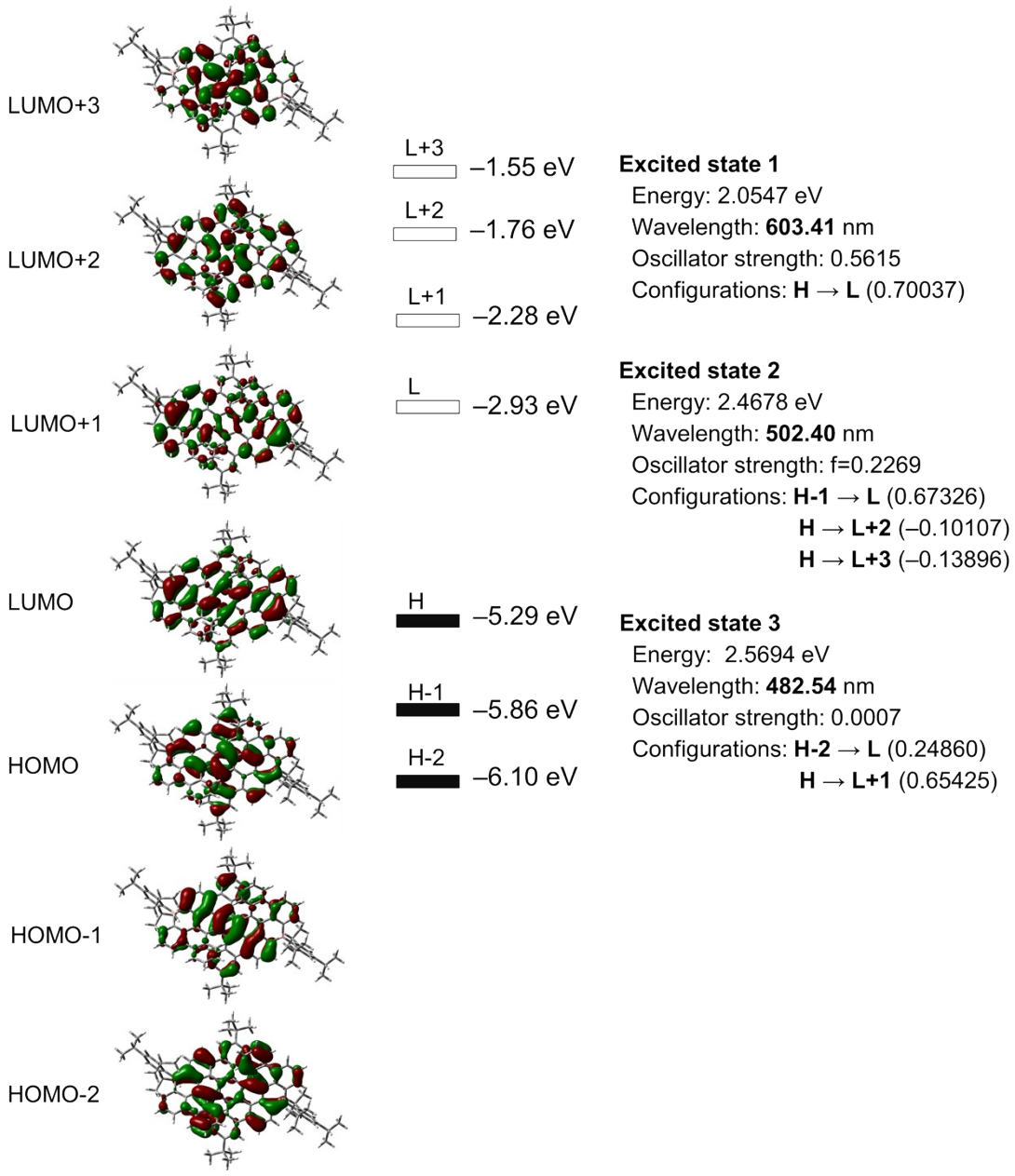

Fig. S15. The molecular orbitals, energy levels, excitation energies and oscillator strengths of **1**.

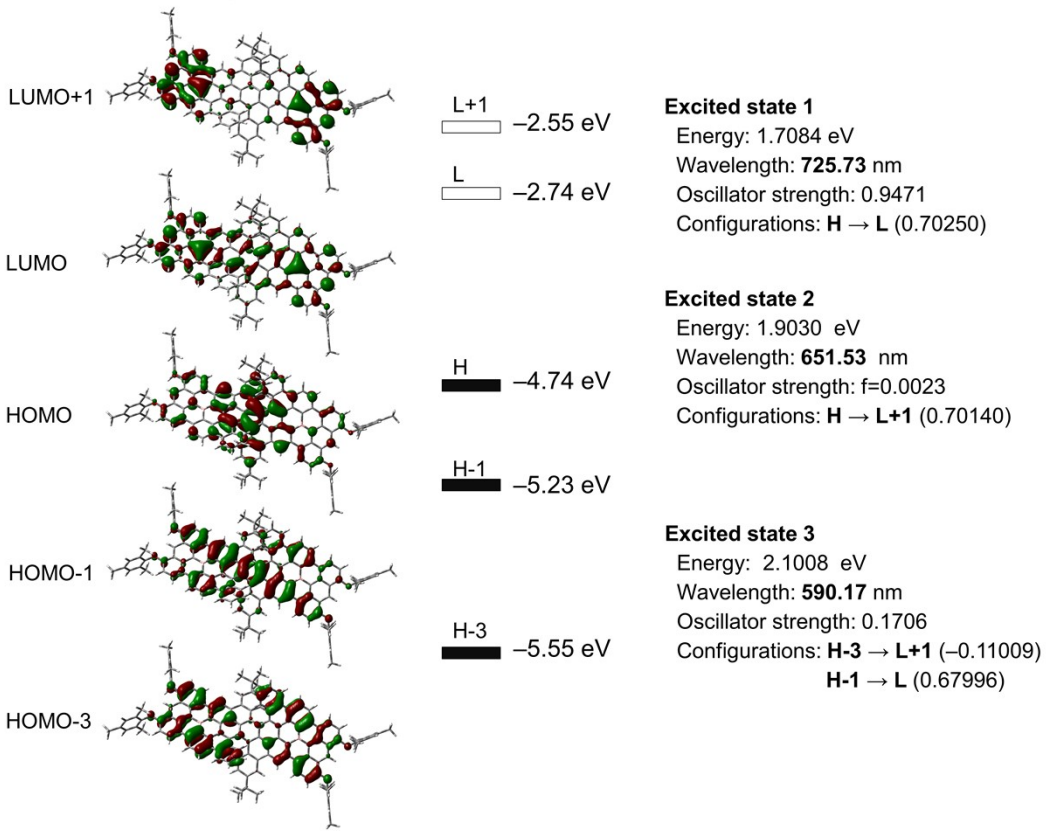

Fig. S16. The molecular orbitals, energy levels, excitation energies and oscillator strengths of **2**.

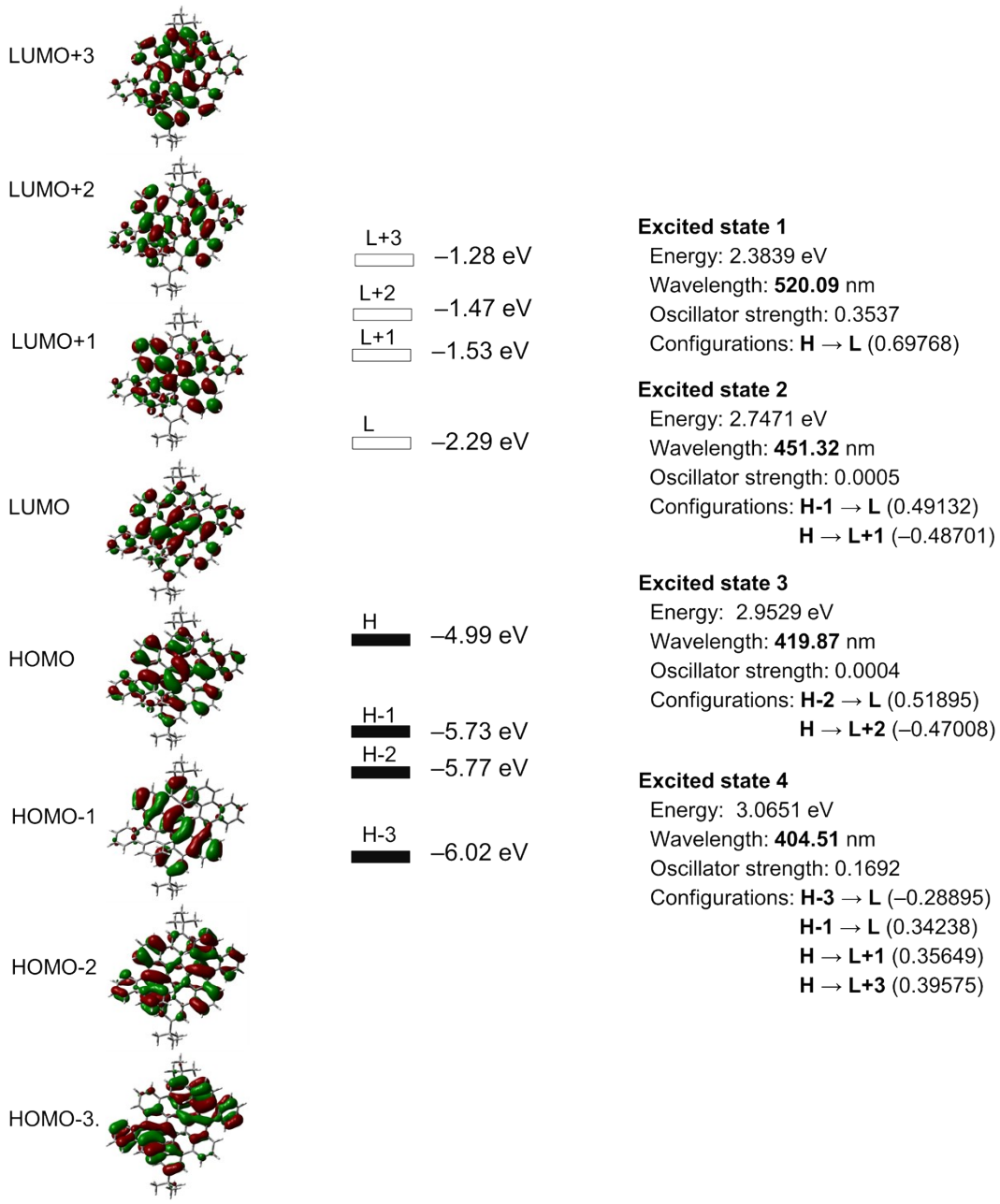

Fig. S17. The molecular orbitals, energy levels, excitation energies and oscillator strengths of **1C**.

9. ^{1}H NMR and ^{13}C NMR spectra

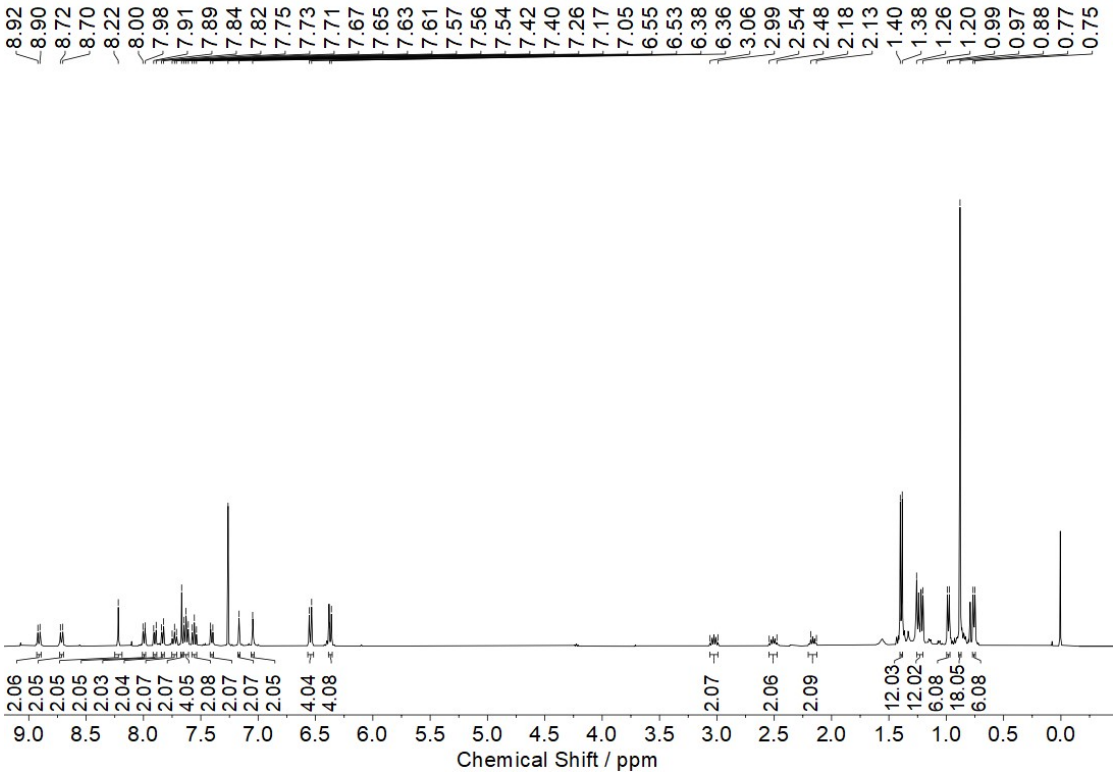

Fig. S18. ^{1}H NMR spectrum of **5** in $CDCl_3$.

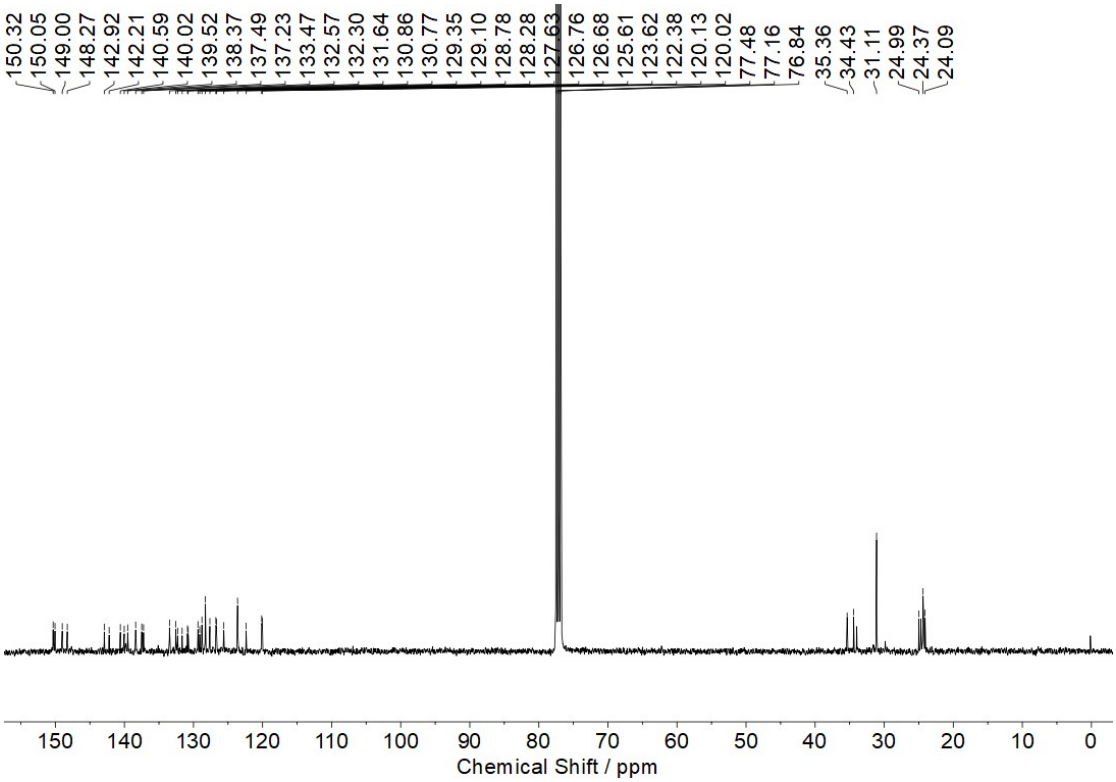

Fig. S19. ^{13}C NMR spectrum of **5** in $CDCl_3$.

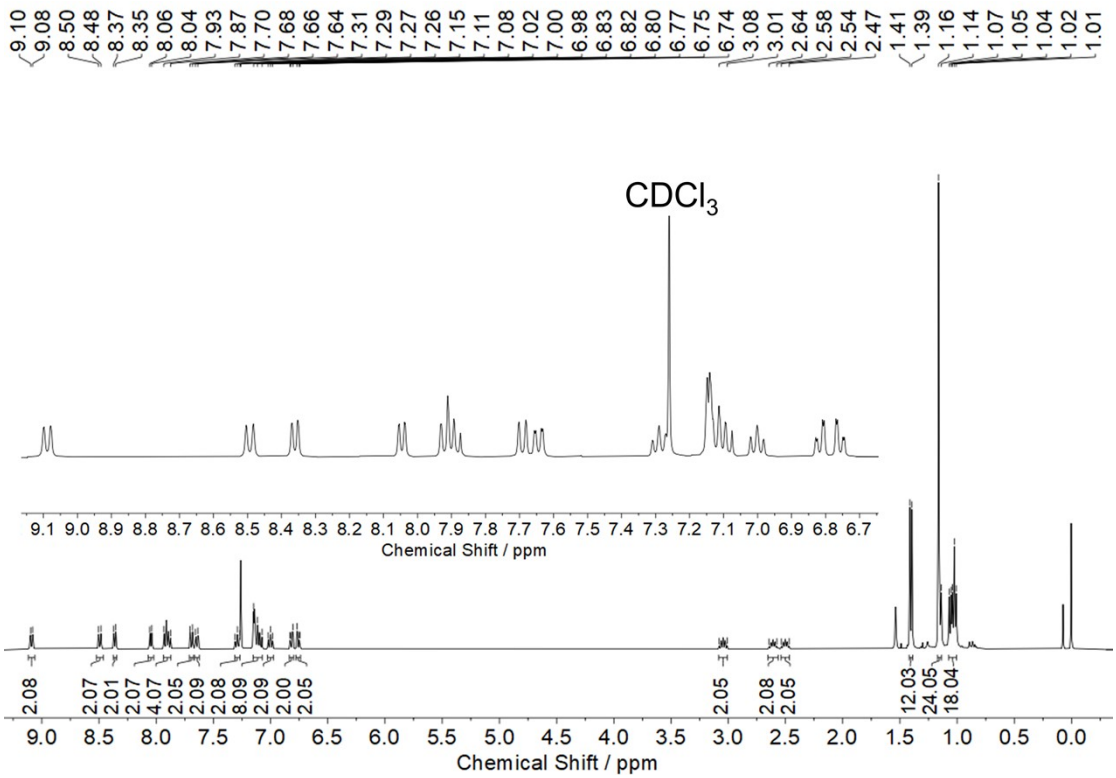

Fig. S20. ^{1}H NMR spectrum of **6** in $CDCl_3$.

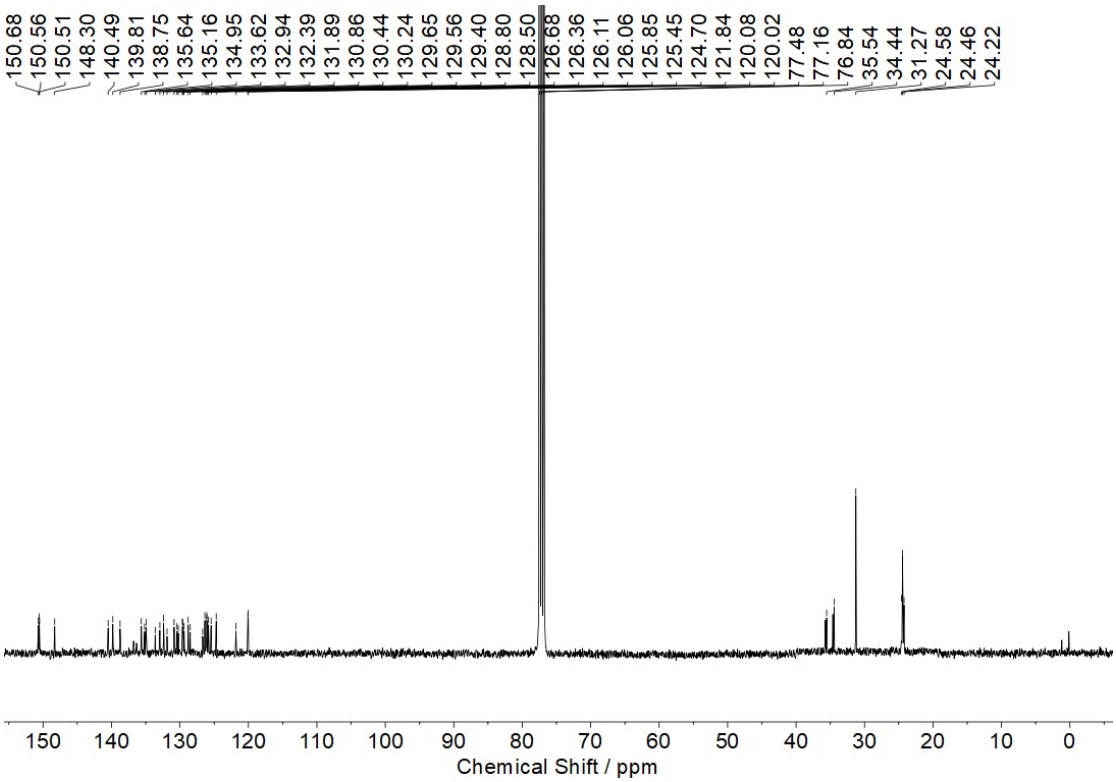

Fig. S21. ^{13}C NMR spectrum of **6** in $CDCl_3$.

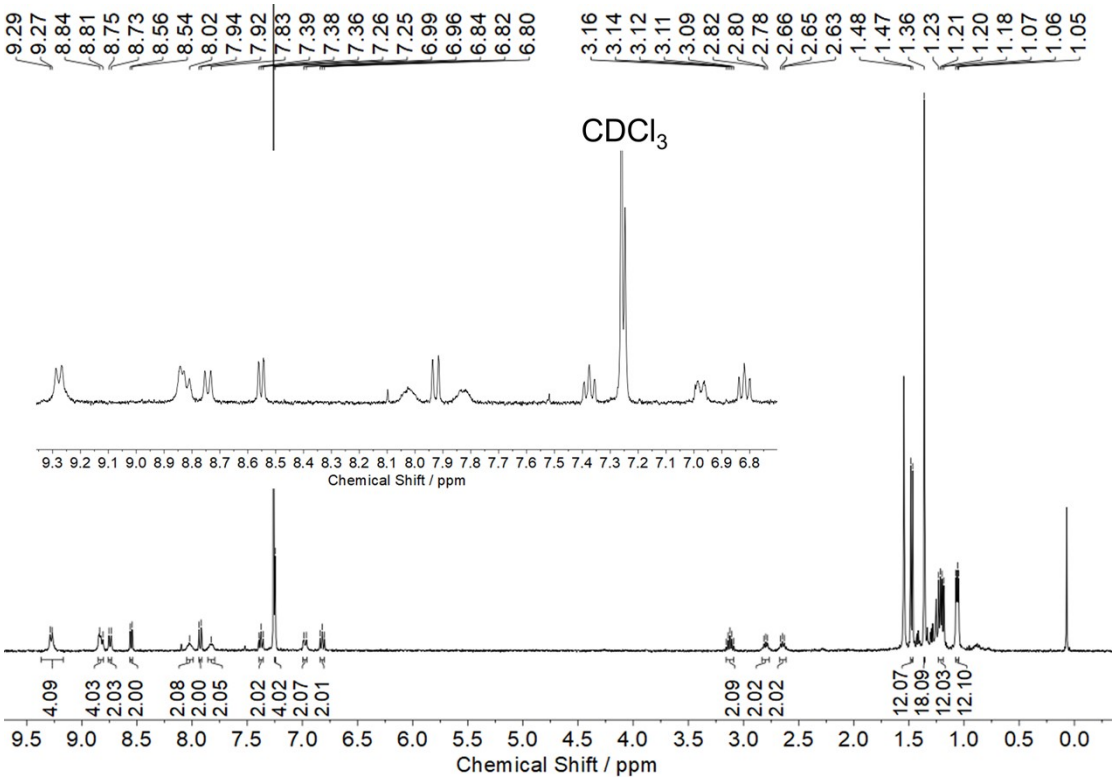

Fig. S22. ^{1}H NMR spectrum of **1** in $CDCl_3$.

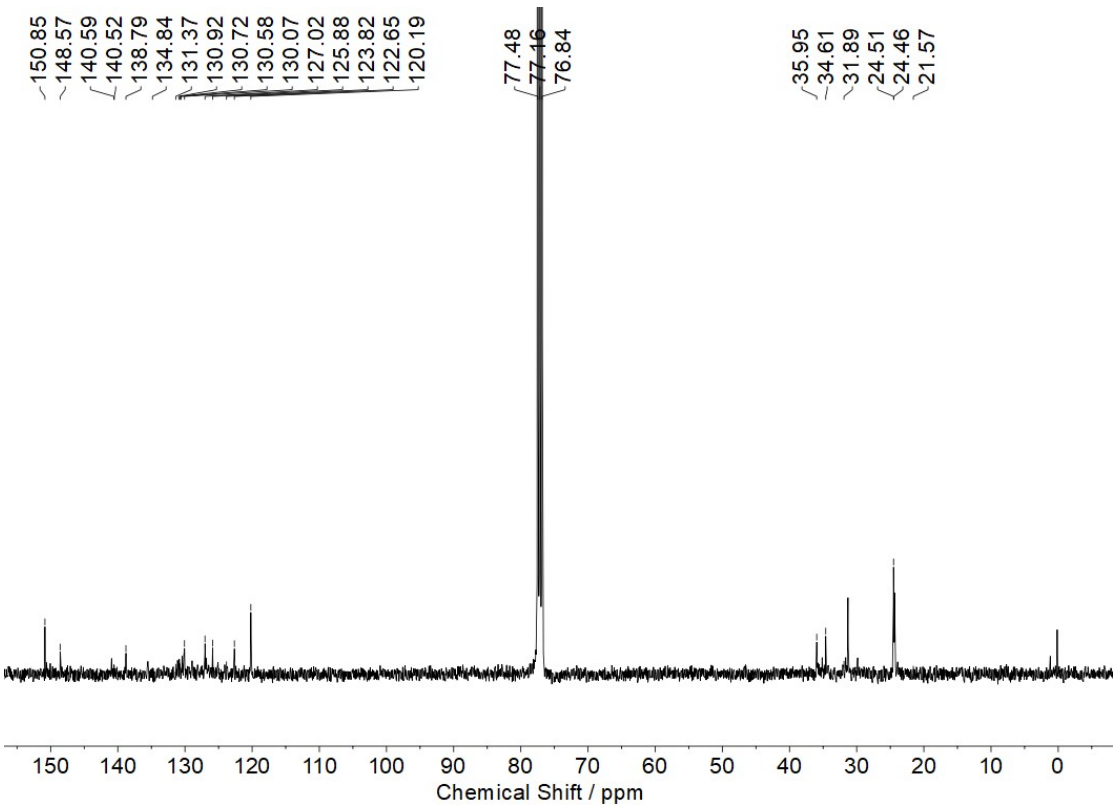

Fig. S23. ^{13}C NMR spectrum of **1** in $CDCl_3$.

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