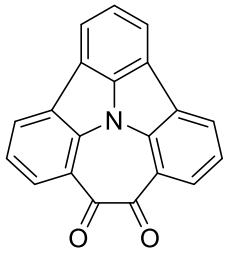
Table of Contents

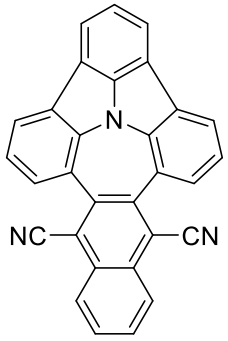
1. General Remarks

All reagents and solvents were commercially available and were used without further purification unless otherwise noted. FTIR-Spectra were recorded on a Tianjin Gangdong FTIR-650 spectrometer on a Ge ATR crystal. NMR spectra were taken on Bruker AVANCE NEO (600MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to traces of DMSO and CH_2Cl_2 in the corresponding deuterated solvent. HRMS experiments were carried out on a ThermoFisher LTQ Orbitrap XL. Crystal structure analysis was accomplished with a XtaLAB Synergy, Dualflex, HyPix diffractometer. Absorption spectra were recorded on a Shimadzu UV2600. The UV-vis-NIR absorption spectrum was measured on a Lambda 950 in dichloromethane. Electrochemical data were obtained in dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) and ferrocene was used as an internal standard. Cyclic voltammagram (CV) and differential pulse voltammagrams (DPV) were obtained using a glassy carbon working electrode, a platinum counter electrode, and a Ag reference electrode tested on CHI660E station. EPR spectrum was measured on a Bruker Magnettech ESR5000 apparatus. Elemental analysis was carried out on a PE 2400 II instrument. Compound **2** was synthesized according to the previously reported method.[S1]

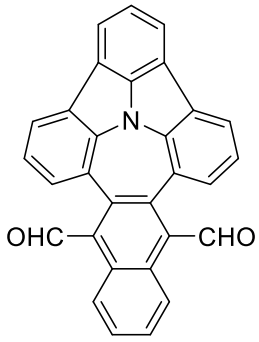
2. Experimental part



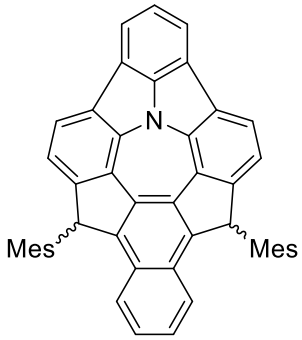
A 120 mL screw capped glass vial was charged with compound **2** (4.08 g, 15.38 mmol) and SeO_2 (3.75 g, 33.84 mmol). Under the protection of argon, dry *o*-dichlorobenzene (30 mL) was added to the glass vial. The vial was bubbled with argon for 3 minutes and quickly sealed. The glass vial was heated in an oil bath at 180 °C for 12 hours. After cooling down to room temperature, the reaction mixture was directly purified by neutral alumina column chromatography (dichloromethane/methanol 10:1) to give product **3** (3.95 g, 13.37 mmol, 87 %) as orange solid. ^{1}H NMR (600 MHz, DMSO) δ (ppm) = 8.61 (d, J = 7.7 Hz, 2H), 8.32 (d, J = 7.3 Hz, 2H), 8.26 (d, J = 7.9 Hz, 2H), 7.76 (t, J = 7.3 Hz, 1H), 7.64 (t, J = 7.7 Hz, 2H). Analytical data are in agreement with those published before.[S1]



A 250 mL flask was charged with compound **3** (2.52 g, 8.55 mmol), 1,2-phenylenediacetonitrile (1.47 g, 9.41 mmol), CH_3ONa (1.15 g, 21.38 mmol), methanol (80 mL) and DMF (80 mL). The flask was heated in an oil bath at 50 °C for 12 hours. After cooling down to room temperature, the reaction mixture was filtered and the solid was washed with water (100 mL), methanol (50 mL) to give the product **4** as orange solid (2.35 g, 5.66 mmol, 66%). m. p. > 400 °C; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.51 (dd, J = 6.3, 3.2 Hz, 2H), 8.17 (d, J = 7.8 Hz, 2H), 8.02 (d, J = 7.8 Hz, 2H), 7.90 (dd, J = 6.4, 3.2 Hz, 2H), 7.88 (d, J = 7.4 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.44 (t, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 154.71, 148.40, 142.80, 133.23, 132.91, 131.08, 129.76, 127.48, 127.09, 127.04, 125.76, 123.96, 123.42, 121.47, 118.03, 117.71; IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 1476, 1432, 1334, 1237, 1215, 1123, 803, 777, 753, 595, 574, 534, 514, 507, 503; HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{30}H_{14}N_3$ 416.1188; found 416.1193.



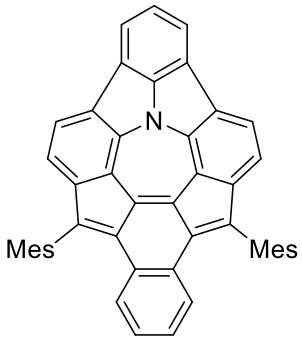
A 38 mL screw capped glass vial was charged with compound **4** (166 mg, 0.40 mmol) and anhydrous dichloromethane (8 mL). Under the protection of argon, the vial was cooled to -42 °C and DIBAl-H (1.5 M in toluene, 1.07 mL, 1.60 mmol) was added dropwise. After 30 minutes, the vial was stirred at room temperature for 16 hours. Diluted HCl (1M, 10 mL) was added and the mixture was further stirred for 1 hour at room temperature. The reaction was then diluted with dichloromethane (100 mL) and washed with water (3×100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/petroleum ether 1:2) to give product **5** (75 mg, 0.18 mmol, 44 %) as brownish yellow solid. m. p. 323-325 ℃; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 9.82 (s, 2H), 8.97 (dd, *J* = 6.6, 3.4 Hz, 2H), 8.03 (dd, *J* = 6.1, 2.6 Hz, 2H), 7.92 (d, *J* = 7.4 Hz, 2H), 7.74 (dd, *J* = 6.7, 3.3 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.41-7.36 (m, 4H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 193.96, 148.40, 140.93, 139.02, 132.77, 132.73, 130.19, 129.58, 127.42, 127.01, 125.50, 125.46, 124.06, 123.57, 121.67, 53.84; IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 1674, 1474, 1431, 1334, 1306, 1242, 1215, 1128, 1053, 805, 773, 752, 712, 658, 591; HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{30}H_{15}NO_2Na$ 444.0995; found 444.0993.



A 38 mL screw capped glass vial was charged with compound **5** (30 mg, 0.07 mmol) and anhydrous THF (3 mL). The vial was cooled at 0 ℃ and mesitylmagnesium bromide (1M in THF, 0.57 mL, 0.57 mmol) was added. The vial was then capped and stirred at room temperature for 12 hours. The reaction was quenched by adding water (5 mL) and diluted with dichloromethane (100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by neutral alumina column chromatography (dichloromethane) to give the intermediate **6** as oily liquid. Anhydrous dichloromethane (3 mL) was added to dissolve **6**. Under the protection of argon, boron trifluoride diethyl etherate (3 mL) was added. After stirring at room temperature for 2 hours, the reaction was quenched by adding water (5 mL) and diluted with dichloromethane (100 mL), which was further washed with water (3×100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by neutral alumina column chromatography (petroleum ether) to give the *anti*-**7** (12 mg, 27%) as colorless solid and *syn*-**7** (23 mg, 51%) as yellow solid.

anti-**7**: m. p. 358-360 ℃; ^{1}H NMR (600 MHz, CD_2Cl_2/CS_2) δ (ppm) = 7.88 (d, *J* = 7.4 Hz, 2H), 7.73 (d, *J* = 8.1 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.33 (dd, *J* = 6.2, 3.3 Hz, 2H), 7.11 (s, 2H), 7.09 (dd, *J* = 6.3, 3.2 Hz, 2H), 7.02 (d, *J* = 8.1 Hz, 2H), 6.63 (s, 2H), 5.93 (s, 2H), 2.83 (s, 6H), 2.30 (s, 6H), 1.24 (s, 6H); ^{13}C NMR (150 MHz, CD_2Cl_2/CS_2) δ (ppm) = 192.94, 145.34, 143.73, 138.45, 137.05, 136.98, 135.82, 133.53, 133.38, 132.65, 130.94, 129.81, 129.13, 128.38, 126.24, 125.92, 125.55, 124.66, 123.43, 121.95, 119.73, 53.84, 22.32, 21.17, 18.95; IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 1482, 1446, 1379, 1323, 1018, 853, 798, 773, 749, 694, 654, 632, 578, 521, 504; HRMS(ESI) (*m/z*): $[M]^+$ calculated for $C_{48}H_{35}N$ 625.2770; found 625.2772.

syn-**7**: m. p. 360-361 ℃; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 7.85 (d, *J* = 7.3 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.3 Hz, 1H), 7.24 (dd, *J* = 6.2, 3.3 Hz, 2H), 7.07 (d, *J* = 2.0 Hz, 2H), 7.04 (dd, *J* = 6.4, 3.2 Hz, 2H), 6.88 (d, *J* = 8.1 Hz, 2H), 6.43 (s, 2H), 6.13 (s, 2H), 2.83 (s, 6H), 2.22 (s, 6H), 0.53 (s, 6H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 149.52, 146.63, 145.20, 138.00, 137.30, 136.84, 135.75, 133.85, 133.39, 132.11, 130.55, 129.50, 128.83, 128.05, 125.95, 125.85, 125.45, 124.47, 123.11, 121.77, 119.32, 53.84, 22.21, 20.93, 18.54; IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 1509, 1478, 1443, 1325, 1032, 1017, 845, 797, 778, 746, 690, 659, 628, 586, 534; HRMS(ESI) (*m/z*): $[M]^+$ calculated for $C_{48}H_{35}N$ 625.2770; found 625.2770



A 38 mL screw capped glass vial was charged with compound **7** (21 mg, 0.03 mmol) and DDQ (14 mg, 0.06 mmol). Under the protection of argon, dry toluene (1 mL) was added to the vial, which was further bubbled with argon for 3 minutes. The vial was quickly sealed and heated in an oil bath at 80 ℃ for 15 hours. After cooling down to room temperature, the reaction was then diluted with dichloromethane (100 mL) and washed with water (3×100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (petroleum ether) to give product **8** (21 mg, 0.0.03 mmol, 99 %) as blue black solid. m. p. 371-372 ℃; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 7.58 (d, J = 7.5 Hz, 2H), 7.34 (d, J = 8.1 Hz, 2H), 7.23 (t, J = 7.5 Hz, 1H), 6.98 (s, 4H), 6.76-6.70 (m, 4H), 6.27 (d, J = 8.1 Hz, 2H), 2.35 (s, 6H), 2.10 (s, 12H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 144.12, 143.45, 141.94, 138.16, 136.40, 135.39, 131.37, 131.27, 129.86, 129.19, 128.86, 127.73, 127.29, 126.46, 125.88, 125.41, 124.62, 122.23, 117.86, 53.84, 21.32, 19.92; IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 1440, 1309, 1194, 1011, 928, 850, 807, 785, 761, 724, 702, 670, 642, 600, 540; HRMS(ESI) (*m/z*): $[M]^+$ calculated. for $C_{48}H_{33}N$ 623.2613; found 623.2614。

Chemical oxidation of **8**: The solution of $AgSbF_6$ (17 mg, 0.067 mmol) in dry dichloromethane (10 mL) was added to the solution of compound **8** (40 mg, 0.064) in dry dichloromethane (10 mL) under the protection of Argon. The solution was stirred at room temperature for 1 hour and the color was changed from dark blue to blackish green. The solution was filtered through a syringe and the solvent was removed under reduced pressure to afford quantitatively $\mathbf{8}^{\bullet+}$ as a dark blue amorphous solid. Elemental anal. calculated for $C_{48}H_{33}F_6NSb$: C 67.07 H 3.87 N 1.63, found: C 66.92 H 3.95 N 1.57.

3. NMR spectra

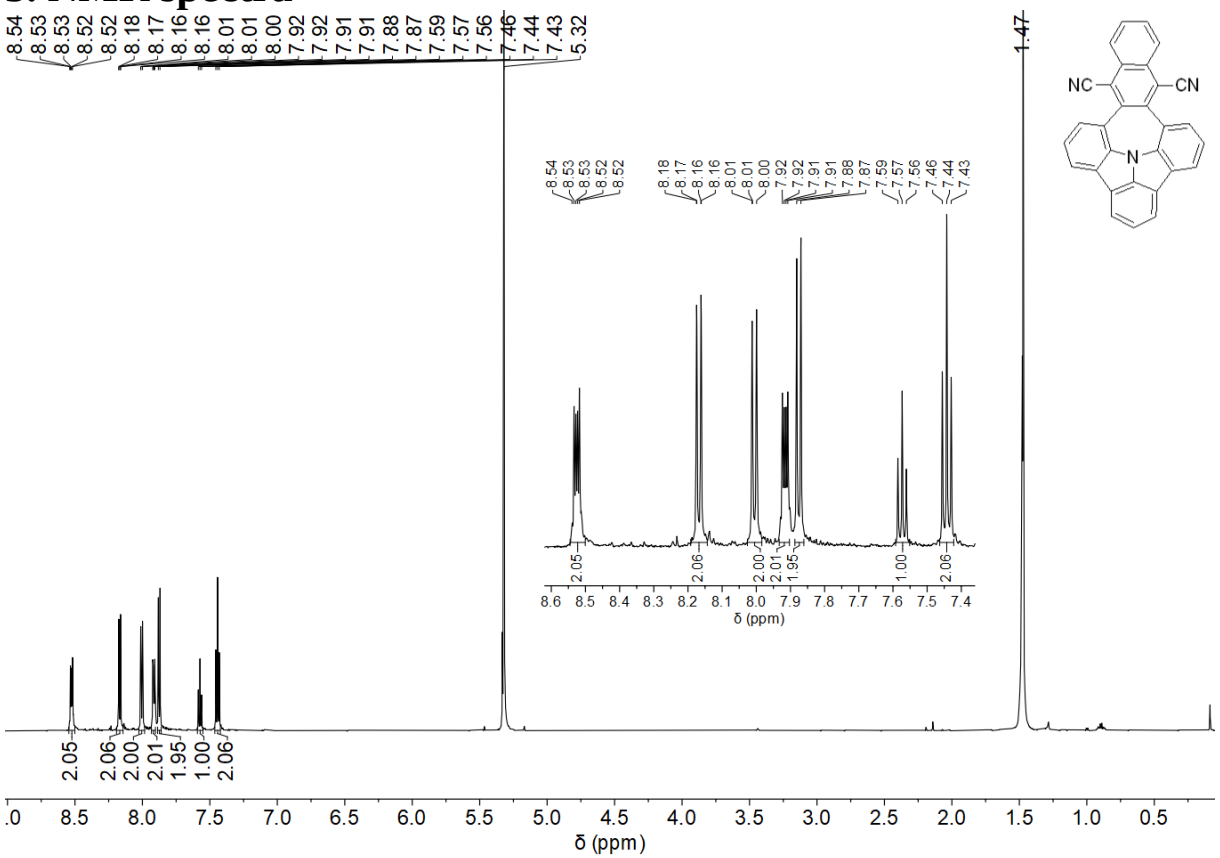


Figure S1. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **4**.

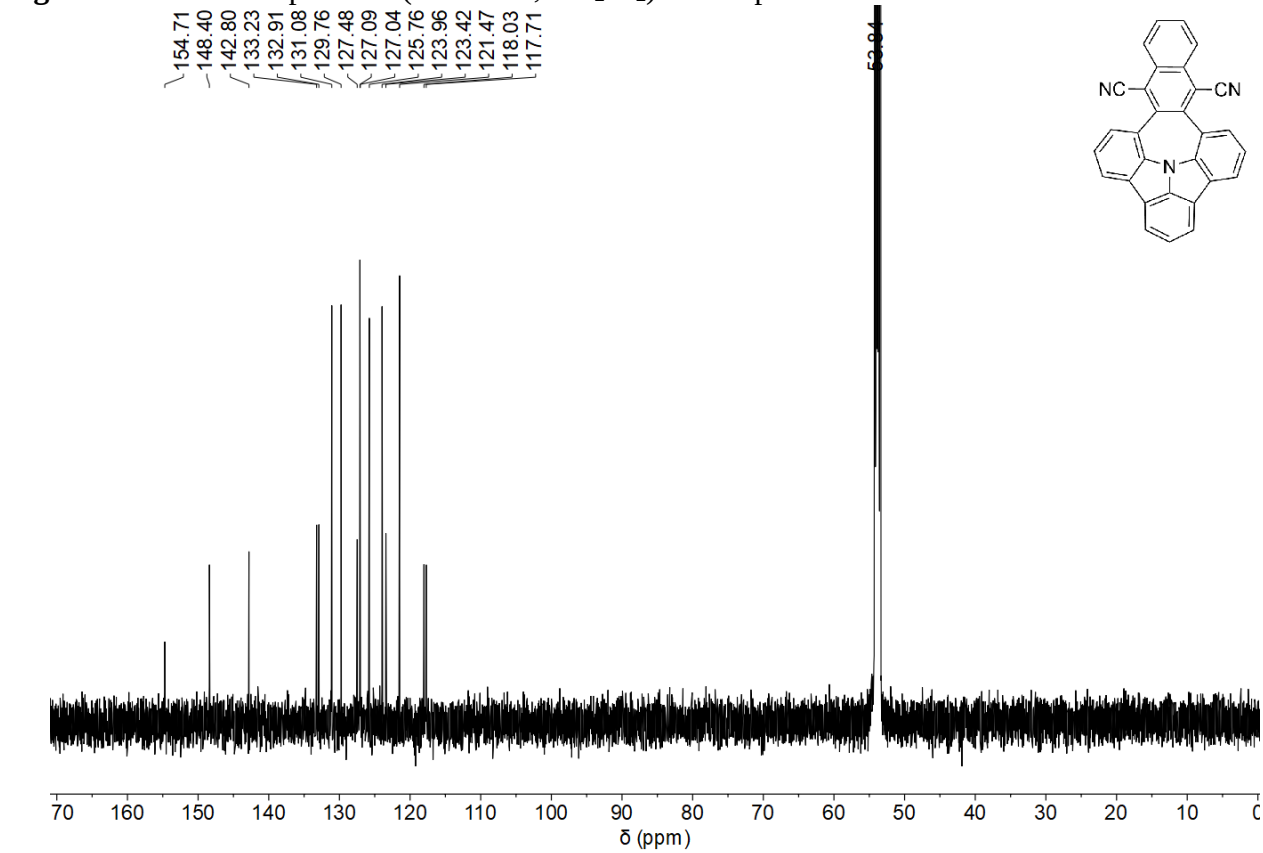


Figure S2. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **4**.

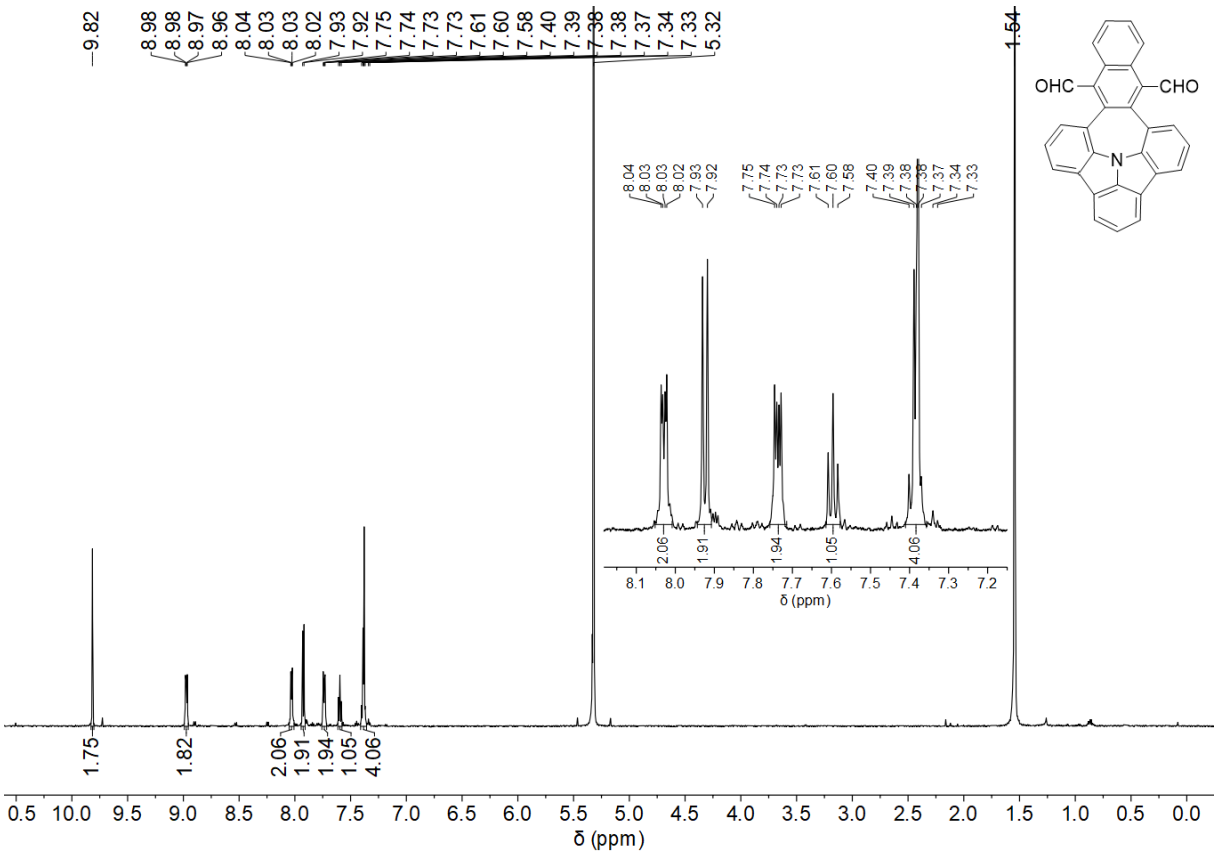


Figure S3. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **5**.

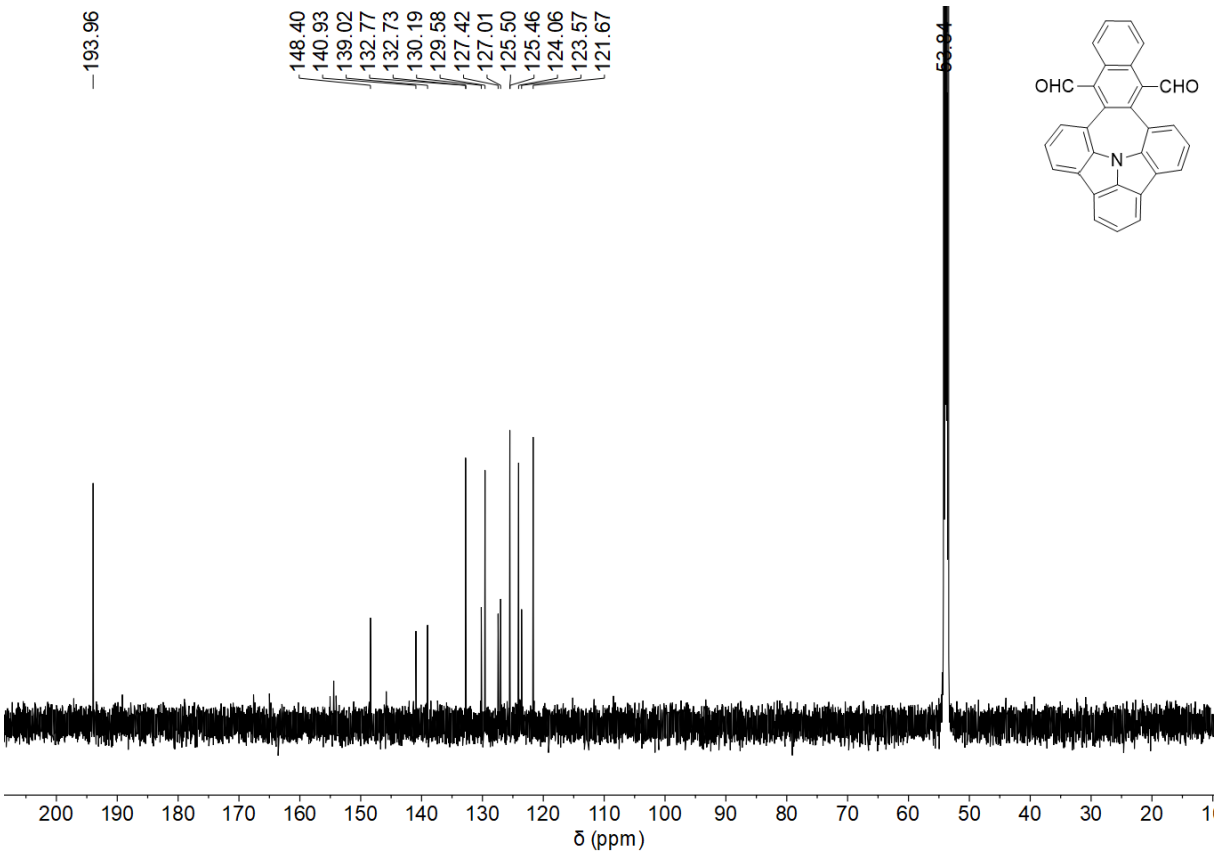


Figure S4. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **5**.

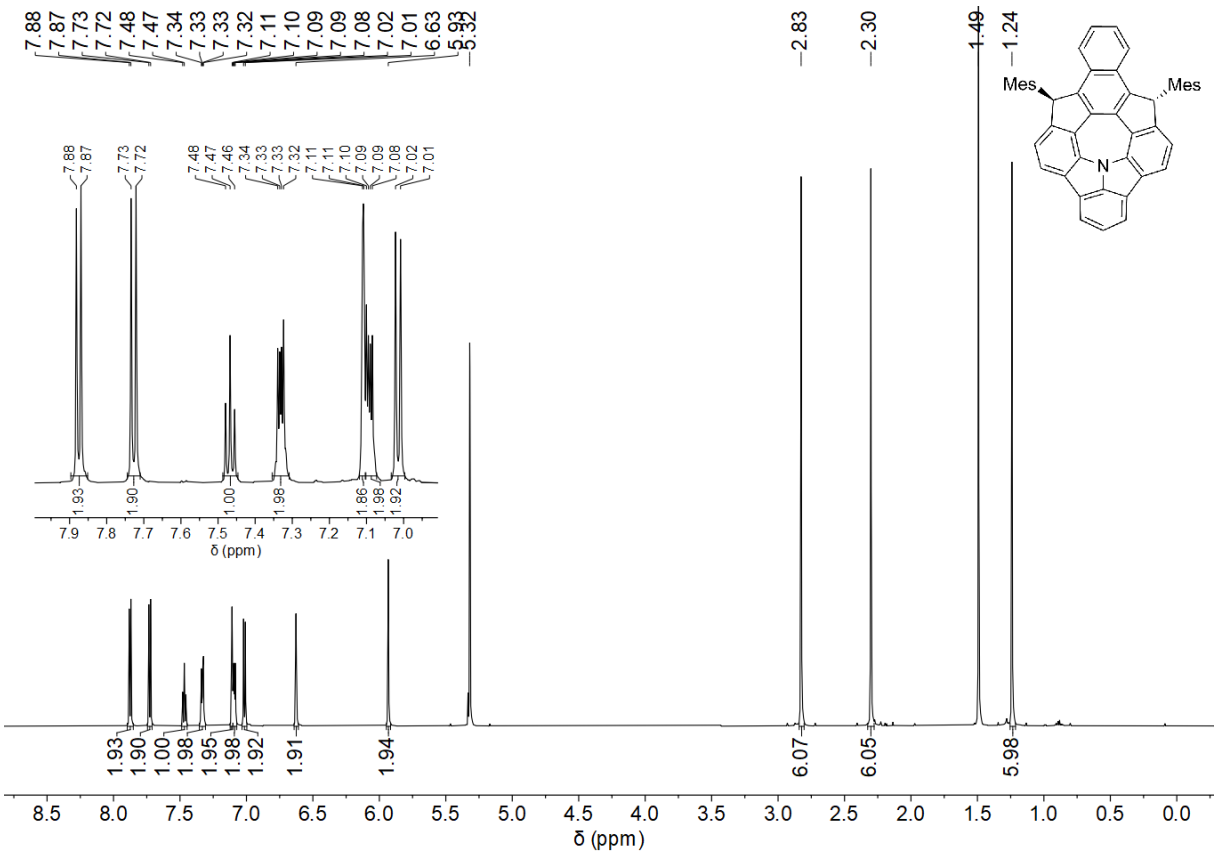


Figure S5. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2/CS_2) of compound *anti*-**7**.

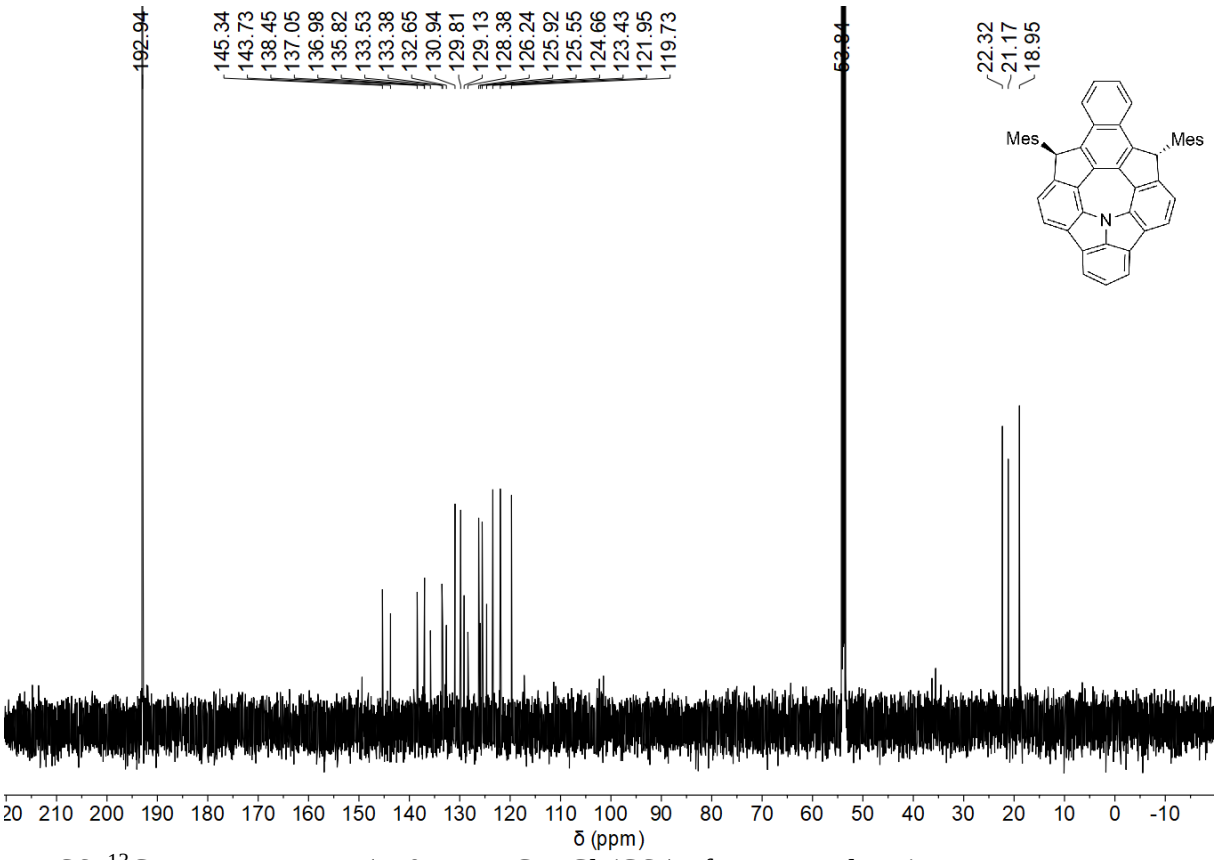


Figure S6. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2/CS_2) of compound *anti*-**7**.

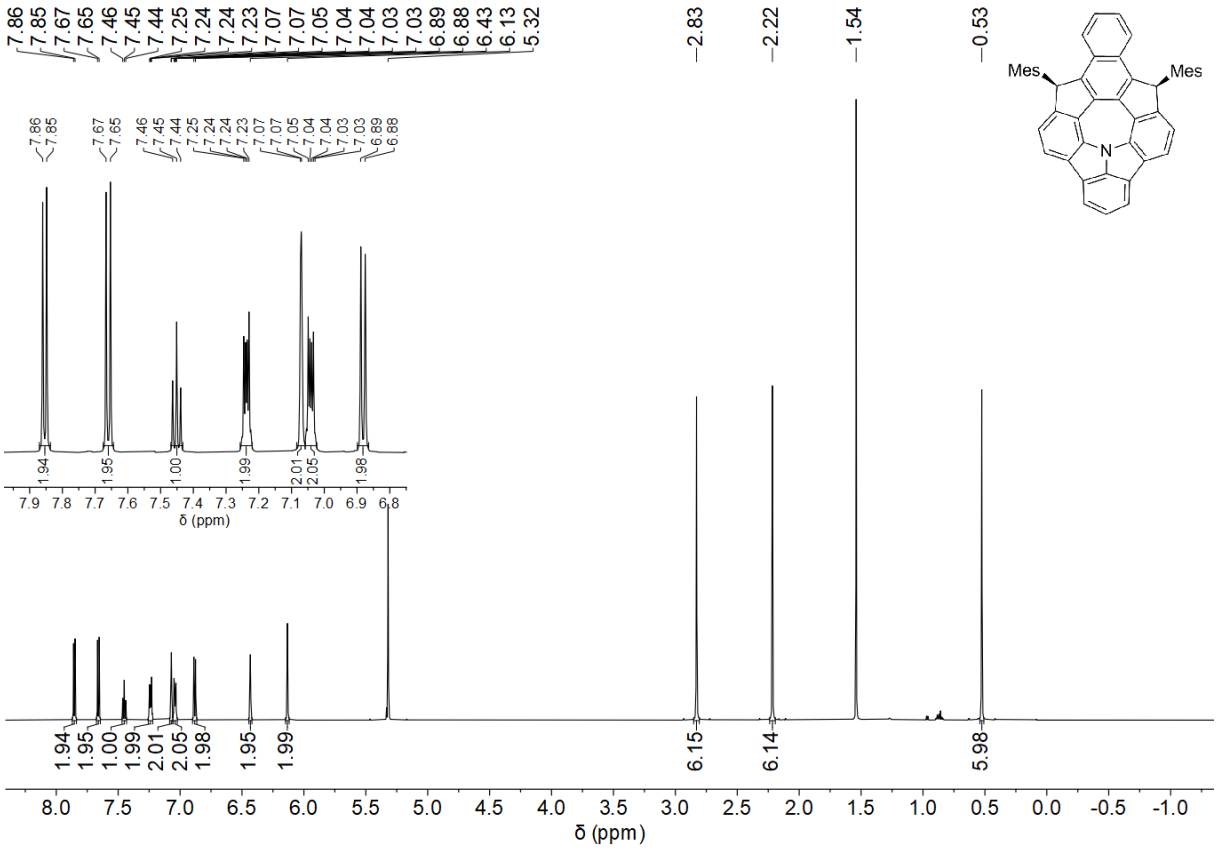


Figure S7. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound *syn*-**7**.

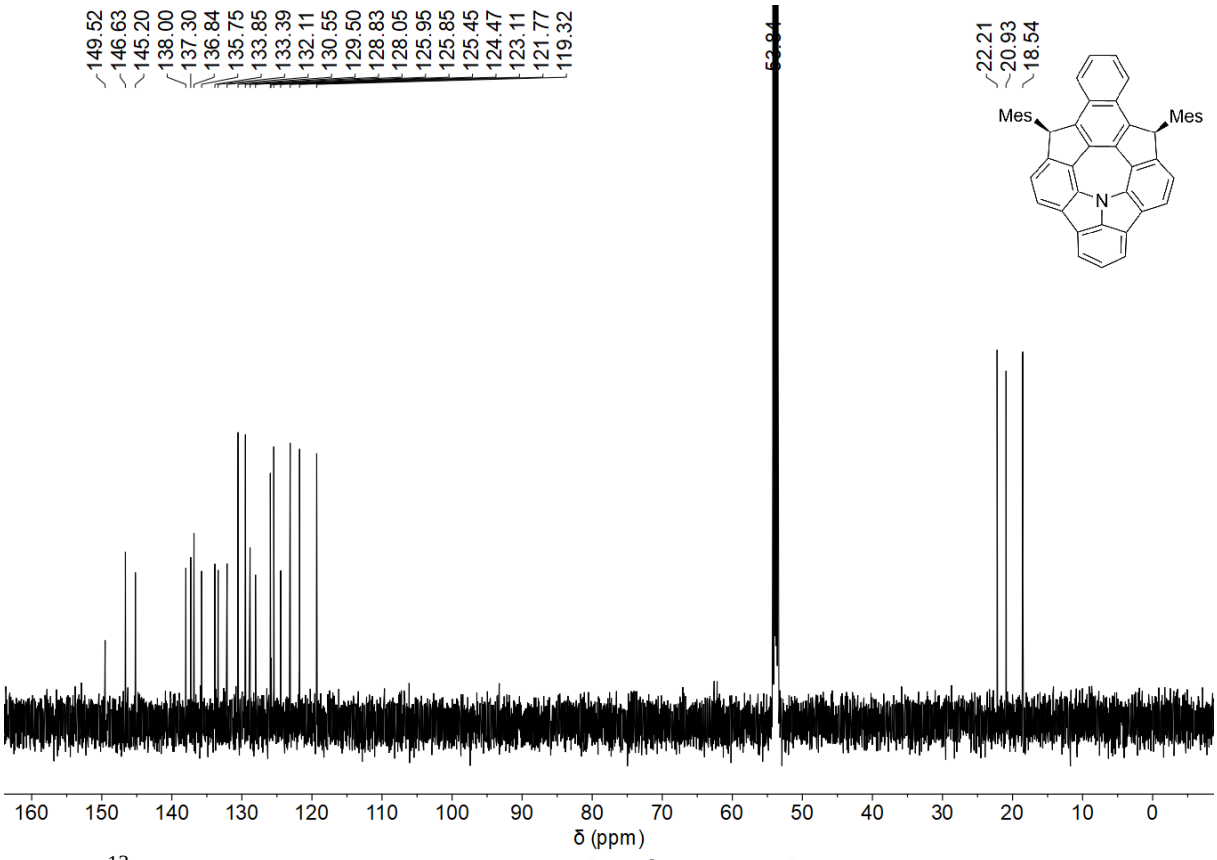


Figure S8. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound *syn*-**7**.

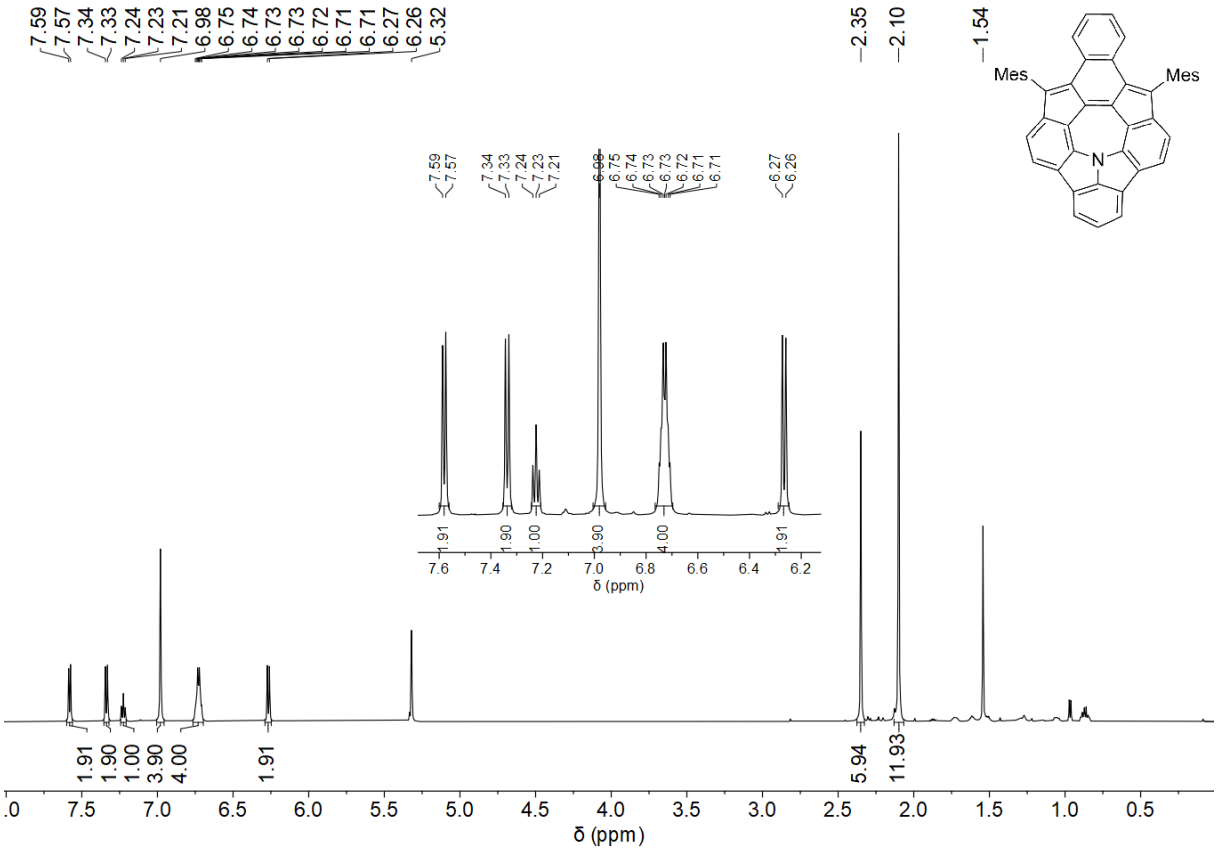


Figure S9. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **8**.

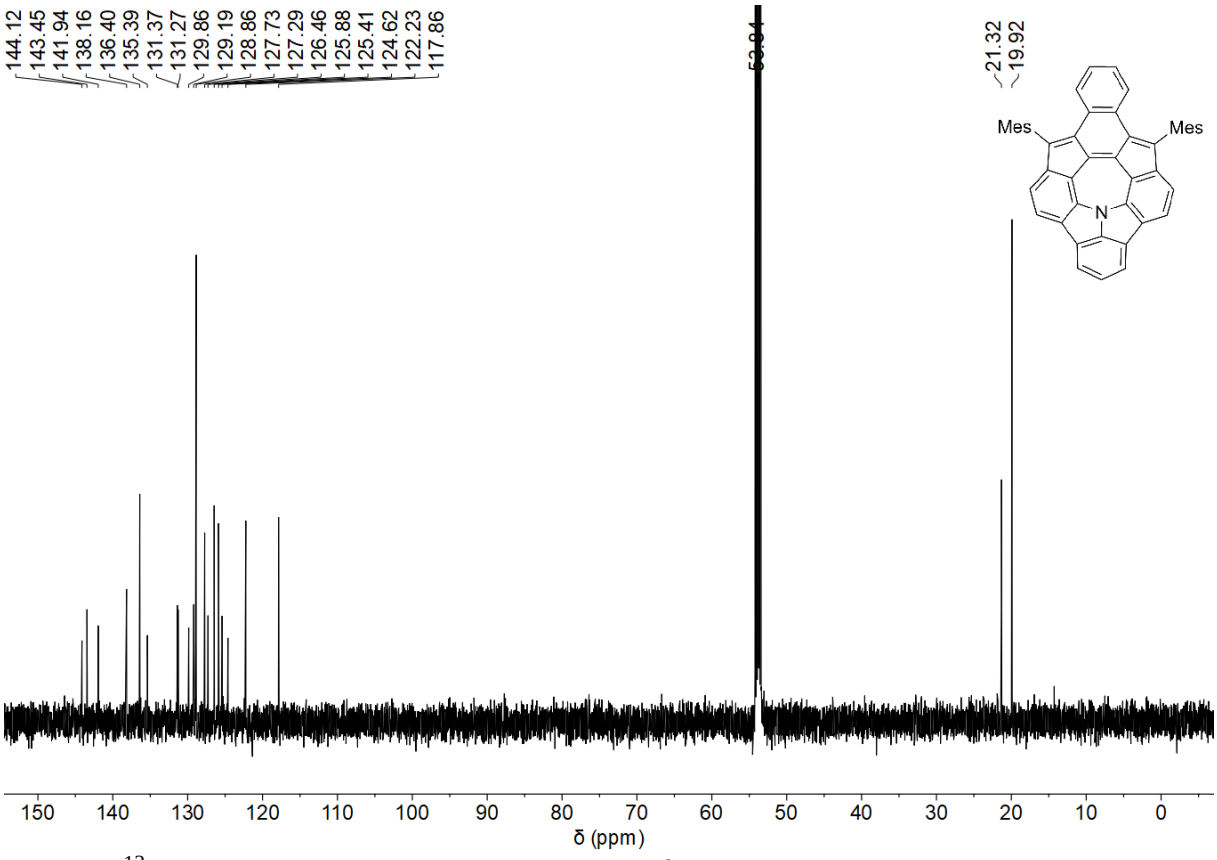


Figure S10. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **8**.

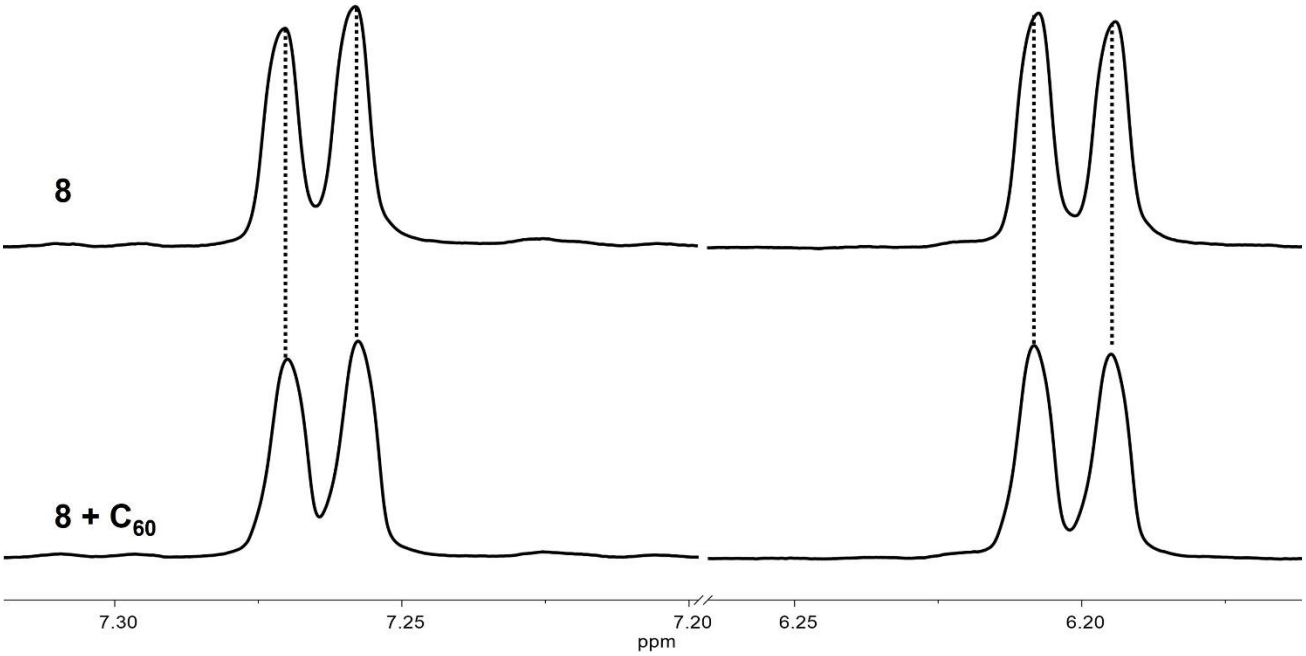


Figure S11. ^{1}H NMR spectra (600 MHz, toluene-d_8, 298 K) of **8** and in the presence of C_{60}.

4. X-ray crystallographic structure determination

Table S1 Crystal data and structure refinement for *anti*-7

Empirical formula	$C_{49}H_{37}Cl_2N$
Formula weight	710.69
Temperature/K	120.01(10)
Crystal system	triclinic
Space group	P-1
a/Å	8.3564(2)
b/Å	11.9727(3)
c/Å	19.0309(5)
α/°	101.659(2)
β/°	99.106(2)
γ/°	103.552(2)
Volume/Å^3	1770.04(9)
Z	2
ρ_{calc}g/cm^3	1.333
μ/mm^{-1}	1.930
F(000)	744.0
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.856 to 153.07
Index ranges	$-10 \leq h \leq 10$, $-15 \leq k \leq 15$, $-23 \leq l \leq 23$
Reflections collected	23444
Independent reflections	7142 [R_{int} = 0.0362, R_{sigma} = 0.0348]
Data/restraints/parameters	7142/0/475
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0624, wR_2 = 0.1695
Final R indexes [all data]	R_1 = 0.0733, wR_2 = 0.1769
Largest diff. peak/hole / e Å^{-3}	1.25/-0.99

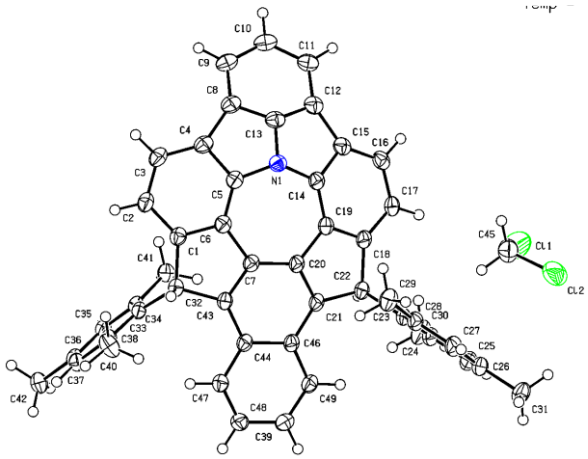


Figure S12. Crystal structure of *anti*-**7** with an ellipsoid contour at the 50% probability level.

Table S2 Crystal data and structure refinement for *syn*-7.

Empirical formula	$C_{50}H_{37}Cl_6N$
Formula weight	864.50
Temperature/K	100.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	11.0574(5)
b/Å	14.7851(5)
c/Å	15.2153(4)
α/°	61.099(4)
β/°	72.149(4)
γ/°	85.623(3)
Volume/Å^3	2065.12(15)
Z	2
ρ_{calc}g/cm^3	1.390
μ/mm^{-1}	4.080
F(000)	892.0
Crystal size/mm^3	0.15 × 0.14 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.854 to 147.154
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 17, -18 ≤ l ≤ 16
Reflections collected	28700
Independent reflections	7974 [R_{int} = 0.0780, R_{sigma} = 0.0723]
Data/restraints/parameters	7974/0/520
Goodness-of-fit on F^2	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0722, wR_2 = 0.1870
Final R indexes [all data]	R_1 = 0.0898, wR_2 = 0.2027
Largest diff. peak/hole / e Å^{-3}	0.80/-0.49

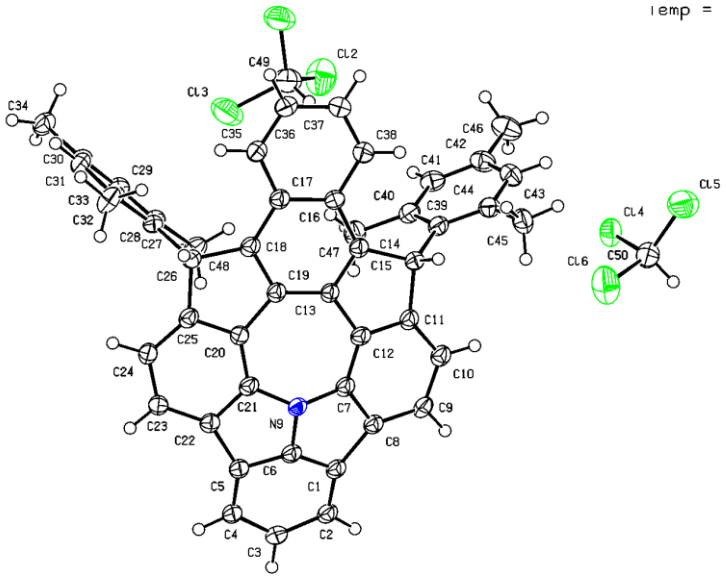


Figure S13. Crystal structure of *syn*-**7** with an ellipsoid contour at the 50% probability level.

Table S3 Crystal data and structure refinement for 8.

Empirical formula	$C_{48}H_{33}N$
Formula weight	623.75
Temperature/K	295.8(3)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.4124(2)
b/Å	24.3763(6)
c/Å	18.1250(5)
α/°	90
β/°	98.549(2)
γ/°	90
Volume/Å^3	3675.49(17)
Z	4
ρ_{calc}g/cm^3	1.127
μ/mm^{-1}	0.491
F(000)	1312.0
Crystal size/mm^3	0.14 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.12 to 153.982
Index ranges	$-10 \le h \le 10$, $-30 \le k \le 28$, $-22 \le l \le 18$
Reflections collected	26239
Independent reflections	7266 [R_{int} = 0.0687, R_{sigma} = 0.0490]
Data/restraints/parameters	7266/0/448
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0747, wR_2 = 0.1957
Final R indexes [all data]	R_1 = 0.1047, wR_2 = 0.2168
Largest diff. peak/hole / e Å^{-3}	0.25/-0.22

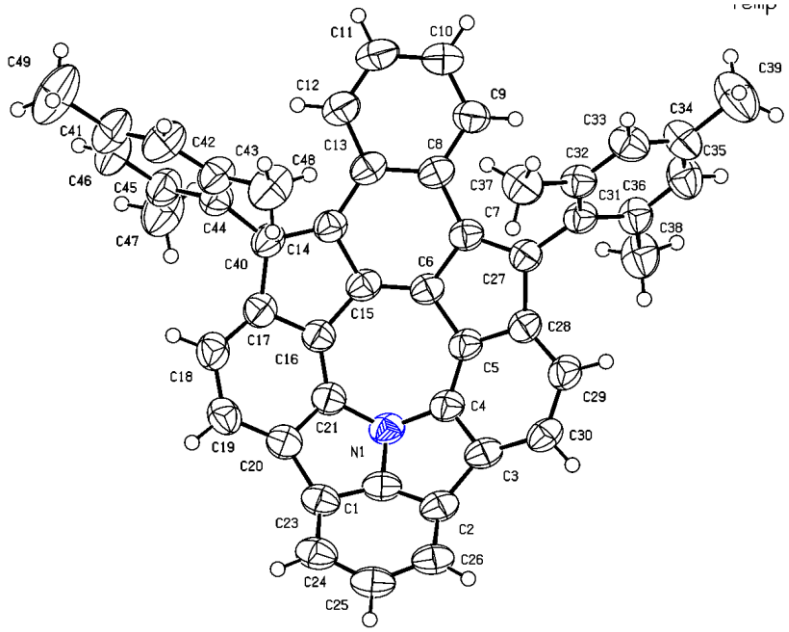


Figure S14. Crystal structure of **8** with an ellipsoid contour at the 50% probability level.

5. UV/vis absorption spectra

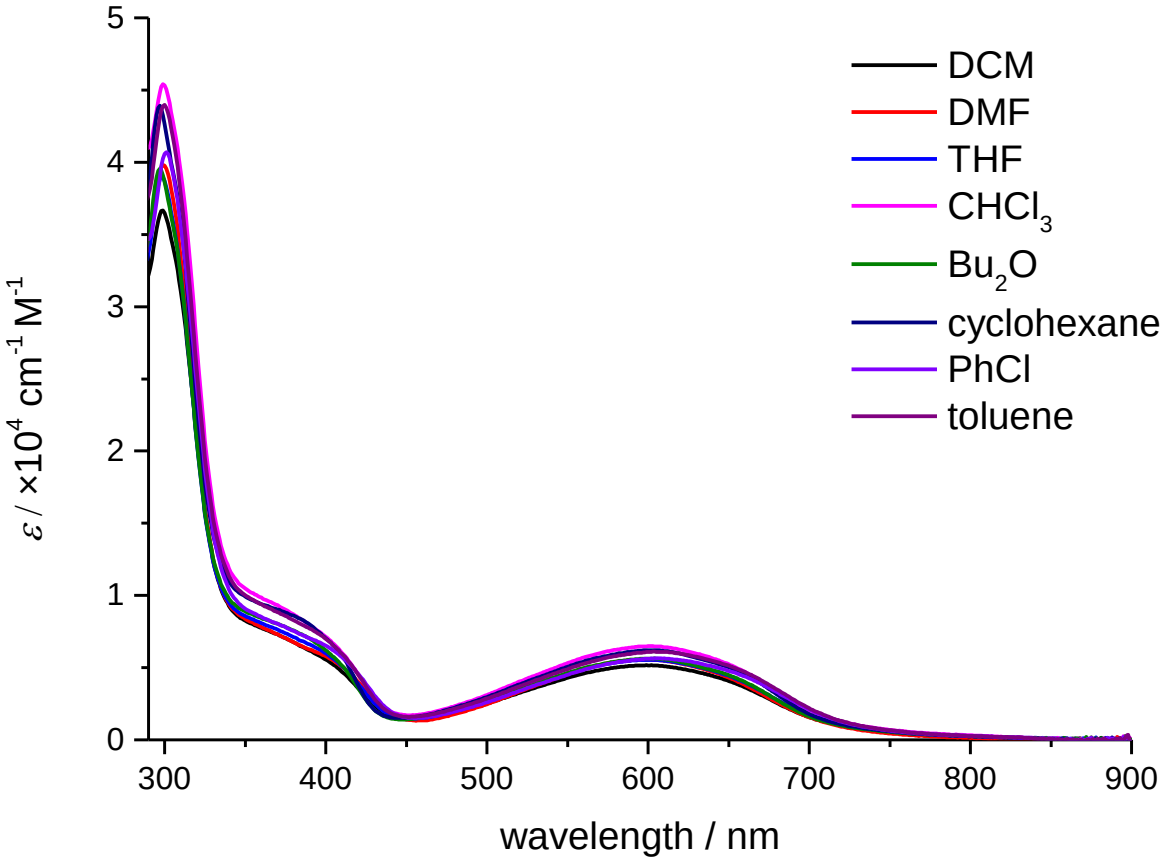


Figure S15. UV/vis absorption spectra of **8** in different solvents.

6. The theoretical calculations

All the theoretical calculations were carried out using a *Gaussian 16* software.[S2] All the calculations were based on the optimized geometries at B3LYP/6-31G(d,p) level of theory. The frontier molecular orbitals are calculated at the B3LYP/6-311+G(d,p) level of theory. The bowl-to-bowl inversion energy was calculated at B3LYP/6-311+G(2d,p) level of theory for the single-point energy, the planar transition state was checked by frequency calculations at B3LYP/6-31G(d,p) level of theory.[S3] The calculation of excited state properties was performed using time-depended DFT methods at B3LYP/6-311G+(d,p) level of theory in the solvent dichloromethane. The nucleus-independent chemical shift (NICS) calculation was done at GIAO-B3LYP/6-311G(d) level of theory. Bq atoms were inserted at the calculated positions and the Bq positions that are at the 1 Å away above the molecule were fixed with the assistant of Multiwfn software, as well as the generation of isotropic chemical shielding surfaces (ICSS), LOL-pi maps and related quantities.[S4]

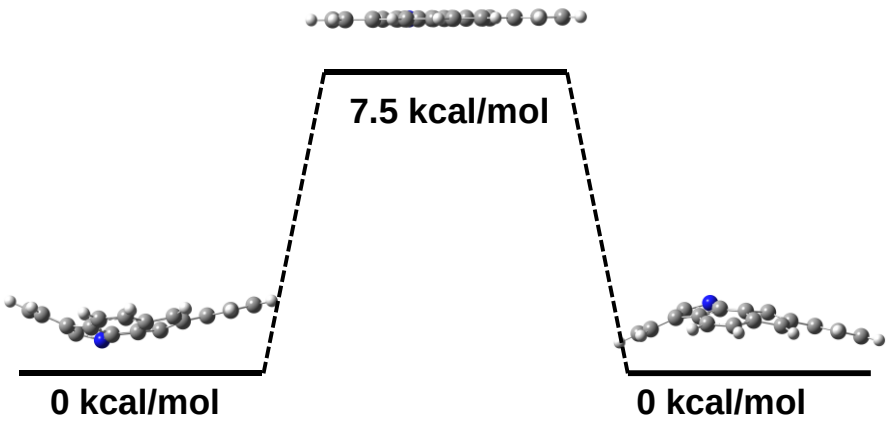


Figure S16. Energy diagram of the inversion process of the non-substituted **8**.

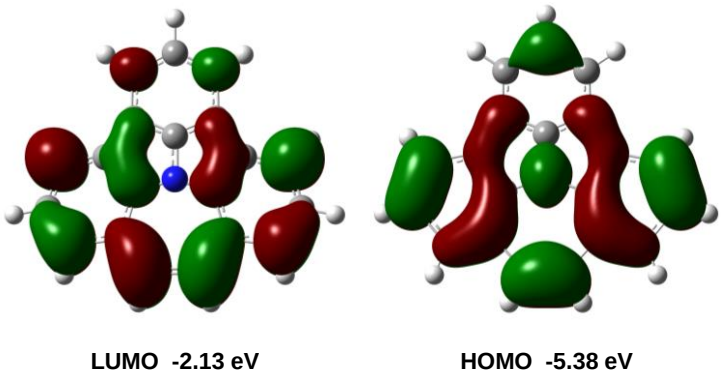


Figure S17. Frontier molecular orbitals and related energy levels of **2** calculated at B3LYP/6-311G+(d,p) level of theory.

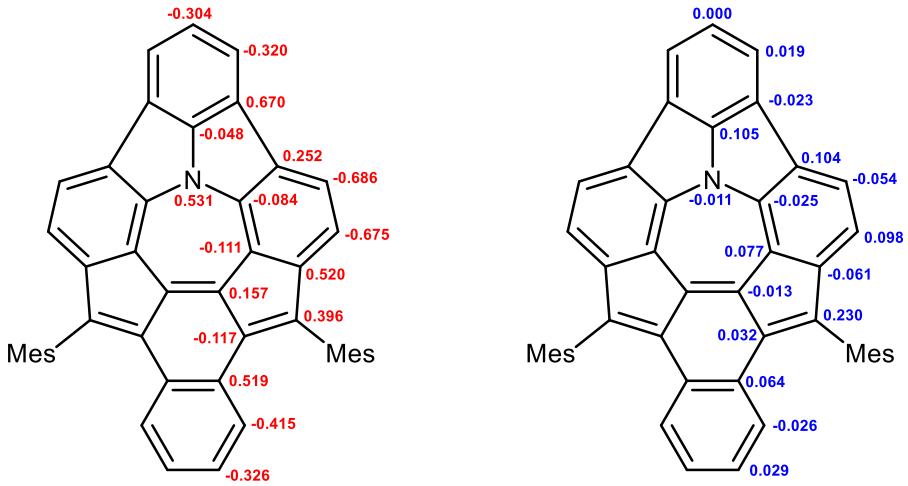


Figure S18. Calculated Mulliken atom charge (red) and spin density (blue) of $\mathbf{8}^{\bullet+}$ at UB3LYP/6-311+G(d,p) level of theory.

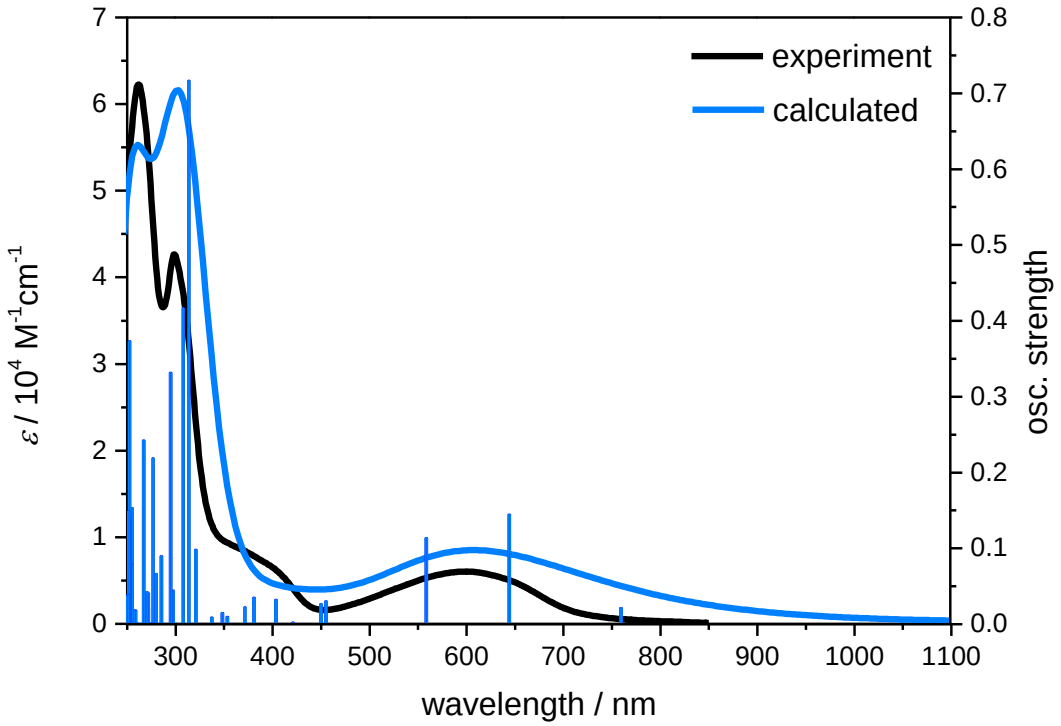


Figure S19. UV/Vis absorption spectrum of compound **8**, TD-DFT calculated spectrum and oscillator strength (column) in dichloromethane at B3LYP/6-311+G(d,p) level.

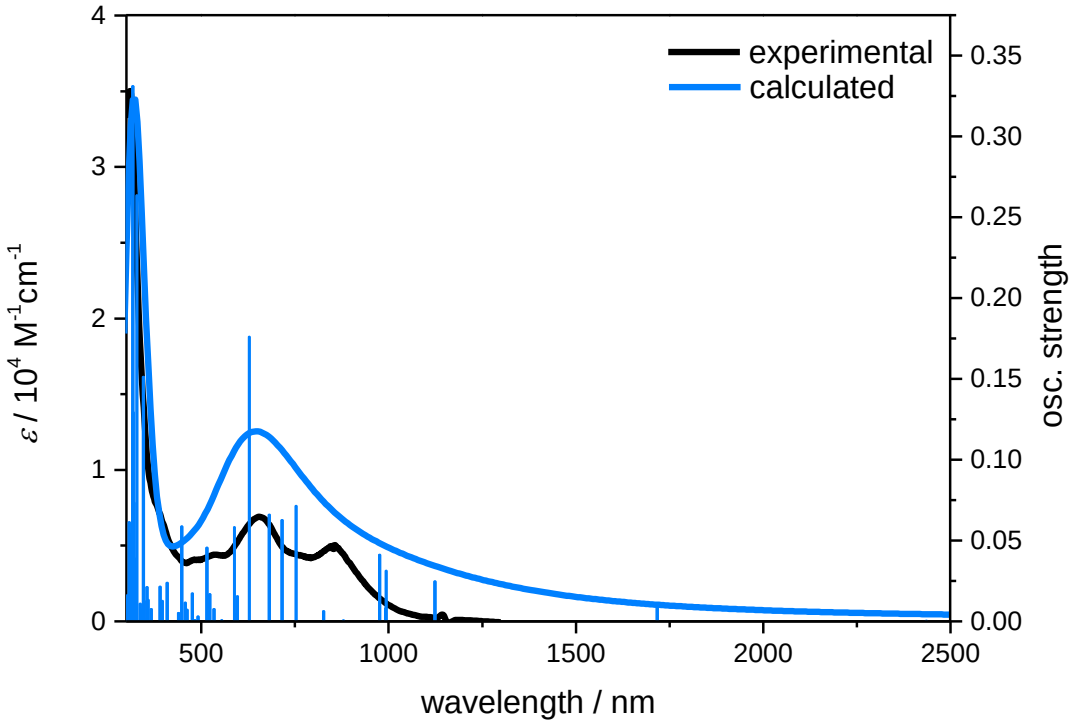


Figure S20. UV/Vis absorption spectrum of compound **8**$^{\bullet+}$, TD-DFT calculated spectrum and oscillator strength (column) in dichloromethane at B3LYP/6-311+G(d,p) level.

Table S4. TD-DFT calculated first ten excited states of compound **8** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State	1:	1.6308 eV	760.26 nm	f=0.0213	<S**2>=0.000
HOMO-1 → LUMO	15.5%				
HOMO → LUMO	84.0%				
Excited State	2:	1.9212 eV	645.33 nm	f=0.1447	<S**2>=0.000
HOMO-1 → LUMO	82.1%				
HOMO → LUMO	14.6%				
Excited State	3:	2.2160 eV	559.50 nm	f=0.1138	<S**2>=0.000
HOMO-2 → LUMO	98.0%				
Excited State	4:	2.7179 eV	456.18 nm	f=0.0303	<S**2>=0.000
HOMO-3 → LUMO	99.1%				
Excited State	5:	2.7497 eV	450.91 nm	f=0.0266	<S**2>=0.000
HOMO-4 → LUMO	99.0%				
Excited State	6:	2.9382 eV	421.98 nm	f=0.0022	<S**2>=0.000
HOMO-6 → LUMO	50.4%				
HOMO-5 → LUMO	49.1%				
Excited State	7:	2.9386 eV	421.92 nm	f=0.0004	<S**2>=0.000

HOMO-6 → LUMO 49.1%

HOMO-5 → LUMO 50.5%

Excited State 8: 3.0661 eV 404.38 nm f=0.0322 <S**2>=0.000

HOMO-7 → LUMO 95.9%

Excited State 9: 3.2457 eV 381.99 nm f=0.0351 <S**2>=0.000

HOMO-8 → LUMO 96.1%

Excited State 10: 3.3284 eV 372.50 nm f=0.0223 <S**2>=0.000

HOMO-1 → LUMO+1 8.2%

HOMO → LUMO+1 87.8%

Table S4. TD-DFT calculated first fifteen excited states of compound **8**$^{\bullet+}$ in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1: 0.5089 eV 2436.40 nm f=0.0005 <S**2>=0.786

HOMO (β) → LUMO (β) 99.2%

Excited State 2: 0.7218 eV 1717.73 nm f=0.0106 <S**2>=0.760

HOMO-1 (α) → LUMO (α) 1.7%

HOMO (α) → LUMO (α) 1.3%

HOMO-1 (β) → LUMO (β) 95.7%

Excited State 3: 1.1023 eV 1124.81 nm f=0.0248 <S**2>=0.829

HOMO (α) → LUMO (α) 93.9%

HOMO-7 (β) → LUMO (β) 1.8%

HOMO-1 (β) → LUMO (β) 1.1%

Excited State 4: 1.2469 eV 994.36 nm f=0.0313 <S**2>=0.822

HOMO-3 (β) → LUMO+1 (β) 1.1%

HOMO-2 (β) → LUMO (β) 96.9%

Excited State 5 1.2487 eV 992.94 nm f=0.0082 <S**2>=2.559

HOMO-1 (α) → LUMO (α) 64.0%

HOMO-8 (β) → LUMO+1 (β) 1.2%

HOMO-3 (β) → LUMO (β) 1.5%

HOMO (β) → LUMO+1 (β) 30.3%

Excited State 6: 1.2695 eV 976.63 nm f=0.0412 <S**2>=0.836

HOMO-1 (α) → LUMO (α) 1.0%

HOMO-3 (β) → LUMO (β) 96.2%

HOMO-2 (β) → LUMO+1 (β) 1.3%

Excited State 7: 1.4078 eV 880.69 nm f=0.0001 <S**2>=0.801

HOMO-5 (β) → LUMO (β) 4.8%

HOMO-4 (β) → LUMO (β) 93.9%

Excited State 8: 1.4082 eV 880.43 nm f=0.0006 <S**2>=0.803

HOMO-5 (β) → LUMO (β) 93.8%

HOMO-4 (β) → LUMO (β) 4.8%

Excited State 9: 1.4986 eV 827.34 nm f=0.0063 <S**2>=2.655

HOMO-2 (α) → LUMO (α) 61.0%

HOMO-1 (β) → LUMO+1 (β) 34.9%

Excited State 10: 1.6446 eV 753.89 nm f=0.0714 <S**2>=0.810

HOMO-2 (α) → LUMO (α) 3.5%

HOMO-6 (β) → LUMO (β) 86.5%

HOMO-1 (β) → LUMO+1 (β) 8.1%

Excited State 11: 1.7312 eV 716.17 nm f=0.0627 <S**2>=0.880

HOMO-1 (α) → LUMO (α) 17.0%

HOMO-7 (β) → LUMO (β) 32.1%

HOMO-1 (β) → LUMO (β) 1.8%

HOMO (β) → LUMO+1 (β) 46.0%

Excited State 12: 1.8162 eV 682.66 nm f=0.0661 <S**2>=0.825

HOMO-9 (α) → LUMO (α) 1.2%

HOMO-1 (α) → LUMO (α) 13.0%

HOMO (α) → LUMO (α) 2.2%

HOMO-7 (β) → LUMO (β) 62.3%

HOMO (β) → LUMO+1 (β) 18.2%

Excited State 13: 1.9710 eV 629.03 nm f=0.1760 <S**2>=0.859

HOMO-8 (α) → LUMO (α) 1.0%

HOMO-3 (α) → LUMO (α) 5.2%

HOMO-2 (α) → LUMO (α) 30.7%

HOMO-8 (β) → LUMO (β) 2.7%

HOMO-6 (β) → LUMO (β) 9.3%

HOMO-1 (β) → LUMO+1 (β) 48.3%

Excited State 14: 2.0767 eV 597.02 nm f=0.0155 <S**2>=1.982

HOMO-4 (α) → LUMO (α) 96.0%

HOMO-2 (β) → LUMO+1 (β) 1.4%

Excited State 15: 2.0829 eV 595.25 nm f=0.0049 <S**2>=1.052

HOMO-8 (α) → LUMO (α) 1.0%

HOMO-3 (α) → LUMO (α)	12.9%
HOMO-2 (α) → LUMO (α)	1.6%
HOMO-8 (β) → LUMO (β)	73.3%
HOMO-7 (β) → LUMO+1 (β)	1.6%
HOMO-1 (β) → LUMO+1 (β)	4.2%

Cartesian coordinates for theoretically optimized structures

8 opt B3LYP/6-31G(d,p) HF = -1903.832224 Hartree imaginary frequency 0

C	1.26016600	2.79118600	-0.67957300
C	1.56896600	1.45904900	-0.77757100
C	0.67728200	0.32200400	-0.89724300
C	-0.67745800	0.32283400	-0.89715800
C	-1.56772900	1.46096500	-0.77725500
C	-1.25725400	2.79271400	-0.67924200
N	0.00176300	3.33787900	-0.87646800
C	1.45450800	-0.87839200	-0.65090300
C	0.72055500	-2.15545900	-0.65214200
C	-0.72367200	-2.15457000	-0.65203100
C	-1.45609400	-0.87662600	-0.65071500
C	1.38940700	-3.39049900	-0.65295600
C	0.69475800	-4.59677100	-0.64956300
C	-0.70087500	-4.59590500	-0.64949000
C	-1.39402800	-3.38877800	-0.65279200
C	0.00259800	4.58259400	-0.31611900
C	2.13784800	3.77083600	-0.13716500
C	3.43604000	3.31390100	0.17542300
C	3.78282300	1.95094900	0.04620300
C	2.83488100	1.00011000	-0.38835800
C	-2.83409700	1.00356000	-0.38773700
C	-3.78072500	1.95552000	0.04724800
C	-3.43222000	3.31804200	0.17645600
C	-2.13358100	3.77341000	-0.13653800
C	-1.27086900	4.96372600	0.13048000
C	-1.24611900	6.13489600	0.90722400

C	0.00411200	6.70987800	1.22631200
C	1.25355200	6.13340300	0.90683200
C	1.27665800	4.96219500	0.13009000
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C	2.76073300	-0.49143700	-0.35991300
C	3.92404800	-1.33385000	0.02277200
C	-3.92567400	-1.32954400	0.02366700
C	4.03617400	-1.84788800	1.33339700
C	5.15936000	-2.61012700	1.66903700
C	6.17703800	-2.87599600	0.74897300
C	6.04781000	-2.35566000	-0.54173800
C	4.94509400	-1.58451900	-0.92096500
C	-4.95057200	-1.57421200	-0.91747000
C	-6.05713000	-2.33834100	-0.53526200
C	-6.18409900	-2.86160100	0.75448400
C	-5.16609400	-2.59547800	1.67415000
C	-4.03902500	-1.84036700	1.33549100
C	7.39508200	-3.67618400	1.14590400
C	2.96418300	-1.59177700	2.36752500
C	4.84645200	-1.04924900	-2.33143000
C	-4.85608000	-1.03318300	-2.32602000
C	-2.96800000	-1.58149900	2.36992700
C	-7.37502000	-3.70878900	1.13575300
H	2.47358300	-3.39724800	-0.66312700
H	1.24331300	-5.53402100	-0.65388500
H	-1.25054700	-5.53250700	-0.65378100
H	-2.47821300	-3.39402200	-0.66287500
H	4.17580900	3.99989200	0.57773100
H	4.77435900	1.63291600	0.35431500
H	-4.77254000	1.63869600	0.35572300
H	-4.17101900	4.00489400	0.57907000
H	-2.14963300	6.57101200	1.32282100
H	0.00474500	7.61123000	1.83236600
H	2.15771700	6.56844300	1.32214500

H	5.24057900	-3.00451300	2.67964500
H	6.82529200	-2.55469100	-1.27618700
H	-6.84096700	-2.52687900	-1.26570800
H	-5.25160400	-2.98149300	2.68762500
H	7.80397300	-4.23124900	0.29621000
H	8.19345800	-3.02368800	1.52136300
H	7.16251500	-4.39282900	1.93920500
H	3.28264700	-1.94355300	3.35241700
H	2.03193200	-2.10738800	2.11203300
H	2.72799200	-0.52574200	2.44662300
H	5.70226900	-1.36916300	-2.93153000
H	3.93407600	-1.39588600	-2.82873500
H	4.81453200	0.04570800	-2.34521800
H	-3.94566600	-1.37904600	-2.82741800
H	-5.71407300	-1.34999100	-2.92465800
H	-4.82293300	0.06178300	-2.33590200
H	-3.28718200	-1.93108500	3.35536600
H	-2.73156000	-0.51534700	2.44679400
H	-2.03569500	-2.09790700	2.11624500
H	-8.27086500	-3.41346200	0.58121500
H	-7.19387900	-4.76897300	0.91816500
H	-7.59616300	-3.63076700	2.20440500

8$^{\bullet+}$ opt B3LYP/6-31G(d,p) HF = -1903.832224 Hartree imaginary frequency 0

C	1.26214700	2.77431500	-0.66389300
C	1.57570200	1.45122300	-0.77180000
C	0.68060800	0.31211200	-0.88132200
C	-0.68079900	0.31266200	-0.88124100
C	-1.57493300	1.45251100	-0.77150400
C	-1.26020700	2.77533500	-0.66351700
N	0.00116800	3.31795200	-0.83776300
C	1.44131700	-0.87716600	-0.64056200
C	0.72904200	-2.14113500	-0.64936900
C	-0.73110400	-2.14053400	-0.64918200

C	-1.44240600	-0.87601700	-0.64034300
C	1.39970400	-3.38235900	-0.65323100
C	0.70067800	-4.57757100	-0.66046800
C	-0.70470300	-4.57699600	-0.66021500
C	-1.40274800	-3.38122100	-0.65277300
C	0.00176700	4.54409100	-0.24472400
C	2.14075700	3.75450400	-0.10118200
C	3.44712600	3.30312300	0.19807000
C	3.79954000	1.94810700	0.04697600
C	2.85066800	0.99405100	-0.40018000
C	-2.85016300	0.99637600	-0.39956000
C	-3.79801700	1.95116700	0.04822800
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C	-2.13779800	3.75620400	-0.10042600
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C	0.00289200	6.66891400	1.29609500
C	1.25455500	6.09790200	0.97457300
C	1.28010700	4.92915500	0.19332600
C	-2.78906800	-0.47471600	-0.35983800
C	2.78829800	-0.47693300	-0.36018200
C	3.94443700	-1.31838200	0.00561800
C	-3.94556100	-1.31540900	0.00642500
C	3.99362600	-1.96711800	1.26435400
C	5.12383600	-2.72181200	1.58402400
C	6.19924400	-2.86573600	0.70116100
C	6.12568900	-2.21657600	-0.53587200
C	5.03035300	-1.43114600	-0.89910000
C	-5.03514800	-1.42223900	-0.89471900
C	-6.13413900	-2.20043800	-0.52726600
C	-6.20552400	-2.85247400	0.70840900
C	-5.12918300	-2.70928500	1.59027400
C	-3.99532100	-1.96184300	1.26636200
C	7.41580700	-3.67066000	1.08374500

C	2.87887400	-1.83154700	2.27697600
C	5.00126900	-0.77278800	-2.26089300
C	-5.00966300	-0.75943800	-2.25442200
C	-2.88041900	-1.82513100	2.27869200
C	-7.39942700	-3.69969500	1.07033000
H	2.48310300	-3.39161600	-0.66726800
H	1.24215000	-5.51788800	-0.67780000
H	-1.24689700	-5.51690300	-0.67734600
H	-2.48615600	-3.38942900	-0.66644600
H	4.18246400	3.98846300	0.60669100
H	4.79375400	1.62925800	0.34306300
H	-4.79235100	1.63314100	0.34481800
H	-4.17899000	3.99173500	0.60843000
H	-2.15147800	6.54055200	1.38552500
H	0.00335800	7.56774900	1.90422200
H	2.15719200	6.53887200	1.38470600
H	5.16857400	-3.20592200	2.55636500
H	6.94503300	-2.32592900	-1.24177400
H	-6.95963300	-2.29955500	-1.22753000
H	-5.17718100	-3.18559400	2.56625400
H	7.88727900	-4.12484400	0.20798800
H	8.16829100	-3.03369300	1.56456800
H	7.16449000	-4.46651200	1.79004600
H	3.19540400	-2.21644200	3.24891500
H	1.98720600	-2.39226100	1.97612100
H	2.57675600	-0.78830300	2.41354000
H	5.88263500	-1.05194300	-2.84205800
H	4.11628400	-1.06722800	-2.83541100
H	4.98542600	0.31967400	-2.18844200
H	-4.12556700	-1.05144900	-2.83148500
H	-5.89188300	-1.03786100	-2.83464700
H	-4.99474000	0.33283400	-2.17897000
H	-3.19639000	-2.21014300	3.25076100
H	-2.57864600	-0.78174200	2.41505700

H	-1.98861900	-2.38547000	1.97757100
H	-8.31366300	-3.32393800	0.60281400
H	-7.26143500	-4.73323200	0.72969100
H	-7.55515200	-3.73175600	2.15197800

1 opt B3LYP/6-31G(d,p) HF = -1205.788535 Hartree imaginary frequency 0
Single point energy at B3LYP/6-311+G(2d,p) -1206.067588 Hartree

C	1.36074400	1.26055400	0.60815200
C	0.02769900	1.57369400	0.55150300
C	-1.11159200	0.67650800	0.54132600
C	-1.11159100	-0.67650800	0.54132600
C	0.02770000	-1.57369400	0.55150300
C	1.36074500	-1.26055300	0.60815300
N	1.87889700	0.00000100	0.86726100
C	-2.27604500	1.44880500	0.14370000
C	-3.53916200	0.72011800	-0.04385300
C	-3.53916200	-0.72011900	-0.04385400
C	-2.27604300	-1.44880600	0.14369700
C	-4.75350200	1.39161900	-0.24821600
C	-5.94314200	0.69866700	-0.45096900
C	-5.94314100	-0.69867000	-0.45097100
C	-4.75350100	-1.39162200	-0.24821800
C	3.18015900	0.00000100	0.45284900
C	2.39749200	2.13600700	0.18040300
C	1.98080900	3.43373500	-0.18525900
C	0.61262600	3.78322300	-0.21874100
C	-0.38659600	2.83911900	0.10141500
C	-0.38659300	-2.83911800	0.10141500
C	0.61262900	-3.78322400	-0.21873800
C	1.98081200	-3.43373500	-0.18525400
C	2.39749400	-2.13600600	0.18040700
C	3.61008700	-1.27338500	0.05287000
C	4.86313100	-1.24956400	-0.58358600

C	5.47205000	0.00000100	-0.83435100
C	4.86312900	1.24956500	-0.58359100
C	3.61008500	1.27338600	0.05286700
C	-1.85128400	-2.74248600	-0.09887700
C	-1.85128800	2.74248800	-0.09886700
H	-4.76001500	2.47783300	-0.23873700
H	-6.86868000	1.24577900	-0.60294200
H	-6.86867900	-1.24578200	-0.60294500
H	-4.76001300	-2.47783600	-0.23874100
H	2.71013700	4.17204500	-0.50557300
H	0.34213400	4.77714700	-0.56305500
H	0.34213800	-4.77714700	-0.56305300
H	2.71014100	-4.17204400	-0.50556700
H	5.34366600	-2.15356300	-0.94563600
H	6.43734100	0.00000000	-1.33221800
H	5.34366300	2.15356300	-0.94564300
H	-2.46630600	-3.55537800	-0.46808600
H	-2.46631200	3.55538100	-0.46807000

Transition state of **1** opt B3LYP/6-31G(d,p) HF = -1205.779379 Hartree
imaginary frequency 1
Single point energy at B3LYP/6-311+G(2d,p) -1206.055684 Hartree

C	1.33700000	-1.27262900	-0.00020200
C	0.01153800	-1.58063900	-0.00032600
C	-1.10968000	-0.67536300	-0.00031600
C	-1.10968000	0.67536300	-0.00032200
C	0.01153800	1.58063900	-0.00032900
C	1.33700000	1.27262900	-0.00020200
N	1.80835600	0.00000000	0.00000600
C	-2.31190800	-1.47559600	-0.00014000
C	-3.58277300	-0.72499300	0.00001900
C	-3.58277300	0.72499300	0.00001700
C	-2.31190800	1.47559600	-0.00014400
C	-4.81737200	-1.39003800	0.00020200
C	-6.02506800	-0.69813000	0.00037600

C	-6.02506800	0.69813000	0.00037400
C	-4.81737200	1.39003800	0.00019900
C	3.14330200	0.00000000	0.00006100
C	2.42127000	-2.18810000	-0.00009600
C	1.98273400	-3.53785100	-0.00003300
C	0.60274000	-3.88669000	-0.00004800
C	-0.42325900	-2.90421000	-0.00020600
C	-0.42325900	2.90421000	-0.00020700
C	0.60274000	3.88669000	-0.00004600
C	1.98273400	3.53785100	-0.00003200
C	2.42127000	2.18810000	-0.00009300
C	3.65742400	1.30573800	0.00002600
C	5.06481600	1.26556600	0.00031600
C	5.70756300	0.00000000	0.00042400
C	5.06481600	-1.26556600	0.00031400
C	3.65742400	-1.30573800	0.00002600
C	-1.91585300	2.80983300	-0.00008400
C	-1.91585300	-2.80983400	-0.00008400
H	-4.82426700	-2.47632700	0.00021100
H	-6.96241400	-1.24621500	0.00051500
H	-6.96241400	1.24621500	0.00050900
H	-4.82426700	2.47632700	0.00020300
H	2.70343900	-4.35042700	0.00002800
H	0.35513200	-4.94414900	0.00008200
H	0.35513200	4.94414900	0.00008700
H	2.70343900	4.35042700	0.00002900
H	5.67781900	2.16194100	0.00040400
H	6.79364600	0.00000000	0.00063300
H	5.67781900	-2.16194100	0.00040100
H	-2.57802600	3.66827700	0.00010100
H	-2.57802600	-3.66827700	0.00009600

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