Electronic Supplementary Information

Cyano disubstituted tetrabenzoindeno[2,1-*a*]fluorene: open-shell or closed-shell?

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1. Experimental section

1.1 General information: Chemicals and reagents were purchased from local and international commercial suppliers (Merck, GLR innovations, BLDpharm, Spectrochem) and used without further purification. Thin layer chromatography (TLC) was performed using pre-coated silica-plates purchased from Merck (silica gel 60 PF254, 0.25 mm). Column chromatography was performed using silica gel 100-200 mesh. NMR spectra were recorded in $CDCl_3$ (Eurisotop, on JEOL JNM-ECS400 spectrometer at operating frequencies of 400 MHz (^1H) or 100 MHz (^{13}C) as indicated in the individual spectrum. Chemical shifts (δ) are given in ppm relative to residual solvent (chloroform δ = 7.26 for ^1H, and δ = 77.16 for proton-decoupled ^{13}C NMR), and coupling constants (*J*) are expressed in hertz (Hz). Multiplicity is tabulated as s for singlet, d for doublet, dd for doublet of doublet, t for triplet, q for quartet, and m for multiplet. Structural assignments were made with additional information from gCOSY, and gNOESY experiments. High-resolution mass spectra (HRMS) were recorded using electronspray ionization (ESI) methods on Waters (XEVO G2-XS QTOF) mass spectrometer. UV-vis-NIR spectra were recorded in JASCO V-770 spectrophotometer. Cyclic voltammetry was performed using an Electrochemical Analyzer potentiostat model CHI-1110C from CH Instruments with a conventional three-electrode cell at room temperature under a nitrogen atmosphere at a scan rate of 50 mV s^{-1}. This electrochemical cell contains a glassy carbon (disc-shaped with 3-mm diameter) as a working electrode, Pt wire as a counter electrode, and Ag wire as a pseudo-reference electrode. The glassy carbon working electrode was polished with 1.0-micron α-alumina polishing powder using a figure-eight motion. Electrolyte solution (0.1 M) was prepared from dichloromethane (DCM) and tetra-*n*-butylammonium hexafluorophosphate (Bu_4NPF_6). The DCM was degassed by nitrogen gas sparging for 15 minutes prior to measurements. The potential was externally calibrated against the ferrocene/ferrocenium couple (0.43 V). Melting points were determined using a Cole-Parmer MP 250D-P melting point analyzer. X-band electron paramagnetic resonance (EPR) spectra were recorded using an EMX MICRO X Bruker EPR instrument.

1.2 Syntheses and characterization data

2,5-di(phenanthren-9-yl)thiophene-3,4-dicarbaldehyde (9): An oven-dried thick-walled glass tube was charged with **7** (715.45 mg, 3.22 mmol), **8** (300 mg, 1.01 mmol), K_2CO_3 (696 mg, 5.03 mmol), THF (12 mL) and water (2.4 mL), and the mixture was purged with nitrogen for 30 mins. Catalyst $Pd(PPh_3)_4$ (100 mg, 10 mol %) was subsequently added under nitrogen, and the glass tube was sealed before being warmed to 85 °C using an oil bath. After 14 h, the flask was cooled to room temperature, and THF was evaporated under reduced pressure. Water was added, and the reaction mixture was extracted with EtOAc (5 x 30 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure. The residue was purified by silica gel column chromatography (hexanes:EtOAc, 94:6) to afford the title product **9** (420 mg, 85% yield) as light brown solid: R_f = 0.19 (5% EtOAc/hexanes); mp 280−281 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.21 (s, 2H), 8.81 (d, *J* = 8.2 Hz, 2H), 8.76 (d, *J* = 8.2 Hz, 2H), 8.00 – 7.90 (m, 6H), 7.80 – 7.73 (m, 4H), 7.72 – 7.65 (m, 4H). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$) δ 186.9, 152.3, 137.1, 131.0 (2 C), 130.7 (2 C), 130.5, 129.2, 128.2, 127.5, 127.4, 127.2, 126.1, 123.3, 122.9; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{34}H_{21}O_2S$ 493.1262, found 493.1262 (error: 0.0 ppm).

18,19-dimesityl-18,19-dihydrodibenzo[4,5:6,7]indeno[1,2-*b*]dibenzo[4,5:6,7]indeno[2,1-*d*]thiophene (2H-DPDCPT): 2-Mesitylmagnesium bromide (1.0 M in diethyl ether, 1.62 mL, 1.62 mmol) was added dropwise to the dry tetrahydrofuran (5 mL) solution of **9** (180 mg, 0.45 mmol) under nitrogen. The mixture was stirred at room temperature for 12 h, and the reaction was quenched with a saturated aqueous NH_4Cl solution. The volatile organics were evaporated under reduced pressure, and the mixture was extracted with dichloromethane (3 x 30 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered, and removed under reduced pressure to afford a crude mixture containing intermediate diol (320 mg) compound. In the next step, $BF_3{\cdot}Et_2O$ (0.1 mL) was added to the solution of crude diol in anhydrous DCM (5 mL) under nitrogen, and the reaction mixture was stirred for 30 min at room temperature. Once diol was completely consumed, as monitored by TLC, a saturated aqueous $NaHCO_3$ solution (12 mL) was added and the reaction mixture was extracted with DCM (3 × 30 mL). The organic

layer was dried over anhydrous Na_2SO_4, filtered, and evaporated under reduced pressure. The residue was subjected to silica gel column chromatography (hexanes/DCM, 90:10) to give title product **2H-DPDCPT** as a light yellow solid (100 mg, 35% over two steps): R_f = 0.27 (5% DCM/hexanes); mp 387 °C dec; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.81 (d, *J* = 8.3 Hz, 2H), 8.70 (d, *J* = 8.2 Hz, 2H), 8.57 (d, *J* = 7.9 Hz, 2H), 7.87 (t, *J* = 7.5 Hz, 2H), 7.80 – 7.73 (m, 2H), 7.50 – 7.44 (m, 4H), 7.34 – 7.28 (m, 2H), 7.00 (s, 2H), 6.60 (s, 2H), 5.29 (s, 2H), 2.33 (s, 6H), 1.80 (s, 6H), 1.32 (s, 6H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 145.2, 144.2, 142.2, 138.4, 138.3, 136.7, 134.5, 133.4, 130.7, 130.3, 130.1, 130.0, 129.4, 127.1, 126.5, 126.4, 125.4, 125.2, 123.6, 123.5, 123.5, 48.2, 21.2, 21.0, 17.6; HRMS (ESI) *m/z*: $[M]^+$ calcd for $C_{52}H_{40}S$ 696.2851, found 696.2858 (error: 1.0 ppm).

19,20-dimesityl-as-indaceno[2,3-l:6,7-l']diphenanthrene-9,10-dicarbonitrile (6): DDQ (68 mg, 0.30 mmol) was added to the solution of **2H-DPDCPT** (52 mg, 0.074 mmol) in dry DCM (5 mL) under nitrogen, and the reaction mixture was stirred at room temperature for 30 min. Once the starting material was consumed (as monitored by TLC), the DCM was removed *in vacuo*, and the crude was purified by silica gel column chromatography (silica gel was treated with triethylamine; hexanes:DCM, 70:30) to afford target compound **6** as dark-purple solid (23 mg, 42% yield over three steps): R_f = 0.15 (5% EtOAc/hexanes). Recrystallization of **6** from a dichloromethane/acetonitrile (1:1) mixture, by solvent diffusion method, at ambient temperature in the dark afforded single crystals suitable for x-ray crystallographic analysis: mp 325−326 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.50 (t, *J* = 7.6 Hz, 4H), 8.39 (d, *J* = 7.9 Hz, 2H), 7.65 (t, *J* = 7.4 Hz, 2H), 7.62 – 7.55 (m, 2H), 7.46 – 7.39 (m, 2H), 7.02 (t, *J* = 7.3 Hz, 2H), δ 6.54 (s, 4H), 6.51 (d, J = 8.3 Hz, 2H), 2.31 (s, 6H), 1.95 (s, 12H); ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 158.0, 137.6, 135.4, 133.5, 131.1, 128.6, 128.1, 127.7, 127.5, 127.4, 126.7, 123.8, 123.5, 123.4, 116.0, 107.4, 21.4, 21.12 [Likely the population of triplet species at 25 °C resulting in weaker intensity for aromatic signals for the π-backbone]; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{56}H_{39}N_2$ 739.3113, found 739.3099 (error: −1.9 ppm). **NOTE:** A DDQ-adduct could be isolated when crude reaction mixture was subjected to silica gel column chromatography under nitrogen (see Appendix).

1.3 NMR spectra

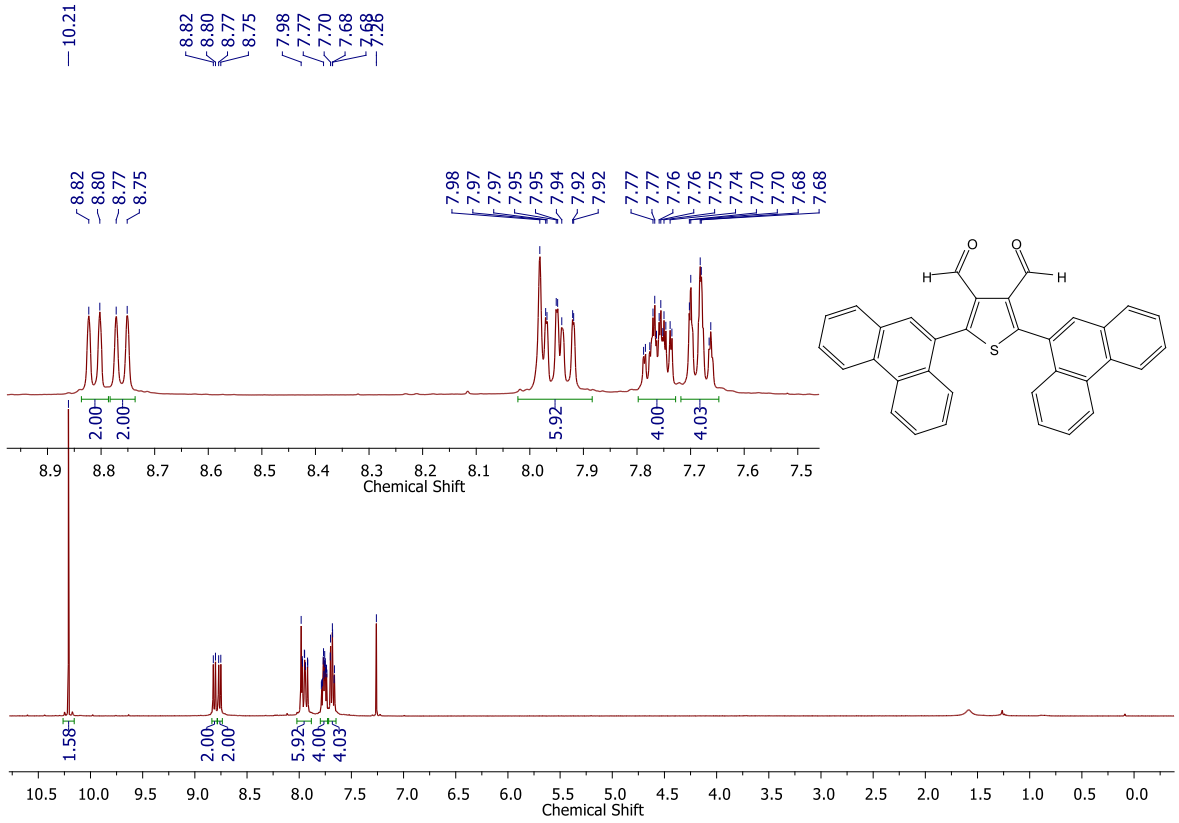


Fig. S1 ^{1}H NMR spectrum of **9** (in $CDCl_3$, 400 MHz, 298 K).

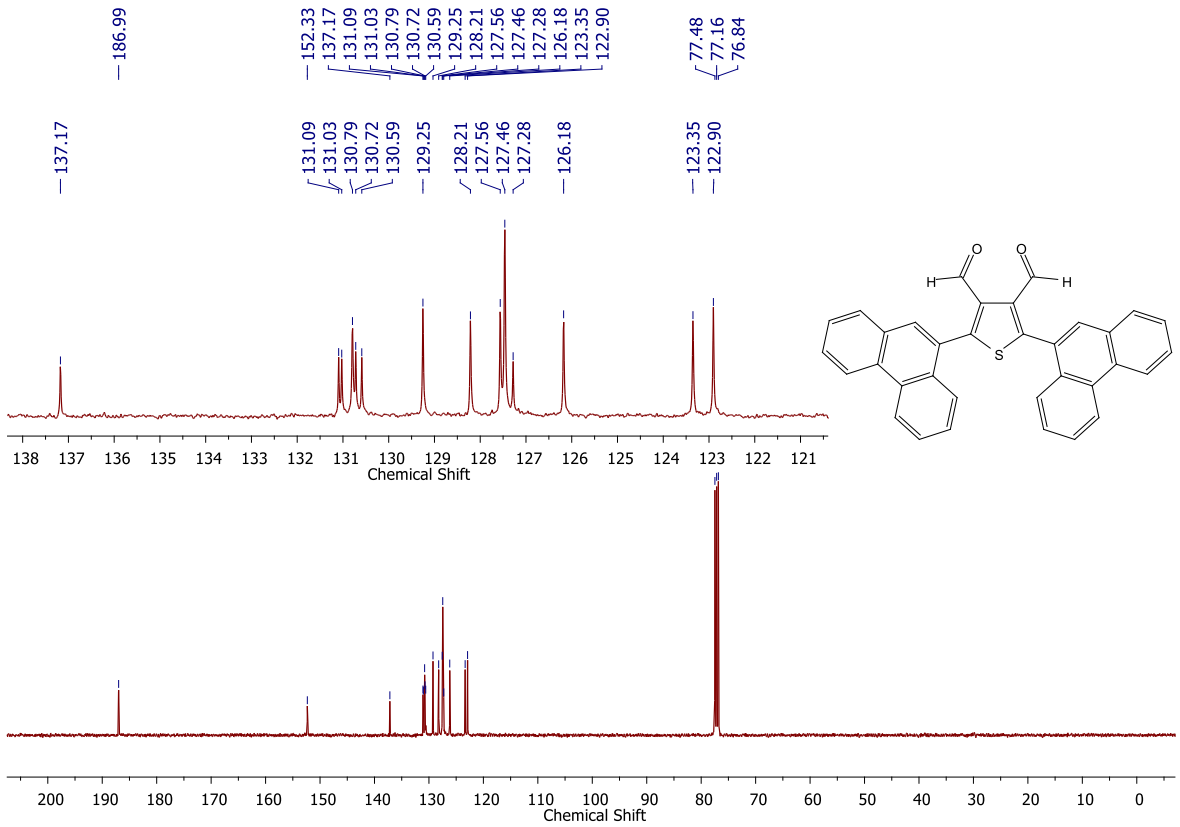


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of **9** (in $CDCl_3$, 100 MHz, 298 K).

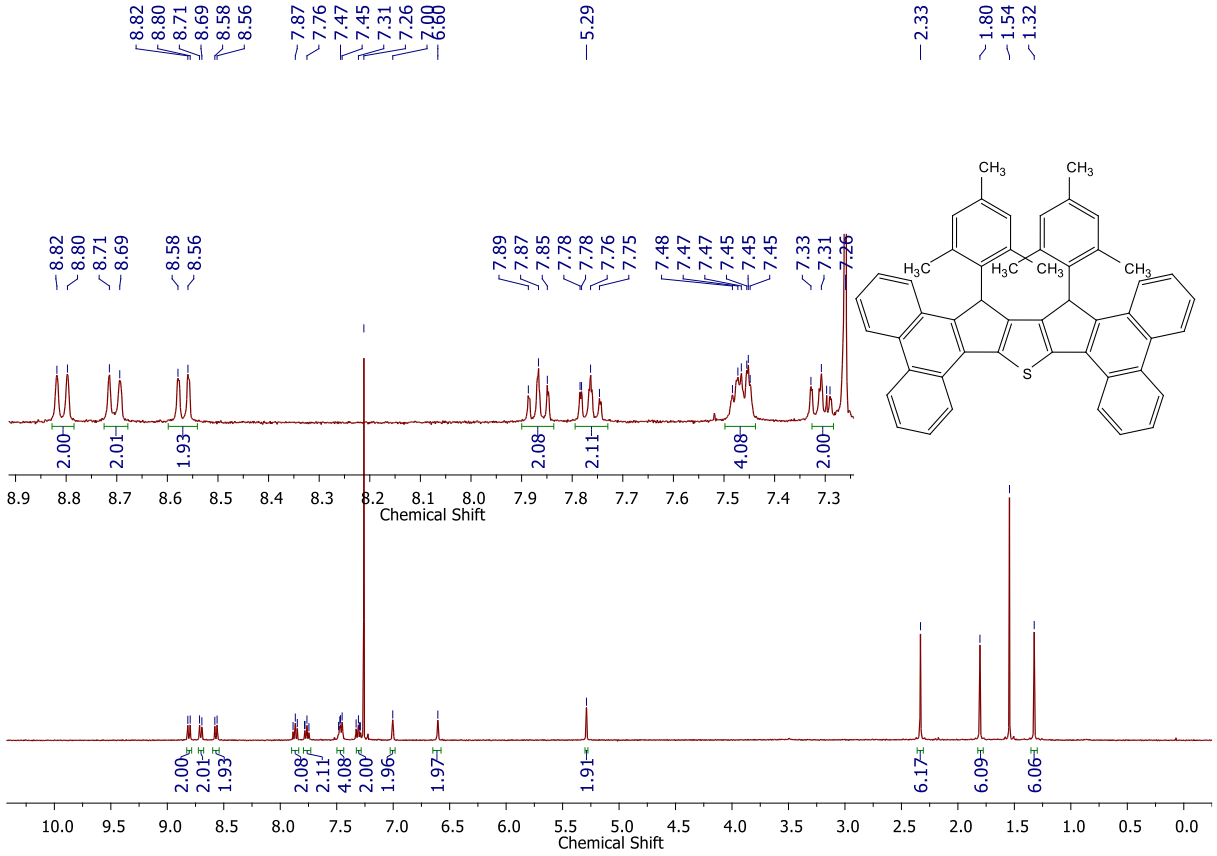


Fig. S3 ^{1}H NMR spectrum of **2H-DPDCPT** (in $CDCl_3$, 400 MHz, 298 K).

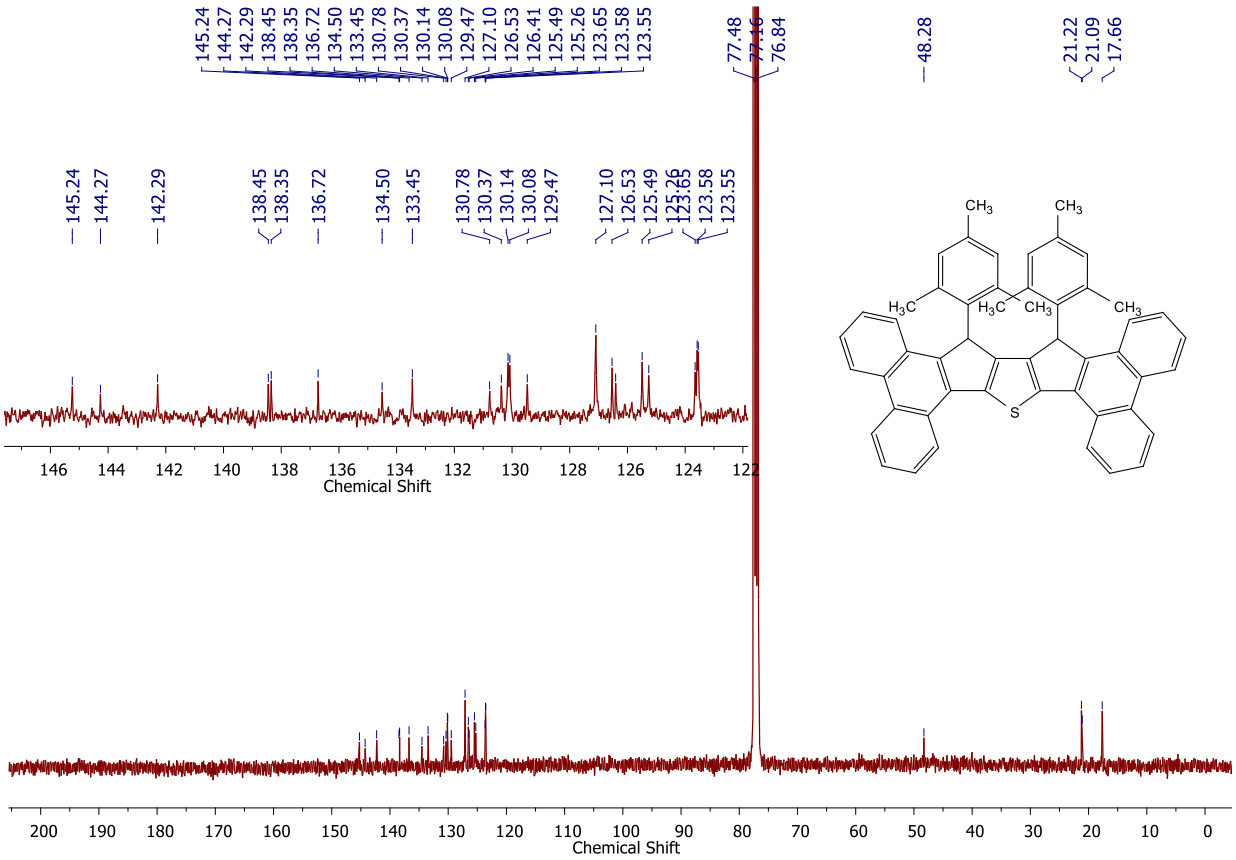


Fig. S4 ^{13}C{^{1}H} NMR spectrum of **2H-DPDCPT** (in $CDCl_3$, 100 MHz, 298 K).

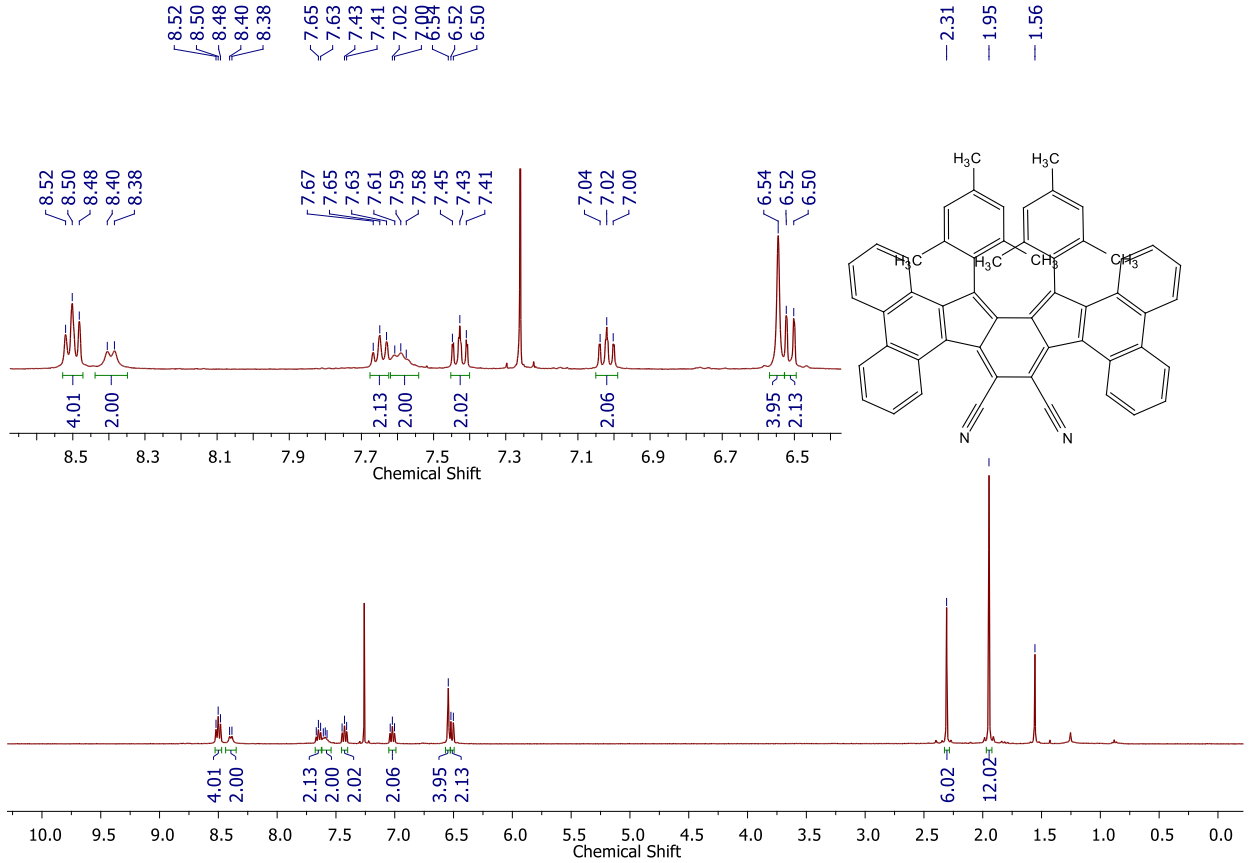


Fig. S5 ^{1}H NMR spectrum of **6** (in $CDCl_3$, 400 MHz, 298 K).

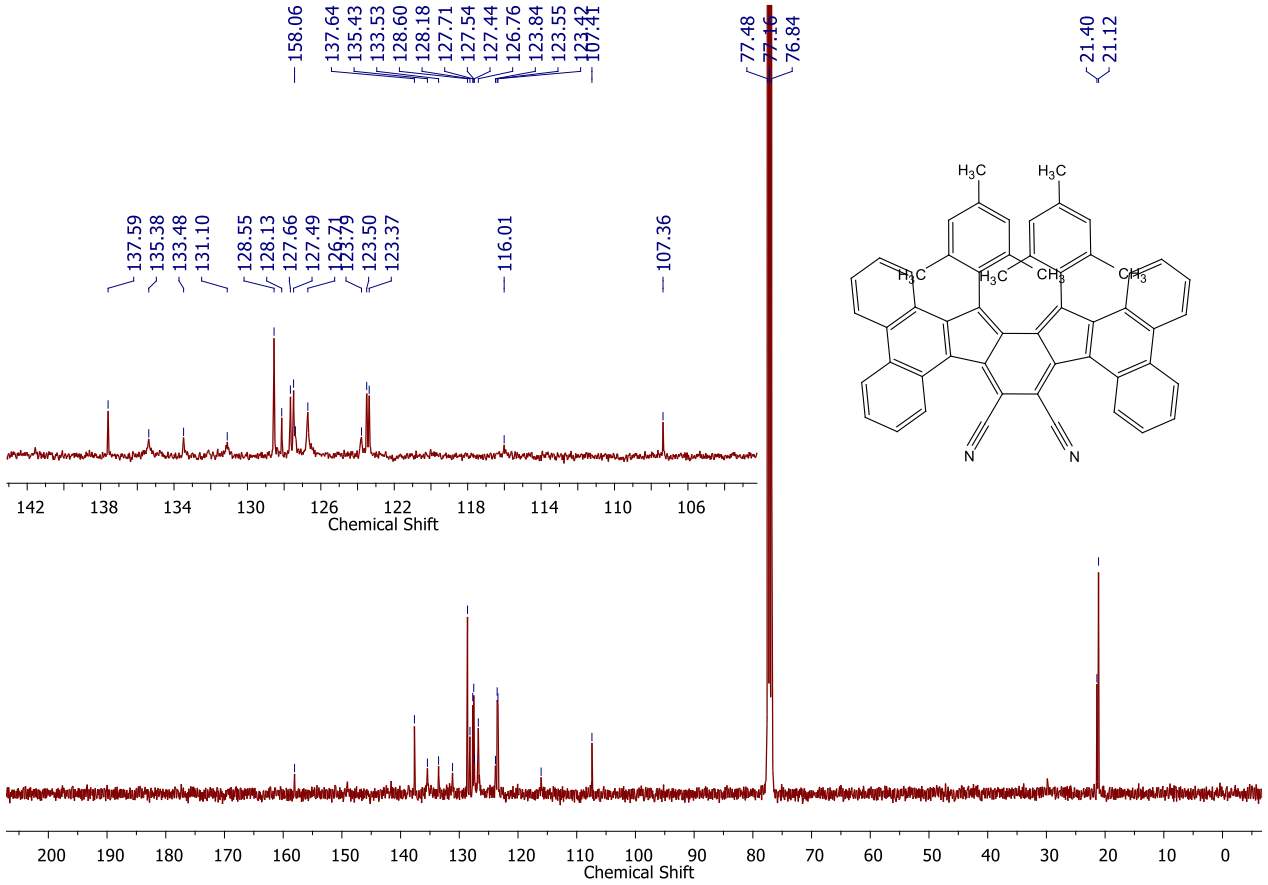


Fig. S6 $^{13}C\{^{1}H\}$ NMR spectrum of **6** (in $CDCl_3$, 100 MHz, 298 K).

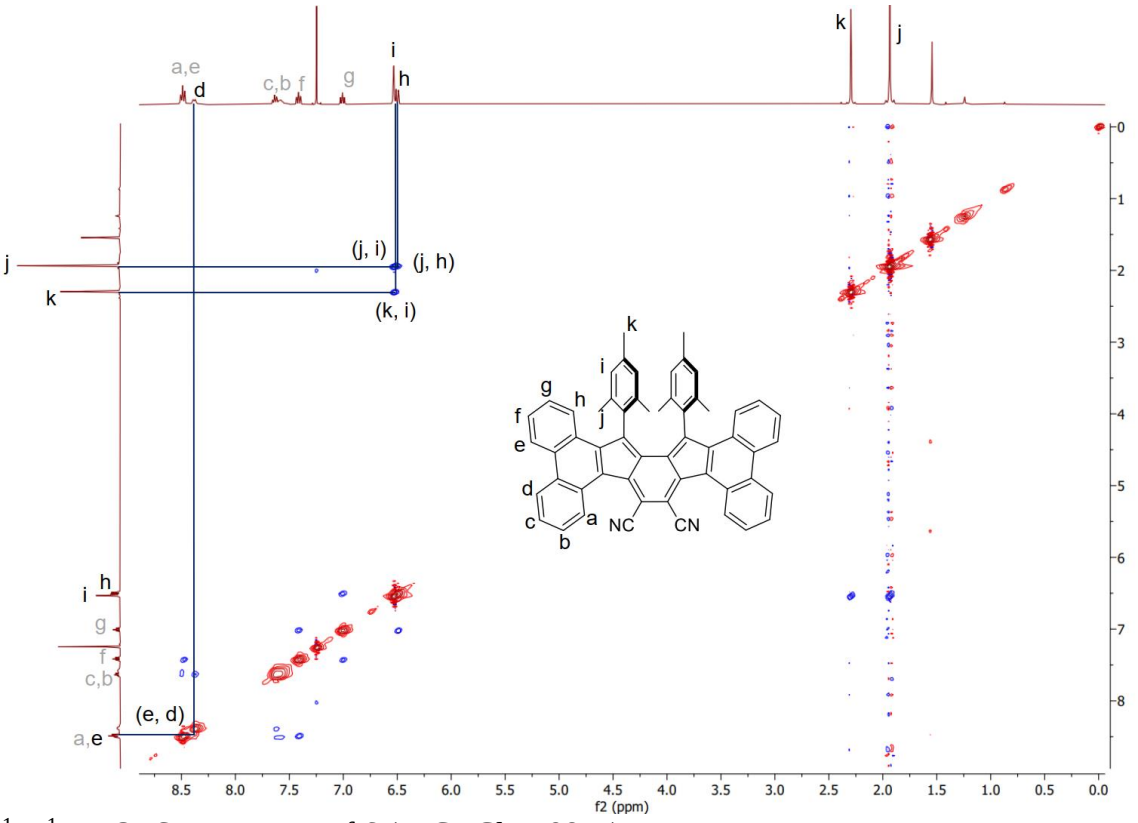


Fig. S7 ^{1}H-^{1}H NOESY spectrum of **6** (in $CDCl_3$, 298 K)

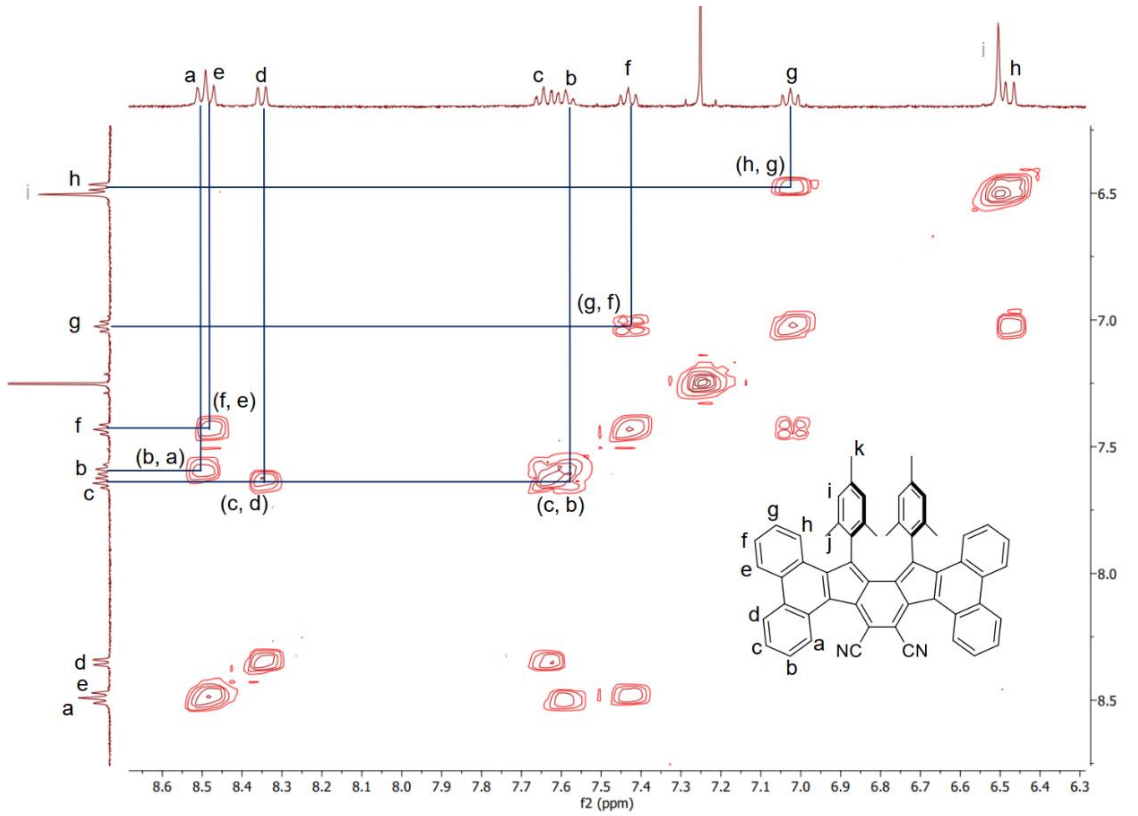


Fig. S8 ^{1}H-^{1}H COSY spectrum of **6** (in $CDCl_3$, 233 K, aromatic region expansion).

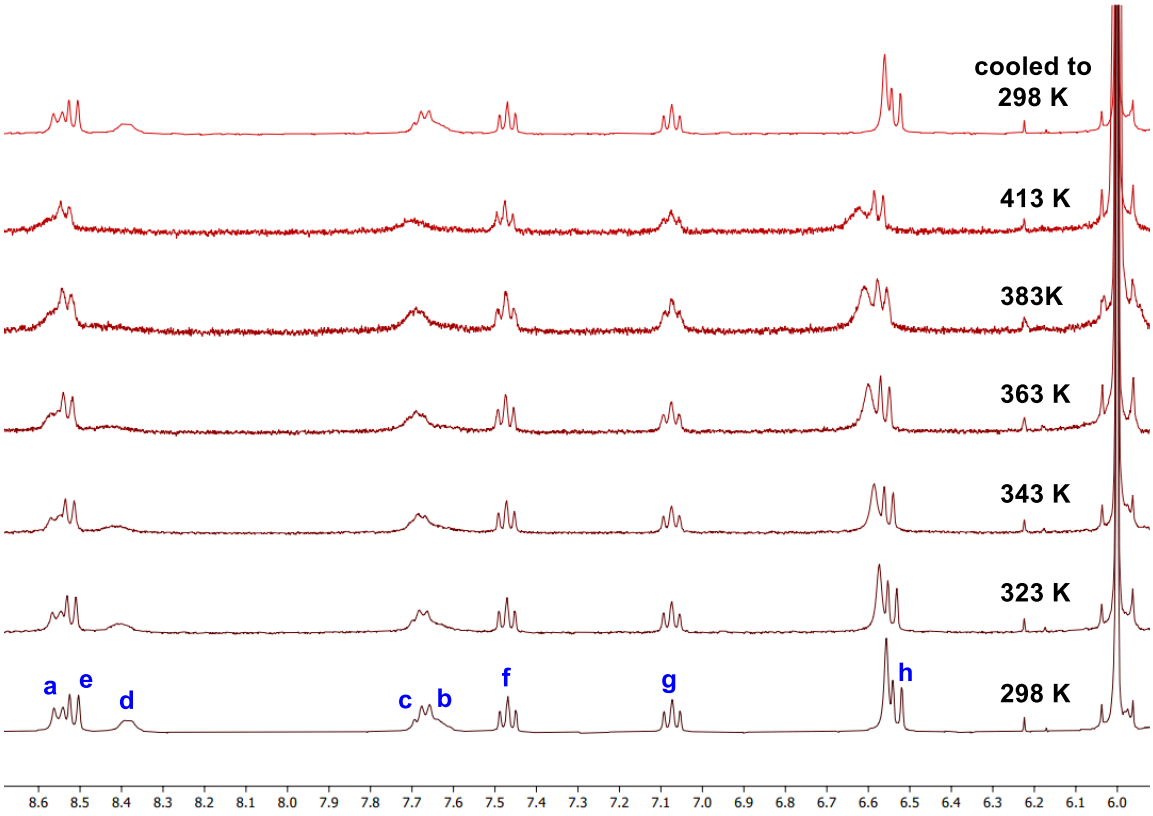


Fig. S9 Variable temperature (VT) ^{1}H NMR spectra for **6** in $C_2D_2Cl_4$ showing the aromatic phenanthrene proton signals were broadened upon heating (up to 413 K), and when cooled back to 298 K, the original spectrum could be recovered.

2. Photostability test

To check the photostability of final compound **6**, solution of known concentration of **6** in toluene was exposed to ambient light (under normal lab light condition and temperature). It leads to the gradual decomposition of **6** in solution, resulting in the decrease of the absorbance at longer wavelength (470-1500 nm) region with simultaneous appearance of new absorbance bands in shorter wavelength region (350-450 nm) (Fig. S10a).

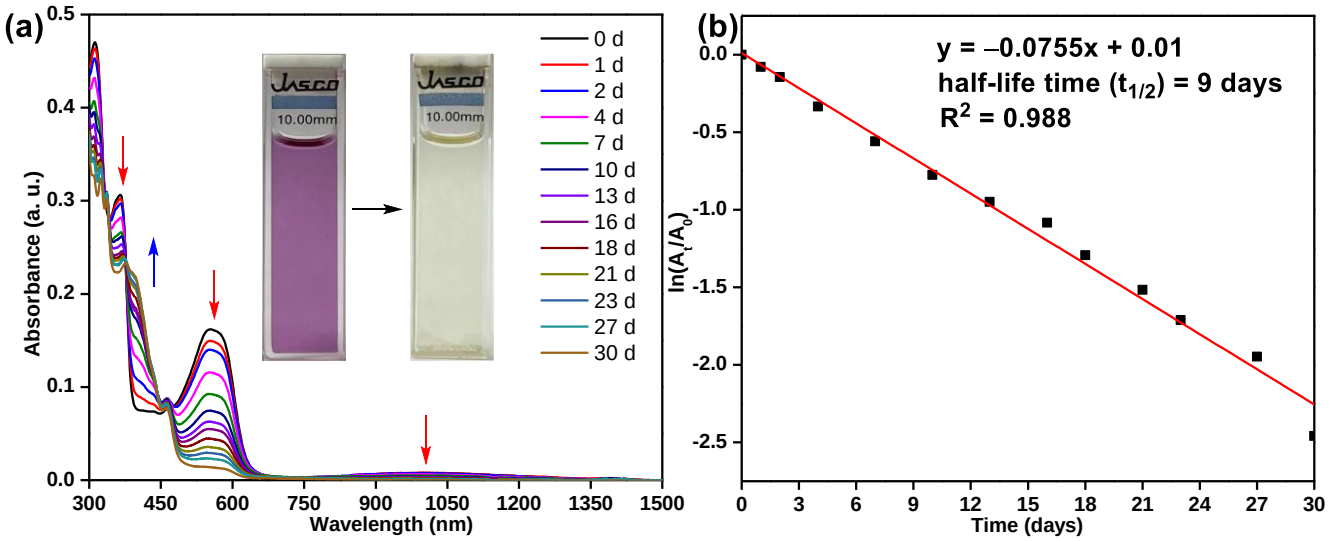


Fig. S10 (a) Absorption spectral changes under ambient light conditions for compound **6** in toluene (0 days to 30 days). (b) Fitting with first-order kinetics.

The half-life ($t_{1/2}$) of **6** was determined according to the following equation:

$$t_{1/2} = \frac{\ln 2}{0.0755} = 9.18 \text{ days}$$

3. Variable temperature (VT) ESR measurement and Bleaney-Bowers plot:

To get the ground sate spin multiplicity and the energy separation between the singlet and triplet state, VT-EPR experiment were carried out using solid sample of **6**, and VT-EPR of **6** in DCM solution was also recorded. The EPR spectra was recorded in a X band EPR instrument (EMX MICRO X, Bruker EPR instrument).

EPR experimental parameters:

Frequency: 9.31 GHz; Power: 8.47 mW; Modulation frequency: 100 KHz; Modulation amplitude: 10G Conversion time: 120 msec, Time constant: 328 msec.

The modified Bleaney-Bowers equation were used to fit the IT against the T data points to get the energy separation between the singlet and triplet spin state of the diradical species.

$$IT = \frac{2\rho N_A g^2 \beta^2}{k_b} * \frac{1}{3 + \exp\left(-\frac{2J}{k_b T}\right)} + \frac{(1-\rho) N_A g^2 \beta^2}{2k_b}$$

Here, '*I*' is the EPR intensity, 'T' is the temperature in Kelvin scale, *g* is the g factor, N_A is the Avogadro constant, β is the Bohr magneton, k_b is the Boltzmann constant, and ρ is the paramagnetic purity

The *IT* vs. *T* data set was fitted according to the below equation using Origin 2021 software package.

$$IT = \frac{a}{3 + \exp\left(-\frac{b}{T}\right)} + c$$

$$a = \frac{2\rho N_A g^2 \beta^2}{k_b}\ ; = \frac{2J}{k_b}\ ;\ \text{c}\quad \text{M}= \frac{(1-\rho) N_A g^2 \beta^2}{2k_b}$$

a = 1.97467e9; b = –490.47654; c = 4.24564e7

The singlet-triplet energy gap ($\Delta E_{S\text{-}T}$) as solid = 2J = –490.47*0.0019872 kcal/mol = –0.97 kcal/mol

VT-EPR in DCM solution:

$\Delta E_{S\text{-}T}$ in solution = −869.3342*0.0019872 = −1.73 kcal/mol

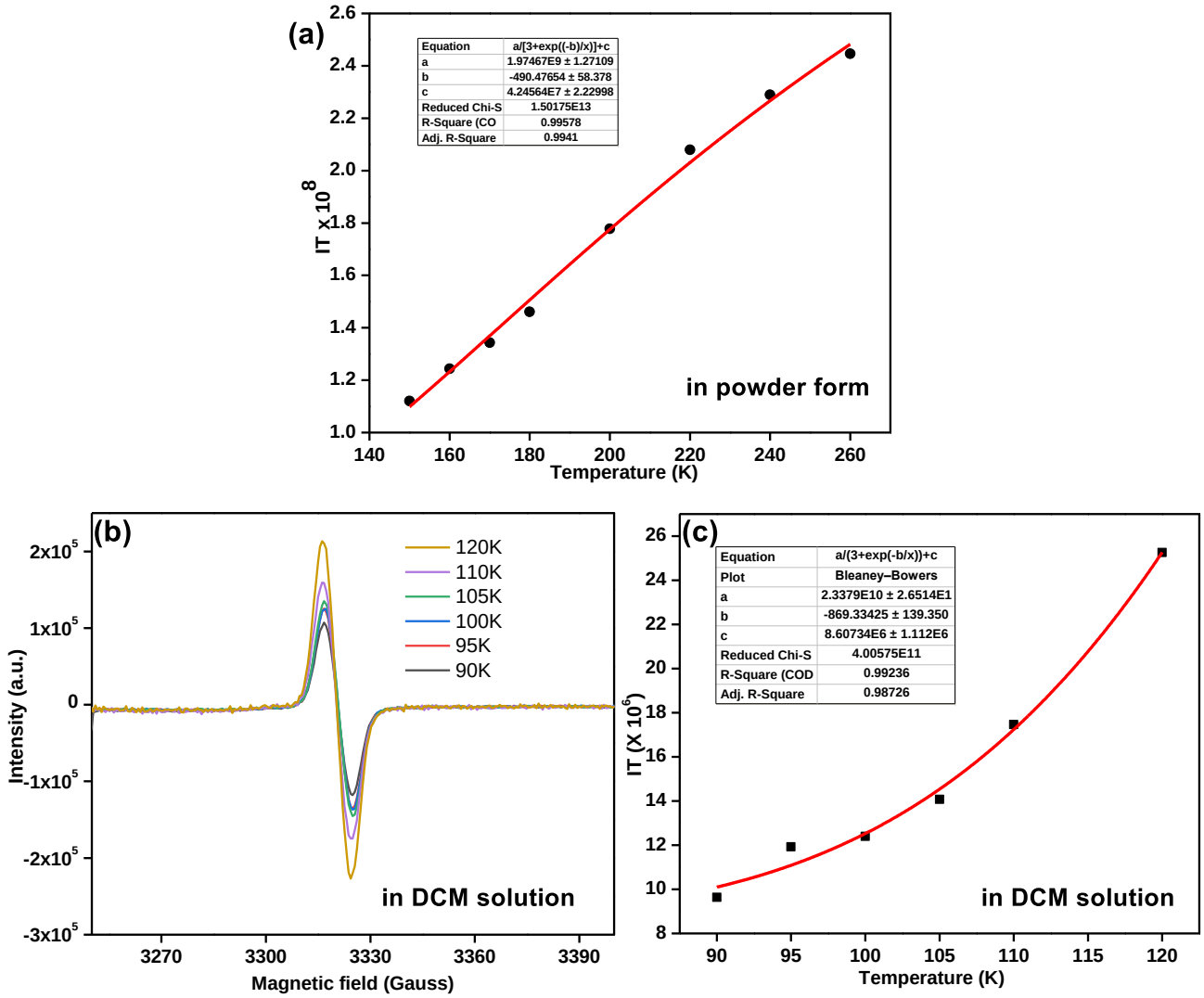


Fig. S11 (a) The Bleaney-Bowers plot for solid sample **6**. (VT-EPR data was shown in the main manuscript, Fig. 3b). (b) VT-EPR spectra and (c) The Bleaney-Bowers plot of **6** in DCM solution.

4. X-ray crystallographic analysis

A suitable single crystal of **6** was selected using paratone oil and mounted on glass fiber with the help of gum. The intensity data and geometric parameters of these crystals were garnered with the help of Bruker D8 Venture X-ray diffractometer having a micro-focus sealed X-ray tube Mo-Kα (λ = 0.71073 Å) source of X-rays along with a PHOTON 100 detector with inclining Phi and Omega (width of 0.5 for one frame)

working at a scan speed of 10 s per frame. The crystal was kept at 298 K during data collection. Data acquisition, as well as extraction of data, was accomplished by utilizing Bruker Apex-3 and Bruker SAINT software packages using a narrow-frame algorithm.[1] By utilizing OLex2[2] the crystal structure was solved with the help of olex2.solve[3] structure solution program by employing intrinsic Phasing methods, and crystal structure refinement was done with the SHELXL[4] refinement package by putting into use Least Squares minimization. Refinement of all non-hydrogen atoms was completed with the help of anisotropic thermal parameters.

Table S1. X-ray crystallographic information of **6**

CCDC No.	2309430
Empirical formula (including disordered acetonitrile)	$C_{58}H_{41}N_3$
Formula weight	779.94
Temperature/K	298
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	12.7061(5)
b/Å	14.0855(4)
c/Å	23.6488(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4232.5(3)
Z	4
ρ_{calc}g/cm^3	1.224
μ/mm^{-1}	0.071
F(000)	1640.0
Crystal size/mm^3	0.231 × 0.214 × 0.123
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.498 to 52.9
Index ranges	$-15 \leq h \leq 15$, $-15 \leq k \leq 17$, $-25 \leq l \leq 29$
Reflections collected	48088
Independent reflections	8683 [R_{int} = 0.0441, R_{sigma} = 0.0299]
Data/restraints/parameters	8683/0/557
Goodness-of-fit on F^2	1.041
Final R indexes [I>=2σ (I)]	R_1 = 0.0384, wR_2 = 0.0921
Final R indexes [all data]	R_1 = 0.0447, wR_2 = 0.0961
Largest diff. peak/hole / e Å^{-3}	0.14/-0.16
Flack parameter	0.1(10)

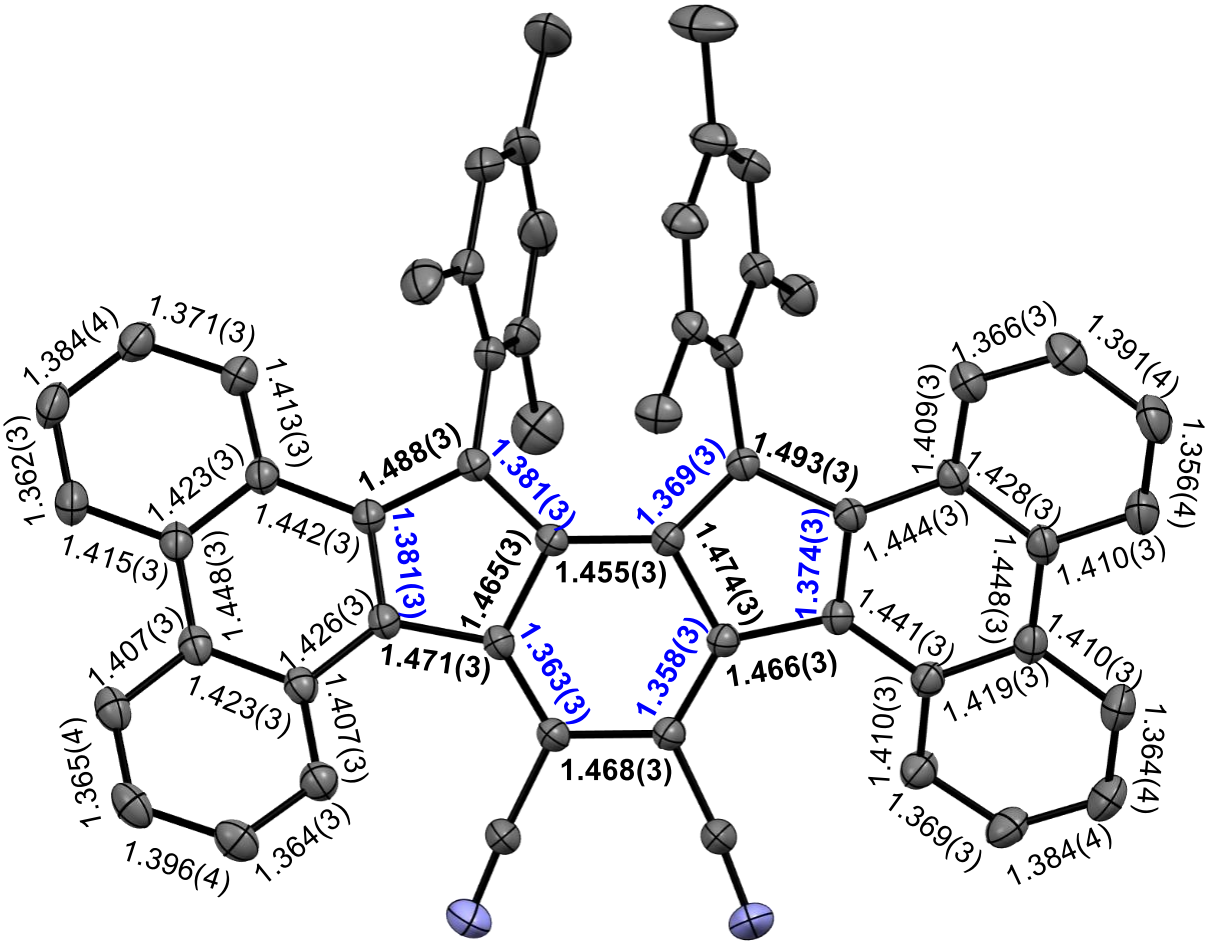


Fig. S12 ORTEP drawing of **6** with thermal ellipsoids at 30% probability level, showing the core bond lengths with e.s.d values (hydrogens, and acetonitrile solvent disorder omitted).

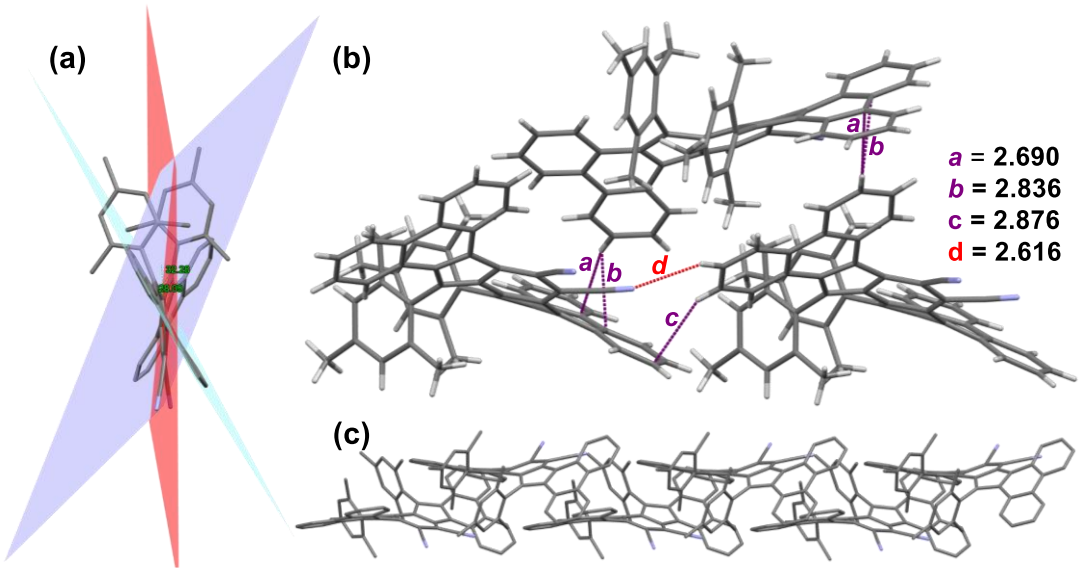


Fig. S13 (a) Side view of **6** showing the twisting of the π-backbone. (b) Non-covalent interactions (Å) are labelled for **6** (C−H···π (*a* = 2.690 Å, *b* = 2.836 Å, *c* = 2.876 Å) and C−H···N (*d* = 2.616 Å) interactions between the neighboring molecules). (c) 1D wave-like packing for **6**.

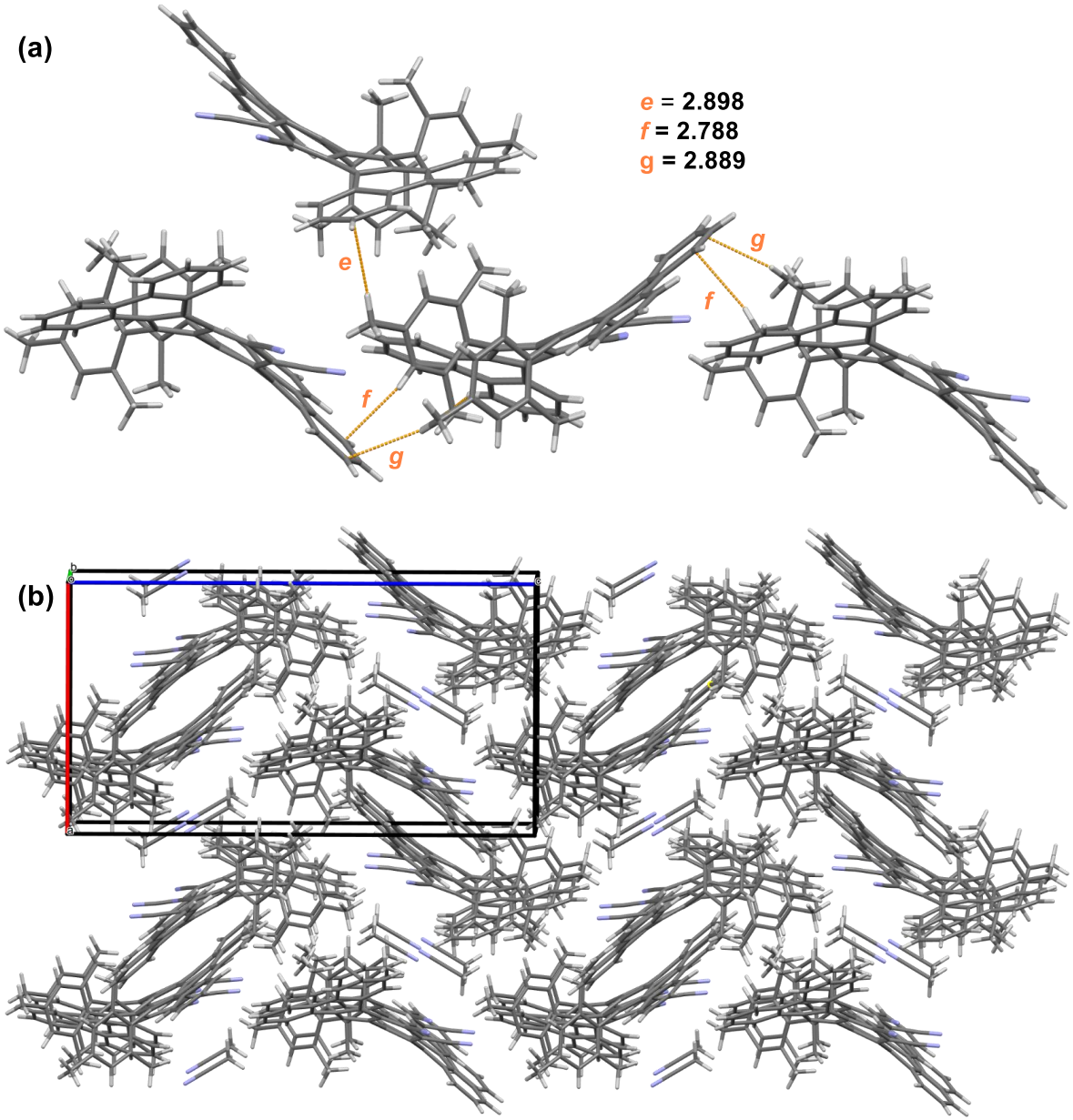


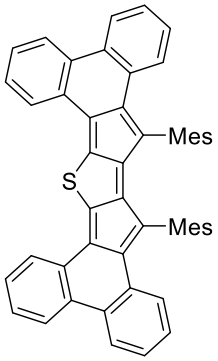
Fig. S14 (a) C–H···π non-covalent interactions (Å) between mesityl groups and π-backbone of neighbouring molecules of **6** (labelled as e, f, g); (b) 3D molecular packing of **6** (with the solvent disorder).

5. DFT calculations

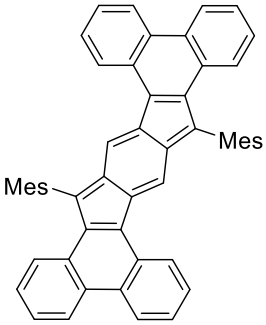
Gas-phase density functional theory (DFT) calculations were performed with Gaussian 09 package using a high-performance computing cluster facility of IIT Ropar at the BHandHLYP level of theory with basis set 6-31G(d).[5] X-ray crystallographic structure of **6** was used for DFT-optimization. The calculated NOON (natural orbital occupation number) value for **DPDCPT**, **4**, **5** and **6** was based on the broken symmetry formalism.[6] NICS (standard GIAO method)[7] and HOMA[8] indices were calculated for the optimized closed-shell structure for **6**. The reported $NICS(1)_{zz}$ indices were the average of two positions (above and below the plane) for non-planar **6**. Excitation energy was computed using time-dependent

density functional theory (TD-DFT) for the optimized closed-shell structure of **6** in toluene. Molecular orbital contributions were determined using the GaussSum 3.0 package.[9]

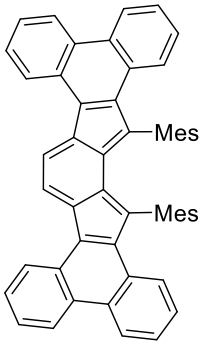
Table S2. Relative electronic energies of optimized geometries for **DPDCPT**, **4**, **5** and **6**.



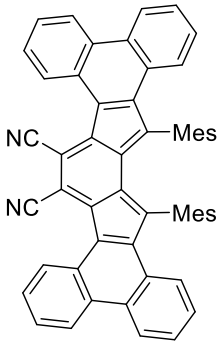
DPDCPT



4



5



6

Compounds	Optimization	hartree	kcal/mol	% diradical character
DPDCPT	Singlet closed-shell BHandHLYP /6-31G(d)	–2401.384192	–1506890.193	51
	Singlet open-shell UBHandHLYP /6-31G(d)	–2401.404936	–1506903.21	
	Triplet open-shell UBHandHLYP /6-31G(d)	–2401.403911	–1506902.567	
4	Singlet closed-shell BHandHLYP /6-31G(d)	–2080.649108	–1305626.041	0
	Singlet open-shell UBHandHLYP /6-31G(d)	–2080.649108	–1305626.041	
	Triplet open-shell UBHandHLYP /6-31G(d)	–2080.638009	–1305619.076	
5	Singlet closed-shell BHandHLYP /6-31G(d)	–2080.623976	–1305610.271	1
	Singlet open-shell UBHandHLYP /6-31G(d)	–2080.623976	–1305610.271	
	Triplet open-shell UBHandHLYP /6-31G(d)	–2080.618459	–1305606.809	
6	Singlet closed-shell BHandHLYP /6-31G(d)	–2264.984351	–1421298.065	30
	Singlet open-shell UBHandHLYP /6-31G(d)	–2264.987479	–1421300.028	
	Triplet open-shell UBHandHLYP /6-31G(d)	–2264.98346	–1421297.506	

DPDCPT: $\Delta E_{\text{Singlet(OS)-Triplet(OS)}}$ = –0.64 kcal/mol; $\Delta E_{\text{OS-CS}}$ = –13.01 kcal/mol; $\Delta E_{\text{CS-T}}$ = 12.37 kcal/mol. Occupation number calculation of the open-shell singlet **DPDCPT** for HOMO = 1.26 and LUMO = 0.74 affords a 51% diradical character (singlet diradical character index (y_0) = 0.51).

Compound 4: $\Delta E_{\text{Singlet(OS)-Triplet(OS)}}$ = –6.96 kcal/mol; $\Delta E_{\text{OS-CS}}$ = 0 kcal/mol; $\Delta E_{\text{CS-T}}$ = –6.96 kcal/mol. Occupation number calculation of the open-shell singlet **5** for HOMO = 2.00 and LUMO = 0.00 affords a 0% diradical character (singlet diradical character index (y_0) = 0).

Compound 5: $\Delta E_{\text{Singlet(OS)-Triplet(OS)}}$ = –3.46 kcal/mol; $\Delta E_{\text{OS-CS}}$ = 0 kcal/mol; $\Delta E_{\text{CS-T}}$ = –3.46 kcal/mol. Occupation number calculation of the open-shell singlet **5** for HOMO = 1.89 and LUMO = 0.11 affords a 1% diradical character (singlet diradical character index (y_0) = 0.01)

Compound 6: $\Delta E_{\text{Singlet(OS)-Triplet(OS)}}$ = –2.52 kcal/mol; $\Delta E_{\text{OS-CS}}$ = –1.96 kcal/mol; $\Delta E_{\text{CS-T}}$ = –0.56 kcal/mol. Occupation number calculation of the open-shell singlet **6** for HOMO = 1.41 and LUMO = 0.59 affords a 30% diradical character (singlet diradical character index (y_0) = 0.30).

Optimized open-shell structure of DPDCPT

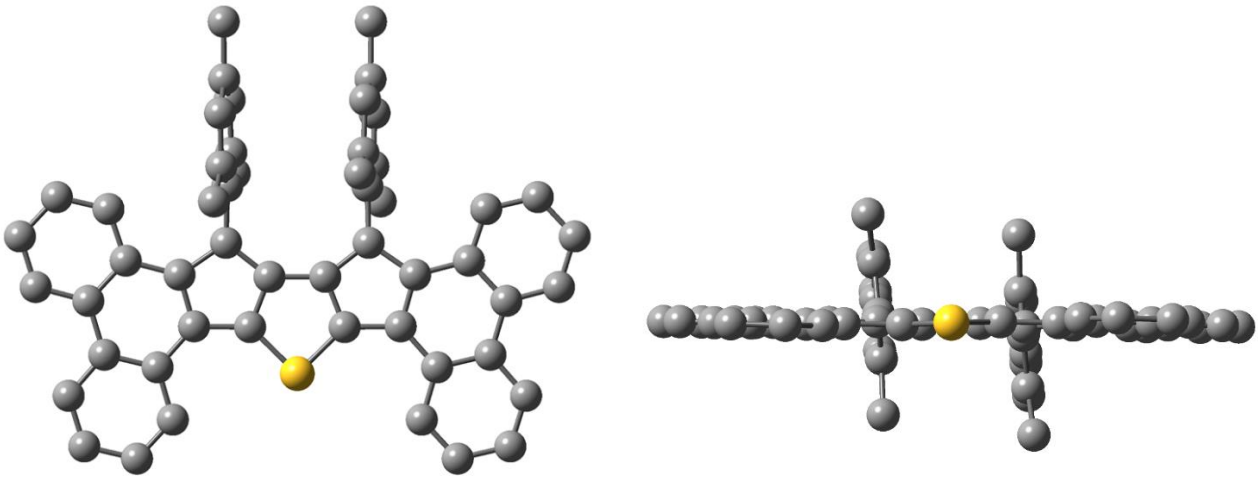


Fig. S15 Optimized structure of **DPDCPT** top-view (left) and side-view (right) in the ground state

Optimized closed-shell structure of 4

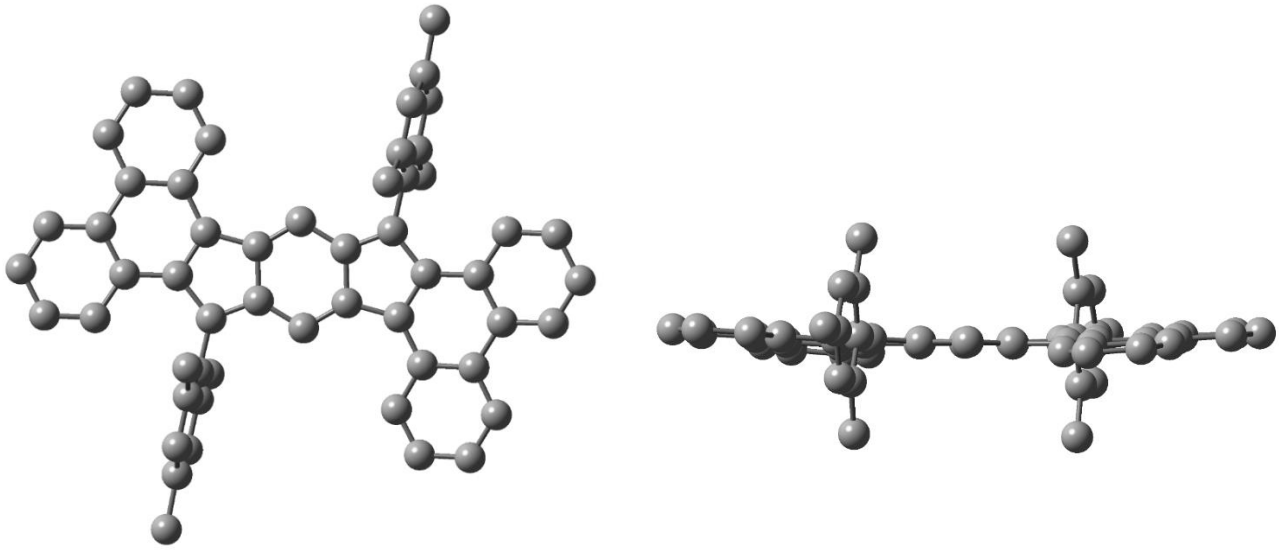


Fig. S16 Optimized structure of **4** top-view (left) and side-view (right) in the ground state

Optimized closed-shell structure of 5

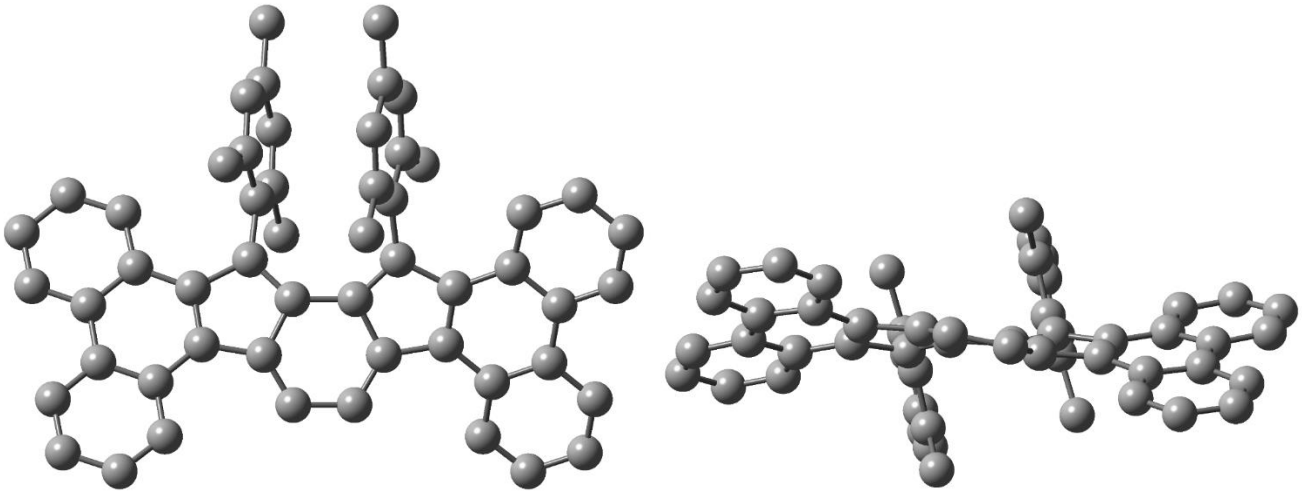


Fig. S17 Optimized structure of **5** top-view (left) and side-view (right) in the ground state

Optimized open-shell structure of 6

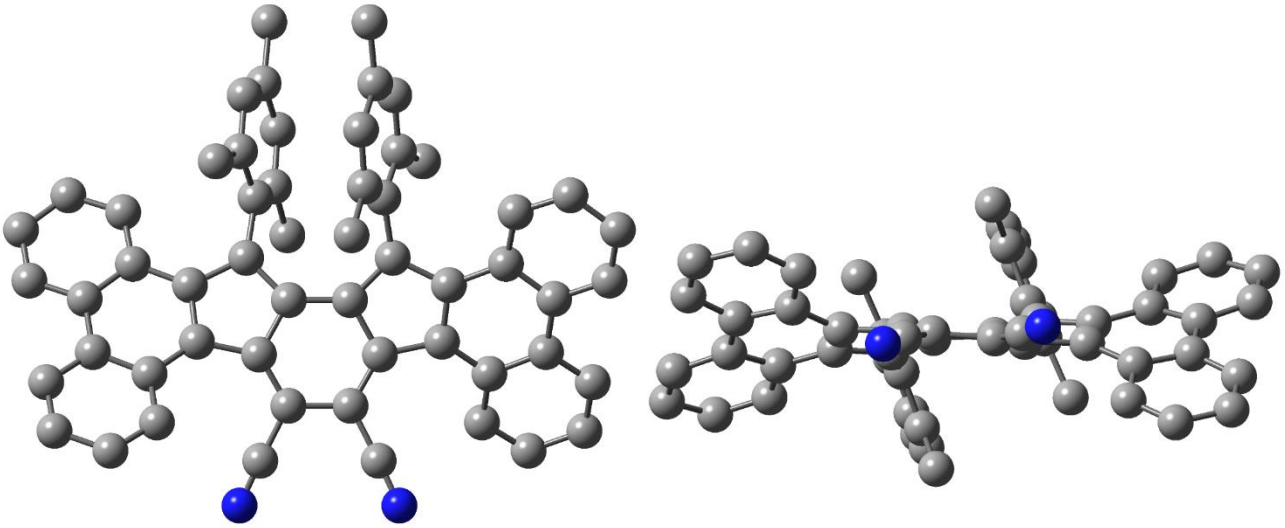


Fig. S18 Optimized structure of **6** top-view (left) and side-view (right) in the ground state.

TDDFT computation of compound 6.

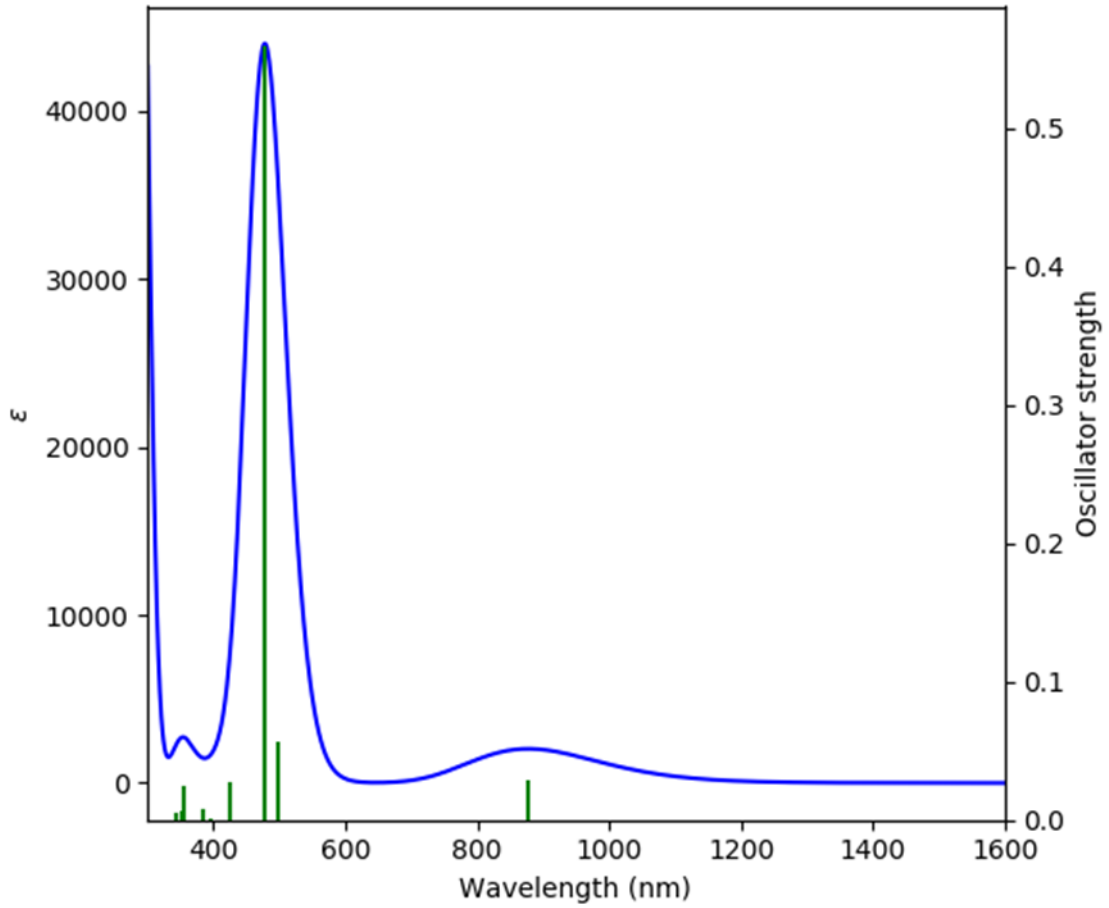


Fig. S19 Theoretical absorption of **6** in the toluene.

Table S3. Summary of TDDFT calculation for **6**

Wavelength (nm)	**Oscillator Strength (*f*)**	**Major contributions**
877	0.0281	HOMO->LUMO (96%)
499	0.0571	H-2->LUMO (85%)
476	0.5599	H-1->LUMO (89%)
424	0.0278	H-4->LUMO (90%)
396	0.0006	H-3->LUMO (88%)
384	0.0086	H-5->LUMO (86%)
367	0	H-6->LUMO (98%)
353	0.0245	H-8->LUMO (72%), H-7->LUMO (21%)
353	0.0071	HOMO->L+1 (85%)
343	0.0051	H-8->LUMO (21%), H-7->LUMO (77%)
297	0.1029	H-10->LUMO (66%)
297	0.0725	H-9->LUMO (84%)
291	0.5117	H-11->LUMO (10%), H-2->L+3 (11%), HOMO->L+2 (57%)
285	0.0117	H-1->L+1 (42%), HOMO->L+3 (24%)

278	0.2266	H-11->LUMO (12%), H-10->LUMO (22%), H-2->L+1 (42%), HOMO->L+4 (10%)
272	0.1661	H-5->L+1 (13%), H-1->L+1 (38%), HOMO->L+3 (28%)
271	0.1689	H-11->LUMO (60%), H-2->L+1 (16%)
268	0.1295	H-14->LUMO (35%), H-12->LUMO (35%)
257	0.5147	H-3->L+1 (20%), HOMO->L+5 (52%)
254	0.002	H-2->L+1 (22%), HOMO->L+4 (53%)
254	0.0139	H-14->LUMO (12%), H-1->L+3 (10%), HOMO->L+6 (39%)
249	0.1024	H-14->LUMO (32%), H-12->LUMO (51%)
246	0.0158	H-4->L+1 (91%)
246	0.0551	H-3->L+1 (53%), HOMO->L+5 (17%)
243	0.0122	H-13->LUMO (83%)
242	0.0946	H-5->L+1 (59%), HOMO->L+3 (14%)
236	0.5504	H-3->L+3 (22%), H-1->L+2 (39%), HOMO->L+4 (14%)
233	1.4557	H-3->L+2 (17%), H-1->L+3 (21%), HOMO->L+6 (36%)
229	0.0634	H-15->LUMO (21%), HOMO->L+7 (24%)
229	0.0018	H-6->L+1 (96%)

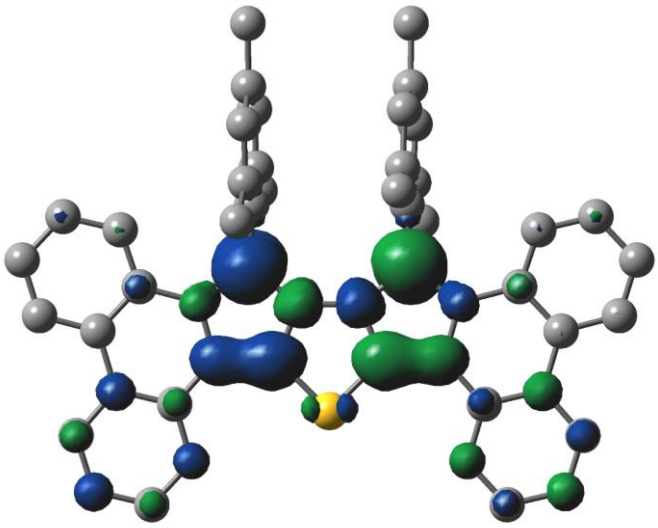


Fig. S20 Spin density distribution of the singlet open-shell stae of **DPDCPT** calculated at the UBHandHLYP/6-31G* level of theory with isovalue of 0.004.

Molecular Orbitals for 6

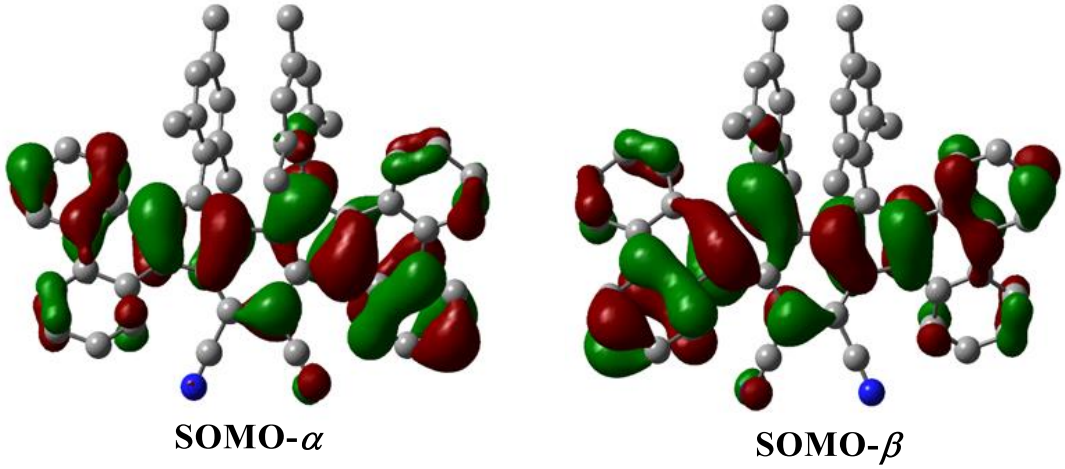


Fig. S21 Calculated (UBHandHLYP/6-31G*) frontier molecular orbital (FMO) profiles for the α-spin and β-spin of **6** (isovalue of 0.02).

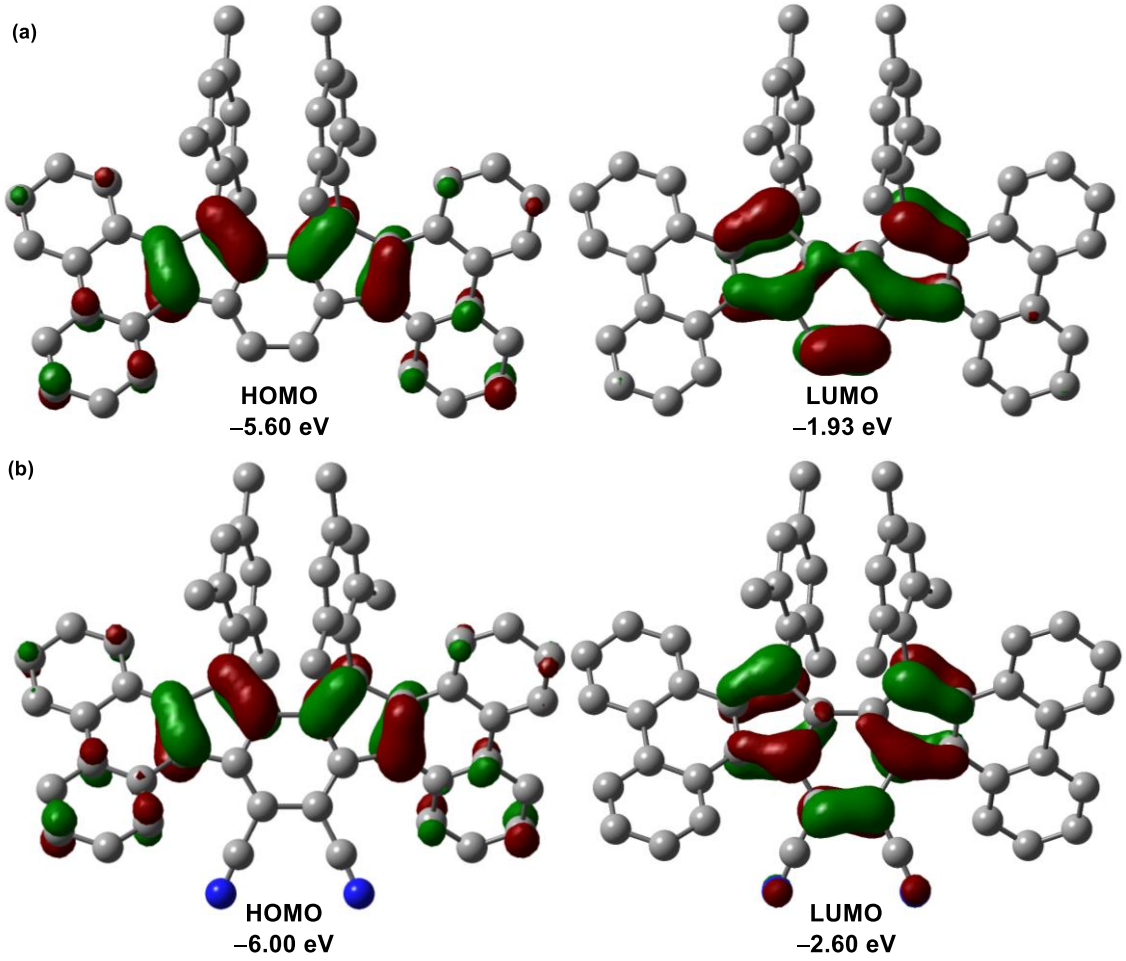


Fig. S22 FMO profiles (isovalue 0.04) of (a) **5** and (b) **6**, calculated at BHandHLYP/6-31G*.

The FMO profile suggests large LUMO coefficients at the *as*-indacene unit of **5**. Therefore, electron-withdrawing cyano substituents on the central six-membered ring may significantly stabilize the LUMO energy level, resulting in a narrower HOMO-LUMO energy gap for **6** than that of **5**.

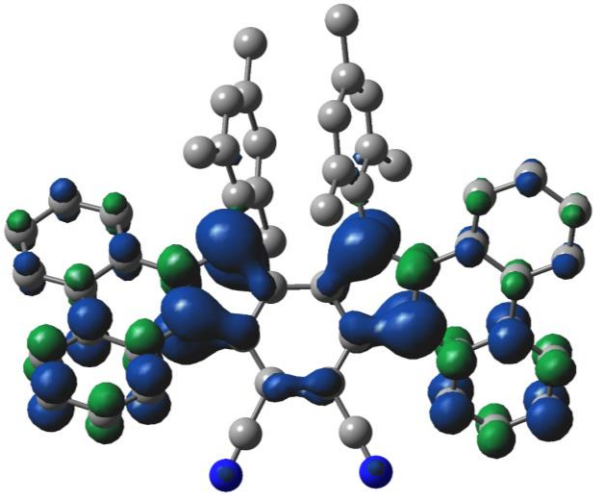
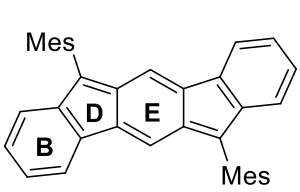
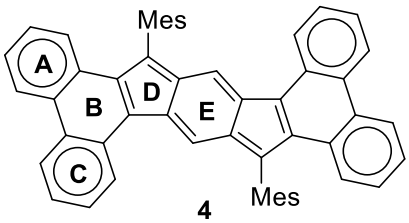


Fig. S23 Spin density distribution of the triplet state of **6** calculated at the UBHandHLYP/6-31G* level of theory with isovalue of 0.004.

NICS Calculations for 1, 2, benzo-2, 4, 5, and 6.



1

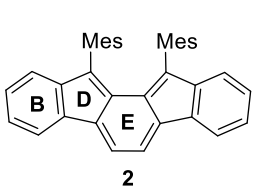


4

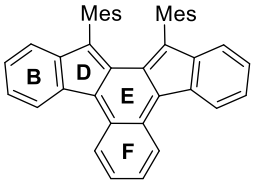
Table S4. NICS(1)$_{zz}$ value comparisons between **1** and **4**, calculated at the (U)BHandHLYP/6-31G(d) level.

Rings	**1**			**4**		
	CS	OS	T	CS	OS	T
A	–	–	–	−27.15	−27.15	−25.26
B	−19.89	−20.04	−15.84	−13.53	−13.52	−5.49
C	–	–	–	−25.82	−25.82	−21.87
D	12.54	10.40	6.60	29.45	29.45	11.62
E	10.33	4.25	−15.74	21.34	21.34	−13.00

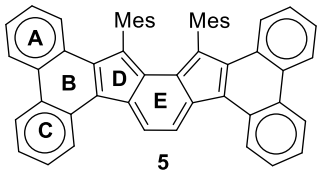
Table S5. NICS(1)$_{zz}$ value comparisons between **2** and **benzo-2**, and **5** and **6**, calculated at the (U)BHandHLYP/6-31G(d) level.



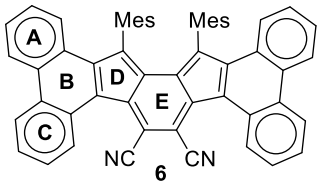
2



Benzo-2



5



6

Rings	**2**			**Benzo-2**		
	CS	OS	T	CS	OS	T
B	−19.39	−19.59	−17.28	−15.86	−18.75	−15.69
D	13.35	11.19	3.08	19.11	11.69	11.46
E	9.99	2.57	−13.82	12.07	−0.63	−11.03
F	–	–	–	2.73	−12.92	−23.48
Rings	**5**			**6**		
	CS	OS	T	CS	OS	T
A	−24.81	−24.76	−23.88	−23.09	−22.02	−22.41
B	−12.15	−11.93	−4.21	−10.20	−5.02	−2.44
C	−24.07	−23.92	−20.77	−21.97	−19.74	−19.11
D	26.81	22.75	0.76	31.79	24.15	−1.04
E	17.44	13.32	−9.94	12.67	−1.67	−9.20

The calculated NICS(1)$_{zz}$ in closed-shell singlet (CS), open-shell singlet (OS), and triplet (T) states clearly indicate that phenanthrene-fused indacenes (*s*-indacene and *as*-indacene) showed a greater degree of paratropicity in the ground state, in comparison to their benzo-fused analogs. In Table S5, the NICS(1)$_{zz}$ values for **2** and **benzo-2**, and **5** and **6** are reported. The data suggested that in the CS and OS states, five-membered rings D of **6** exhibit a significantly greater degree of paratropicity than other compounds, which indicated enhanced antiaromaticity for **6**. Further, ring E showed small negative NICS value for the OS state (−1.67) for **6**, implying weak aromatic character, while the NICS value of ring E for **5** in the OS state displayed greater antiaromatic character.

Since reactions in which aromaticity is gained are normally highly favorable, it is quite likely that OS state for **6** should be the ground state. However, the small negative NICS value for ring E in **6** may not be reflected in its singlet ground state, thus a dominance of quinoidal CS state (which can be accessible at room temperature) was observed by single-crystal analysis, reflecting a pronounced ground state antiaromaticity for **6**.

Furthermore, as reported by Ottosson and Solà *et al.*[10] for a diphenanthro-pentalene system, its triplet excited state (T_1) was significantly stabilized (going down near the parent pentalene) due to the retention of five aromatic cycles in the excited state, comprising four disjoint Clar sextets and one disjoint triplet biradical Baird π-octet.

Following the same logic reported by Ottosson and Solà *et al.*, for compound **6**, the T_1 state may also go down (stabilized T_1) as a result of combination of Baird and Clar aromatic stabilization of the first excited triplet state. Indeed, NICS indices for the rings A-E for the triplet state of **6** (Table S5) were found to be negative, suggesting aromatic stabilization of T_1 state. The total number of aromatic cycles within the molecule **6** in the triplet exited state may be represented in four disjoint Clar cycles (shown in red) and one disjoint triplet biradical Baird aromatic 12πe cycle (shown in green, Fig S24b).

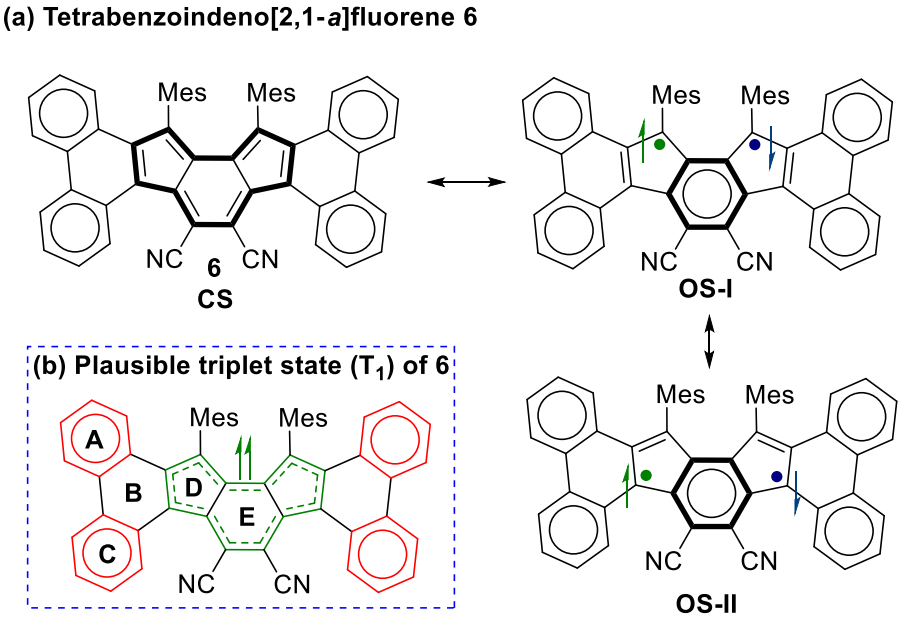


Fig. S24 (a) Plausible CS and OS resonance forms for **6**; (b) Representation of four aromatic Clar cycles in the peripheral benzene rings and one aromatic Baird cycle in the central *as*-indacene ring for **6**.

Calculated proton chemical shifts data:

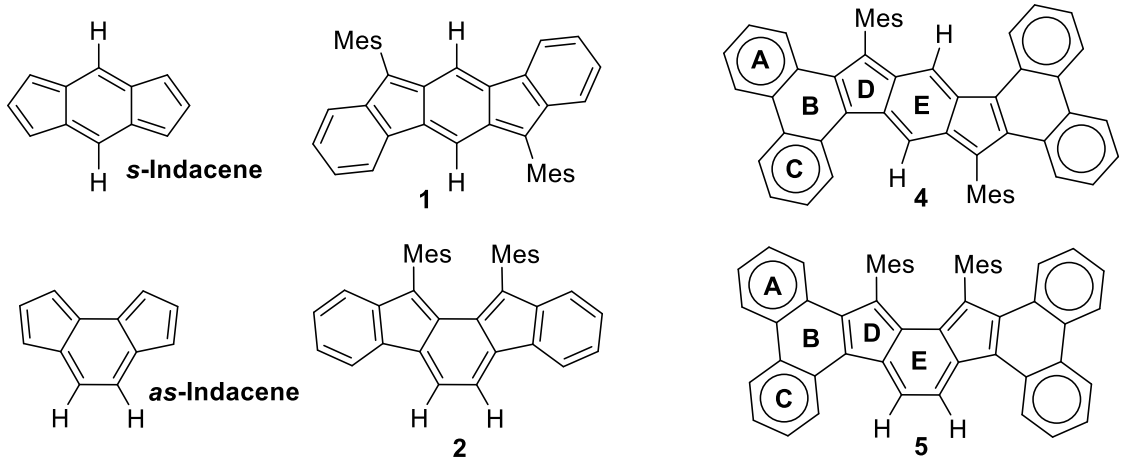


Table S6. Comparison of ^{1}H NMR chemical shifts (calculated) of core indacene protons at BHandHLYP/6-31G(d). *s*-indacene units for **1** and **4**, and *as*-indacene units for **2** and **5**. (Reference: TMS B3LYP/6-311+G(2d,p) GIAO)

Compound	Closed-Shell singlet (ppm)
***s*-Indacene**	4.00
1	6.06
4	6.22
***as*-Indacene**	4.43
2	5.89
5	6.06

Table S6 clearly indicates that the *s*-indacene protons of **4** and **5** experience a downfield shift compared to **1** and **2**, respectively, despite the enhancement of antiaromatic character in **4** and **5** due to diphenanthro-fusion. This observation may be attributed to the deshielding ring-current effect of the outer benzene rings of the phenanthrene units which are closer to the indacene protons in space. These findings are consistent with our previous observation,[11a] and also observed by Haley *et al.* for compound **4**[11b] showing downfield chemical shift despite greater antiaromaticity of *s*-indacene.

Cartesian coordinates (in Angstroms) for the optimized structures:

Singlet closed-shell structure of DPDCPT

Atom type	**x**	**y**	**z**
C	-4.42276200	-0.19000700	-0.07227700
C	-5.39250600	-1.22951000	-0.12208200
C	-4.97954300	-2.62155200	-0.17284200
C	-3.60328200	-2.94718700	-0.18375500
C	-2.65987500	-1.88298800	-0.11371000
C	-3.03489800	-0.54939700	-0.05221800
C	-1.22569700	-1.88839600	-0.10731600
C	-0.72962000	-0.54501900	-0.04067600
C	-1.82150000	0.29112900	0.02177200
C	1.22576000	-1.88837200	0.10743000
C	0.72965200	-0.54500300	0.04078800
C	2.65994000	-1.88293400	0.11377300
C	3.03492800	-0.54933600	0.05224200
C	1.82150900	0.29116500	-0.02171300
C	3.60337500	-2.94710900	0.18379600

C	4.97962900	-2.62144100	0.17279700
C	5.39255600	-1.22939100	0.12197000
C	4.42278400	-0.18991200	0.07220600
C	6.75215700	-0.87048900	0.13168700
C	7.15819900	0.43755100	0.10095900
C	6.20480400	1.45710300	0.06343300
C	4.87122500	1.14787400	0.05043500
C	3.21227800	-4.29709000	0.25528500
C	4.13759600	-5.30358800	0.30415500
C	5.50033300	-4.99020800	0.28305700
C	5.90361000	-3.68194400	0.22078400
C	-4.87124000	1.14776800	-0.05057700
C	-6.20482600	1.45696500	-0.06367600
C	-7.15819300	0.43738900	-0.10124000
C	-6.75211500	-0.87064200	-0.13190400
C	-5.90349600	-3.68207800	-0.22084900
C	-5.50018500	-4.99033500	-0.28306300
C	-4.13743900	-5.30368200	-0.30407400
C	-3.21214800	-4.29716100	-0.25518000
S	0.00004500	-3.02189800	0.00004800
C	-1.80654700	1.75706500	0.22686400
C	-1.71716400	2.62857700	-0.86340800
C	-1.76673800	3.99715300	-0.63775900
C	-1.89831700	4.52492700	0.63796700
C	-1.99336600	3.64288700	1.70456800
C	-1.95608100	2.26794700	1.52243100
C	-2.13242800	1.35240800	2.70283500
C	-1.63926700	2.10115200	-2.26855600
C	-1.91397800	6.01038900	0.86338000
C	1.80651900	1.75709900	-0.22682800
C	1.95593200	2.26798200	-1.52238600
C	1.99313900	3.64294200	-1.70452100
C	1.89812500	4.52496300	-0.63792400
C	1.76669700	3.99717300	0.63783100
C	1.71721400	2.62861100	0.86347300
C	1.63938700	2.10112700	2.26860200
C	2.13225500	1.35246500	-2.70281000
C	1.91365500	6.01043300	-0.86327700
H	7.50632700	-1.63551200	0.16775700
H	8.20953700	0.67505100	0.11057800
H	6.51478500	2.48944400	0.04667600
H	4.15218600	1.94307100	0.02627400
H	2.16496800	-4.54655300	0.27846500
H	3.81776500	-6.33140500	0.35900100
H	6.23615600	-5.77690500	0.31848300
H	6.95850400	-3.47627600	0.20940500
H	-4.15222500	1.94298500	-0.02638800
H	-6.51483400	2.48929900	-0.04696900
H	-8.20953600	0.67486200	-0.11094200
H	-7.50626400	-1.63568300	-0.16801200
H	-6.95839500	-3.47643400	-0.20953000
H	-6.23598700	-5.77704900	-0.31850600
H	-3.81758000	-6.33149400	-0.35887000
H	-2.16483000	-4.54660000	-0.27828200
H	-1.70463700	4.66611000	-1.48286400

H	-2.11004400	4.03317200	2.70468500
H	-2.07313800	1.90743200	3.63438000
H	-3.10221400	0.85854400	2.67096100
H	-1.38027100	0.56892700	2.72552500
H	-0.82713800	1.39132900	-2.38664300
H	-2.55778100	1.58413300	-2.54252400
H	-1.48667800	2.90975000	-2.97691200
H	-2.29073100	6.54040400	-0.00742300
H	-2.53524100	6.27701300	1.71444000
H	-0.91088400	6.38541900	1.06414100
H	2.10973000	4.03323100	-2.70464500
H	1.70467400	4.66612900	1.48294400
H	1.48816800	2.90983800	2.97712300
H	0.82639900	1.39233300	2.38701700
H	2.55736600	1.58290200	2.54205600
H	1.38010000	0.56898300	-2.72549800
H	2.07294200	1.90750100	-3.63434600
H	3.10204500	0.85860600	-2.67096200
H	0.91021800	6.38570800	-1.06186100
H	2.29236900	6.54031400	0.00676200
H	2.53317100	6.27696000	-1.71563300

Singlet open-shell structure of DPDCPT

Atom type	**x**	**y**	**z**
C	4.43725200	-0.17576000	0.09025200
C	5.40524500	-1.21405700	0.12853900
C	4.99120700	-2.60759400	0.15051100
C	3.61315400	-2.93443100	0.14435800
C	2.67177300	-1.87208200	0.09477800
C	3.04599500	-0.53767300	0.05870600
C	1.22206900	-1.89092300	0.07101100
C	0.72121200	-0.59000200	0.03114500
C	1.84379100	0.28781600	-0.00786300
C	-1.22207700	-1.89092000	-0.07098500
C	-0.72121600	-0.58999800	-0.03111000
C	-2.67178000	-1.87207200	-0.09476000
C	-3.04599900	-0.53766100	-0.05869100
C	-1.84379100	0.28782000	0.00789800
C	-3.61315900	-2.93442200	-0.14435100
C	-4.99121100	-2.60758400	-0.15053400
C	-5.40524700	-1.21404400	-0.12858200
C	-4.43725300	-0.17574800	-0.09026800
C	-6.76488100	-0.85620800	-0.15395100
C	-7.17100700	0.45246800	-0.14765100
C	-6.21754400	1.47111200	-0.12008300
C	-4.88320400	1.16108700	-0.09326900
C	-3.21986300	-4.28653000	-0.18062400
C	-4.14531900	-5.29347200	-0.21561100
C	-5.50759700	-4.97838400	-0.21507800
C	-5.91329200	-3.66856500	-0.18419600
C	4.88319200	1.16107800	0.09323900

C	6.21753200	1.47110700	0.12001400
C	7.17099800	0.45246500	0.14755300
C	6.76487800	-0.85621400	0.15386400
C	5.91328600	-3.66857700	0.18416800
C	5.50759000	-4.97839600	0.21507500
C	4.14531200	-5.29348200	0.21564200
C	3.21985700	-4.28653800	0.18066000
S	-0.00000300	-3.09478500	0.00000700
C	1.81152600	1.75308500	-0.20760100
C	1.70746600	2.61812400	0.88566400
C	1.75180400	3.98796300	0.66696900
C	1.89166700	4.52165500	-0.60547000
C	1.99657400	3.64503800	-1.67592600
C	1.96438800	2.26935700	-1.50030400
C	2.15313400	1.35847900	-2.68244500
C	1.61971500	2.08051300	2.28635200
C	1.90444700	6.00806600	-0.82472100
C	-1.81151800	1.75308800	0.20763700
C	-1.96440400	2.26935700	1.50032600
C	-1.99659800	3.64504800	1.67594700
C	-1.89166200	4.52165900	0.60550300
C	-1.75176400	3.98796300	-0.66694300
C	-1.70742200	2.61813500	-0.88563400
C	-1.61966100	2.08052200	-2.28632100
C	-2.15318600	1.35848800	2.68246800
C	-1.90440900	6.00807600	0.82470600
H	-7.51872800	-1.62193800	-0.18237300
H	-8.22213000	0.69013600	-0.16834300
H	-6.52656600	2.50390900	-0.12182900
H	-4.16369300	1.95638700	-0.07691500
H	-2.17283200	-4.53540000	-0.18373800
H	-3.82593300	-6.32239700	-0.24309900
H	-6.24340100	-5.76558500	-0.24020600
H	-6.96845300	-3.46420200	-0.18608700
H	4.16367100	1.95637100	0.07690300
H	6.52655100	2.50390500	0.12175300
H	8.22212100	0.69013700	0.16821000
H	7.51873100	-1.62193700	0.18225900
H	6.96844600	-3.46421800	0.18603900
H	6.24339400	-5.76559700	0.24019800
H	3.82592300	-6.32240600	0.24315400
H	2.17282600	-4.53540800	0.18381000
H	1.67895400	4.65281000	1.51442000
H	2.11765300	4.04056600	-2.67347100
H	2.06218100	1.90979600	-3.61362300
H	3.13921400	0.89726500	-2.66424600
H	1.42648500	0.55076700	-2.69442900
H	0.83636800	1.33516500	2.38225300
H	2.55344300	1.60274600	2.57981900
H	1.41513800	2.87717000	2.99506200
H	2.25501500	6.53677600	0.05767200
H	2.54650700	6.28153300	-1.65801200
H	0.90493200	6.37804400	-1.05082700
H	-2.11770200	4.04057700	2.67348700
H	-1.67889700	4.65281200	-1.51439300

H	-1.41485100	2.87714400	-2.99500300
H	-0.83647200	1.33500300	-2.38216400
H	-2.55347100	1.60296400	-2.57987200
H	-1.42657200	0.55074500	2.69445400
H	-2.06221000	1.90980300	3.61364600
H	-3.13928700	0.89731600	2.66427200
H	-0.90451200	6.37835900	1.04861800
H	-2.25702000	6.53664800	-0.05696100
H	-2.54475500	6.28138800	1.65935900

Triplet structure of DPDCPT

Atom type	**x**	**y**	**z**
C	-4.43031800	-0.15789600	-0.09711800
C	-5.39788800	-1.19310600	-0.12693400
C	-4.98609100	-2.59442500	-0.14030900
C	-3.60897700	-2.93073200	-0.13433500
C	-2.65565200	-1.87982600	-0.09425400
C	-3.02935700	-0.51931100	-0.06635400
C	-1.21800500	-1.91704500	-0.06057800
C	-0.71230500	-0.62746400	-0.02507500
C	-1.85900800	0.27920300	0.00053300
C	1.21796000	-1.91706600	0.06057900
C	0.71228200	-0.62747700	0.02507500
C	2.65560700	-1.87987400	0.09425500
C	3.02933000	-0.51936100	0.06635400
C	1.85900400	0.27917200	-0.00053100
C	3.60892100	-2.93078900	0.13433600
C	4.98604000	-2.59449700	0.14030900
C	5.39785400	-1.19318000	0.12692600
C	4.43029300	-0.15796200	0.09711300
C	6.75528600	-0.83788400	0.15305700
C	7.16446200	0.47265400	0.15481100
C	6.21205700	1.48780900	0.13570400
C	4.87490200	1.17532900	0.10920400
C	3.22344200	-4.28523900	0.16078700
C	4.15493400	-5.28910600	0.18676800
C	5.51277100	-4.96409600	0.18633000
C	5.91133000	-3.64815600	0.16435500
C	-4.87492500	1.17539700	-0.10921100
C	-6.21207800	1.48788300	-0.13572000
C	-7.16448900	0.47273400	-0.15483500
C	-6.75531900	-0.83780500	-0.15307800
C	-5.91139500	-3.64807200	-0.16434800
C	-5.51285200	-4.96401600	-0.18632000
C	-4.15501800	-5.28904200	-0.18676300
C	-3.22351400	-4.28518600	-0.16078700
S	-0.00003500	-3.12815600	0.00000600
C	-1.80903800	1.74470700	0.19471900
C	-1.69750200	2.60437600	-0.90167000
C	-1.73862600	3.97550900	-0.68975900
C	-1.88160300	4.51533200	0.57960300

C	-1.98981600	3.64391800	1.65413400
C	-1.96100000	2.26747400	1.48504600
C	-2.15627900	1.36368600	2.67161300
C	-1.60748700	2.05919400	-2.29918400
C	-1.89391900	6.00266600	0.79261200
C	1.80907400	1.74467800	-0.19471200
C	1.96106300	2.26744200	-1.48504100
C	1.98992200	3.64388200	-1.65412900
C	1.88172700	4.51530100	-0.57959600
C	1.73872100	3.97548300	0.68976200
C	1.69755400	2.60434900	0.90167200
C	1.60752200	2.05917600	2.29918900
C	2.15630700	1.36364700	-2.67160900
C	1.89409800	6.00263500	-0.79261100
H	7.50920800	-1.60372000	0.17552900
H	8.21588000	0.70878400	0.17548900
H	6.51830200	2.52144000	0.14391600
H	4.15616000	1.97139600	0.10028800
H	2.17786700	-4.53895700	0.16349800
H	3.84166600	-6.31994200	0.20689600
H	6.25501600	-5.74546600	0.20431500
H	6.96552800	-3.43971200	0.16568200
H	-4.15618400	1.97146100	-0.10028900
H	-6.51831800	2.52151500	-0.14393300
H	-8.21590500	0.70886800	-0.17552400
H	-7.50924400	-1.60364000	-0.17555800
H	-6.96559100	-3.43961200	-0.16566900
H	-6.25510600	-5.74537700	-0.20429900
H	-3.84176200	-6.31988200	-0.20689000
H	-2.17794100	-4.53891600	-0.16350200
H	-1.66100900	4.63618800	-1.54003700
H	-2.11147800	4.04452500	2.64962400
H	-2.04648300	1.91637900	3.60001200
H	-3.15107800	0.92157900	2.66317800
H	-1.44534100	0.54204300	2.68056300
H	-0.83973700	1.29619000	-2.38411700
H	-2.54836700	1.60057100	-2.59990100
H	-1.37782300	2.84792400	-3.00912000
H	-2.22154000	6.52903600	-0.09989900
H	-2.55471600	6.28173400	1.60931900
H	-0.89887400	6.37005400	1.04130700
H	2.11160000	4.04448700	-2.64961800
H	1.66110800	4.63616400	1.54003900
H	1.37773800	2.84789100	3.00910300
H	0.83985200	1.29608900	2.38409400
H	2.54843800	1.60065900	2.59996100
H	1.44533500	0.54203300	-2.68056100
H	2.04653500	1.91634700	-3.60000700
H	3.15108800	0.92149800	-2.66317300
H	0.89912200	6.37002000	-1.04158300
H	2.22147700	6.52900900	0.09998500
H	2.55511800	6.28169800	-1.60914000

Singlet closed-shell structure of 4

Atom type	x	y	z
C	2.35962800	-1.62168000	-0.10013400
C	3.31581100	-0.62389600	-0.02737700
C	2.64471000	0.67767200	-0.01931000
C	1.29862300	0.45422200	-0.07718500
C	1.04455200	-0.97533700	-0.10838900
C	0.23547400	1.41161300	-0.07847800
C	-1.04453600	0.97530300	-0.10840400
C	-1.29861000	-0.45425400	-0.07719200
C	-0.23546100	-1.41164500	-0.07851100
C	-2.35960400	1.62165200	-0.10013200
C	-3.31579100	0.62387900	-0.02730000
C	-2.64469900	-0.67769500	-0.01927600
C	2.72844600	-3.00153400	-0.16457600
C	4.10167300	-3.34072000	-0.07826900
C	5.10590800	-2.29593500	0.03351400
C	4.71675600	-0.93424500	0.03855000
C	-2.72840500	3.00150700	-0.16461700
C	-4.10161200	3.34072100	-0.07812000
C	-5.10584800	2.29595400	0.03383000
C	-4.71672200	0.93425500	0.03881000
C	6.47737800	-2.59393500	0.12312700
C	7.42767700	-1.60987800	0.20618300
C	7.04101600	-0.26876500	0.20158400
C	5.71309600	0.05801600	0.11995400
C	1.78443300	-4.03445300	-0.32704600
C	2.15923900	-5.34975300	-0.37081500
C	3.50948800	-5.68847300	-0.25715400
C	4.45120500	-4.70232500	-0.12110800
C	-6.47729900	2.59398000	0.12364300
C	-7.42760500	1.60994200	0.20684400
C	-7.04097000	0.26882200	0.20220300
C	-5.71306800	-0.05798500	0.12038200
C	-1.78439600	4.03439000	-0.32734300
C	-2.15918300	5.34969700	-0.37111600
C	-3.50940200	5.68845200	-0.25720600
C	-4.45112000	4.70233300	-0.12095200
C	-3.24480700	-2.03263600	0.04240100
C	3.24479300	2.03262500	0.04236200
C	3.46989300	2.64310100	1.28217900
C	4.01135800	3.92072300	1.31640300
C	4.33057100	4.61201900	0.15629700
C	4.10018600	3.98847500	-1.06136300
C	3.56035500	2.71168000	-1.14022600
C	-3.46922900	-2.64340600	1.28210700
C	-4.01081600	-3.92106100	1.31627600
C	-4.33071900	-4.61197900	0.15622700
C	-4.10095800	-3.98808900	-1.06146100
C	-3.56111200	-2.71138100	-1.14026000
C	3.15180200	1.92471300	2.56457100
C	3.34144400	2.06847200	-2.48205700
C	4.88846600	6.00620800	0.21772700
C	-3.34291700	-2.06773600	-2.48199500
C	-3.15036800	-1.92547100	2.56456600

C	-4.88864900	-6.00617300	0.21724900
H	0.50737900	2.45070800	-0.03815500
H	-0.50738100	-2.45073900	-0.03825500
H	6.80530800	-3.61750100	0.12721900
H	8.47041500	-1.87476200	0.27313700
H	7.78300700	0.51073400	0.26337500
H	5.42721100	1.09248300	0.11899600
H	0.74750800	-3.78845300	-0.44498700
H	1.41459900	-6.11850100	-0.49853000
H	3.81445100	-6.72182500	-0.28780300
H	5.48360900	-4.99320400	-0.05331900
H	-6.80520700	3.61755400	0.12778500
H	-8.47032800	1.87484700	0.27395200
H	-7.78296600	-0.51066300	0.26412200
H	-5.42719800	-1.09245700	0.11943600
H	-0.74750900	3.78834700	-0.44552600
H	-1.41455400	6.11842000	-0.49904000
H	-3.81434600	6.72181000	-0.28784100
H	-5.48350600	4.99323900	-0.05299900
H	4.18981900	4.38550700	2.27442000
H	4.34934800	4.50617000	-1.97544800
H	-4.18877600	-4.38608500	2.27425700
H	-4.35068300	-4.50551800	-1.97555400
H	3.69383600	0.98403800	2.63584600
H	3.41904800	2.53202400	3.42399700
H	2.09331700	1.68616900	2.63605700
H	3.67500400	2.72192100	-3.28246300
H	3.88632900	1.13043400	-2.56473300
H	2.29151100	1.83969600	-2.64882700
H	5.49196100	6.15271800	1.10951400
H	5.50801300	6.22387300	-0.64797000
H	4.09059800	6.74764000	0.24106100
H	-3.67644600	-2.72112400	-3.28246400
H	-3.88826000	-1.12992300	-2.56424700
H	-2.29314100	-1.83843900	-2.64902900
H	-3.69184800	-0.98450900	2.63621600
H	-3.41769500	-2.53282900	3.42393300
H	-2.09172600	-1.68753900	2.63581100
H	-5.48051700	-6.15725000	1.11599500
H	-5.51960000	-6.21873600	-0.64149300
H	-4.09102200	-6.74818500	0.22585500

Singlet open-shell structure of 4

Atom type	**x**	**y**	**z**
C	2.35961800	-1.62170600	-0.10003300
C	3.31582100	-0.62393500	-0.02738900
C	2.64472900	0.67764700	-0.01927300
C	1.29863700	0.45420100	-0.07697900
C	1.04455400	-0.97535300	-0.10817400
C	0.23550200	1.41160800	-0.07823400
C	-1.04451700	0.97531700	-0.10811500

C	-1.29860100	-0.45423600	-0.07692000
C	-0.23546700	-1.41164400	-0.07830000
C	-2.35957000	1.62167900	-0.09987400
C	-3.31577200	0.62391900	-0.02707600
C	-2.64469100	-0.67767300	-0.01908700
C	2.72841700	-3.00156900	-0.16452700
C	4.10165300	-3.34076900	-0.07835900
C	5.10590600	-2.29599200	0.03339500
C	4.71676900	-0.93429500	0.03840400
C	-2.72836400	3.00153600	-0.16448300
C	-4.10158000	3.34076100	-0.07812500
C	-5.10581500	2.29601200	0.03405600
C	-4.71669400	0.93430900	0.03912500
C	6.47737200	-2.59400600	0.12302200
C	7.42768700	-1.60995600	0.20598800
C	7.04104600	-0.26884000	0.20128400
C	5.71312900	0.05795600	0.11968900
C	1.78437900	-4.03447700	-0.32692200
C	2.15917200	-5.34977800	-0.37078200
C	3.50943200	-5.68850900	-0.25731300
C	4.45117200	-4.70237500	-0.12133200
C	-6.47724700	2.59405500	0.12409900
C	-7.42754500	1.61002900	0.20754400
C	-7.04091900	0.26890800	0.20295900
C	-5.71303300	-0.05791700	0.12096600
C	-1.78434500	4.03440200	-0.32725900
C	-2.15913700	5.34969800	-0.37130100
C	-3.50937300	5.68846000	-0.25765100
C	-4.45109900	4.70236000	-0.12131200
C	-3.24484100	-2.03259400	0.04238900
C	3.24483600	2.03257900	0.04234600
C	3.47039600	2.64292200	1.28216800
C	4.01186300	3.92052700	1.31634000
C	4.33067700	4.61195500	0.15618500
C	4.09985100	3.98855700	-1.06145000
C	3.55997100	2.71176600	-1.14026600
C	-3.46886100	-2.64375800	1.28196400
C	-4.01053600	-3.92139500	1.31590000
C	-4.33091600	-4.61189400	0.15574700
C	-4.10153600	-3.98761400	-1.06182600
C	-3.56163100	-2.71093200	-1.14039600
C	3.15282000	1.92436200	2.56459100
C	3.34053300	2.06874700	-2.48210400
C	4.88866900	6.00610300	0.21766500
C	-3.34387200	-2.06684400	-2.48198600
C	-3.14953100	-1.92628400	2.56456700
C	-4.88898300	-6.00604500	0.21649500
H	0.50742600	2.45069700	-0.03790100
H	-0.50740300	-2.45073300	-0.03806000
H	6.80527800	-3.61757800	0.12723800
H	8.47042200	-1.87485100	0.27295700
H	7.78305100	0.51065300	0.26298100
H	5.42725500	1.09242600	0.11866900
H	0.74744700	-3.78846000	-0.44474700
H	1.41451300	-6.11851500	-0.49844100

H	3.81438700	-6.72186000	-0.28806300
H	5.48358600	-4.99325600	-0.05373500
H	-6.80513500	3.61763300	0.12829500
H	-8.47025300	1.87494600	0.27483000
H	-7.78290800	-0.51056700	0.26509500
H	-5.42715800	-1.09238700	0.12012200
H	-0.74744500	3.78834500	-0.44528300
H	-1.41449800	6.11840400	-0.49926300
H	-3.81432700	6.72180600	-0.28856200
H	-5.48350100	4.99326200	-0.05361800
H	4.19067300	4.38519700	2.27434900
H	4.34868900	4.50635700	-1.97556100
H	-4.18819600	-4.38671200	2.27379400
H	-4.35161800	-4.50473400	-1.97599600
H	3.69529000	0.98392500	2.63574100
H	3.41995300	2.53176200	3.42398800
H	2.09445500	1.68535200	2.63624600
H	3.67414400	2.72214800	-3.28252700
H	3.88504800	1.13051500	-2.56499300
H	2.29047800	1.84037100	-2.64866100
H	5.49418900	6.15179000	1.10822200
H	5.50624400	6.22458700	-0.64922500
H	4.09083300	6.74748000	0.24355000
H	-3.67734800	-2.72010500	-3.28258000
H	-3.88952300	-1.12917600	-2.56387500
H	-2.29419800	-1.83717600	-2.64913300
H	-3.69083600	-0.98525500	2.63666200
H	-3.41673100	-2.53387600	3.42380800
H	-2.09083200	-1.68855200	2.63561900
H	-5.47913700	-6.15788400	1.11623600
H	-5.52163900	-6.21765000	-0.64123100
H	-4.09147800	-6.74820900	0.22281400

Triplet structure of 4

Atom type	**x**	**y**	**z**
C	2.35166300	-1.61030400	-0.07005400
C	3.34720000	-0.60792100	-0.01250400
C	2.72884600	0.65539700	-0.00640400
C	1.29059200	0.43883600	-0.04741400
C	1.03930200	-0.94675400	-0.06801900
C	0.27761500	1.38778600	-0.04508500
C	-1.03924900	0.94671700	-0.06773000
C	-1.29054000	-0.43887400	-0.04720100
C	-0.27756100	-1.38782500	-0.04516200
C	-2.35160500	1.61027600	-0.06946000
C	-3.34713700	0.60789700	-0.01180000
C	-2.72878700	-0.65542900	-0.00594400
C	2.69865000	-2.98840700	-0.13365700
C	4.07198100	-3.35414700	-0.06819000
C	5.10523600	-2.32632000	0.02544100
C	4.74883000	-0.95898700	0.03350300

C	-2.69859000	2.98838500	-0.13292900
C	-4.07190400	3.35413400	-0.06719200
C	-5.10514900	2.32631200	0.02661600
C	-4.74875400	0.95897500	0.03454200
C	6.46778600	-2.65651000	0.09383100
C	7.44492800	-1.69340600	0.15994000
C	7.08933400	-0.34699900	0.15807300
C	5.76416300	0.00884900	0.09627800
C	1.73308900	-4.00715300	-0.27417200
C	2.08390600	-5.33091700	-0.31982600
C	3.42826700	-5.69090400	-0.22865600
C	4.39290000	-4.71748800	-0.11146500
C	-6.46767900	2.65651500	0.09533000
C	-7.44481700	1.69342100	0.16162700
C	-7.08923800	0.34701000	0.15963800
C	-5.76408500	-0.00885100	0.09752800
C	-1.73304500	4.00712600	-0.27359200
C	-2.08385900	5.33089400	-0.31914500
C	-3.42820100	5.69089000	-0.22772000
C	-4.39282000	4.71747800	-0.11037600
C	-3.31071500	-2.01475500	0.03932300
C	3.31073800	2.01473300	0.03900000
C	3.54971800	2.63346700	1.27213600
C	4.06334400	3.92265100	1.29210500
C	4.33905100	4.61858500	0.12344500
C	4.09121400	3.98897100	-1.08777500
C	3.57772700	2.70066600	-1.15148300
C	-3.54909500	-2.63386700	1.27228800
C	-4.06291200	-3.92306700	1.29205500
C	-4.33933000	-4.61849800	0.12336500
C	-4.09202300	-3.98845300	-1.08783500
C	-3.57842100	-2.70027300	-1.15133800
C	3.27892600	1.90636500	2.56027000
C	3.33733500	2.04705300	-2.48435500
C	4.86670000	6.02517500	0.16966900
C	-3.33862100	-2.04615100	-2.48406400
C	-3.27759700	-1.90730500	2.56058100
C	-4.86713700	-6.02504900	0.16898300
H	0.55068000	2.42565200	-0.00386900
H	-0.55062000	-2.42569500	-0.00399400
H	6.77272400	-3.68720400	0.09508600
H	8.48177500	-1.98354100	0.21115400
H	7.84844000	0.41684400	0.20610000
H	5.49977400	1.04957900	0.09648800
H	0.69925000	-3.74309900	-0.37092700
H	1.32347100	-6.08664600	-0.42988400
H	3.71637200	-6.72904700	-0.25945000
H	5.42000600	-5.02926400	-0.05947700
H	-6.77260400	3.68721300	0.09670300
H	-8.48164900	1.98356500	0.21309200
H	-7.84834000	-0.41682600	0.20782600
H	-5.49970900	-1.04958400	0.09766800
H	-0.69922600	3.74306600	-0.37055400
H	-1.32343800	6.08661900	-0.42932700
H	-3.71630300	6.72903500	-0.25843600

H	-5.41991500	5.02926100	-0.05819800
H	4.25294100	4.39365700	2.24500200
H	4.30392700	4.51156400	-2.00832500
H	-4.25207000	-4.39438300	2.24487400
H	-4.30531700	-4.51068800	-2.00846600
H	3.90963600	1.02464700	2.65482500
H	3.46989100	2.54820100	3.41502400
H	2.24715200	1.56729000	2.61654800
H	3.56240900	2.73062000	-3.29747700
H	3.95887000	1.16247400	-2.60729400
H	2.30347700	1.72616700	-2.58960100
H	5.49269600	6.18530500	1.04346300
H	5.45560100	6.25688500	-0.71360200
H	4.05340900	6.74851900	0.21702900
H	-3.56405400	-2.72941000	-3.29734700
H	-3.96021200	-1.16152600	-2.60638900
H	-2.30480900	-1.72522300	-2.58963700
H	-3.90815500	-1.02554900	2.65578700
H	-3.46823300	-2.54945300	3.41517300
H	-2.24575600	-1.56837800	2.61650800
H	-5.48023100	-6.19002900	1.05093500
H	-5.46919100	-6.25117400	-0.70688500
H	-4.05371600	-6.74914800	0.19974900

Singlet closed-shell structure of 5

Atom type	**x**	**y**	**z**
C	1.54291600	1.49769600	0.67127100
C	3.03075700	-0.57421500	0.08307100
C	1.82246000	2.55138800	-0.20864900
C	-3.89491000	-2.74544100	0.67064300
C	-0.72908200	-0.82425800	0.02316300
C	-1.38702300	-2.11740500	0.24765400
C	-5.22007100	-2.28968500	0.48163500
C	-2.82613600	-1.87493400	0.30182100
C	-1.70857800	0.09281300	-0.23181300
C	0.72928200	-0.82421000	-0.02341800
C	4.36446200	-0.09393900	0.33636700
C	2.82642900	-1.87471100	-0.30200400
C	1.70870600	0.09294800	0.23157000
C	-6.27280300	-3.14189800	0.86160900
H	-7.29224500	-2.82328400	0.74082700
C	3.89529800	-2.74515800	-0.67068600
C	-3.03058600	-0.57447100	-0.08329800
C	-1.21884800	1.76876800	-2.00520900
C	-4.64167400	1.17482700	-0.88513800
H	-3.83311500	1.83948700	-1.11359900
C	-1.54306900	1.49765200	-0.67130200
C	1.38733300	-2.11730700	-0.24785700
C	1.21867800	1.76846600	2.00526100
C	0.70857500	-3.27371800	-0.12792100
C	-4.36434500	-0.09436400	-0.33667500

C	1.75070500	3.85518300	0.25687300
H	1.96688100	4.66389700	-0.42541100
C	3.68238300	-4.00144900	-1.27184100
H	2.67966200	-4.31352200	-1.49747500
C	-0.70817200	-3.27376900	0.12780900
C	-5.45302100	-0.96928200	-0.07660700
C	-1.82289500	2.55110400	0.20884100
C	0.98462100	0.65828700	2.99401200
H	0.13275200	0.04246100	2.71768200
H	0.80045900	1.06102800	3.98556300
H	1.84573600	-0.00384100	3.05605800
C	5.45322900	-0.96878000	0.07643600
C	-6.04058000	-4.37584600	1.41123000
H	-6.87088800	-5.00159800	1.69534600
C	4.64164700	1.17539300	0.88457300
H	3.83299900	1.83998900	1.11292000
C	-5.92309000	1.57688500	-1.15482600
H	-6.09897200	2.55246200	-1.57820800
C	-4.72946600	-4.80661800	1.63006300
H	-4.54263600	-5.76023400	2.09662900
C	-3.68184500	-4.00164600	1.27192400
H	-2.67907700	-4.31363100	1.49747000
C	6.75390400	-0.52245600	0.37068500
H	7.59269000	-1.17190800	0.19780700
C	-6.75374300	-0.52316900	-0.37096000
H	-7.59244900	-1.17269900	-0.19799000
C	5.22041200	-2.28928800	-0.48160900
C	4.73009200	-4.80641000	-1.62974800
H	4.54336800	-5.76009800	-2.09620700
C	1.16331900	3.08967200	2.43145900
H	0.92208800	3.29430600	3.46378600
C	-6.99290100	0.72007400	-0.89385200
H	-8.00308200	1.02773300	-1.11036900
C	6.99292200	0.72091700	0.89333200
H	8.00307200	1.02873600	1.10976800
C	5.92301800	1.57766000	1.15415500
H	6.09880000	2.55335100	1.57731700
C	-1.75147200	3.85499600	-0.25644000
H	-1.96787300	4.66353400	0.42598600
C	2.26924000	2.29041200	-1.61976300
H	3.31375900	1.98286000	-1.64337300
H	2.17246900	3.18588500	-2.22582700
H	1.69009000	1.50208600	-2.08786600
C	-2.26951800	2.28975300	1.61993200
H	-3.31386800	1.98164300	1.64355300
H	-2.17319600	3.18522400	2.22607200
H	-1.68991800	1.50169900	2.08793900
C	1.41954700	4.14724200	1.57255700
C	6.04115500	-4.37554100	-1.41079800
H	6.87153400	-5.00129200	-1.69471000
C	-1.42037600	4.14740200	-1.57207200
C	6.27323900	-3.14150300	-0.86132300
H	7.29264800	-2.82282600	-0.74043800
C	-1.16382800	3.09007400	-2.43116500
H	-0.92259900	3.29495900	-3.46344200

C	-0.98450600	0.65882000	-2.99415200
H	-0.13260600	0.04303600	-2.71782100
H	-0.80025000	1.06177100	-3.98560100
H	-1.84553400	-0.00339900	-3.05644500
C	1.32035600	5.57077700	2.04293800
H	2.08535700	6.19448800	1.58709800
H	1.42708400	5.64143600	3.12186700
H	0.35450500	6.00193300	1.78104100
C	-1.32163500	5.57106200	-2.04216900
H	-0.35625200	6.00276000	-1.77944200
H	-2.08736700	6.19426200	-1.58685200
H	-1.42755200	5.64180600	-3.12117200
H	-1.21050800	-4.22369300	0.16431600
H	1.21098600	-4.22360600	-0.16433400

Singlet open-shell structure of 5

Atom type	**x**	**y**	**z**
C	1.54308000	1.49775500	0.67136400
C	3.03066800	-0.57423800	0.08295900
C	1.82272900	2.55134300	-0.20863300
C	-3.89502300	-2.74517400	0.67103500
C	-0.72917900	-0.82406300	0.02343700
C	-1.38716300	-2.11719400	0.24803700
C	-5.22018500	-2.28958900	0.48159600
C	-2.82625500	-1.87464700	0.30224000
C	-1.70865700	0.09300400	-0.23163000
C	0.72915200	-0.82406600	-0.02341600
C	4.36443900	-0.09422100	0.33640200
C	2.82621200	-1.87466900	-0.30224200
C	1.70864600	0.09298600	0.23166300
C	-6.27290800	-3.14190000	0.86134900
H	-7.29237100	-2.82349500	0.74015400
C	3.89494600	-2.74524000	-0.67099600
C	-3.03068600	-0.57421900	-0.08299500
C	-1.21880700	1.76866000	-2.00529900
C	-4.64180200	1.17509400	-0.88470500
H	-3.83326600	1.83990700	-1.11282600
C	-1.54305600	1.49777200	-0.67132300
C	1.38712200	-2.11718700	-0.24809100
C	1.21888300	1.76865400	2.00534800
C	0.70832900	-3.27355600	-0.12810100
C	-4.36444000	-0.09418300	-0.33648100
C	1.75111500	3.85518600	0.25682900
H	1.96737800	4.66385000	-0.42548800
C	3.68179300	-4.00129500	-1.27254000
H	2.67900200	-4.31301000	-1.49838500
C	-0.70837300	-3.27355900	0.12794200
C	-5.45309700	-0.96923000	-0.07672700
C	-1.82269700	2.55136900	0.20866200
C	0.98469200	0.65852300	2.99411900
H	0.13220800	0.04333300	2.71823000

H	0.80140000	1.06126600	3.98583200
H	1.84536700	-0.00422200	3.05555100
C	5.45307500	-0.96930500	0.07666700
C	-6.04066100	-4.37571200	1.41127700
H	-6.87097900	-5.00153500	1.69521200
C	4.64183400	1.17507100	0.88457300
H	3.83331600	1.83991400	1.11267100
C	-5.92320900	1.57706900	-1.15459600
H	-6.09909700	2.55274400	-1.57775100
C	-4.72956700	-4.80624600	1.63066300
H	-4.54275900	-5.75970400	2.09755900
C	-3.68194000	-4.00120100	1.27266900
H	-2.67917700	-4.31293900	1.49858600
C	6.75377900	-0.52333300	0.37126800
H	7.59242000	-1.17304300	0.19863500
C	-6.75379000	-0.52323900	-0.37135000
H	-7.59244600	-1.17292300	-0.19869100
C	5.22012200	-2.28968800	-0.48159300
C	4.72938300	-4.80639900	-1.63050800
H	4.54253100	-5.75988100	-2.09733700
C	1.16366000	3.08987300	2.43146900
H	0.92251300	3.29459000	3.46380100
C	-6.99297700	0.72006800	-0.89409100
H	-8.00314100	1.02763100	-1.11082500
C	6.99299900	0.71998900	0.89395900
H	8.00317100	1.02753600	1.11067600
C	5.92325300	1.57702600	1.15443800
H	6.09916800	2.55271500	1.57755000
C	-1.75102500	3.85521100	-0.25679900
H	-1.96727900	4.66388200	0.42551200
C	2.26939400	2.29025400	-1.61975700
H	3.31368500	1.98193800	-1.64339500
H	2.17329500	3.18589600	-2.22567800
H	1.68966800	1.50243600	-2.08800800
C	-2.26942200	2.29030800	1.61977300
H	-3.31379500	1.98226600	1.64338900
H	-2.17308800	3.18588600	2.22575200
H	-1.68990600	1.50230600	2.08797300
C	1.41996800	4.14736800	1.57247200
C	6.04049800	-4.37589600	-1.41117600
H	6.87078800	-5.00176800	-1.69508600
C	-1.41982600	4.14738100	-1.57243000
C	6.27280500	-3.14206000	-0.86131900
H	7.29228300	-2.82369300	-0.74015600
C	-1.16352400	3.08987600	-2.43141900
H	-0.92233000	3.29458600	-3.46374100
C	-0.98460500	0.65852300	-2.99406000
H	-0.13213200	0.04332600	-2.71815300
H	-0.80128900	1.06126100	-3.98577100
H	-1.84528400	-0.00421400	-3.05550800
C	1.32069900	5.57092800	2.04275100
H	2.08335700	6.19540700	1.58407600
H	1.43101900	5.64208000	3.12129400
H	0.35340700	6.00080700	1.78406300
C	-1.32048800	5.57093800	-2.04270700

H	-0.35320400	6.00079100	-1.78394800
H	-2.08316400	6.19543700	-1.58409000
H	-1.43072600	5.64208900	-3.12125800
H	1.21067300	-4.22348100	-0.16471100
H	-1.21071200	-4.22348700	0.16444200

Triplet structure of 5

Atom type	**x**	**y**	**z**
C	-1.55338500	1.49999700	-0.56188500
C	-2.99771300	-0.55607300	-0.08317700
C	-1.80055900	2.52763100	0.35628200
C	3.87891600	-2.77501800	-0.57483400
C	0.70070800	-0.93482900	-0.00464500
C	1.37347500	-2.18653400	-0.14200700
C	5.20216700	-2.28781700	-0.43437700
C	2.79762900	-1.91802400	-0.21279200
C	1.74095800	0.08402500	0.17487600
C	-0.70084800	-0.93478000	0.00470100
C	-4.34731400	-0.05842800	-0.30321700
C	-2.79783600	-1.91782200	0.21284300
C	-1.74102100	0.08414800	-0.17483700
C	6.25800900	-3.12516700	-0.81795500
H	7.27297300	-2.78067700	-0.74007400
C	-3.87918000	-2.77473800	0.57489900
C	2.99759400	-0.55627300	0.08313900
C	1.27921900	1.80887900	1.89968400
C	4.62650600	1.23006500	0.78764400
H	3.82243300	1.90923600	0.98520400
C	1.55348600	1.49988900	0.56194400
C	-1.37370000	-2.18643300	0.14208800
C	-1.27906000	1.80897100	-1.89961600
C	-0.68960400	-3.38380800	0.08618700
C	4.34722000	-0.05867000	0.30305700
C	-1.74939800	3.84401900	-0.07600100
H	-1.94274700	4.63300000	0.63560100
C	-3.68061500	-4.05351400	1.13293700
H	-2.68192100	-4.39435000	1.32508200
C	0.68929700	-3.38385900	-0.08607300
C	5.43299800	-0.93962400	0.07997700
C	1.80086000	2.52750200	-0.35619000
C	-1.10549000	0.72469100	-2.92852000
H	-0.32612500	0.01994000	-2.65230900
H	-0.85037000	1.14859400	-3.89521400
H	-2.02208200	0.14958900	-3.04760400
C	-5.43314100	-0.93932100	-0.08011500
C	6.03920900	-4.38436000	-1.32703700
H	6.87714300	-4.99802000	-1.61515300
C	-4.62654700	1.23026600	-0.78795200
H	-3.82245400	1.90939100	-0.98555900
C	5.91253400	1.64495300	1.03995800
H	6.08633400	2.64004800	1.41627600

C	4.73619800	-4.84935800	-1.49709300
H	4.55634600	-5.81969800	-1.93032800
C	3.68025800	-4.05381800	-1.13278600
H	2.68153700	-4.39461200	-1.32486600
C	-6.73185100	-0.48958700	-0.35840200
H	-7.56759400	-1.15153800	-0.22209900
C	6.73173500	-0.48990500	0.35816700
H	7.56745300	-1.15189300	0.22188700
C	-5.20239800	-2.28747900	0.43435600
C	-4.73661300	-4.84897400	1.49725200
H	-4.55683100	-5.81929600	1.93055600
C	-1.24078700	3.14066500	-2.29143300
H	-1.03914900	3.37383900	-3.32626200
C	6.97783500	0.77784100	0.82568000
H	7.98886500	1.08944600	1.03201700
C	-6.97789100	0.77812100	-0.82604600
H	-7.98890100	1.08973900	-1.03246000
C	-5.91255100	1.64517200	-1.04036400
H	-6.08630000	2.64023400	-1.41679400
C	1.74991700	3.84388900	0.07612200
H	1.94341200	4.63285300	-0.63545900
C	-2.20365400	2.22586300	1.77224300
H	-3.24857300	1.92227600	1.81811700
H	-2.08356300	3.10203700	2.40213500
H	-1.61585800	1.42039300	2.19881600
C	2.20394000	2.22569500	-1.77214700
H	3.24880700	1.92192300	-1.81800100
H	2.08402000	3.10190400	-2.40202300
H	1.61601200	1.42033800	-2.19875500
C	-1.46914100	4.17323900	-1.39465700
C	-6.03959300	-4.38391900	1.32711200
H	-6.87757100	-4.99751600	1.61523000
C	1.46969800	4.17312700	1.39478000
C	-6.25830200	-3.12474700	0.81793900
H	-7.27324500	-2.78020800	0.73998400
C	1.24116600	3.14057000	2.29153100
H	1.03956700	3.37375400	3.32636500
C	1.10548200	0.72460600	2.92856800
H	0.32598400	0.02000100	2.65236100
H	0.85046100	1.14853300	3.89527800
H	2.02197300	0.14933700	3.04761800
C	-1.38997800	5.60927100	-1.82889400
H	-2.11808900	6.22377100	-1.30531900
H	-1.56678600	5.71283400	-2.89595500
H	-0.40520400	6.02601200	-1.61912700
C	1.39077800	5.60916100	1.82905300
H	0.40604200	6.02604400	1.61938700
H	2.11892600	6.22356800	1.30542100
H	1.56770000	5.71267900	2.89610000
H	-1.20605500	-4.32484000	0.11608200
H	1.20568400	-4.32492800	-0.11595800

Singlet closed-shell structure of 6

Atom type	**x**	**y**	**z**
C	1.46873300	1.73296300	0.84909000
C	3.01281100	-0.28832700	0.20612600
C	1.82505100	2.82411700	0.04498900
C	-3.94150300	-2.30532300	0.82708100
C	-0.72546300	-0.55376100	-0.00118600
C	-1.40904900	-1.83198800	0.25124500
C	-5.24999200	-1.82656500	0.57999700
C	-2.84724900	-1.55112800	0.30305300
C	-1.67649100	0.35327300	-0.35458100
C	0.72556900	-0.55370900	0.00115800
C	4.32284300	0.18895400	0.54996400
C	2.84741500	-1.55091800	-0.30313500
C	1.67653400	0.35341100	0.35449500
C	-6.33101500	-2.53593800	1.13293400
H	-7.33676200	-2.19202600	0.97267000
C	3.94173200	-2.30508300	-0.82709000
C	-3.01272300	-0.28855700	-0.20624200
C	-1.01617800	1.94327300	-2.15674300
C	-4.54711200	1.36832200	-1.28993900
H	-3.71294900	1.96950000	-1.59303300
C	-1.46884400	1.73287000	-0.84911200
C	1.40924400	-1.83188900	-0.25129400
C	1.01602500	1.94324800	2.15672700
C	0.72879900	-2.99379700	-0.10998200
C	-4.32279100	0.18864400	-0.55005200
C	1.70017900	4.10576600	0.55740200
H	1.97440800	4.94388200	-0.06573300
C	3.76802400	-3.41808100	-1.67004300
H	2.77657200	-3.73621600	-1.93052100
C	-0.72852500	-2.99384600	0.10990100
N	-1.83660700	-5.30998100	-0.10832300
C	-5.43846600	-0.61442300	-0.19377000
C	-1.36911600	-4.26873200	0.01725800
C	-1.82529600	2.82393300	-0.04495000
C	0.68594300	0.79372200	3.07042200
H	-0.18523700	0.24116600	2.72679100
H	0.47716000	1.15128300	4.07403900
H	1.50793700	0.08427000	3.13250200
C	5.43856800	-0.61411000	0.19382700
C	-6.13743000	-3.64607900	1.91236600
H	-6.98603700	-4.16467000	2.32756400
C	4.54708400	1.36870800	1.28974600
H	3.71288900	1.96991000	1.59270100
C	-5.80943600	1.75047200	-1.65769300
H	-5.95006600	2.65244200	-2.23058100
C	-4.84098000	-4.08338800	2.19689900
H	-4.68312900	-4.93280500	2.84053600
C	1.36945000	-4.26865400	-0.01735100
C	-3.76770600	-3.41831400	1.67003200
H	-2.77622700	-3.73641600	1.93044500
C	6.71833400	-0.19284400	0.59611100
H	7.57596300	-0.79717700	0.36274000
C	-6.71828300	-0.19317800	-0.59593300

H	-7.57589500	-0.79746400	-0.36238500
C	5.25018600	-1.82627300	-0.57993700
C	4.84135600	-4.08312300	-2.19684100
H	4.68357300	-4.93255700	-2.84047400
C	0.91409700	3.24492500	2.63144600
H	0.57560800	3.40428800	3.64405800
N	1.83695400	-5.30989900	0.10821600
C	-6.90732300	0.96179600	-1.30748100
H	-7.90146300	1.25193200	-1.60627700
C	6.90729600	0.96219600	1.30757900
H	7.90140000	1.25235000	1.60647300
C	5.80937300	1.75091000	1.65757900
H	5.94993700	2.65295200	2.23036900
C	-1.70063600	4.10562100	-0.55731900
H	-1.97495200	4.94367300	0.06586700
C	2.39687100	2.63074900	-1.33191400
H	3.45232100	2.36869900	-1.27914200
H	2.30983000	3.54225600	-1.91472500
H	1.89187900	1.83796400	-1.87289900
C	-2.39702900	2.63042400	1.33197000
H	-3.45242300	2.36815500	1.27922900
H	-2.31016100	3.54194700	1.91478800
H	-1.89184900	1.83774400	1.87292900
C	1.24384800	4.33948800	1.84697300
C	6.13777000	-3.64575400	-1.91225200
H	6.98642100	-4.16430700	-2.32740900
C	-1.24441100	4.33946400	-1.84690300
C	6.33126900	-2.53559300	-1.13282300
H	7.33698800	-2.19160400	-0.97254600
C	-0.91448700	3.24498200	-2.63142200
H	-0.57603900	3.40444200	-3.64403400
C	-0.68589200	0.79382200	-3.07045700
H	0.18542700	0.24146200	-2.72686500
H	-0.47723800	1.15142700	-4.07408400
H	-1.50772900	0.08418400	-3.13249400
C	1.09419600	5.74068800	2.36823800
H	1.89845300	6.38294000	2.01841200
H	1.09344000	5.76268200	3.45433600
H	0.15776700	6.18436100	2.03156100
C	-1.09509900	5.74070300	-2.36816100
H	-0.15916000	6.18491500	-2.03083700
H	-1.89995600	6.38255700	-2.01898100
H	-1.09356500	5.76260500	-3.45426000

Singlet open-shell structure of 6

Atom type	**x**	**y**	**z**
C	-1.47858400	1.74403900	-0.75670300
C	-2.99126900	-0.28226000	-0.21752000
C	-1.83439500	2.81001100	0.07974500
C	3.92676000	-2.32928600	-0.76994400
C	0.70767900	-0.62596400	0.01387000

C	1.39874900	-1.88529500	-0.17389700
C	5.23485100	-1.82760500	-0.55292400
C	2.83034100	-1.58796200	-0.23688500
C	1.69365800	0.34872900	0.31447700
C	-0.70765600	-0.62600800	-0.01411600
C	-4.30975000	0.20900100	-0.54289100
C	-2.83022800	-1.58820800	0.23672700
C	-1.69376700	0.34865100	-0.31448800
C	6.31338500	-2.52348100	-1.11779700
H	7.31606800	-2.16046200	-0.98243200
C	-3.92647400	-2.32957900	0.77005300
C	2.99124600	-0.28208500	0.21756400
C	1.04685300	1.99400300	2.06516500
C	4.53485100	1.40307600	1.25362000
H	3.70270800	2.01346800	1.54320200
C	1.47840800	1.74414900	0.75653700
C	-1.39861100	-1.88540900	0.17352800
C	-1.04718300	1.99374400	-2.06543000
C	-0.71785100	-3.06895400	0.08029800
C	4.30964300	0.20919000	0.54324800
C	-1.72719900	4.10606200	-0.40058600
H	-2.00122900	4.92497800	0.24767200
C	-3.75611200	-3.45313000	1.60055700
H	-2.76663100	-3.78803600	1.84356900
C	0.71805300	-3.06890300	-0.08098100
N	1.84740700	-5.37366200	0.14405300
C	5.42373000	-0.59941200	0.20479800
C	1.36758000	-4.33818300	0.01500400
C	1.83433500	2.81004100	-0.08000300
C	-0.74203600	0.86987500	-3.01883800
H	0.08760300	0.25686100	-2.67625000
H	-0.48578800	1.25868800	-3.99954800
H	-1.59753300	0.20776500	-3.13616500
C	-5.42372900	-0.59961500	-0.20413500
C	6.12348300	-3.64735300	-1.88478600
H	6.97354300	-4.15531100	-2.31003900
C	-4.53515000	1.40283600	-1.25328000
H	-3.70308400	2.01322300	-1.54310800
C	5.80018700	1.79271700	1.61499900
H	5.93981800	2.70772500	2.16713700
C	4.83129800	-4.10687400	-2.14251200
H	4.67411100	-4.96358800	-2.77637700
C	-1.36742100	-4.33818300	-0.01606800
C	3.75659400	-3.45268700	-1.60069300
H	2.76715600	-3.78738300	-1.84418100
C	-6.70232100	-0.17682000	-0.59912300
H	-7.55759500	-0.79083900	-0.38231200
C	6.70222100	-0.17651700	0.60000900
H	7.55759200	-0.79044500	0.38332600
C	-5.23462400	-1.82777000	0.55359500
C	-4.83067700	-4.10722700	2.14277400
H	-4.67331600	-4.96406500	2.77643100
C	-0.96244800	3.30763200	-2.50717400
H	-0.64158700	3.49656100	-3.52052000
N	-1.84737300	-5.37356700	-0.14543800

C	6.89519700	0.99548400	1.28744500
H	7.88971300	1.28818000	1.58232000
C	-6.89549000	0.99513900	-1.28658100
H	-7.89007400	1.28776100	-1.58129700
C	-5.80058500	1.79241100	-1.61439300
H	-5.94037400	2.70738600	-2.16654400
C	1.72713200	4.10612000	0.40019600
H	2.00129900	4.92497100	-0.24808600
C	-2.39500900	2.57726100	1.45512000
H	-3.45026300	2.31442300	1.40186700
H	-2.30646300	3.47304100	2.06174800
H	-1.88660300	1.77074400	1.97214200
C	2.39501500	2.57707900	-1.45531300
H	3.45002000	2.31328800	-1.40196800
H	2.30735700	3.47306400	-2.06176700
H	1.88593500	1.77113600	-1.97257500
C	-1.29090200	4.37812100	-1.68913600
C	-6.12291000	-3.64745600	1.88576700
H	-6.97283900	-4.15529100	2.31142500
C	1.29066700	4.37833300	1.68867600
C	-6.31299400	-2.52348100	1.11896200
H	-7.31566300	-2.16021100	0.98417200
C	0.96207200	3.30795100	2.50677000
H	0.64105600	3.49698000	3.52004900
C	0.74167700	0.87023200	3.01867700
H	-0.08772700	0.25696500	2.67597900
H	0.48509800	1.25914500	3.99925900
H	1.59730100	0.20834000	3.13632800
C	-1.15845000	5.79360800	-2.17470100
H	-1.94490900	6.42717000	-1.77269000
H	-1.20277000	5.84786900	-3.25884700
H	-0.20677600	6.22429200	-1.86476100
C	1.15826500	5.79387800	2.17408400
H	0.20679200	6.22474000	1.86377100
H	1.94499500	6.42726200	1.77232500
H	1.20219500	5.84820100	3.25824400

Triplet structure of 6

Atom type	**x**	**y**	**z**
C	-1.47714600	1.74528800	-0.72914900
C	-2.96876700	-0.26994200	-0.22624200
C	-1.83628300	2.80954100	0.10800700
C	3.91053700	-2.32998400	-0.75005500
C	0.69718800	-0.67064700	0.02624700
C	1.39077200	-1.91416700	-0.13220900
C	5.21660000	-1.81278800	-0.55324000
C	2.81095400	-1.60432000	-0.20201100
C	1.70514700	0.34820300	0.30005700
C	-0.69717800	-0.67062600	-0.02608400
C	-4.29695600	0.22359700	-0.55088900
C	-2.81102200	-1.60419500	0.20205800
C	-1.70501800	0.34818600	-0.30010500

C	6.29148800	-2.48879100	-1.14001600
H	7.29104900	-2.11095300	-1.02323000
C	-3.91072300	-2.32976600	0.74999000
C	2.96881000	-0.26997400	0.22605600
C	1.04265700	1.99857100	2.03689300
C	4.52177200	1.41205200	1.26236100
H	3.69075000	2.02369100	1.55277900
C	1.47726400	1.74525100	0.72928400
C	-1.39082600	-1.91411300	0.13251500
C	-1.04254800	1.99879100	-2.03672000
C	-0.70748500	-3.11692600	0.06791900
C	4.29707700	0.22355000	0.55042100
C	-1.72872200	4.10659800	-0.36999600
H	-2.00551600	4.92415700	0.27881100
C	-3.74161500	-3.45279900	1.58118000
H	-2.75324300	-3.79957200	1.80964000
C	0.70739200	-3.11695900	-0.06737800
N	1.86051000	-5.41049000	0.15037300
C	5.40747200	-0.58333400	0.21176900
C	1.36590200	-4.38113700	0.02635100
C	1.83640200	2.80963500	-0.10770200
C	-0.74237500	0.87684300	-2.99398100
H	0.07461600	0.24896300	-2.64809200
H	-0.47133300	1.26784400	-3.96984200
H	-1.60629900	0.22784700	-3.12318000
C	-5.40743300	-0.58324400	-0.21238700
C	6.10337400	-3.61490500	-1.90942600
H	6.95344200	-4.10805800	-2.35176600
C	-4.52151600	1.41205200	-1.26296800
H	-3.69045300	2.02369400	-1.55325100
C	5.78959000	1.79991100	1.62736400
H	5.92863600	2.71356100	2.18189900
C	4.81551000	-4.09206500	-2.14513700
H	4.65816000	-4.94894100	-2.77856300
C	-1.36598700	-4.38113300	-0.02552900
C	3.74125400	-3.45315700	-1.58101700
H	2.75283600	-3.79997200	-1.80921300
C	-6.68497500	-0.16839300	-0.61068600
H	-7.53806200	-0.78627000	-0.39559200
C	6.68509200	-0.16844600	0.60975500
H	7.53813600	-0.78634500	0.39455200
C	-5.21673800	-1.81260000	0.55281100
C	-4.81598700	-4.09161300	2.14517600
H	-4.65877300	-4.94837400	2.77879000
C	-0.95733100	3.31324500	-2.47590800
H	-0.63464600	3.50422900	-3.48831000
N	-1.86054900	-5.41053600	-0.14930700
C	6.88145200	1.00272800	1.30146200
H	7.87636200	1.29103400	1.59922100
C	-6.88119000	1.00270900	-1.30254000
H	-7.87603200	1.29098700	-1.60055600
C	-5.78925400	1.79987000	-1.62826900
H	-5.92818700	2.71347000	-2.18291400
C	1.72878400	4.10662900	0.37045200
H	2.00556400	4.92427500	-0.27824900

C	-2.40231600	2.57607900	1.48099500
H	-3.45668500	2.31076700	1.42317700
H	-2.31857900	3.47286800	2.08691200
H	-1.89502400	1.77102000	2.00121600
C	2.40249800	2.57635400	-1.48069700
H	3.45674700	2.31057100	-1.42283200
H	2.31922500	3.47336000	-2.08634900
H	1.89492500	1.77166900	-2.00122100
C	-1.28909700	4.38178900	-1.65662100
C	-6.10380500	-3.61450300	1.90909200
H	-6.95396700	-4.10758900	2.35132600
C	1.28912600	4.38163900	1.65710800
C	-6.29175700	-2.48852500	1.13945400
H	-7.29129700	-2.11072500	1.02237200
C	0.95739900	3.31297200	2.47624500
H	0.63472500	3.50380700	3.48867700
C	0.74252200	0.87653400	2.99406100
H	-0.07439600	0.24859900	2.64809200
H	0.47138800	1.26745700	3.96992700
H	1.60649500	0.22760700	3.12327600
C	-1.15593300	5.79827000	-2.13886500
H	-1.93758300	6.43300000	-1.72943200
H	-1.20757300	5.85598800	-3.22254900
H	-0.20068100	6.22498200	-1.83439300
C	1.15591100	5.79804600	2.13954800
H	0.20054100	6.22468200	1.83535700
H	1.93739300	6.43291500	1.73000300
H	1.20780500	5.85565100	3.22322800

6. Appendix

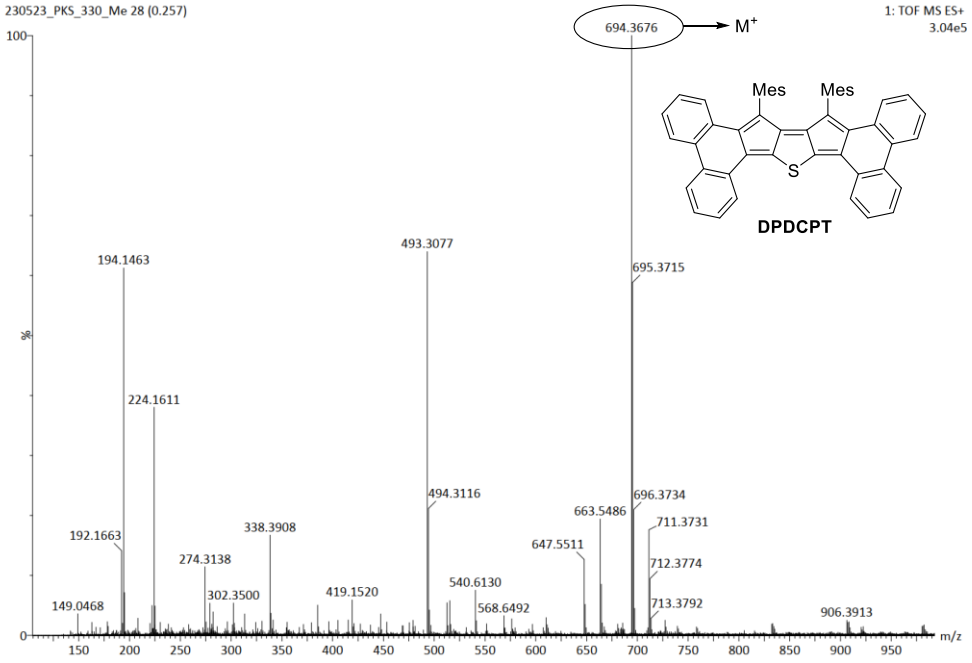


Fig. S25 Compound **DPDCPT** was detected by direct mass spectrometric analysis ((ESI) *m/z*: $[M]^+$ (z = 1) value of 694.3 (calcd 694.3) from the crude reaction mixture.

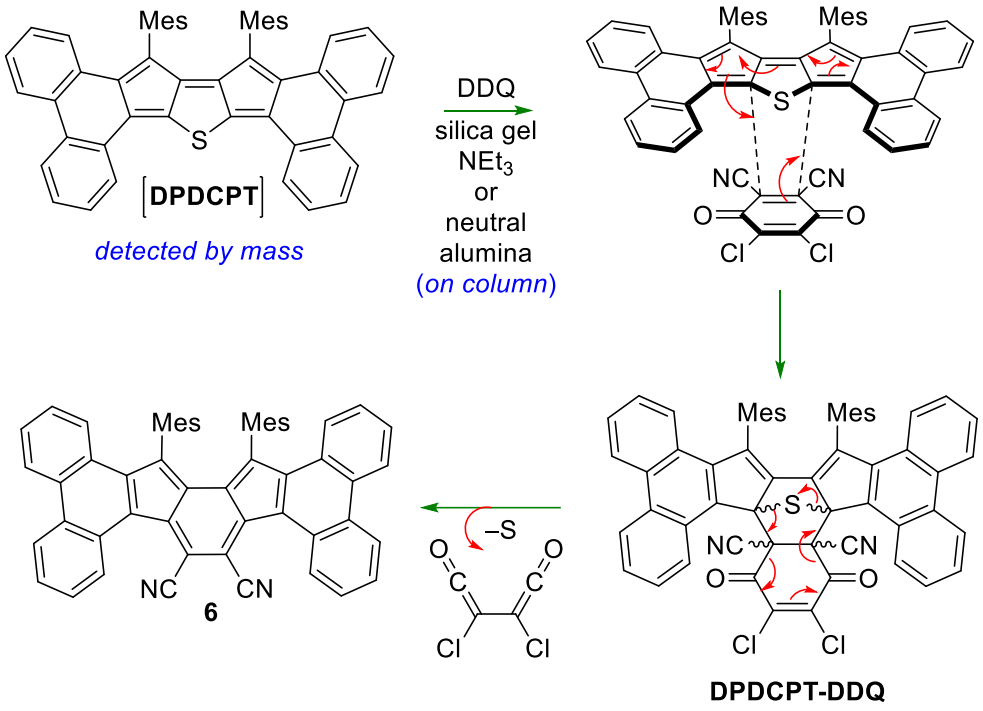


Fig. S26 Plausible mechanism for the conversion of intermediate **DPDCPT** to **6** via an intermediate 10+2 cycloadduct **DPDCPT-DDQ** during column chromatographic purification using triethylamine treated silica or neutral alumina stationary phase.

Compound **DPDCPT** was detected by mass spectroscopic analysis from the crude reaction mixture, as depicted in Fig. S25. Upon subjecting the crude reaction mixture to column chromatographic purification using either triethylamine (NEt_3) treated silica gel or neutral alumina stationary phase, compound **6** was isolated. As shown in Fig. S26, **DPDCPT** and DDQ may undergo a 10+2 cycloaddition reaction resulting in the formation of **DPDCPT-DDQ** adduct, which subsequently afforded **6** by removal of sulfur atom[12] and ClC(=C=O)C(Cl)=C=O unit,[13] in accordance to previous reports. Notably, on performing a quick silica gel (not treated with triethylamine) column chromatographic purification of crude **DPDCPT** containing DDQ in the reaction mixture under nitrogen, the **DPDCPT-DDQ** adduct could be successfully isolated and characterized using ^{1}H NMR, ^{13}C NMR, and HRMS analysis. However, the **DPDCPT-DDQ** adduct was unstable and had low solubility.

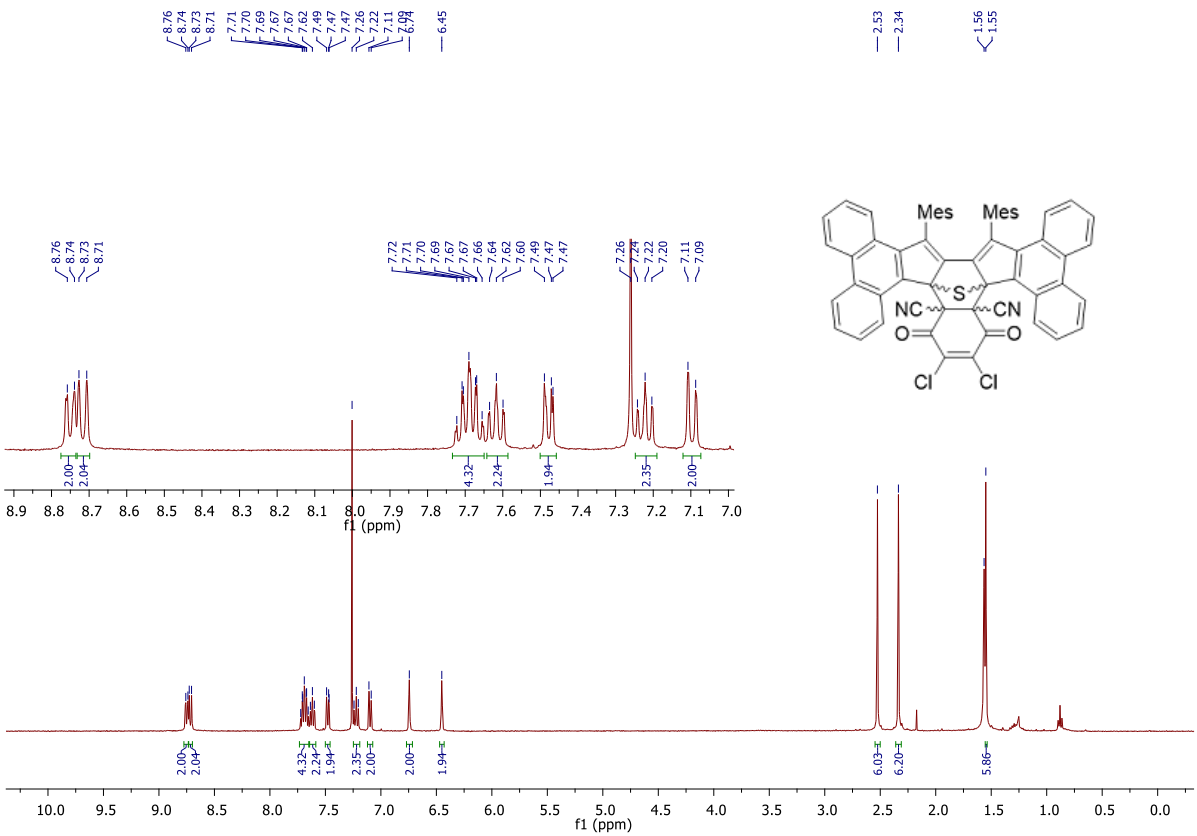


Fig. S27 ^{1}H NMR spectrum of **DPDCPT-DDQ** ($CDCl_3$, 400 MHz, 298 K).

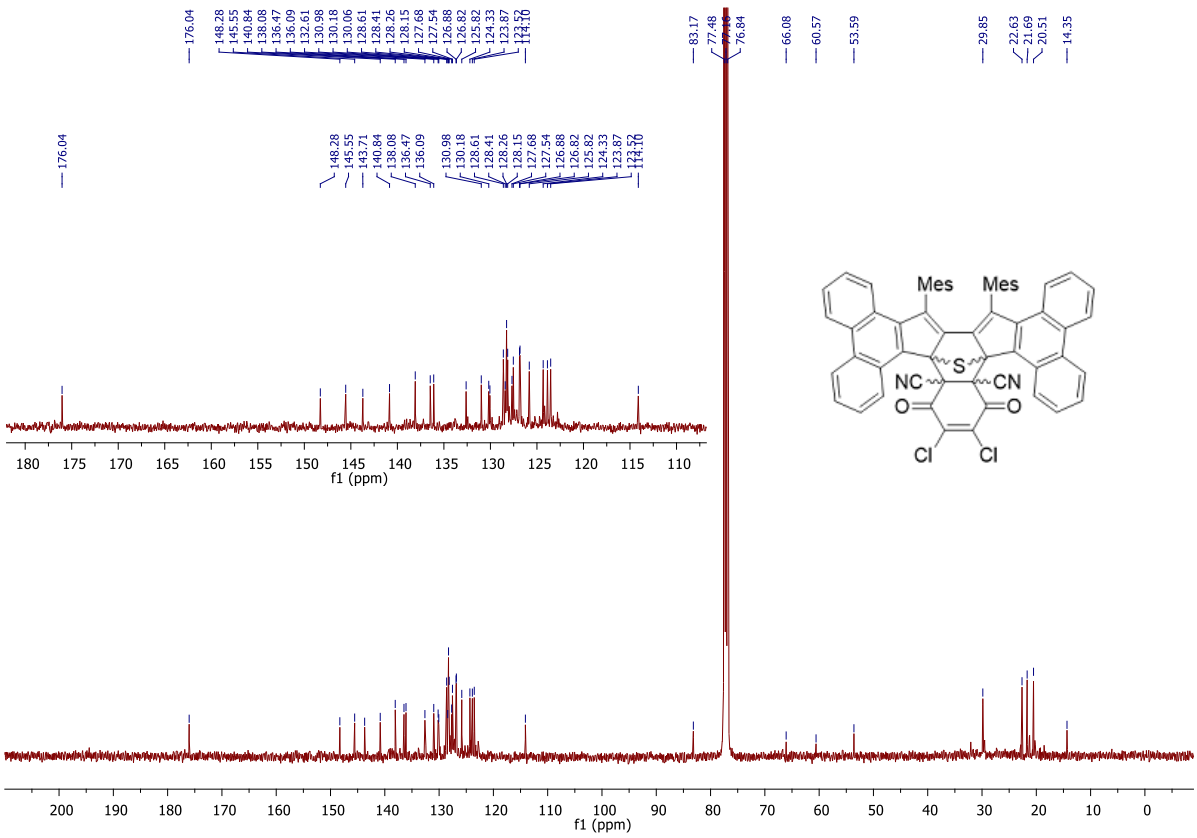


Fig. S28 ^{13}C{^{1}H} NMR of **DPDCPT-DDQ** ($CDCl_3$, 100 MHz, 298 K) (residual hexanes: 14.35, 29.85).

Characterization data of **DPDCPT-DDQ**:

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 7.6 Hz, 2H), 8.72 (d, *J* = 8.3 Hz, 2H), 7.73 – 7.65 (m, 4H), 7.62 (t, *J* = 7.2 Hz, 2H), 7.49 – 7.46 (m, 2H), 7.22 (t, *J* = 7.7 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 6.74 (s, 2H), 6.45 (s, 2H), 2.53 (s, 6H), 2.34 (s, 6H), 1.55 (s, 6H).

^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$) δ 176.0, 148.2, 145.5, 143.7, 140.8, 138.0, 136.4, 136.0, 132.6, 130.9, 130.1, 130.0, 128.6, 128.4, 128.2, 128.1, 127.6, 127.5, 126.8 (2), 125.8, 124.3, 123.8, 123.5, 114.1, 83.1, 66.0, 60.5, 53.5, 22.6, 21.6, 20.5.

HRMS (ESI) *m/z*: $[M + Na]^+$ calcd for $C_{60}H_{38}N_2O_2NaSCl_2$ 943.1929, found 943.1907 (error: −2.3 ppm).

Experimental UV-vis absorption and TDDFT plot for DPDCPT-DDQ adduct.

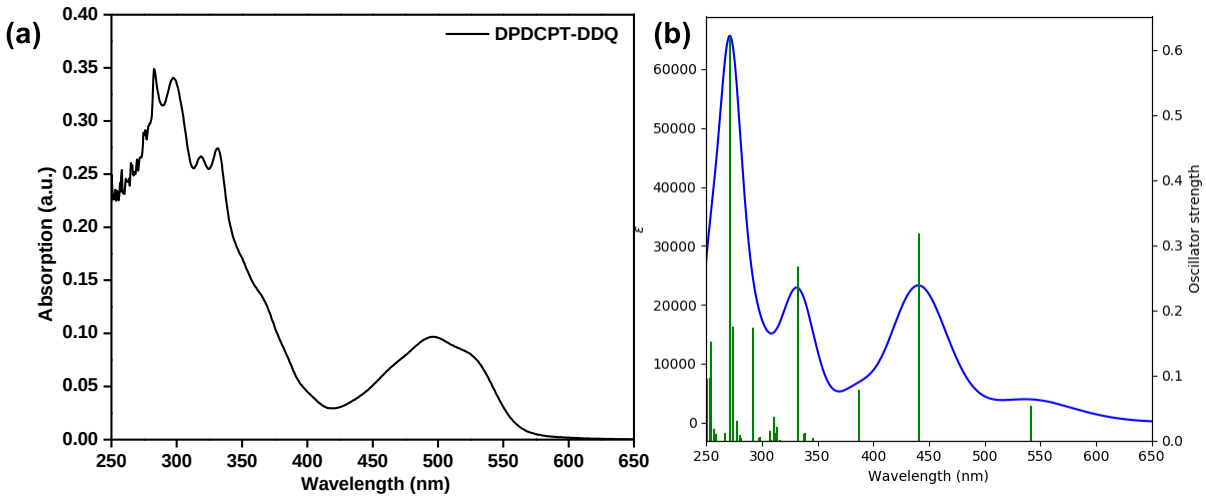


Fig. S29 (a) UV-Vis absorption spectrum of **DPDCPT-DDQ** in toluene (b) Theoretical absorption of **DPDCPT-DDQ** in the toluene at BHandHLYP/6-31G* level of theory.

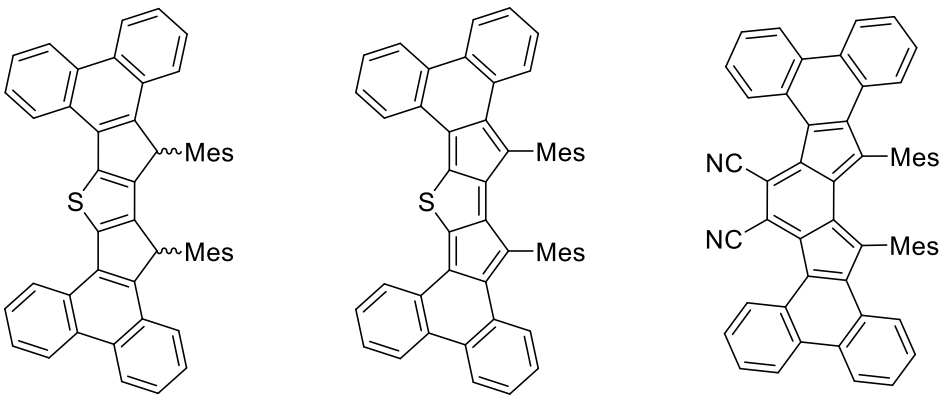


Table S7. Failed attempts for the synthesis of **DPDCPT** from its precursor **2H-DPDCPT**.

Entry	Reaction conditions	Results
1.	*p*-chloranil (4 equiv), DCM, rt, 24 h	starting material intact (no product formation)
2.	*p*-chloranil (4 equiv), TFA, 1,2-DCE rt, 24 h	starting material intact (no product formation)
3.	*p*-chloranil (4 equiv), TFA, 1,2-DCE, 70 °C, 14 h	starting material decomposed
4.	*p*-chloranil (4 equiv), $Sc(OTf)_3$(4 equiv), 1,2-DCE, 70 °C, 12 h	starting material decomposed
5.	*p*-chloranil (4 equiv), toluene, 80 °C, 24 h	starting material intact (no product formation)
6.	*n*-BuLi, *p*-chloranil, Dry THF, −35 °C to rt, 12 h	starting material decomposed
7.	*t*-BuOK, 18-crown-6, *p*-chloranil, Dry THF, 0 °C to rt, 8 h	starting material decomposed
8.	DDQ (4 equiv), 30 min, rt, (Solvent)	Indenofluorene **6** was isolated after column purification of crude mixture, using triethylamine treated silica gel or neutral alumina stationary phase. However, a **DPDCPT-DDQ** adduct was isolated using silica stationary phase under nitrogen.

As shown in Table S7, we have tried oxidative dehydrogenation of **2H-DPDCPT** using *p*-chloranil, under various reaction conditions as stated above. The reactant either remained unconsumed or decomposed, and neither the formation of **DPDCPT** nor indenofluorene structure was detected.

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