

Supporting Information

Modulation of conductance using light-induced morphological change of a layered π -structure

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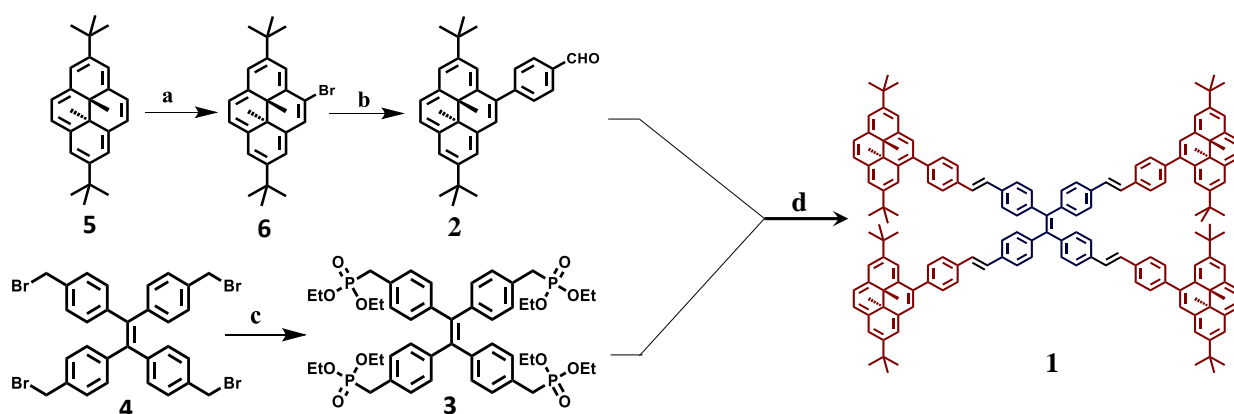
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Materials and instruments:

All the reagents employed were commercially available from commercial sources and were used without further purification. Solvents were purified and dried by standard methods. Tetrahydrofuran (THF) and 1,2-dichloromethane (DCM) were distilled freshly over sodium/benzophenone and anhydride CaH_2 , respectively, prior to use. All other solvents used for synthesis and purification were freshly distilled prior to use. (i.e. DMF). A dry nitrogen/argon atmosphere was maintained during the reactions using flame-dried glassware, unless otherwise indicated. Column chromatography was carried out with a silica-gel of 100-200 mesh, Merck. Reactions were monitored by thin-layer chromatography (TLC) using Merck plates (TLC Silica Gel 60 F254). Yields refer to use chromatographically and spectroscopically pure compounds. The structures of the compounds were determined by NMR spectroscopy, mass spectrometry, XRD analysis and a plethora of other spectroscopic techniques. ^1H NMR spectra were recorded on 400 MHz Jeol and 500 MHz Bruker spectrometer. Chemical shifts are reported as δ values relative to an internal reference of tetramethylsilane (TMS) for ^1H NMR or the solvent peak. In the case of ^{13}C NMR the solvent peak was used for calibration. ^{13}C NMR spectra were recorded on 100 MHz Jeol and 125 MHz Bruker spectrometers with complete proton decoupling. The SEM images were recorded on ZEISS (SUPRA 40 VP) scanning electron microscope with tungsten filament as electron source. The spectroscopic-grade solvents for the spectroscopic experiments were distilled and checked prior to their use to ensure that they were free from any fluorescent impurity. The solid state *I-V* characteristics were measured with Keithley 2450 Source Meter. DLS data were recorded with HORIBA Scientific Nano Partica Nano Particle Analyzer SZ-100. The cyclic voltammetry was performed using BioLogic SP-300.



Scheme S1: (a) NBS (0.9eq), dry DCM/DMF, 0 °C to rt, 14 h; (b) 4-formylphenyl boronic acid (1.5 eq), Pd(PPh₃)₂Cl₂ (10 mol%), Et₃N, dry DMF, N₂, 80 °C, 16 h. (c) P(OEt)₃ (5 mL), N₂, 120 °C, 30 h; (d) compound **2** (4.5 eq), ^tBuOK (4.5 eq), dry THF, reflux, N₂, 30 h;

The unsubstituted DHP **5** was synthesized according to the reported literature¹. The purity of the synthesized compound was confirmed from ¹H NMR data which was consistent with the reported values. Bromination of the parent DHP was done following the reported procedure to afford the bromo-DHP **6** and the ¹H data was consistent with the literature.²

Synthesis of 1,1,2,2-tetrakis(4-(bromomethyl)phenyl)ethene (4**):** HBr in acetic acid (33% v/v) (5 mL) was added to TPE (0.2 g, 0.60 mmol) and the mixture was stirred at 80 °C for 48 h under N₂ atmosphere. The excess acid was neutralised with a 0.1 M solution of Na₂CO₃ followed by washing with water and extraction in dichloromethane. The organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. Upon column chromatography over silica gel (ethylacetate/hexane 1:19), 0.35 g (yield 82%) of pure product **4** was isolated as a white solid. ¹H NMR (CDCl₃, 400MHz) δ 7.13 (d, J = 7.9 Hz, 8H), 6.97 (d, J = 7.9 Hz, 8H), 4.41 (s, 8H). ¹³C{¹H} NMR (CDCl₃, 125 MHz) δ 143.2, 140.6, 136.2, 131.6, 128.6, 33.4.

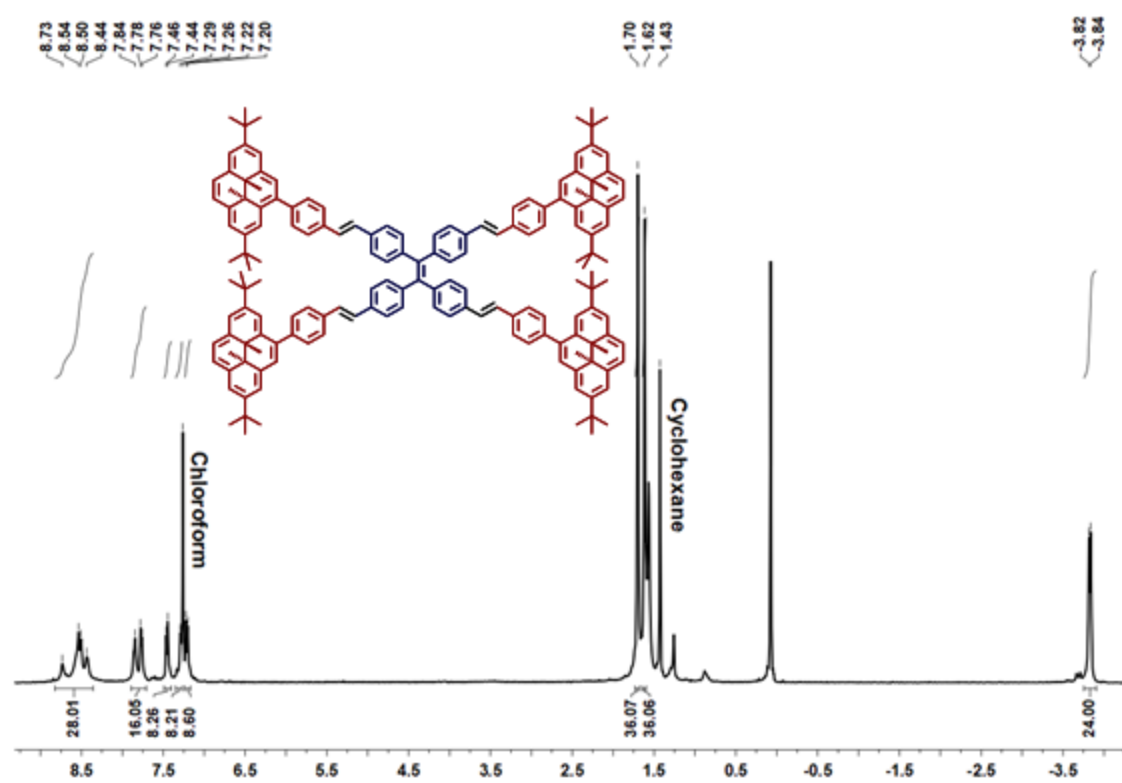


Figure S1: ^1H NMR (CDCl_3 , 400 MHz) spectrum of TPE-DHP 1

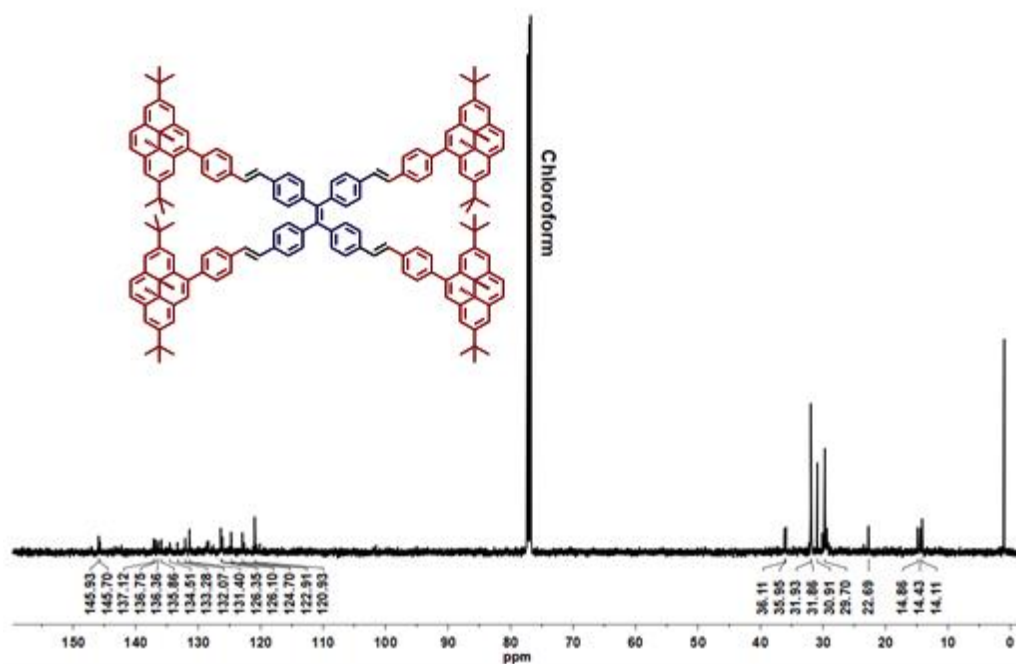


Figure S2: ^{13}C NMR (CDCl_3 , 100 MHz) spectrum of TPE-DHP 1

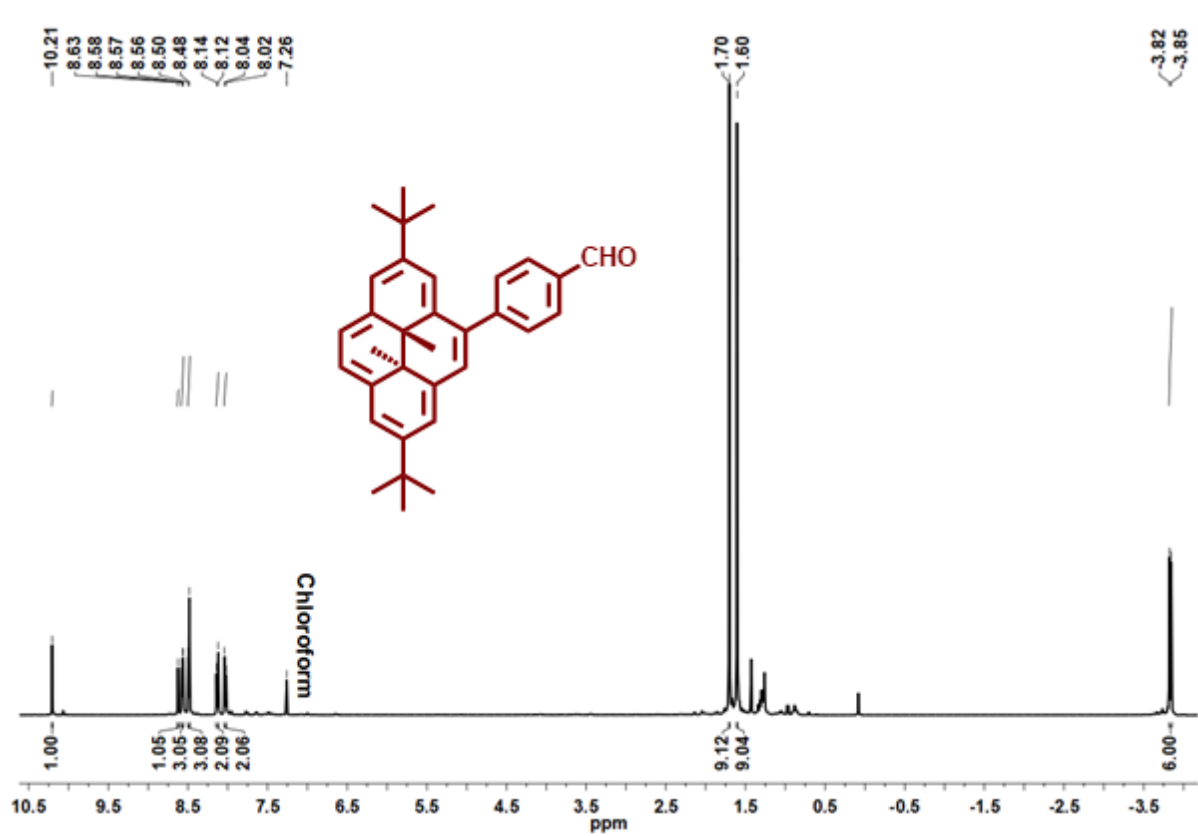


Figure S3: ^1H NMR (CDCl_3 , 400 MHz) spectrum of 2

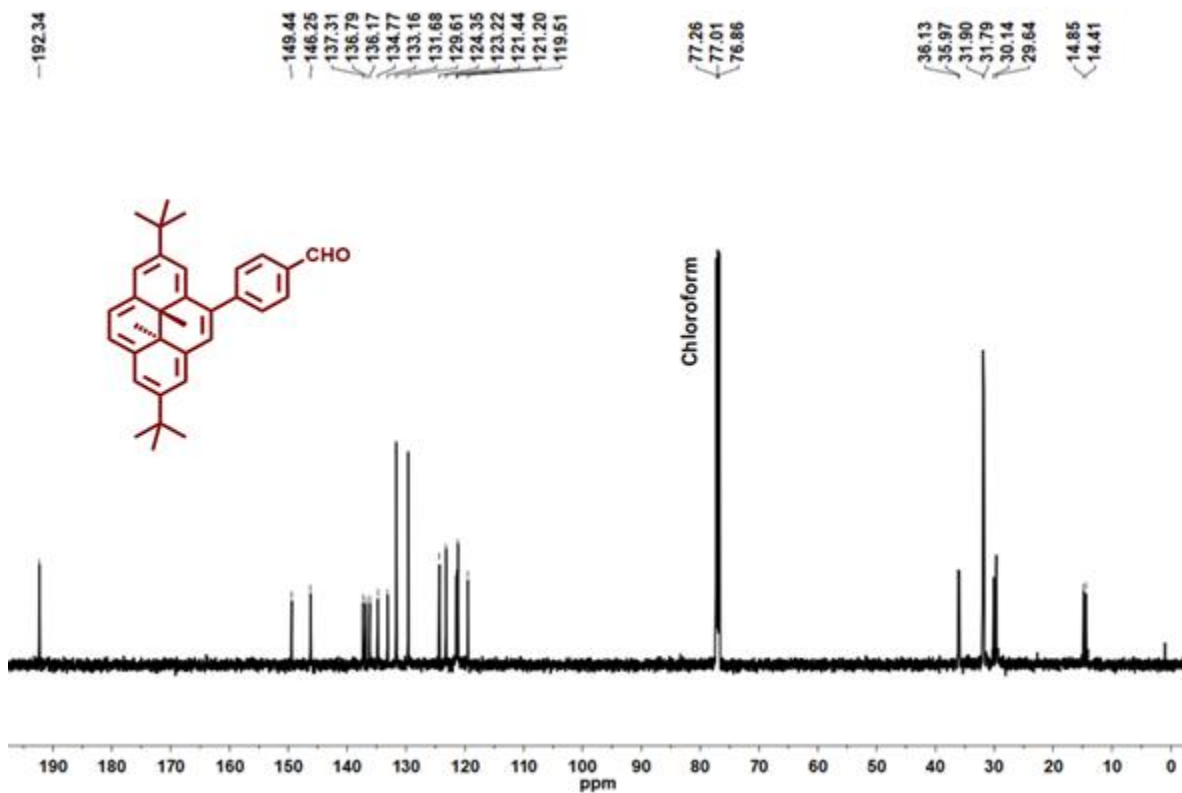


Figure S4: ^{13}C NMR (CDCl_3 , 125 MHz) spectrum of 2

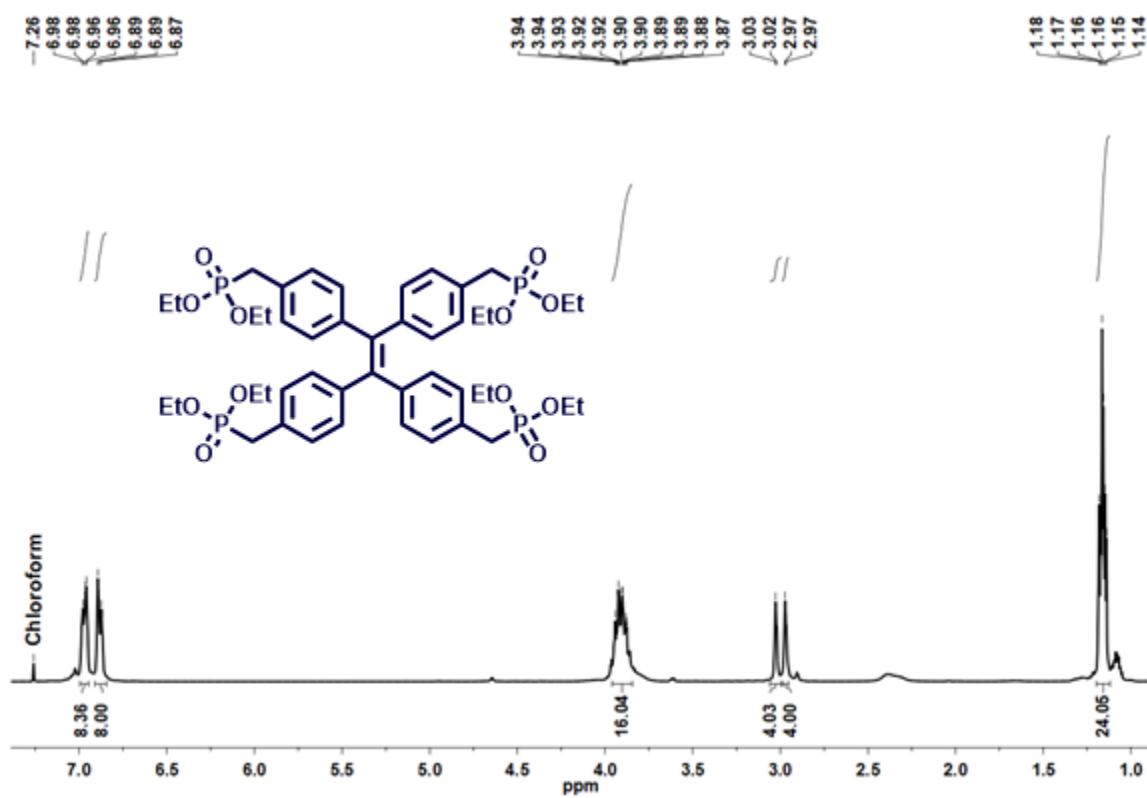


Figure S5: ¹H NMR (CDCl₃, 400 MHz) spectrum of 3

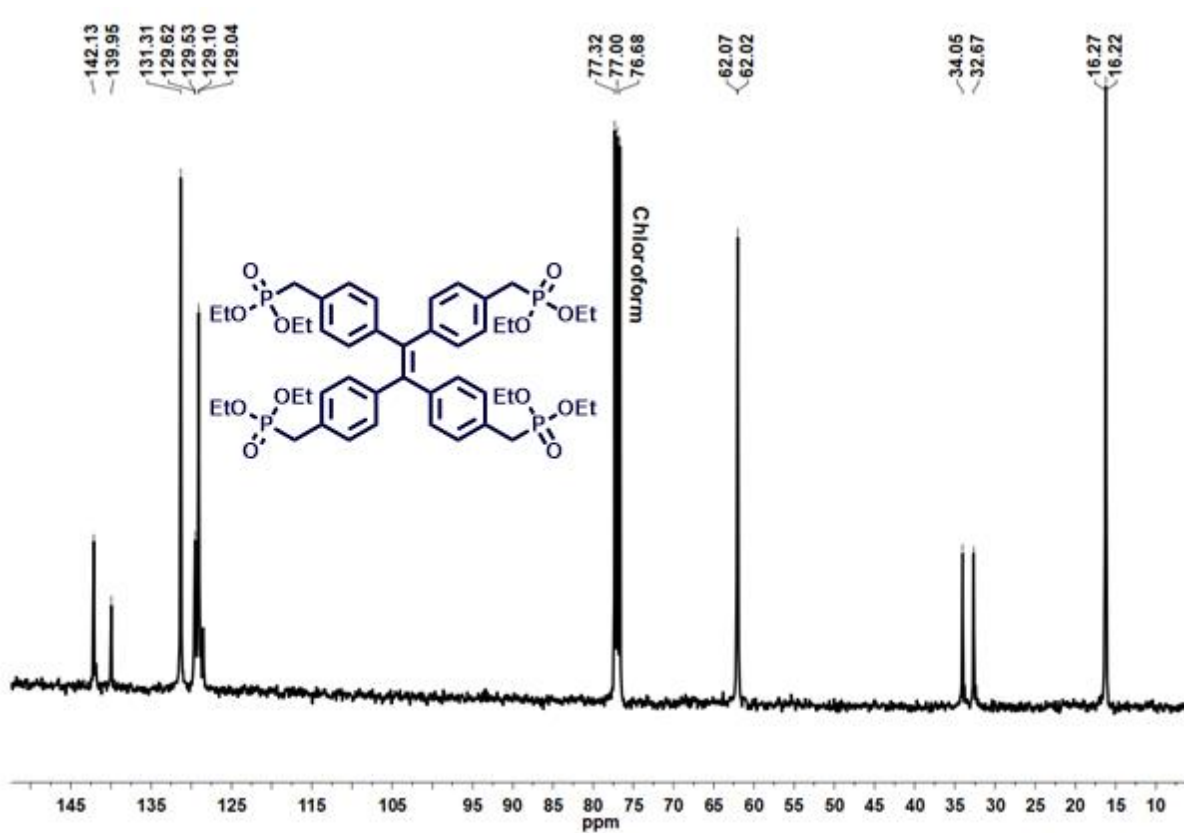


Figure S6: ¹³C NMR (CDCl₃, 100 MHz) spectrum of 3

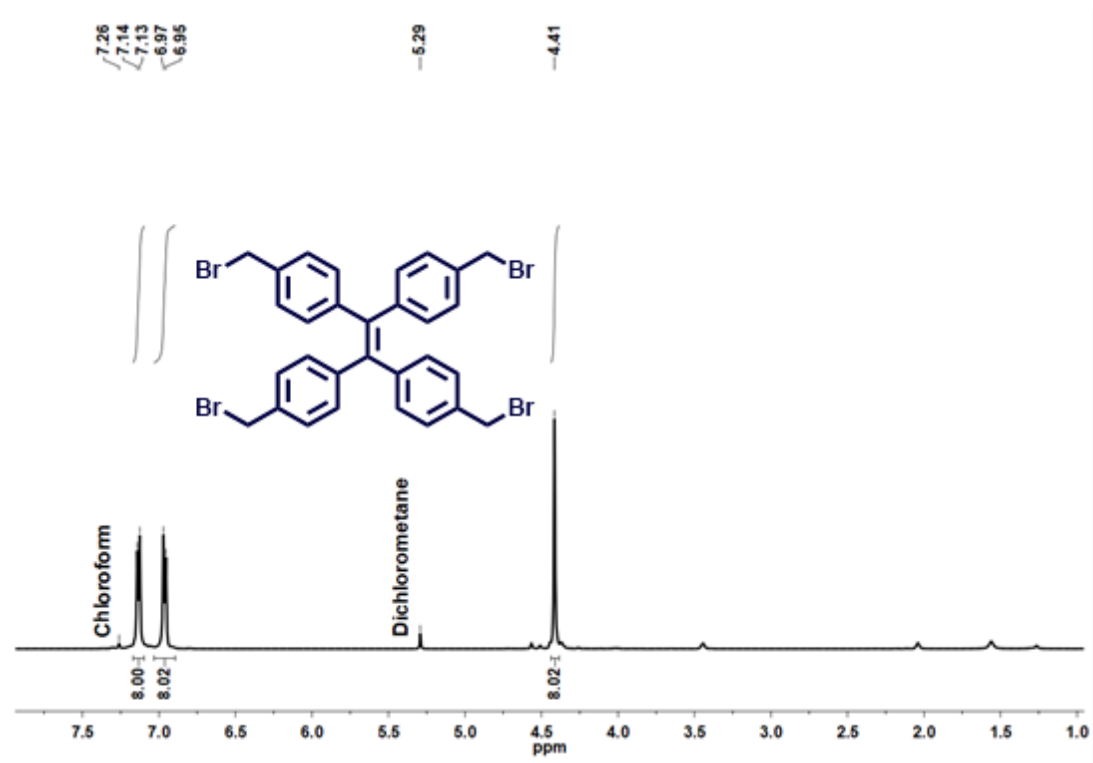


Figure S7: ¹H NMR (CDCl₃, 400 MHz) spectrum of **4**

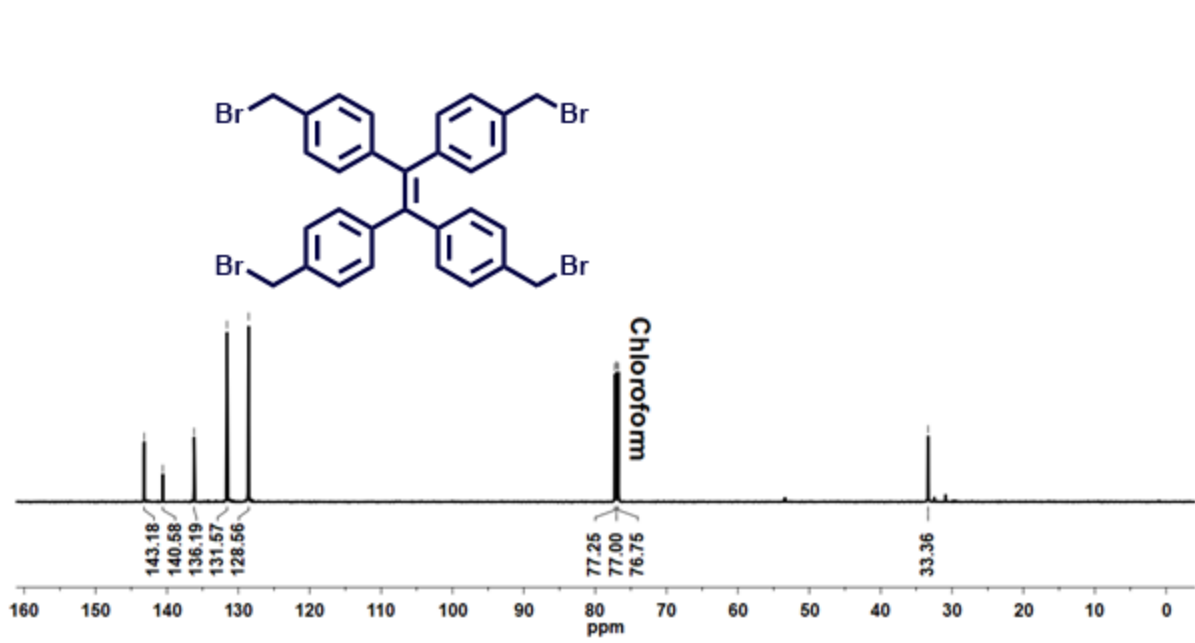


Figure S8: ¹³C NMR (CDCl₃, 100 MHz) spectrum of **4**

Photoisomerization in DMF:

The photoisomerization of compound **1c** ($10\mu\text{M}$ in DMF, degassed under argon) was monitored with UV-Vis spectroscopy. The reverse isomerization was achieved upon heating at $65\text{ }^\circ\text{C}$.

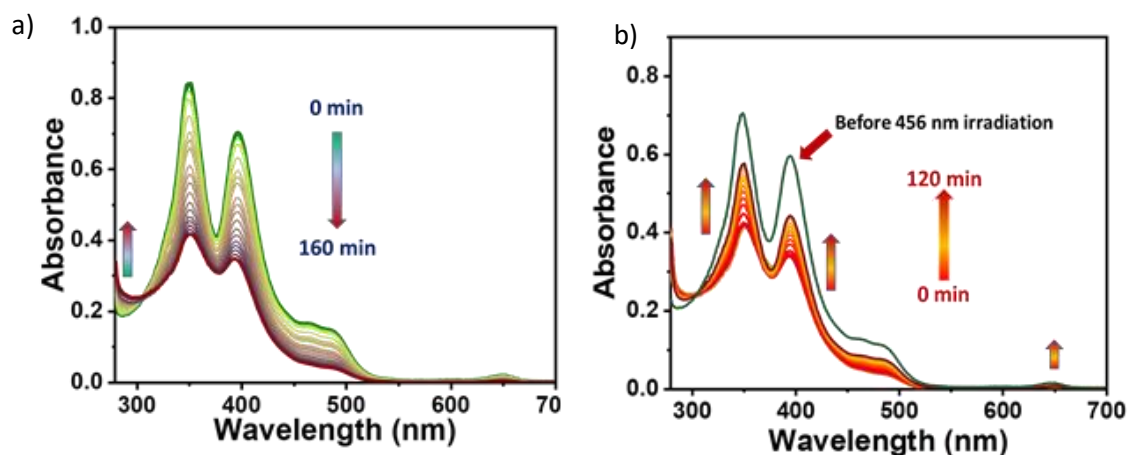


Figure S9: a) closed to open isomerization under 525 nm light in DMF b) thermal reversal at $65\text{ }^\circ\text{C}$ in DMF.

Kinetics of ring closing:

The thermodynamic parameters obtained from the variable temperature (VT) studies of the reversal of the open-form **1o** to the closed-form **1c** were reported. The UV-vis VT experiments (Figure S10) provide the data which helps to calculate the thermodynamic parameters such as the activation energy, and also the enthalpy and the entropy change of the thermal-reversal process using the Arrhenius plot (Figure S11 a) and the Eyring plot (Figure S11 b). The thermal **1o** \rightarrow **1c** conversion is the ground-state reaction and the thermodynamic parameters (Table S1) namely, activation energy, enthalpy, and entropy, correspond to the ground state-thermal parameters. The high activation energy indicates that the open and the closed isomers are good photochromes with very low thermal reversibility at the room temperature (300 K)

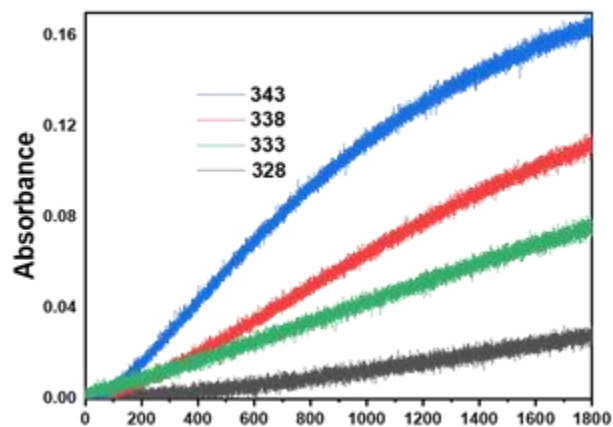


Figure S10: Kinetics of ring closing at different temperatures from 55 °C to 70 °C at 5°C temperature interval.

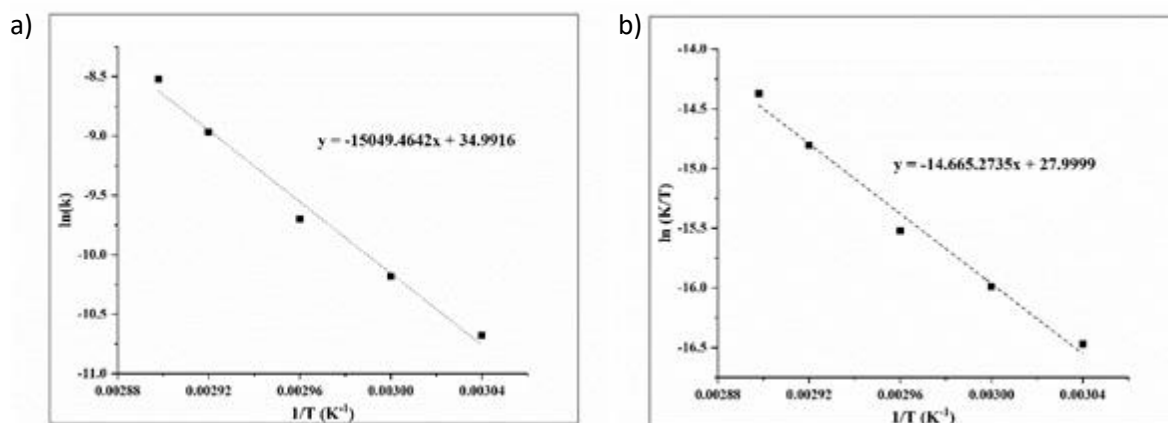


Figure S11: a) Arrhenius plot b) Eyring plot of compound 1.

Compound	DHP-TPE (1)
Activation Energy (E_a) for open to closed conversion; (kcal/mol)	29.79 kcal/mol
Enthalpy of activation (ΔH^\ddagger) for open to closed conversion; (kcal/mol)	29.03 kcal/mol
Entropy of activation (ΔS^\ddagger) for open to closed conversion; (cal/mol)	8.33 cal/mol

Table S1. Thermodynamic parameters for open to closed isomerization.

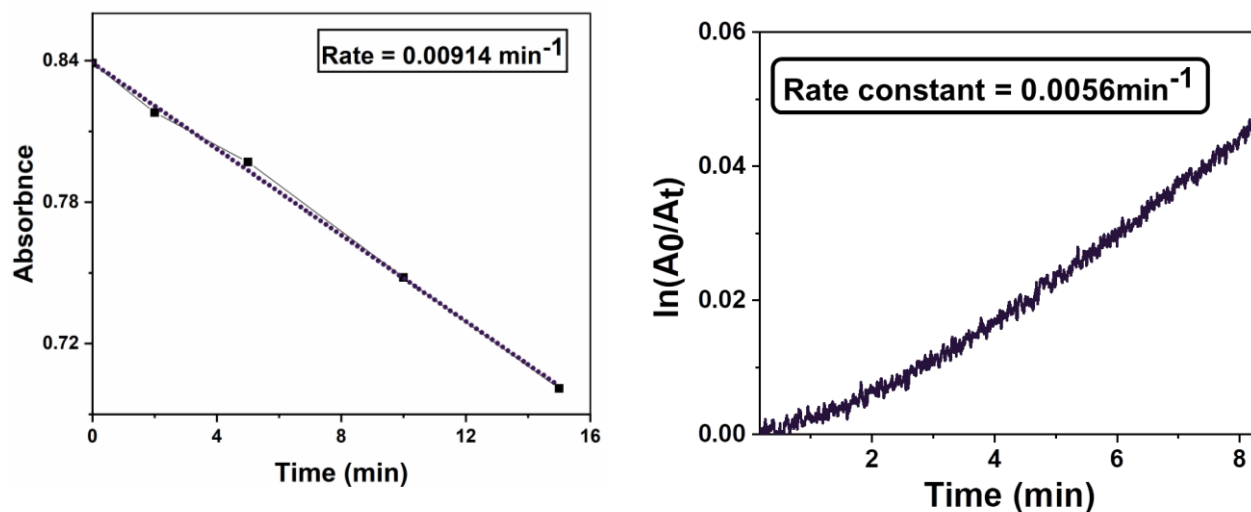


Figure S12. a) Rate of **1c** to **1o** photoisomerization (10 μM in THF), b) kinetics of thermal ring closing at 65 $^{\circ}\text{C}$ (10 μM in THF)

The aggregation behaviour of **1o** was also monitored in different DMF/water solvent systems (10 μM) through UV-Vis spectroscopy, but no significant result was found.

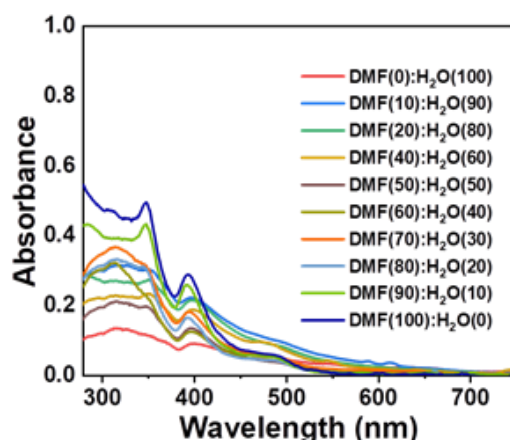


Figure S13. Absorption spectra of **1o** in different DMF/water solvent system.

The aggregation induced emission behaviour of **1c** was also monitored in THF/water systems with increasing water percentage in THF. The maximum emission was obtained in 80:20 THF/water system (10 μM of **1c**).

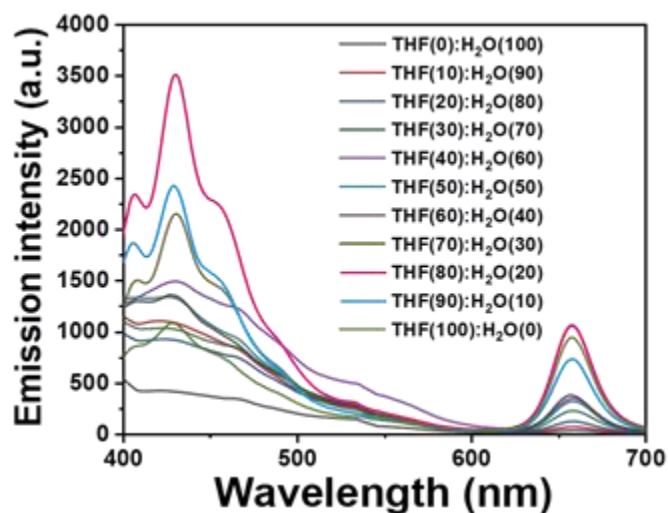
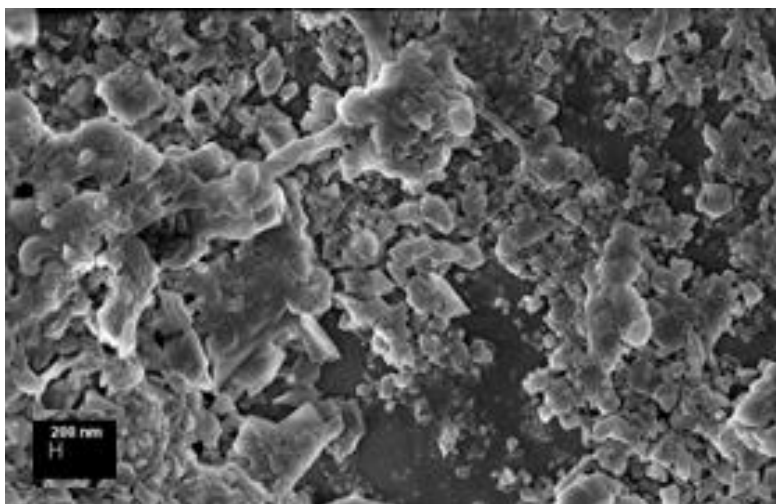


Figure S14. Emission spectra of **1c** in different THF/water system.

Samples for microscopic imaging of **1** (both **1c** and **1o**) were prepared through drop cast method followed by spin coating after dissolving the compound in pure solvents.

a)



b)

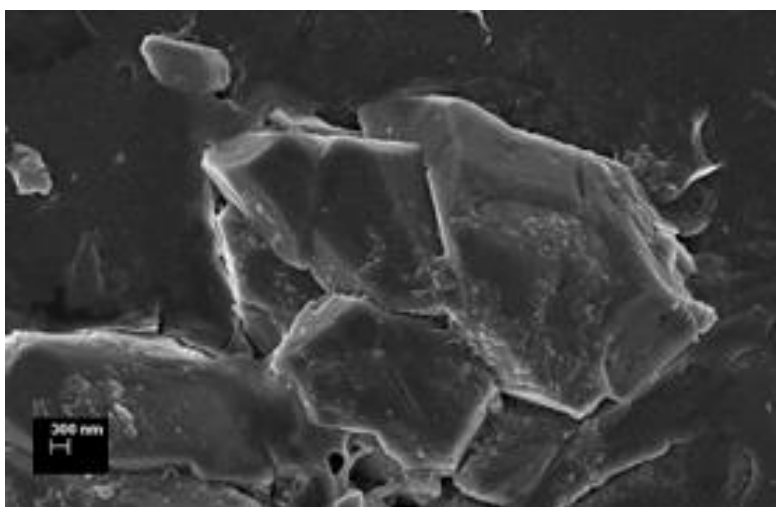


Figure S15: SEM images of **1c** in pure a) DMF; b) THF.

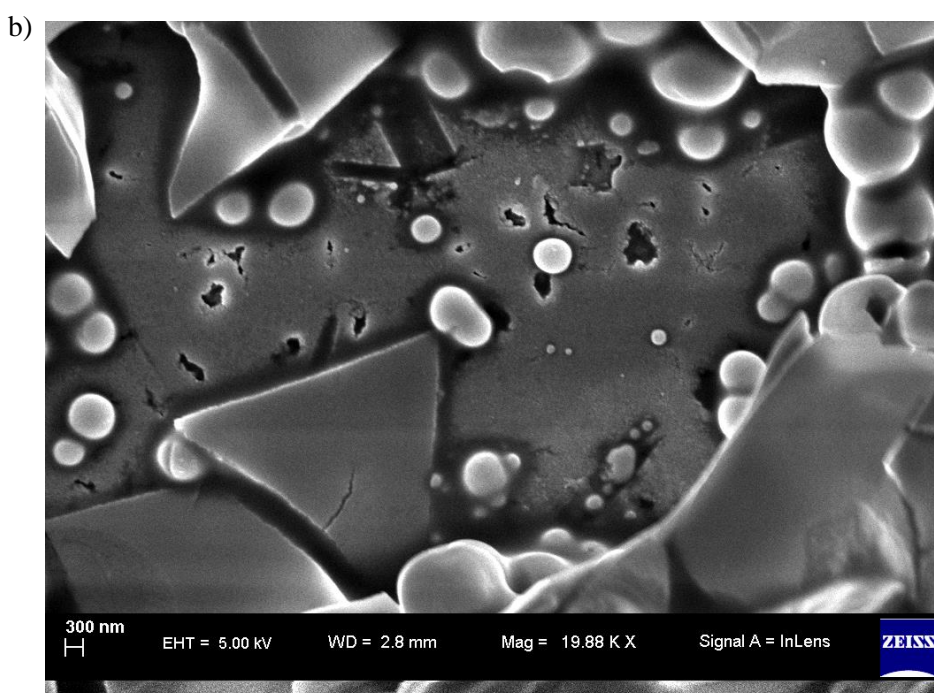
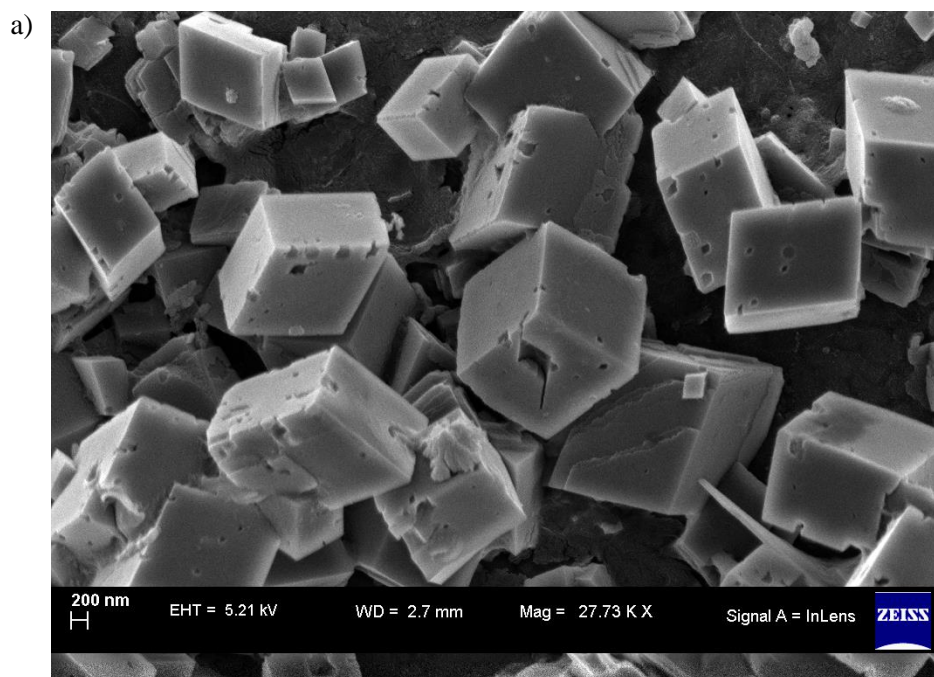


Figure S16: a) SEM images of **1c** in 80:20 THF/H₂O; b) SEM images of **1o** after irradiation of 525 nm light.

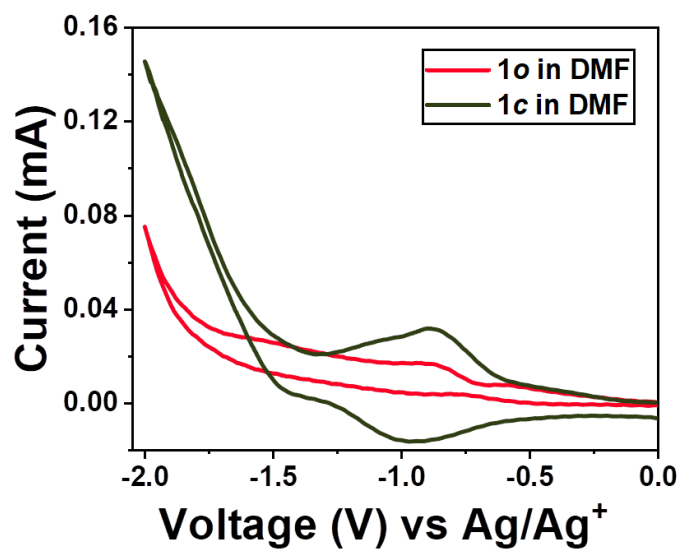


Figure S17. Conductance measurement in solution phase for **1c** and **1o** in DMF through cyclic voltammetry.

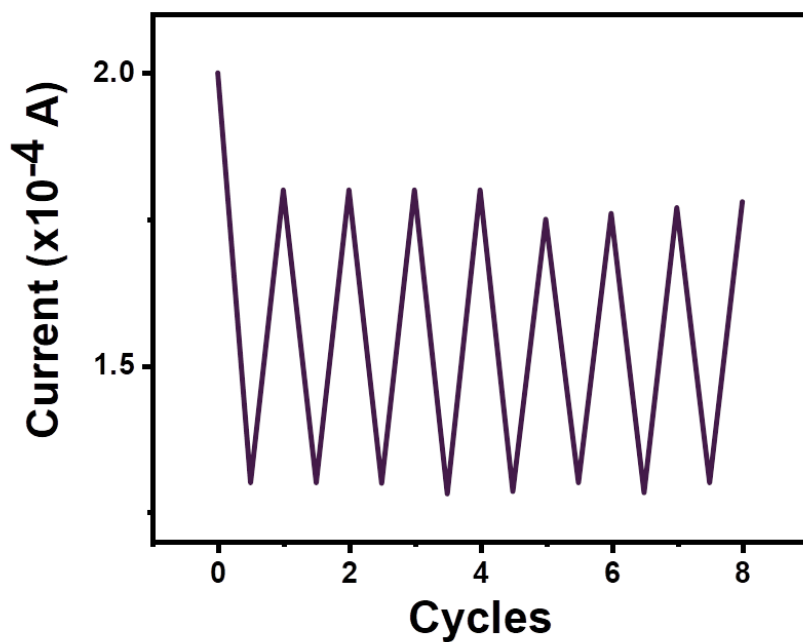


Figure S18. Changes in current observed under cyclic voltammetry before and after isomerization in visible light and heating alternatively (**1c**→**1o** and **1o**→**1c**) over multiple cycles.

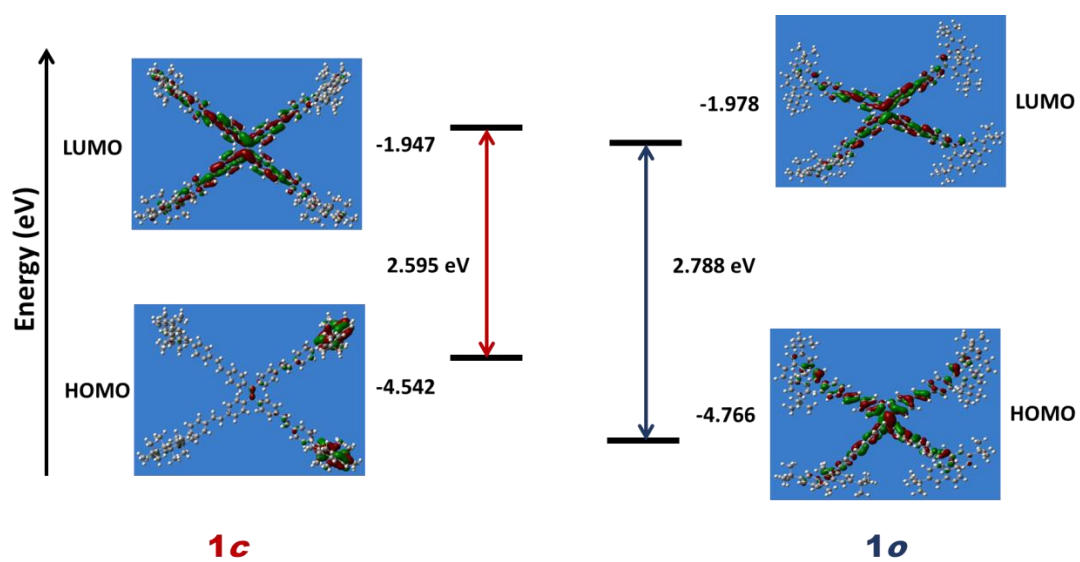


Figure S19. HOMO-LUMO energy difference for **1c** and **1o** calculated through DFT.

Table S2: Cartesian coordinate of DHP-TPE (1c)

0 1			
C	-0.05087000	-0.69501700	-0.57268600
C	-1.35297500	-1.40755000	-0.73281700
C	1.14040100	-1.58313800	-0.42803100
C	0.04419600	0.67829800	-0.56209400
C	-1.14508200	1.56448400	-0.39176100
C	1.34499300	1.39317300	-0.72337800
C	-2.27770100	-1.04073700	-1.73099700
C	-3.47425900	-1.73519600	-1.89089000
C	-3.81157800	-2.82942100	-1.06410800
C	-2.87764800	-3.20205500	-0.07077200
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C	1.30603700	-2.71341900	-1.25432300
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H	8.61474500	7.84888700	0.55336500
H	6.50519000	6.61009000	0.84858500
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H	8.46349800	-10.09278100	7.76536300
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H	8.22336000	-6.94095800	5.78588000
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H	13.61154200	5.08466600	3.05824300
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H	-16.49177000	-11.14252200	1.85758400
H	-17.35716300	-9.61456100	1.57856600
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H	-0.58256800	2.93458200	-1.96341800
H	0.98458800	2.78995900	0.88455800
H	3.09486000	4.00309700	0.62058600
H	4.13611100	1.45310400	-2.69348100
H	2.02426600	0.22026000	-2.40272200
H	1.99904200	-0.50837400	1.23579400
H	3.92071800	-1.99781600	1.51278600
H	2.51510600	-4.41160100	-1.76856300
H	0.56717400	-2.92465400	-2.02029700
H	-0.97584400	-2.83119300	0.84749400
H	-3.09031900	-4.03792800	0.58737500
H	-4.16558000	-1.43318400	-2.67288300
H	-2.04981700	-0.20647400	-2.38486300
C	13.71173300	7.02897000	-1.34002800
C	-13.45264800	7.80183600	2.16383700
C	-12.07660300	-10.45655300	-1.26324000
C	10.93306900	-10.72458200	1.99616300
C	11.81528500	10.54138200	-1.14396800
C	-10.90049300	10.66898700	1.04821000
C	-13.42747500	-6.94351700	-2.60965000
C	13.41644700	-7.59503800	2.09852300
C	7.74602900	4.91325900	-1.82184500
C	8.94067000	5.60968300	-1.98253500
C	9.29467800	6.67386700	-1.12531500
C	8.38737700	7.01565900	-0.10315100
C	7.19023300	6.31862300	0.05689800
C	6.86870700	-6.21672200	0.12495600
C	7.97119300	-7.05400000	0.27212900
C	8.94249000	-6.82517200	1.27052800
C	8.76237000	-5.70822900	2.11009400

C	7.65876100	-4.86891500	1.96154200
C	6.83701700	5.24918400	-0.79376500
C	6.68191700	-5.09936500	0.96918800
C	-11.07553700	9.23556400	-4.11568700
C	-10.92707500	-7.45463800	-7.32922800
C	12.18482700	11.54354400	-6.32900300
C	15.28663600	-8.34313500	-2.79704200
C	-6.80664500	6.24955100	0.36310800
C	-7.90543200	7.08734100	0.53092900
C	-8.93911400	6.77282900	1.44110000
C	-8.81037800	5.58184400	2.18325500
C	-7.71157400	4.74154400	2.01311800
C	10.21824400	-7.99129700	7.37099800
C	9.03306600	-10.16570200	6.83057100
C	8.05181200	-7.97537400	6.10430500
C	9.37818300	-8.74519600	6.30153400
C	14.02371400	-10.49497000	-3.24502200
C	16.21324500	-10.54025300	-2.02010000
C	14.90807400	-9.73475000	-2.21683200
C	12.91612600	-8.81324600	-0.92538700
C	14.12525100	-9.54197300	-0.89872700
C	14.54974600	-10.12780800	0.31442400
C	11.42246400	-9.56784300	5.02539400
C	10.19376600	-8.87072700	4.99515000
C	9.77427300	-8.25868900	3.79567400
C	10.48965000	-8.35958000	2.59484600
C	10.13698600	-7.71059900	1.38088100
C	10.90946700	-7.92049300	0.21496000
C	12.14507000	-8.58211600	0.21769500
C	13.44639700	-10.42534800	3.88999700
C	12.20275800	-9.76449400	3.88753900
C	11.61243800	-9.40052400	2.52398800
C	12.73834800	-8.92077900	1.57961900
C	13.85711000	-9.95896300	1.51610800
C	14.20718600	-10.58673600	2.72552800
C	12.07689700	7.90799300	4.44088300
C	13.49223700	5.91871800	3.75929700

C	10.99492200	5.82576600	3.55148000
C	12.22585700	6.75110200	3.41262700
C	13.56906400	9.49899600	-6.90340600
C	14.67820700	11.58679900	-6.06283300
C	13.42243600	10.69563300	-5.92171600
C	12.11417700	9.34601200	-4.20346600
C	13.22779600	10.16801200	-4.48256900
C	14.16427400	10.43007600	-3.45814000
C	13.46564700	8.19025800	1.71678800
C	12.37323400	7.33682100	1.99035400
C	11.41763100	7.09060600	0.98264100
C	11.52737300	7.60328900	-0.31698100
C	10.56012400	7.43140600	-1.34373400
C	10.79677800	7.95713300	-2.63516600
C	11.85378700	8.82874000	-2.93094100
C	14.75846400	9.60931100	0.15615200
C	13.69904500	8.73027000	0.45340400
C	12.87127300	8.21640600	-0.72596600
C	12.65940900	9.35510500	-1.74965800
C	14.00104800	9.96565200	-2.15051900
C	14.94738700	10.14282800	-1.12465200
C	-11.90035500	11.10313500	7.06355600
C	-13.39294100	9.06780900	7.29963300
C	-14.37369200	11.29323000	6.68645000
C	-13.14719900	10.37227500	6.49053300
C	-12.63105200	7.26530900	-3.76378900
C	-10.15655400	6.99920500	-3.44836800
C	-11.34341100	7.97070500	-3.25215700
C	-12.57764200	9.27836300	-1.45160700
C	-11.53041900	8.39281200	-1.77731400
C	-10.72341900	7.86385900	-0.74449200
C	-11.81839600	9.17229100	4.67831500
C	-12.90536100	10.01411600	5.00734500
C	-13.69537000	10.55284700	3.97041200
C	-13.49144300	10.23574100	2.62326200
C	-14.20668600	10.81294800	1.56062800
C	-13.93803300	10.48399300	0.22439300

C	-12.83599300	9.69145400	-0.14360500
C	-10.40869100	8.02355200	3.00393000
C	-11.52929000	8.78424200	3.36818100
C	-12.54503200	9.08702900	2.27409800
C	-11.80743800	9.38349200	0.94562800
C	-10.85566600	8.23189600	0.59729600
C	-10.09489900	7.68281200	1.66925200
C	-7.79116500	-4.87175600	-1.78657500
C	-8.98847200	-5.56289900	-1.94792100
C	-9.31157100	-6.67523300	-1.13912900
C	-8.37894300	-7.05328000	-0.15273800
C	-7.17867800	-6.36301200	0.00682200
C	-15.67698400	-7.94668700	2.98527300
C	-14.45975900	-10.12173100	3.44750700
C	-16.66316100	-10.13347300	2.24955500
C	-15.33820300	-9.35472400	2.41960300
C	-9.81920400	-9.66516100	-6.77111800
C	-8.75134300	-7.50215100	-6.08225600
C	-10.10647200	-8.22601800	-6.25747600
C	-12.18050600	-8.92435000	-4.95891000
C	-10.92008300	-8.29337400	-4.94531600
C	-10.40478000	-7.80053000	-3.72495600
C	-13.32434200	-8.52436600	1.09881100
C	-14.56080500	-9.20966500	1.09251100
C	-15.07800700	-9.68224600	-0.13167300
C	-14.38508100	-9.56160600	-1.34092200
H	13.19660800	6.58782400	-2.19710300
H	13.83966600	6.25804500	-0.57470600
H	14.69948300	7.37460400	-1.65599100
H	-13.94151600	7.63288800	3.12784400
H	-12.85157200	6.92195400	1.91894100
H	-14.22321200	7.93235100	1.39973900
H	-12.34458600	-11.01248400	-0.35993100
H	-11.00592900	-10.23703300	-1.23260400
H	-12.28844000	-11.08226900	-2.13402700
H	10.47406800	-10.56488000	1.01721400
H	10.15365200	-11.02391400	2.70278800

H	11.66469100	-11.53321700	1.92012600
C	2.40596900	-3.55587800	-1.10773000
C	3.38577200	-3.32637800	-0.11720000
C	3.20403200	-2.20597400	0.72545100
C	2.11206900	-1.35836500	0.57217800
C	2.25895200	1.04356900	-1.73747100
C	3.45333200	1.74150100	-1.89895000
C	3.79896100	2.82219400	-1.05802600
C	2.87594000	3.17743200	-0.04831100
C	1.67787900	2.48710700	0.10666000
C	-1.31535400	2.71044800	-1.19529900
C	-2.41163400	3.55270800	-1.02299400
C	-3.38377000	3.30633300	-0.02893000
C	-3.19672700	2.17053900	0.79175800
C	-2.10837200	1.32331200	0.61278500
C	-5.08747300	-3.51417600	-1.28061100
C	-5.57181100	-4.57365600	-0.59085200
C	-6.84936700	-5.25667200	-0.80566200
C	4.51744200	-4.24953600	-0.01170000
C	5.54661400	-4.17951400	0.86479200
C	-4.51183000	4.23004900	0.10433800
C	-5.55494700	4.12351900	0.96075700
C	-6.68235500	5.04820500	1.09703800
C	5.07135900	3.51260100	-1.27816400
C	5.56463700	4.55750200	-0.57307300
C	-10.60923800	-7.39352100	-1.26607100
C	-11.11597600	-7.83440500	-2.52231800
C	-12.58492600	-8.27511600	-2.55763500
C	-12.92043200	-9.12471800	-1.30777400
C	-12.54564400	-8.35450300	-0.04808700
C	-11.36065800	-7.60524800	-0.08864500
C	-12.97014400	-9.05536500	-3.81538000
C	-14.17783800	-9.77498900	-3.77551200
C	-14.90271900	-9.94958400	-2.58808100

Ground state P.E = -6270.484254 Hartree; Number of imaginary frequency = 0

Table S3: Cartesian coordinate of DHP-TPE (1o)

0 1			
H	-11.65554100	-11.35645700	1.52817000
H	-12.24224200	-10.94184500	3.14054800
C	-0.05230000	1.02951000	0.17267900
C	1.22183600	1.80353000	0.24969800
C	13.62738700	8.41749800	0.08517300
C	-9.34399500	6.78231400	-1.39165300
H	-11.61365200	5.39352800	-0.61937800
H	-9.48791900	9.35531300	-0.92384500
H	9.56412200	-4.60047600	-3.66188500
C	-7.24701400	6.21313600	-0.26638300
C	8.09498700	-6.40114200	-1.17926500
C	8.53231900	6.64954000	0.58098700
H	-12.26466100	3.11962300	-0.69105100
C	6.72981700	-10.87556600	-3.17543500
C	2.62616700	3.65023100	-0.50737200
C	-6.64884500	-5.20037800	0.84583200
H	-12.54982600	-6.11771500	1.85411000
H	-10.82615000	-10.11597600	2.46442600
H	-13.25049400	-5.80738400	3.44627200
H	-13.97073500	-7.02503700	2.39650900
C	-0.08504500	-0.34673700	0.19174300
H	12.73393300	-8.29519300	-5.33685500
H	11.23580800	-8.50929000	-4.43512800
C	5.91992900	3.97125500	1.27928700
C	-10.28794200	-7.46703700	1.56851500
C	3.15069800	-1.71725900	-1.29650500
C	3.42967800	-2.82748500	-0.46689700
C	2.51861800	-3.09936400	0.57725200
C	-1.34244200	-1.11489500	0.43215100
C	-4.93887000	-3.38223900	1.21145100
C	2.03430100	-0.91700900	-1.07845800
C	-3.37183500	-1.53142900	1.71913900
H	9.78986700	8.89855700	1.20822800

H	-4.85903700	-4.85100900	-0.29745600
C	1.44780000	2.91206600	-0.59188800
C	-1.66740900	-2.23841400	-0.36077500
C	4.84559500	4.14922600	0.47440100
C	-10.00501500	13.68845100	-3.21954300
C	4.59198800	-3.70051200	-0.63898900
C	-3.71088400	-2.64232000	0.91553300
C	-14.98111600	9.82986000	-2.71905800
C	-5.84319800	4.26101100	-1.07967800
C	-9.35664300	-10.88582600	6.31715900
C	7.13452900	4.78695200	1.32205100
C	11.54764700	10.56388900	2.42755300
C	-2.82447300	-2.97684800	-0.13344100
C	-9.12600200	5.69189700	-2.25954100
C	-7.98999000	4.89471300	-2.14367900
C	13.04933300	-8.23065700	-3.23841500
H	16.45809000	7.24686400	3.10209400
C	9.34386700	5.17127300	2.30539300
C	9.55374000	6.30742200	1.49621500
C	2.21908000	1.49254900	1.20054700
C	-11.74957500	13.31876900	-4.98738900
C	-5.41967900	-4.46223800	0.55108700
C	5.59261300	-3.55650900	-1.53994900
C	-11.50336800	13.38901000	-3.45489900
C	-15.21303900	4.60512100	0.42790500
C	11.20000200	12.25490100	4.99816400
C	7.35452100	5.91436200	0.49821100
C	11.14509500	-9.15960000	-1.52277500
H	-14.52897100	-6.08598700	-1.79200400
H	-8.35667100	-7.91671600	-0.34740600
H	16.89479800	-4.29521700	-0.33804000
C	-10.72483200	-7.67443900	2.99653700
C	9.20767200	-10.40793500	-3.19655600
C	12.82396300	-6.93127000	-2.72080700
C	-12.08590600	-7.58861300	3.36980600
H	13.07069400	14.26344900	4.91475800
C	-14.10945000	-9.46036400	1.93890700

C	-4.79531400	4.36970200	-0.22887500
H	-0.70499700	3.25138900	1.61737000
H	6.50475600	-9.81114900	-3.04975700
C	-14.17071400	4.21585800	-0.65654100
H	-1.98827700	0.05983000	2.12340600
H	-16.23968400	-6.05134100	-2.25171800
C	3.39058200	2.23660100	1.29207800
H	12.40704600	-9.83666800	-4.54218600
H	11.70331300	-7.57021900	-0.16574100
C	-9.19972100	-9.34778000	6.16279800
H	-7.30186500	-4.03993100	2.55857700
C	-13.03910700	3.41385500	0.02630400
C	11.37853900	-10.45975500	-2.03854100
C	-12.87738700	9.82894500	-1.30105000
C	8.16341900	4.43684600	2.22370300
H	7.58279900	-3.19606200	-3.28029000
H	6.79352300	-11.32719800	-2.17867600
H	-17.23374500	-9.34781200	-0.77040400
H	-7.56310400	-7.97351600	5.64405200
H	-16.02759600	8.19164000	-3.50468200
C	13.38687000	13.34193300	4.41272600
C	7.72860500	-4.08868600	-2.67791100
C	-12.30813800	-8.66463900	0.53833700
C	15.04532400	-6.96689700	-1.65066000
C	15.43532700	8.98711400	2.53361200
H	9.16543800	-12.82571300	-4.73147400
C	13.88793800	-10.47804300	-2.41275800
C	12.53991200	11.34827300	3.04422800
H	-11.05467900	8.64083300	-3.96055100
H	18.37941800	-6.02738300	-1.28906000
H	13.92758500	2.94304700	-1.93827200
C	-13.02034500	-6.59558000	2.71529400
C	-2.21918300	-0.78565000	1.48522200
C	-12.74275700	-9.53318900	1.57514700
C	1.13307800	-1.18226400	-0.02355700
C	-1.28923300	1.85969600	0.07285600
H	-10.36713400	-11.16013600	6.63850700

C	3.63092800	3.33334700	0.43302700
C	-3.43044800	2.36974300	-0.99112800
C	-13.74078900	10.48710000	-2.21633600
C	-14.64363000	-8.39714700	-0.21333600
H	7.41513600	-13.05672800	-4.62883700
H	-5.50033300	-2.99240500	2.05883700
C	13.22121400	9.18964200	1.31840000
C	-15.04580100	-8.95874300	1.00892200
H	-3.03999400	-3.82383800	-0.77626300
H	2.70229500	-3.94939900	1.22880100
H	-12.80742900	13.15695200	-5.22051800
C	-7.01561100	5.13434300	-1.15014000
C	-15.53470900	-6.38864700	-1.48169100
H	-11.17531600	12.49971500	-5.43546800
C	-12.30600700	5.90264000	-1.27847300
C	-8.67536700	-5.62353300	2.14335400
C	8.27889200	-12.60894100	-4.12427500
H	8.68075600	7.48813400	-0.09138900
C	-10.96382200	-8.02997500	0.51439400
C	13.26095300	2.36552200	0.68953800
H	13.90489700	12.72272900	5.15421900
H	-13.40502700	14.41467100	-3.01794400
H	8.83371600	-10.60001400	-5.95481200
C	-14.54112700	-9.59843600	3.35889500
H	-6.54235900	6.41910600	0.53250700
H	6.60284400	6.21098300	-0.22578200
H	10.27992700	11.78112600	4.63976300
H	-16.09418800	-8.97328600	1.28574800
H	10.49889500	10.78511400	2.60595300
C	12.29754800	-8.75636100	-4.43858500
C	12.08524800	6.37647100	1.91664700
H	-13.39043800	9.60233800	0.74614400
H	-12.85743000	8.08616400	0.02435400
C	10.29570800	-6.88293200	-2.29992200
C	10.79842800	7.10836100	1.62894400
H	13.46342900	1.47020200	0.08861100
C	14.19028300	9.73435900	2.19588600

H	8.39553900	-13.10445100	-3.15357500
C	-11.94413100	12.06925700	-2.78825900
C	13.05420400	6.90965400	2.80366900
C	13.86313500	-6.29790300	-1.99970200
H	-15.77132100	-5.86687000	-0.54724700
H	-5.84586700	3.45183900	-1.80807100
H	5.56695900	-2.70729800	-2.22080900
C	-11.80956500	-10.52401700	2.23044600
H	14.10314600	13.61406900	3.62903000
H	17.27174100	-6.38760200	0.97821600
H	2.06240100	0.65883100	1.87580200
C	12.64595400	7.68153600	4.03869800
H	15.86012500	-8.96359600	-1.44754800
H	7.70156200	-9.38964700	-5.32537500
H	8.02687100	3.57299800	2.86862400
H	-12.04318000	15.50854300	-3.32780000
H	-7.84484900	4.06907700	-2.83512400
C	11.85890700	9.44350100	1.63048500
H	5.89136500	-11.33924300	-3.70993900
H	-9.85436100	5.48026700	-3.03508300
C	15.49550300	7.65278400	2.79218100
H	12.83906200	7.04971700	4.91741500
H	-15.67979800	3.80635700	-2.21091500
C	8.85720100	-4.87749800	-2.88684100
C	-6.99211800	-6.30807200	0.03975600
C	-11.48608900	10.03289100	-1.47487000
H	-15.82047400	10.48144400	-2.95982600
H	-6.32911400	-6.59307100	-0.77275600
C	-13.90520300	-9.03948100	4.42377300
H	13.52568200	2.14743500	1.73064400
H	-1.00119900	-2.52577700	-1.16767300
C	-12.13035900	8.48971100	-4.06776300
H	4.12333100	1.96725700	2.04532600
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C	-12.52810700	-8.45908600	4.40375100
H	-4.02622500	-1.25749800	2.54215800

C	10.37404400	-11.08417200	-2.80609300
C	-17.10124000	-8.27113400	-0.92688500
H	-4.17403100	2.11477500	-1.73874200
C	-15.63933100	-7.92742100	-1.29433400
C	12.73313300	-11.08978700	-2.03459700
H	-15.98866300	-8.30009800	-3.42481900
C	-9.49266900	-8.66517500	7.52735900
C	-15.29928800	-8.62994500	-2.63759800
H	-8.74950500	-8.23510800	3.61570300
H	-14.47251900	8.72415300	-0.33629000
C	7.91260700	-10.46300400	-5.37659700
C	14.41597300	6.66388900	2.49297400
C	17.52020400	-6.50114200	-1.78002000
C	-3.62266500	3.49625800	-0.15895200
H	-8.80291500	-9.03783400	8.29484700
C	-1.46808000	2.99462300	0.89001700
C	-2.61062900	3.78445300	0.78287300
C	14.74351800	5.57878600	1.65483600
H	10.11446400	4.87362600	3.00850800
C	-2.29541200	1.57414000	-0.87636700
H	15.91015200	3.01376300	1.24133000
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H	12.77202900	-12.16445400	-1.85856700
H	-9.15402900	-11.39392400	5.36733400
H	12.18470200	2.56430000	0.64979100
H	14.79485000	-11.08168200	-2.42503500
H	8.39335100	-8.41429900	-3.39275400
H	0.69283100	3.18895800	-1.32026300
H	15.79400700	5.37279100	1.48125800
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H	-2.72793100	4.64540100	1.43546200
C	-8.14623900	-7.05187600	0.27306400
C	16.42776600	-6.87490400	0.47428800
H	10.54928800	-12.10213800	-3.13651100
H	6.24538300	-5.92083400	-0.22264700
C	10.15394000	-8.37887400	-2.16955500
H	-11.94232100	-9.61782900	6.10749600

H	15.85458900	-4.27271700	-1.77265000
H	-13.97256600	12.15749800	-3.54247300
H	-8.54224700	7.80736400	0.33585200
C	-14.07997300	7.45781600	-2.76469600
H	1.84538600	-0.07452600	-1.73429600
H	5.91653700	3.13999100	1.98234800
C	-11.58148700	-8.99849000	5.29079000
H	-10.51534700	-8.86526700	7.86484800
H	14.26834700	4.67529600	-1.73480400
H	17.41521000	-6.06897000	-2.78177800
H	11.67263500	4.87500200	0.44233700
C	-13.42895000	8.99394400	-0.16955200
C	-12.68186500	7.65450600	-2.93372300
H	-16.06800200	5.13648900	-0.00375200
H	15.15018000	-4.52332400	-0.15994800
H	13.02608200	7.52648400	-0.09638500
C	16.22985500	-6.27456800	-0.94501900
C	1.39446000	-2.30438200	0.78932400
C	14.08206700	3.57086400	0.15401300
C	9.17301200	-9.02378500	-2.94744800
C	-7.52361600	-4.87996400	1.90881000
C	-14.84898300	3.29749400	-1.71027900
H	16.63646500	-7.94932500	0.43388300
H	-15.59399200	3.70574800	0.92752800
C	-10.53590900	7.65311800	-1.56049800
C	15.06930700	-8.35687600	-1.88012300
H	16.32590900	9.57935900	2.74145700
H	17.74129200	-7.56770900	-1.89504100
H	-15.38507600	-9.71819200	-2.53918100
C	-9.02679500	-6.72015900	1.32362800
H	-9.32711200	-5.35443000	2.96793800
H	-4.78757900	5.18485100	0.49288300
H	-17.42619300	-7.74776000	-0.02019300
H	-14.37159500	-9.15591600	5.40164500
H	-14.12970800	2.99057800	-2.47826400
H	-14.75993200	5.25328900	1.18681700
H	7.09000000	-10.94144900	-5.92254100

C	13.75966000	4.81706600	1.00463700
C	12.44196700	5.30378300	1.07621300
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C	-13.26314000	-8.17629800	-0.37611000
C	8.05312800	-11.08824700	-3.96122600
C	15.58128700	3.19803600	0.21212300
H	11.68844400	11.56177200	5.69272600
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H	12.63564300	4.04927400	-1.44258000
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C	-9.79438900	-8.23548300	3.90059200
H	16.21290500	3.98467800	-0.21672000
C	-7.73282700	-9.04791200	5.77757500
C	16.01110200	-4.75108000	-0.79902200
H	0.71093200	-2.54682400	1.59629400
H	-9.76855700	13.73864500	-2.15052600
H	-9.98167500	11.37130000	-2.21398800
H	-11.44013700	14.25682400	-5.46486800
C	13.85156900	10.84959500	2.99203900
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C	12.15166500	12.62072000	3.82578000
C	-8.38063700	7.01041800	-0.38253500
C	-14.52773700	6.33954800	-2.04117100
H	15.75505300	2.28292800	-0.36543800
C	6.75612300	-4.42782600	-1.71157000
C	11.48209400	-6.29528200	-2.66374300
C	10.76955700	8.46046800	1.39228000
H	-9.36883600	-7.57870800	7.45248100
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H	-9.74865100	14.65561100	-3.66687600
H	11.53766100	-9.16780600	0.57017700
C	-13.64155600	5.48323700	-1.35942600
H	13.49613900	9.07846000	-0.78417000
H	-13.45186400	2.50060300	0.46993400

H	-12.60779100	9.46453200	-4.17352900
H	-10.57814400	-7.81073800	-0.48003100
H	-12.90987700	-7.56484100	-1.20189700
H	-12.56320700	3.98660200	0.83049200
H	11.13008500	14.51286400	3.40656700
H	8.23026900	-7.30565000	-0.59563500
H	13.70011000	-5.27648200	-1.67409200
H	11.48675700	-5.20765600	-2.71636900
C	14.05360000	-9.00830200	-2.60338200
C	-10.19614400	-8.81800100	5.11087100
C	-11.04985500	11.19472800	-2.15330200
C	-15.07941100	8.52240700	-3.08175100
H	4.62623000	-4.53961400	0.05393600
H	2.77905100	4.49095400	-1.17868700
H	-7.06503200	-9.39821000	6.57292300
H	13.19959100	8.60992400	4.18285000
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C	13.70231100	3.82816200	-1.33042700
H	-12.29603000	7.94485300	-5.00803300
H	11.57921400	7.91199800	4.02856900
H	-14.27885200	-8.40068100	-2.96281800
H	-15.24456800	2.39431100	-1.22920600
H	3.80787300	-1.48264600	-2.12714700
C	11.89704300	-8.63309200	-0.32059600
H	-17.76702600	-7.96487200	-1.74182700
C	-11.82651400	7.01390900	-2.00783800
H	-2.17550300	0.71792000	-1.53072200
H	-15.59931100	6.17416700	-1.96886100
H	14.67928700	8.13040500	0.11994900
H	-15.51919300	-10.04452600	3.53639200
C	9.07823600	-6.04791900	-2.13147300
C	-12.33132200	14.56004200	-2.85762400
H	12.97578600	-8.78449200	-0.37232900

Ground state P.E = -6270.366058 Hartree; Number of imaginary frequency = 0

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- 1 M. Tashiro and T. Yamato, *J. Am. Chem. Soc.*, 1982, **104**, 3701–3707.
- 2 R. H. Mitchell, Y. H. Lai and R. V. Williams, *J. Org. Chem.*, 1979, **44**, 4733–4735.