Supplemental Information

Wavy-shaped Polycyclic Hydrocarbons with Controlled Aromaticity

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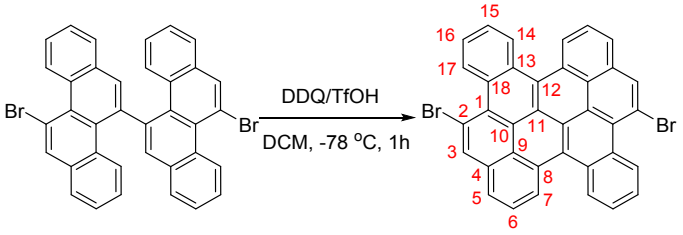
1. Experimental Procedures

1.1 General methods and materials

^{1}H (500.13 MHz) and ^{13}C (125.77 MHz) nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III 500 spectrometer using a 5 mm $^{1}H/^{13}C/^{19}F/^{31}P$ gradient probe. CD_2Cl_2 ($\delta(^{1}H)$ = 5.33 ppm, $\delta(^{13}C)$ = 53.7 ppm), $CDCl_3$ ($\delta(^{1}H)$ = 7.26 ppm, $\delta(^{13}C)$ = 77.0 ppm) or $C_2D_2Cl_4$ ($\delta(^{1}H)$ = 5.98 ppm, $\delta(^{13}C)$ = 73.7 ppm) were used as solvent, lock and internal standard. The 2D NMR spectra were recorded using the standard pulse sequences of the Bruker software package (TOPSPIN 3.2). The sample temperature was controlled by the Bruker variable temperature accessory BVT-3000. The mass spectrometry analysis was performed on a Bruker Autoflex Speed MALDI TOF MS (Bruker Daltonics, Bremen, Germany) using dithranol as matrix. High-resolution ESI mass spectra were recorded in the positive mode with a Finnigan LTQ-FT from Fisher Thermo Scientific. Elemental analysis (EA) was carried out using an Euro EA 3000 CHNS-O Elemental Analyzer from Eurovector Instruments & Software (Italy). UV/visible (UV/Vis) spectra were measured on an Agilent Cary 5000 UV-VIS-NIR spectrophotometer by using 10 mm optical-path quartz cell at room temperature. Electron paramagnetic resonance (EPR) spectra were recorded in the solid form by using a Bruker X-band spectrometer ESP300 E, equipped with an NMR gauss meter (Bruker ER035), a frequency counter (Bruker ER 041 XK) and a variable temperature control continuous flow N_2 cryostat (Bruker B-VT 2000). The temperature dependent magnetization measurement was assessed using a SQUID-VSM (Superconducting Quantum Interference Device - Vibrating Sample Magnetometer, Quantum Design, Inc.). Powder sample with a weight of 5~10 mg was sealed in a plastic capsule. Magnetic moment was measured in the temperature range of 5 to 400 K. Bleaney-Bowers equation was used to fit the $\chi T-T$ plot. Cyclic voltammetry (CV) measurements were carried out on a CHI 760 E potentiostat (CH Instruments, USA) in a three-electrode cell in a dichloromethane solution of nBu$_4$NPF$_6$ (0.1 M) with a scan rate of 50 mV/s at room temperature. A Pt wire, Ag/AgCl (3M KCl solution), and a glassy carbon electrode were used as the counter electrode, the reference electrode, and the working electrode, respectively. 11,11'-Dibromo-5,5'-bichrysene (**3**),[1] 2,5-dibromoterephthalaldehyde (**5**)[2] and 4,6-dibromoisophthalaldehyde (**10**)[3] were synthesized according to the literature.

1.2 Detailed synthetic procedure and characterization data

9,18-Dibromobenzo[*a*]dinaphtho[2,1,8-*cde*:1',2',3',4'-*ghi*]perylene (4)

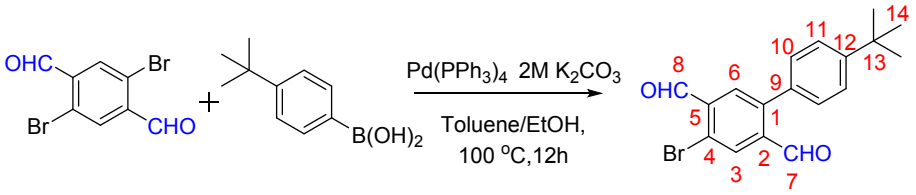


3 **4**

To a mixture of 11,11'-dibromo-5,5'-bichrysene (**3**) (50 mg, 0.08 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (41 mg, 0.18 mmol) in dry dichlormethane (DCM) (9.5 mL) at -78 °C was added trifluoromethanesulfonic acid (0.5 mL). After 1 h, the resulting mixture was quenched by triethylamine and was concentrated under reduced pressure, then the residue was dispersed in methanol. The solid was filtrated, washed with methanol to afford 35 mg (72%) of compound **4** as a red solid. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 9.75 (d, 8.3 Hz, 2H; 17), 8.92 (d, 8.0 Hz, 2H; 14), 8.77 (d, 7.5 Hz, 2H; 7), 8.55 (s, 2H; 3), 8.03 (d, 7.7 Hz, 2H; 5), 7.95 (t, 7.7 Hz, 2H; 6), 7.73 (t, 8.0 Hz, 2H; 15), 7.69 ppm (t, 8.2 Hz, 2H; 16). ^{13}C NMR (125 MHz, $C_2D_2Cl_4$): δ 134.0 (3), 132.0 (4), 128.7 (18), 128.6 (8), 128.5 (13), 128.4 (7), 127.5 (15), 127.0 (14), 126.8 (17), 126.7 (6), 125.4 (5), 124.8 (1), 124.5 (10 or 11), 124.2 (12), 124.1 (9), 124.0 (16), 123.9 (10 or 11), 117.9 ppm (2). HR-MS (MALDI):

m/z = 605.9618, calcd. for $C_{36}H_{16}Br_2$ ([M] $^+$): m/z = 605.9619, error = -0.1 ppm. EA calculated for $C_{36}H_{16}Br_2$: C 71.08%, H 2.65%, found: C 70.04%, H 2.43%.

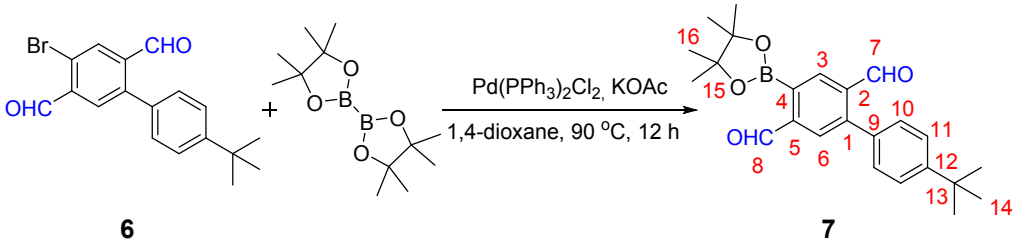
4-Bromo-4'-(*tert*-butyl)-[1,1'-biphenyl]-2,5-dicarbaldehyde (6)



5 **6**

A suspension of compound **5** (4.8 g, 16.44 mmol), (4-(tert-butyl)phenyl)boronic acid (1.46 g, 8.22 mmol), $Pd(PPh_3)_4$ (190 mg, 0.16 mmol) and 2M aqueous solution of K_2CO_3 (8 mL) in toluene (60 mL) and EtOH (8 mL) was degassed by three freeze–pump–thaw cycles. The reaction mixture was heated at 100 °C overnight under argon. After cooling to room temperature, the mixture was extracted with DCM and washed with water. The organic layer was dried over anhydrous $MgSO_4$. The solvent was removed under vacuum and the residue was purified by silica gel column chromatography using DCM/hexane (3/1, v/v) as eluent to give the crude product as a yellow solid then recrystallization with chloroform for two times to get compound **6** (1.85 g) as a white solid in 65% yield. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 10.43 (s, 1H; 8), 9.96 (s, 1H; 7), 8.22 (s, 1H; 3), 7.97 (s, 1H; 6), 7.54 (d, 8.4 Hz, 2H; 11), 7.33 (d, 8.4 Hz, 2H; 10), 1.37 ppm (s, 9H; 14). ^{13}C NMR (125 MHz, CD_2Cl_2): δ 191.3 (8), 190.8 (7), 152.3 (12), 145.1 (1), 138.2 (2), 136.4 (5), 133.2 (3), 133.0 (9), 132.5 (6), 129.9 (10), 126.1 (11), 125.3 (4), 35.0 (13), 31.3 ppm (14). HR-MS (ESI): m/z = 344.0407, calcd. for $C_{18}H_{17}BrO_2$ ([M] $^+$): m/z = 344.0412, error = -1.51 ppm.

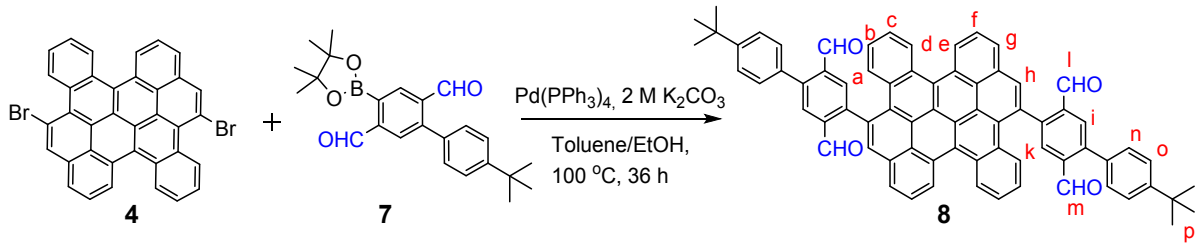
4'-(*tert*-Butyl)-4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1'-biphenyl]-2,5-dicarbaldehyde (7):



6 **7**

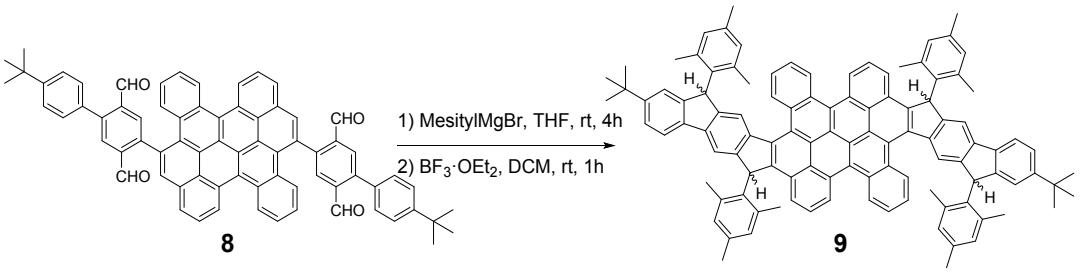
Compound **6** (300 mg, 0.87 mmol), bis(pinacolato)diboron (441 mg, 1.74 mmol), $Pd(PPh_3)_2Cl_2$ (30 mg, 0.045 mmol), KOAc (170 mg, 1.74 mmol) and dry 1,4-dioxane (10 mL) were added to a Schlenk flask equipped with a magnetic stirrer. The reaction mixture was purged with argon by 30 min and then stirred at 90 °C for 20 h. After cooling to room temperature, the mixture was diluted with ethyl acetate and washed with water and brine before drying with $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified by short column chromatography over silica gel (ethyl acetate) to give compound **7** (341 mg, 91%) as a white waxy solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.67 (s, 1H; 8), 10.08 (s, 1H; 7), 8.50 (s, 1H; 3), 8.05 (s, 1H; 6), 7.52 (d, 8.4 Hz, 2H; 11), 7.3 (d, 8.4 Hz, 2H; 10), 1.41 (s, 12H; 16), 1.38 ppm (s, 9H; 14). ^{13}C NMR (125 MHz, $CDCl_3$): δ 194.08 (8), 192.16 (7), 152.06 (12), 147.62 (1), 144.11 (5), 136.04 (2), 135.63 (3), 133.66 (9), 130.8 (very br; 4; identified by HMBC correlation to H_6), 129.98 (6), 129.78 (10), 125.68 (11), 84.78 (15), 34.75 (13), 31.29 (14), 24.90 ppm (16). HR-MS (ESI): m/z = 391.2193, calcd. for $C_{24}H_{29}BO_4$ ([M] $^+$): m/z = 391.2195, error = -0.45 ppm.

4,4''-(Benzo[*a*]dinaphtho[2,1,8-cde:1',2',3',4'-*ghi*]perylene-9,18-diyl)bis(4'-(*tert*-butyl)-[1,1'-biphenyl]-2,5-dicarbaldehyde) (8)



In a two-necked round-bottom flask equipped with a condenser, a mixture of compound **4** (100 mg, 0.16 mmol) and compound **7** (258 mg, 0.66 mmol) in toluene (15 mL), 2 M aqueous solution of K_2CO_3 (1.5 mL) and EtOH (1.5 mL) was degassed with argon for 30 minutes. Then, $Pd(PPh_3)_4$ (19 mg, 0.16 mmol) was added. After deoxygenation by three "freeze-pump-thaw" cycles, the reaction mixture was heated to 100 °C for 36 h under argon. After cooling to room temperature, the reaction solvent was removed under vacuum and the residue was purified by silica gel column chromatography using EtOAc/hexane (1/4, v/v) as eluent to obtain the title compound **8** (98 mg, 61%) as an orange solid. Final purification was done by recycling gel permeation chromatography using $CHCl_3$ as the eluent. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 120°C): *δ* 10.30 (br, 2H; m), 10.08 and 9.87 (br, 2H; l), 9.28 (d, 8.5 Hz, 2H; d), 9.16 (d, 7.8 Hz, 2H; e), 8.52 and 8.41 (br, 2H; h, i or k), 8.8-8.25 (6H; h, i or k and g), 8.25 8.1 (2H; a , f), 7.73 (t, 7.8 Hz, 2H; b), 7.68 (d, 8.0 Hz, 4H; o), 7.60 (d, 8.0 Hz, 4H; n), 7.40 (t, 7.8 Hz, 2H; c), 1.44 ppm (s, 18H; p). ^{13}C NMR (125 MHz, $C_2D_2Cl_4$, 30°C): *δ* 192.2, 191.3, 191.0 (all CHO), 152.0, 146.4, 146.3, 144.9, 144.8, 137.4, 137.2, 136.2, 136.0, 133.3, 133.0, 132.5, 132.4, 131.1, 131.0, 130.6, 130.5, 130.2, 129.8, 129.3, 129.2, 129.1, 128.9, 128.6, 128.4, 128.0, 127.9, 127.6, 127.0, 126.8, 126.7, 126.5, 126.2, 126.0, 125.9, 125.7, 125.3, 124.9, 124.7, 124.6, 124.4, 123.9, 123.7, 34.5 (C_{tBu}), 31.2 ppm (CH_3). HR-MS (MALDI): m/z = 978.3702, calcd. for $C_{72}H_{50}O_4$ ([M]$^+$): m/z = 978.3709, error = -0.7 ppm. EA calculated for $C_{72}H_{50}O_4$: C 88.32%, H 5.15%, found: C 88.01%, H 5.45%.

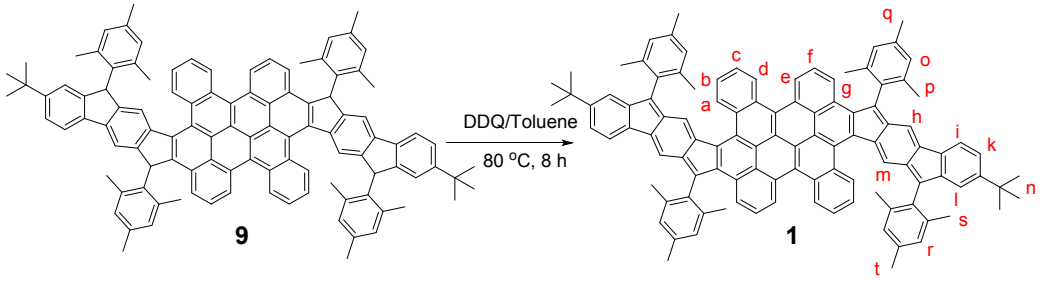
5,20-Di-*tert*-butyl-1,7,16,22-tetramesityl-1,7,16,22-tetrahydrobenzo[*a*]benzo[5,6]-*s*-indaceno[1,2-*k*]benzo[5',6']-*s*-indaceno[1',2':3,4]naphtho[2,1,8-*cde*]naphtho[1,2,3,4-*ghi*]perylene (9)



Compound **8** (30 mg, 0.03 mmol) was dissolved in 15 mL of dry THF under argon atmosphere. To the solution was added 0.6 mL mesitylmagnesium bromide solution (1M in THF, 0.6 mmol) and the mixture was stirred at room temperature for 4 hours. The reaction mixture was then poured into 30 mL water and extracted by chloroform. The organic layer was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The residue was then redissolved in 30 mL dry DCM under argon atmosphere and 1 mL of BF_3•OEt_2 was added. The mixture was stirred for 1 h and then washed with $NaHCO_3$ solution (3x20 mL) and water (3x20 mL). The organic layer was dried over $MgSO_4$ and the solvent was removed under reduced pressure. The residue was purified by column chromatography (silica gel, n-hexane/DCM (1/1, v/v)) to give compound **9** as a red solid (36 mg, 87% in two steps). The ^{1}H NMR spectrum of compound **9** is very complex. VT measurements (-50°C – 120°C) reveal internal motions by line narrowing and line broadening effects. Signals of different intensity point to minor and

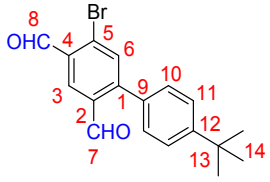
major isomers. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 120°C): selected signals δ 9.25, 9.10, 8.35, 8.00. 7.89. 7.76, 7.45, 7.31, 7.08, 6.81, 6.67. 6.31, 5.72, 5.64, 3.15, 2.79, 2.73, 2.42, 2.31, 1.37 ppm. ^{13}C NMR (125 MHz, $C_2D_2Cl_4$, 30°C): selected signals 150.5, 147.8, 139.9, 137.8, 136.0, 135.5, 130.7, 130.2, 129.2, 128.7, 127.1, 123.8, 121.0, 119.6, 114.8, 50.2, 49.6, 34.7, 31.4, 22.5, 22.3, 21.7, 21.1, 20.9, 18.5 ppm. HR-MS (MALDI): m/z = 1386.7039, calcd. for $C_{108}H_{90}$ ([M]$^+$): m/z = 1386.7043, error = -0.2 ppm. EA calculated for $C_{108}H_{90}$: C 93.46%, H 6.54%, found: C 93.21%, H 6.75%.

5,20-Di-*tert*-butyl-1,7,16,22-tetramesitylbenzo[*a*]benzo[5,6]-*s*-indaceno[1,2-*k*]benzo[5',6']-*s*-indaceno[1',2':3,4]naphtho[2,1,8-*cde*]naphtho[1,2,3,4-*ghi*]perylene (1)



To a 25 mL flask with a stir bar was added **9** (30 mg, 0.02 mmol) and dry toluene (10 mL). The mixture was degassed by three freeze-thaw cycles and then brought to 80 °C. Then, DDQ (36 mg) in toluene (1.8 mL) was added dropwise via a syringe. After stirring for 8 hours, the reaction was cooled down. After evaporation of the solvent, the residue was purified by column chromatography (n-hexane/DCM = 1/1) to yield compound **1** as a dark-brown coloured solid (23 mg, 76 %). ^{1}H NMR (500 MHz, $C_2D_2Cl_4$): δ 9.52 (d, 8.0 Hz, 2H; a), 8.92 (d, 8.0 Hz, 2H; d), 8.76 (d, 7.5 Hz, 2H; e), 7.75 (s, 2H; m), 7.61 (t, 7.5 Hz, 2H; c), 7.57 (t, 8.0 Hz, 2H; f), 7.47 (d, 8.4 Hz, 2H; g), 7.43 (t, 7.6 Hz, 2H; b), 7.18 (d, 7.8 Hz, 2H; i), 7.14 (s, 4H; o or r) 7.00 (s, 4H; o or r), 6.99 (d, 7.8 Hz, 2H; k), 6.66 (4H; h and l), 2.52 (s, 6H; q or t) 2.39 (s, 6H; q or t) 2.31 (br, 24H; p and s) 1.21 ppm (s, 18H; n). At 120 °C line broadening is observed for several signals of the core whereas the signals of the mesitylene groups become narrower and the broad signal of the methyl groups p and s results in two signals at 2.37 and 2.33 ppm, respectively. ^{13}C NMR (125 MHz, $C_2D_2Cl_4$): δ 150.9 (C_{ar} ipso to tBu), 149.6, 146.1, 143.9, 139.9, 137.4 and 137.2 (C_{ar} ipso to q / t), 136.8, 136.3, 135.6, 132.6, 129.5, 128.9, 128.7, 128.1 (o or r), 128.0 (a and o or r), 127.3 (c and d), 126.9 (e), 126.2 (f), 125.7, 125.4 (m), 125.2, 124.9 (k), 123.7 (b), 123.4, 121.4 (g), 120.1 (h or l), 119.9 (i), 118.9 (h or l), 34.4 (C of tBu), 31.0 (n), 21.3 and 21.2 (q and t), 20.8 and 20.5 ppm (p and s). Due to broad signals only few correlations could be observed in the HMBC spectrum. Therefore, assignments are given only for protonated carbons, which could be assigned by their HSQC correlations. HR-MS (MALDI): m/z = 1382.6743, calcd. for $C_{108}H_{86}$ ([M]$^+$): m/z = 1382.6730, error = 0.9 ppm. EA calculated for $C_{108}H_{86}$: C 93.74%, H 6.26%, found: C 93.92%, H 6.04%.

5-Bromo-4'-(*tert*-butyl)-[1,1'-biphenyl]-2,4-dicarbaldehyde (11)

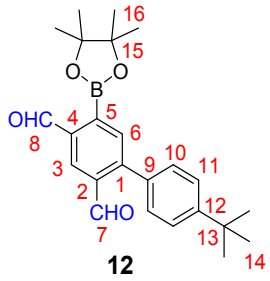


11

Starting from compound **10** and following a procedure similar to that for compound **6**, compound **11** was obtained as a white solid in 68% yield. ^{1}H NMR (500 MHz, CD_2Cl_2): δ 10.38 (s, 1H; 8), 9.96 (s, 1H; 7), 8.42 (s, 1H; 3), 7.81 (s, 1H; 6), 7.54 (d, 8.7 Hz, 2H; 11), 7.33 (d, 8.7 Hz, 2H; 10), 1.37 ppm (s, 9H; 14). ^{13}C NMR (125 MHz, CD_2Cl_2): δ

190.8 (7), 190.7 (8), 153.1 (12), 151.4 (1), 136.6 (6), 133.6 (2), 132.9 (4), 132.7 (9), 131.2 (5), 129.9 (10), 129.8 (3), 126.1 (11), 35.0 (13), 31.3 ppm (14). HR-MS (ESI): m/z = 344.0406, calcd. for $C_{18}H_{17}BrO_2$ ([M]$^+$): m/z = 344.0412, error = -1.61 ppm.

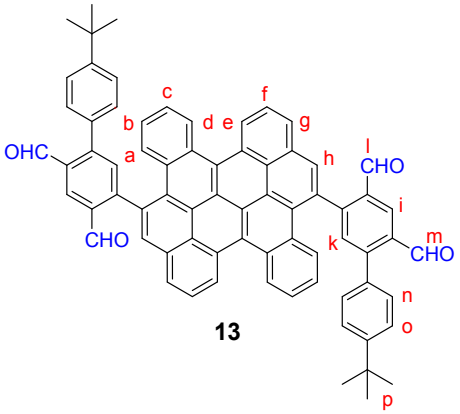
4'-(tert-Butyl)-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-[1,1'-biphenyl]-2,4-dicarbaldehyde (12)



12

Starting from compound **11** and following a procedure similar to that for compound **7**, compound **12** was obtained as a white solid in 88% yield. ^{1}H NMR (500 MHz, $CDCl_3$): δ 10.46 (s, 1H; 8), 10.05 (s, 1H; 7), 8.51 (s, 1H; 3), 7.87 (s, 1H; 6), 7.52 (d, 8.3 Hz, 2H; 11), 7.35 (d, 8.3 Hz, 2H; 10), 1.42 (s 12H; 16), 1.38 ppm (s, 9H; 14). ^{13}C NMR (125 MHz, $CDCl_3$): δ 193.0 (8), 191.7 (7), 152.1 (12), 149.3 (1), 139.9 (4), 137.7 (6), 137.2 (very br; 5, identified by HMBC correlation to H_3), 135.0 (2), 133.8 (9), 129.7 (10), 128.3 (3), 125.6 (11), 84.8 (15), 34.8 (13), 31.3 (14), 24.9 ppm (16). HR-MS (ESI): m/z = 391.2197, calcd. for $C_{24}H_{29}BO_4$ ([M]$^+$): m/z = 391.2195, error = 0.67 ppm.

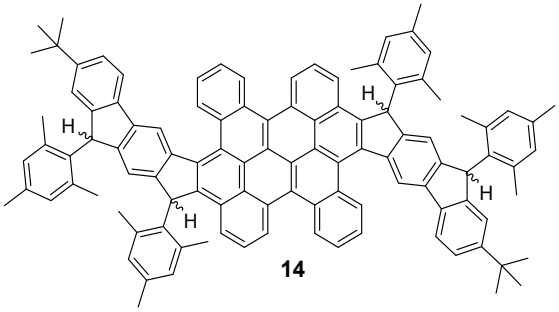
5,5''-(Benzo[a]dinaphtho[2,1,8-cde:1',2',3',4'-ghi]perylene-9,18-diyl)bis(4'-(tert-butyl)-[1,1'-biphenyl]-2,4-dicarbaldehyde) (13):



13

Starting from compound **4** and compound **12**, following a procedure similar to that for compound **8**, compound **13** was obtained as a yellow coloured solid in 66% yield. Final purification was done by recycling gel permeation chromatography using $CHCl_3$ as the eluent. Similar to compound **8**, the ^{1}H NMR spectrum of **13** is much more complex than expected from the chemical structure due to several isomers. VT measurements (30°C – 120°C) reveal internal motions by line narrowing and line broadening effects. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 120°C): δ 10.28 (s, 2H; m), 10.06 and 10.01 (br, 2H; l), 9.29 (d, 8.6 Hz, 2H; d), 9.15 (d, 7.6 Hz, 2H; e), 8.82 (s, 2H; h, i or k), 8.33 (d, 8.3 Hz, 2H; g), 8.30 (s, 2H; h, i or k), 8.21 (d, 8.6 Hz, 2H; a), 8.17 (t, 8.3 Hz, 2H; f), 7.96 and 7.94 (br s, 2H; h, i or k), 7.58 (d, 8.3 Hz, 4H; o), 7.49 (br d, 4H; n), 7.44 (t, 8.0 Hz, 2H; c), 1.44 ppm (s, 18H; p). ^{13}C NMR (125 MHz, $C_2D_2Cl_4$, 30°C): δ 191.6, 190.8, 190.7 and 190.6 (all CHO), 152.3, 151.9, 151.8, 150.6, 150.5, 133.5, 133.1, 133.0, 132.8, 132.7, 132.4, 130.9, 129.7, 129.4, 129.1, 129.0, 128.7, 128.6, 128.5, 128.0, 127.6, 126.8, 126.6, 125.8, 125.7, 125.6, 125.4, 125.1, 124.8, 124.4, 123.9, 123.8, 34.5 (C_{tBu}), 31.1 ppm (CH_3). HR-MS (MALDI): m/z = 978.3701, calcd. for $C_{72}H_{50}O_4$ ([M]$^+$): m/z = 978.3709, error = -0.8 ppm. EA calculated for $C_{72}H_{50}O_4$: C 88.32%, H 5.15%, found: C 88.60 %, H 4.99%.

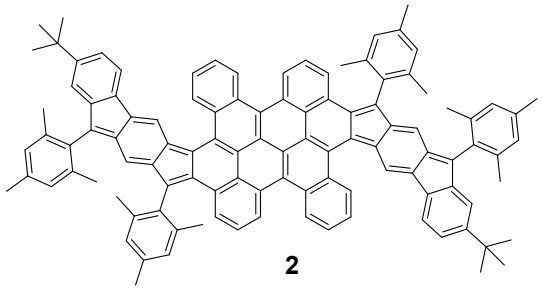
5,20-Di-*tert*-butyl-1,3,16,18-tetramesityl-1,3,16,18-tetrahydrobenzo[*a*]benzo[6,7]-*s*-indaceno[1,2-*k*]benzo[6',7']-*s*-indaceno[1',2':3,4]naphtho[2,1,8-*cde*]naphtho[1,2,3,4-*ghi*]perylene (14)



14

Starting from compound **13** and following a procedure similar to that for compound **9**, compound **14** was obtained as a yellow coloured solid in 88% yield. Similar to compound **9**, the ^{1}H NMR spectrum of compound **14** is very complex owing to diastereomers. VT measurements (-50°C – 120°C) reveal internal motions by line narrowing and line broadening effects. Signals of different intensity point to minor and major isomers. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 120°C): selected signals 9.62, 9.39, 9.18, 9.04, 8.0-7.7, 7.46, 7.25, 7.21, 7.17, 7.04,, 7.01, 6.71, 6.58, 6.31, 6.15, 5.65, 5.55, 3.03, 2.94, 2.75, 2.67, 2.5-2.2, 1.36 ppm. ^{13}C NMR (125 MHz, $C_2D_2Cl_4$, 30°C): selected signals 150.3, 146.9, 139.1, 137.7, 137.4, 136.1, 135.5, 130.3, 128.6, 127.5, 123.8, 122.6, 120.8, 119.6, 119.1, 115.1, 114.9, 50.5, 49.7, 34.6, 31.4, 22.5, 22.2, 21.7, 19.4, 19.0 ppm. HR-MS (MALDI): m/z = 1386.7043, calcd. for $C_{108}H_{90}$ ([M]$^{+}$): m/z = 1386.7043, error = 0 ppm. EA calculated for $C_{108}H_{90}$: C 93.46%, H 6.54%, found: C 93.48%, H 6.46%.

5,20-Di-*tert*-butyl-1,3,16,18-tetramesitylbenzo[*a*]benzo[6,7]-*s*-indaceno[1,2-*k*]benzo[6',7']-*s*-indaceno[1',2':3,4]naphtho[2,1,8-*cde*]naphtho[1,2,3,4-*ghi*]perylene (2)



2

Starting from compound **14** and following a procedure similar to that for compound **1**, compound **2** was obtained as a deep-green colored solid in 67% yield. ^{1}H NMR (500 MHz, $C_2D_2Cl_4$, 90°C): δ 9.12 (br, 2H; a), 8.81 (br, 2H; d), 8.50 (d, 8.0 Hz, 2H; e), 7.63 (4H; b, c), 7.29 (t, 8.0 Hz, 2H; f), 7.26 (br, 2H; h), 7.01 (s, 4H; o or r), 6.95 (d, 8.0 Hz, 2H; g), 6.92 (br s, 4H; o or r), 6.81 (br s, 4H; i and k), 6.34 (br s, 2H; l), 6.03 (br s, 2H; m), 2.41 (s, 6H; t or q), 2.34 (br s, 18H; t or q, p or s), 2.22 (s, 12H; p or s), 1.18 ppm (s, 18H; n). Recording a ^{13}C NMR spectrum was not successful in a reasonable measuring time due to the limited amount of substance and signal broadening also for ^{13}C NMR signals in the available temperature range. ^{1}H NMR (500 MHz, toluene-d_8, 70°C): δ 9.20 (br, 2H; a), 8.73 (br, 2H; d), 8.34 (d, 7.8 Hz, 2H; e), 7.49 (br, 2H; h), 7.36 (4H; b, c), 7.28 (d, 7.8 Hz, 2H; g), 7.00 (t, 7.8 Hz, 2H; f), 6.79 (s, 4H; o), 6.74 (d, 7.9 Hz, 2H; i), 6.70 (d, 7.9 Hz, 2H; k), 6.61 (br s, 4H; r), 6.54 (br s, 2H; l), 6.27 (br s, 2H; m), 2.42 (vbr s, 12H; p), 2.19 (br s, 12H; s), 2.06 (s, 6H; q), 1.03 ppm (s, 18H; n). HR-MS (MALDI): m/z = 1382.6731, calcd. for $C_{108}H_{86}$ ([M]$^{+}$): m/z = 1382.6730, error = 0.07 ppm. EA calculated for $C_{108}H_{86}$: C 93.74%, H 6.26%, found: C 93.64%, H 6.32%.

2. HR MALDI-TOF MS for 1 and 2

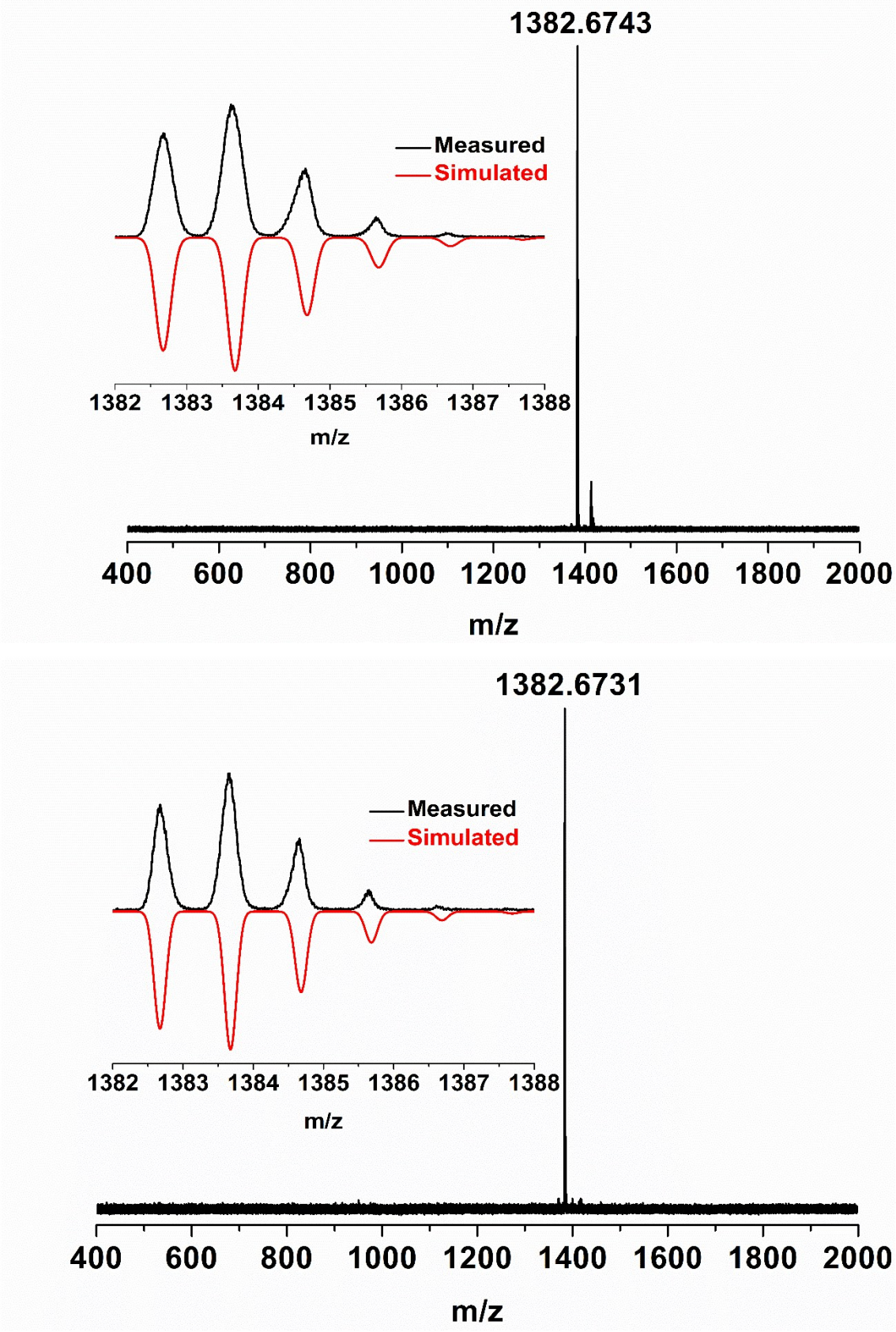


Figure S1. HR-MALDI-TOF mass spectra of **1** and **2**.

3. NMR spectra of 1 and 2

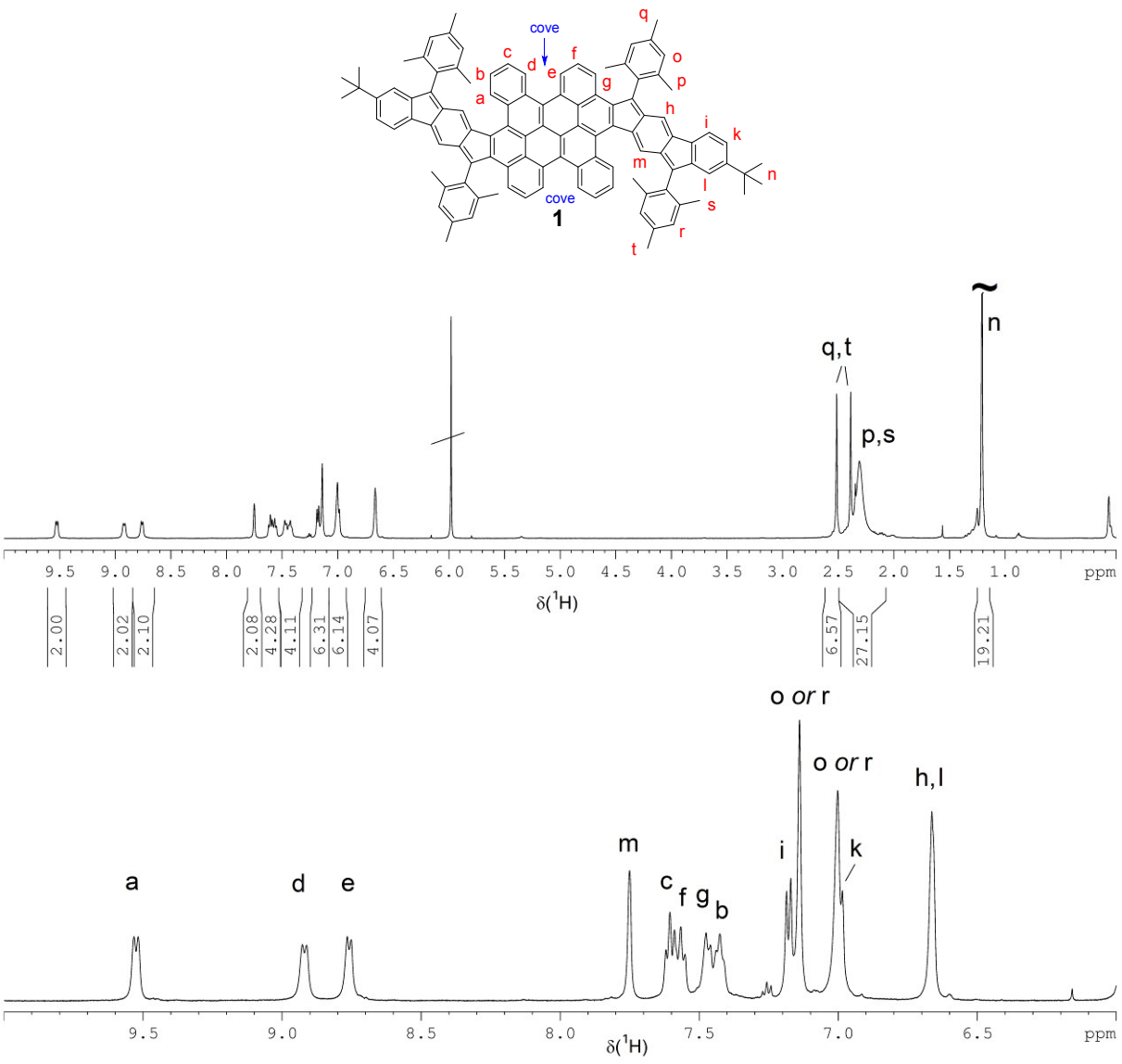


Figure S2. ^{1}H NMR spectrum of **1** (solvent: $C_2D_2Cl_4$, 303 K).

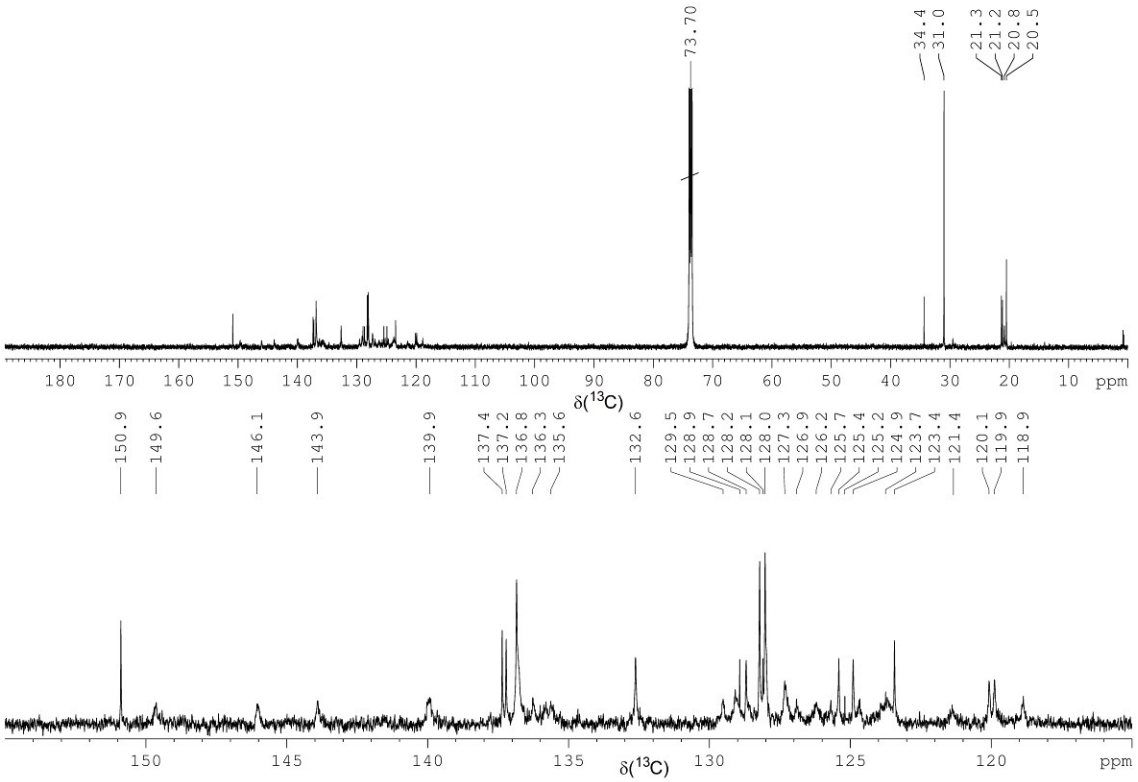


Figure S3. ^{13}C NMR spectrum of **1** (solvent: $C_2D_2Cl_4$, 303 K).

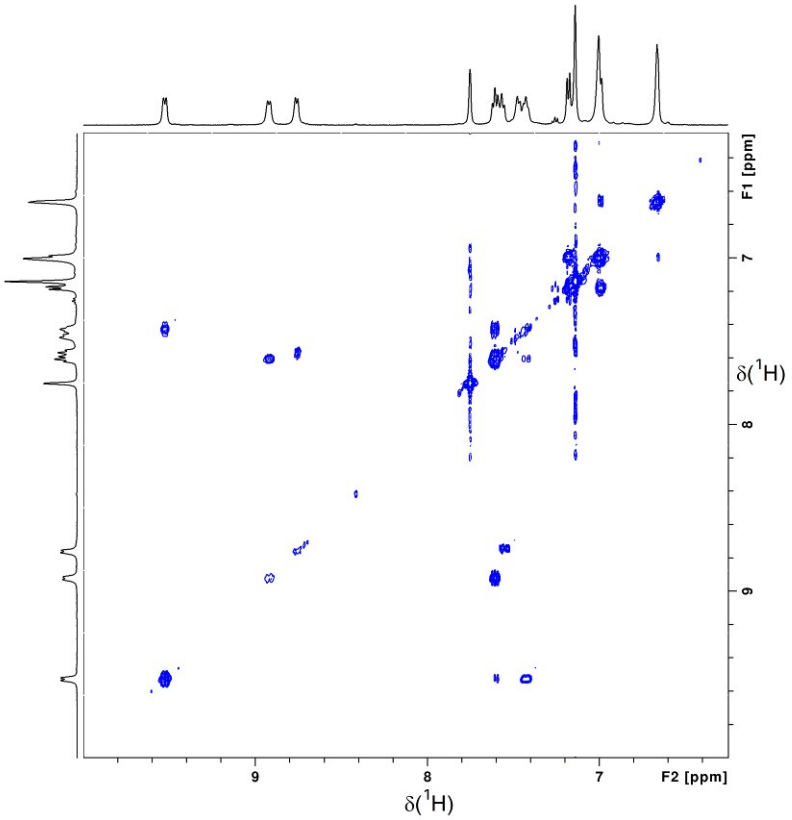


Figure S4. COSY spectrum (region) of **1** (solvent: $C_2D_2Cl_4$, 303 K).

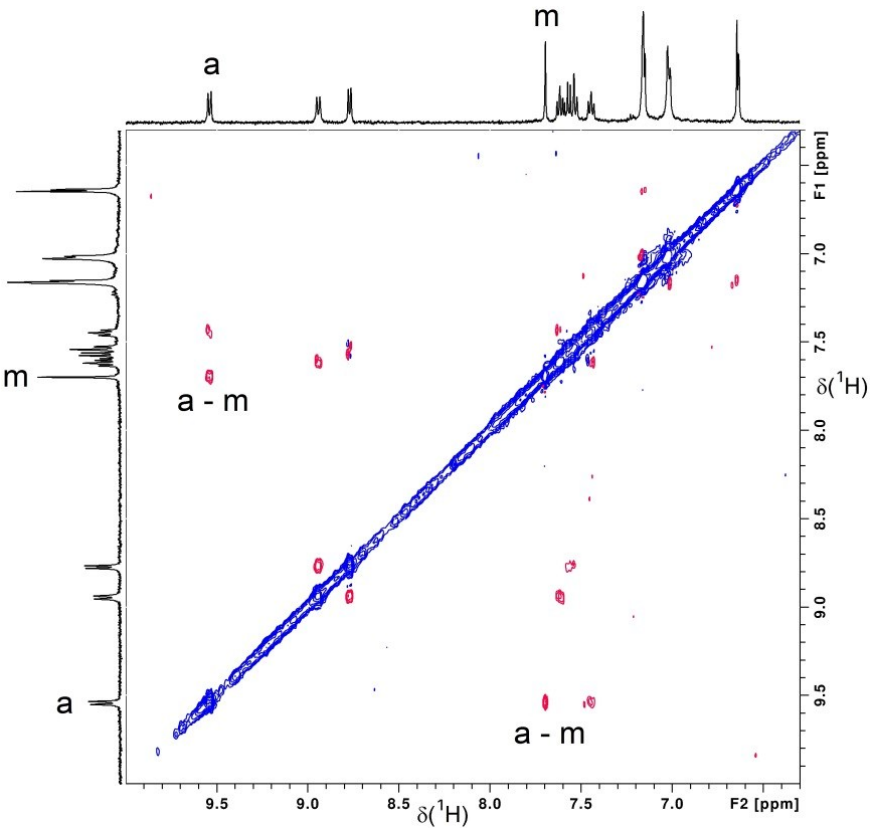


Figure S5. ROESY spectrum (region) of **1** (solvent: CD_2Cl_2, 303 K).

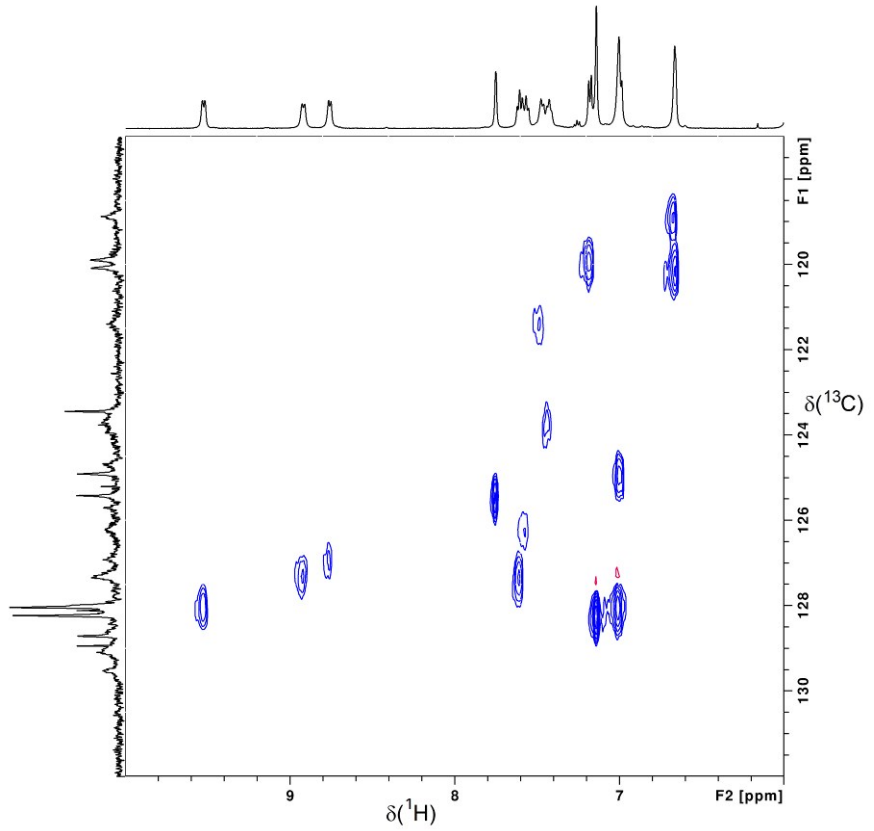


Figure S6. HSQC spectrum (region) of **1** (solvent: $C_2D_2Cl_4$, 303 K).

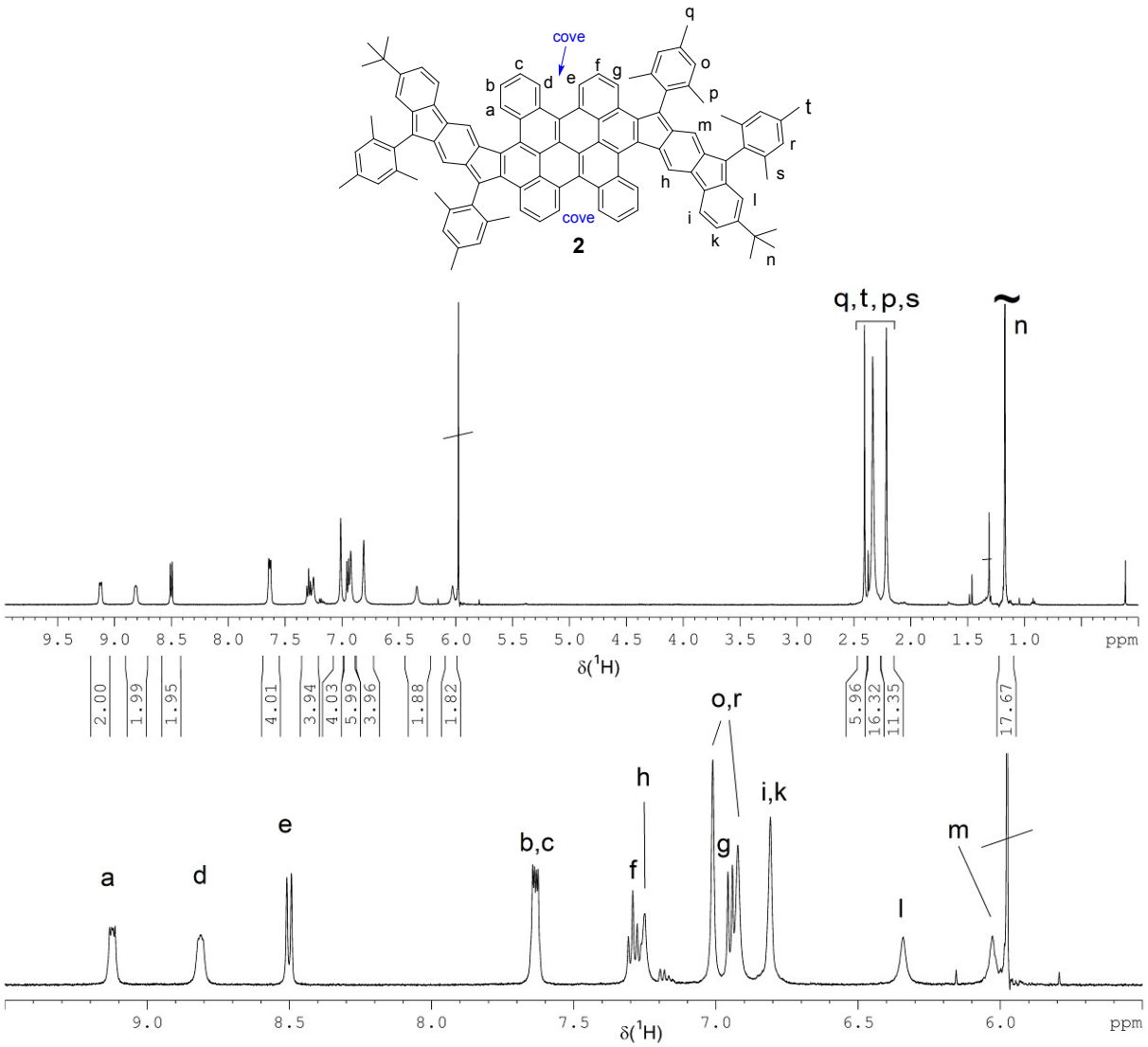


Figure S7. ^{1}H NMR spectrum of **2** (solvent: $C_2D_2Cl_4$, 363 K).

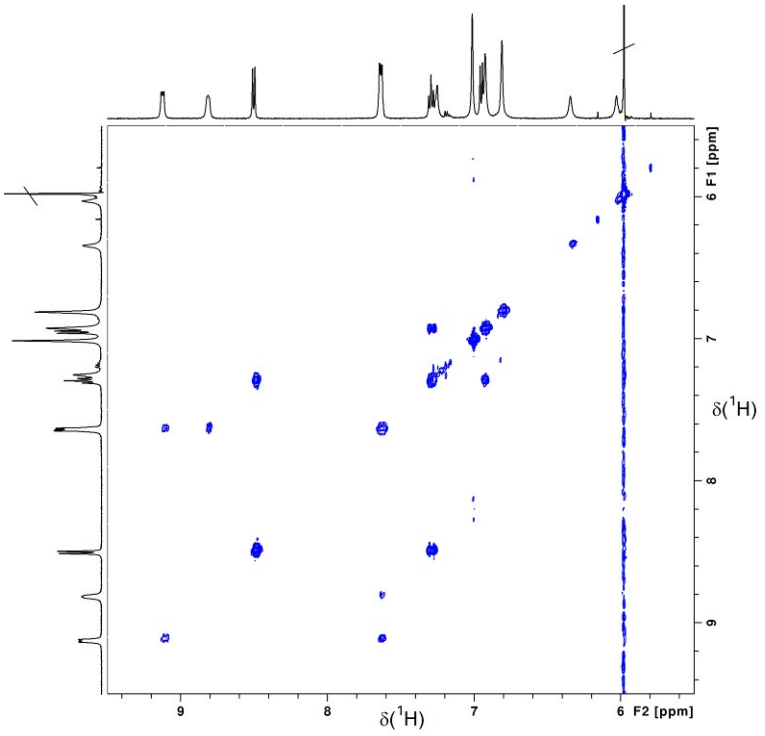


Figure S8. COSY spectrum (region) of **2** (solvent: $C_2D_2Cl_4$, 363 K).

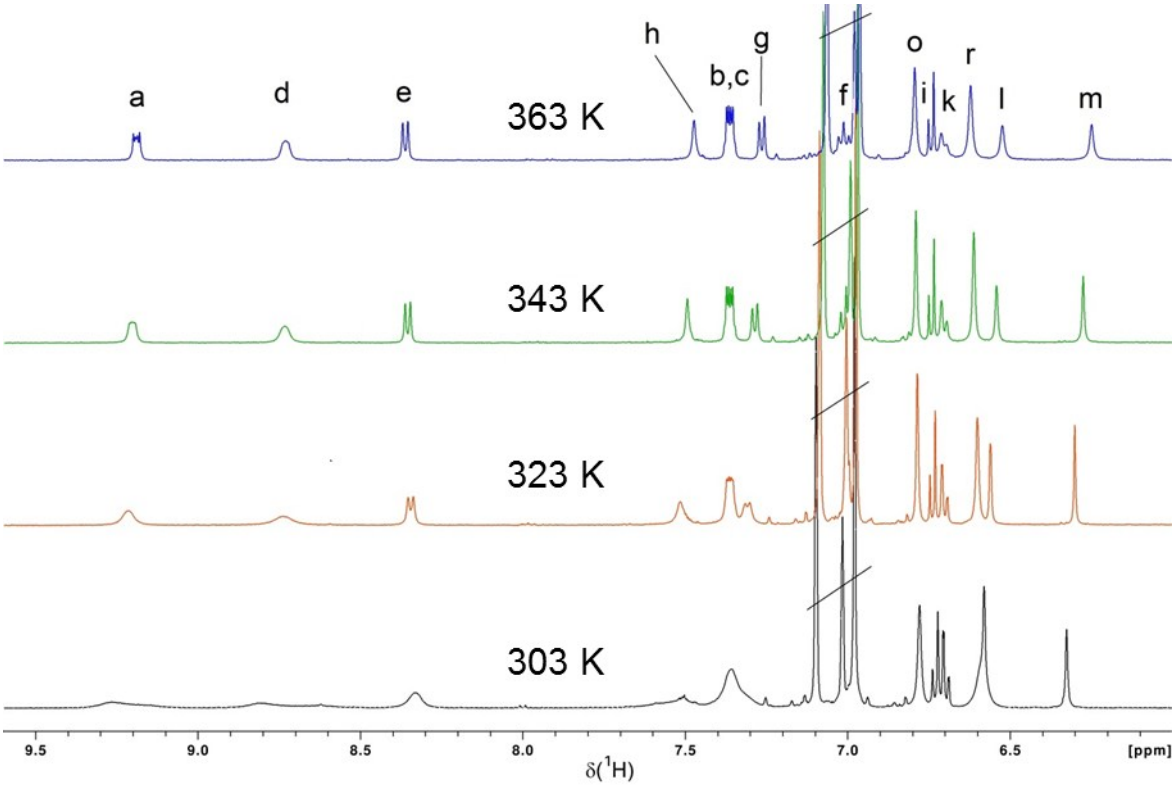


Figure S9. ^{1}H NMR spectra (region of aromatic protons) of **2** recorded in toluene-d_8 at different temperatures.

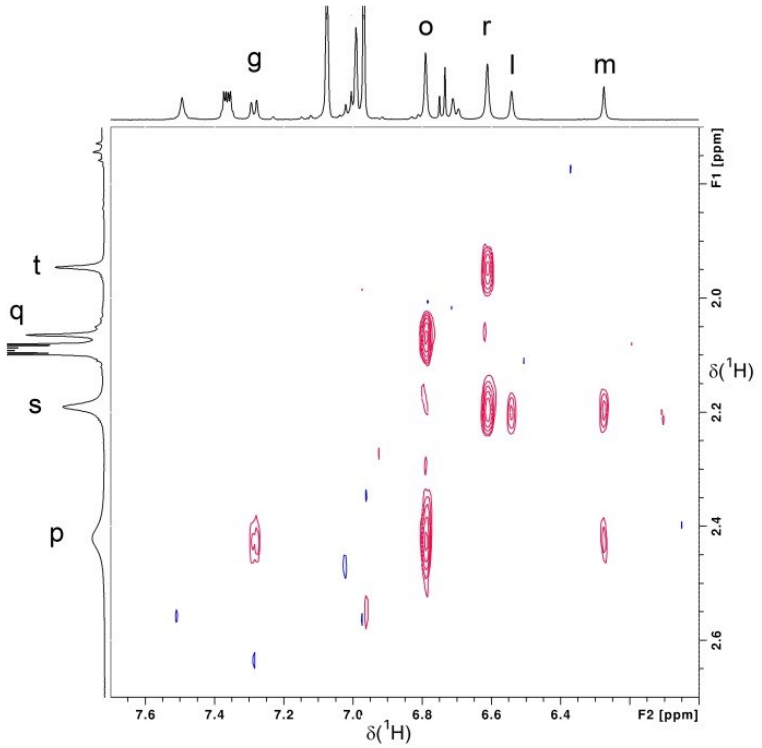


Figure S10. ROESY spectrum of **2** recorded in toluene-d_8 at 343 K. The depicted region shows the correlations that allow the assignment of the mesityl group signals o – q and r – t.

Temperature-dependent NMR measurement of 1 and 2 in different solvent

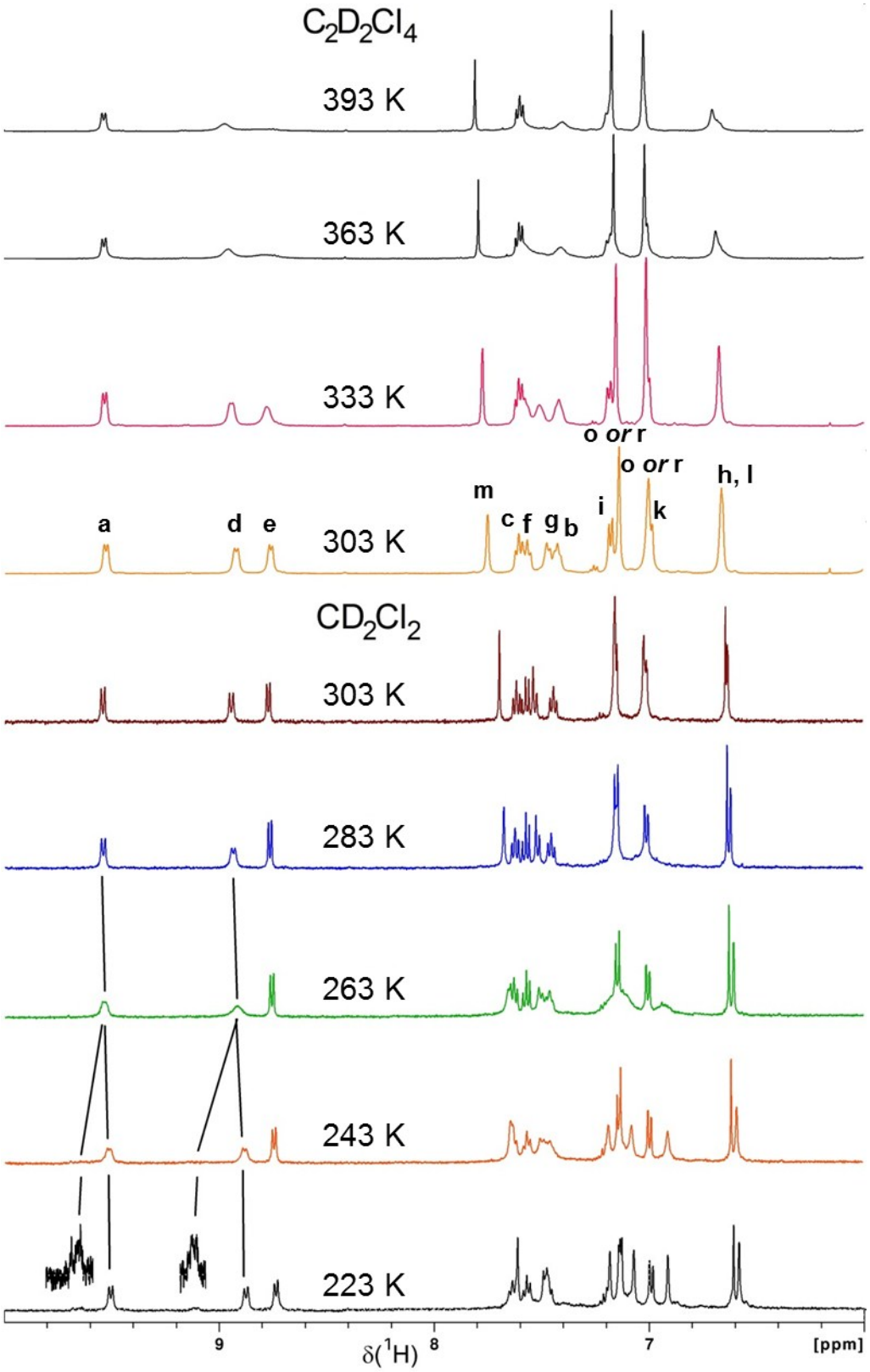


Figure S11. ^{1}H NMR spectra (region of aromatic protons) of **1** recorded in CD_2Cl_2 at 223, 243, 263, 283 and 303 K and recorded in $C_2D_2Cl_4$ at 303, 333, 363 and 393 K. The lines, which represent a guide for the eye, indicate coalescence processes of selected signals.

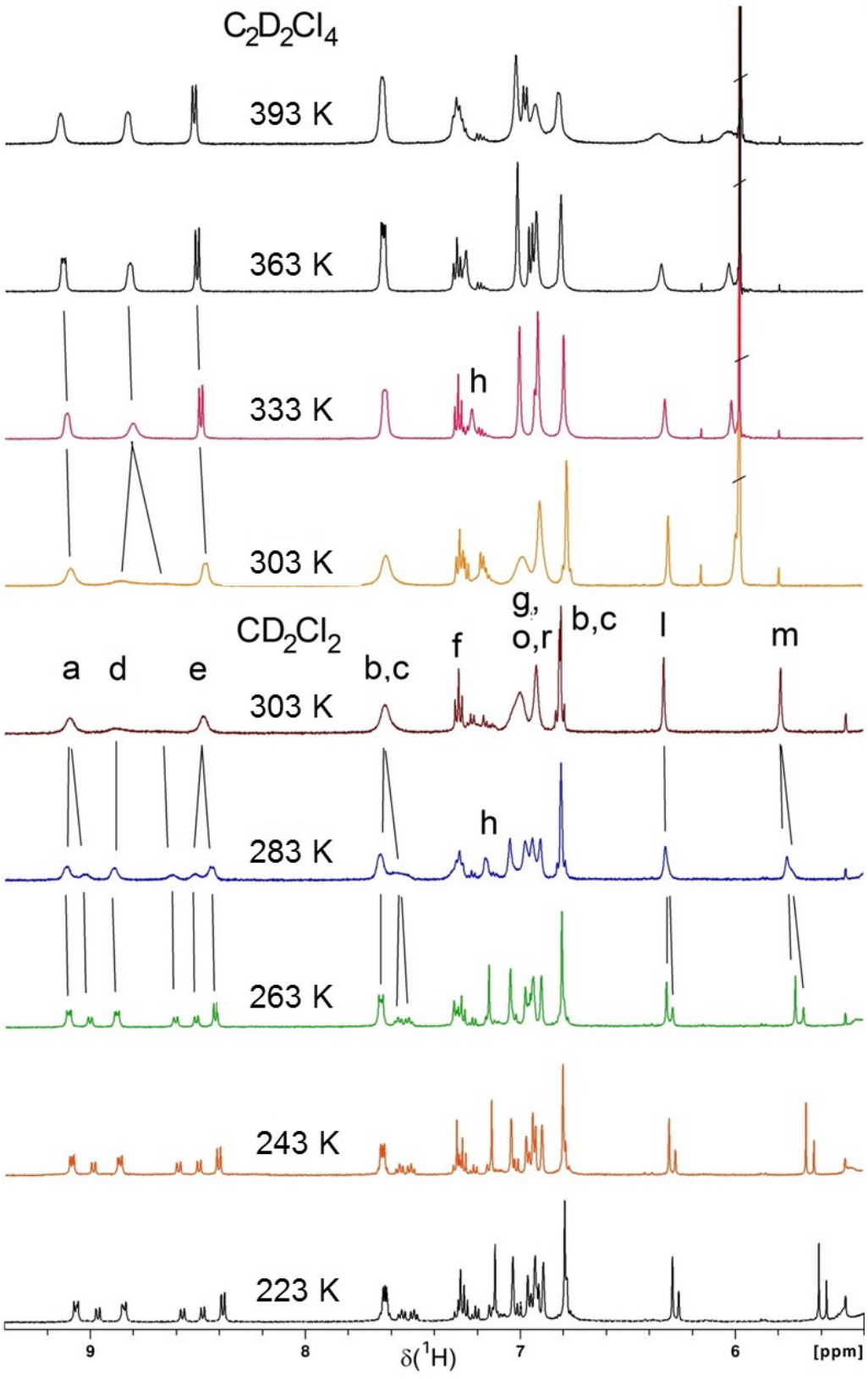


Figure S12. ^{1}H NMR spectra (region of aromatic protons) of **2** recorded in CD_2Cl_2 at 223, 243, 263, 283 and 303 K and recorded in $C_2D_2Cl_4$ at 303, 333, 363 and 393 K. The solid lines, which represent a guide for the eye, indicate coalescence processes for selected signals.

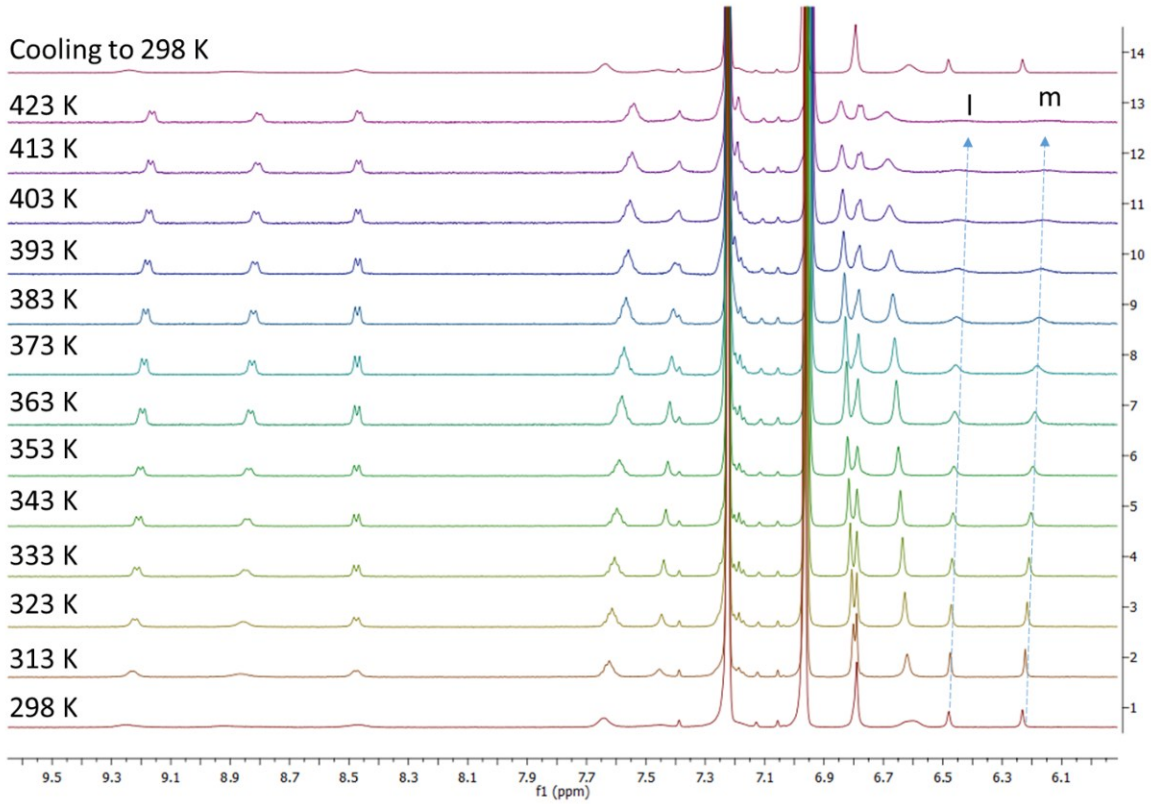


Figure S13. VT ^{1}H NMR spectra (region of aromatic protons) of **2** recorded in *o*-$C_6D_4Cl_2$.

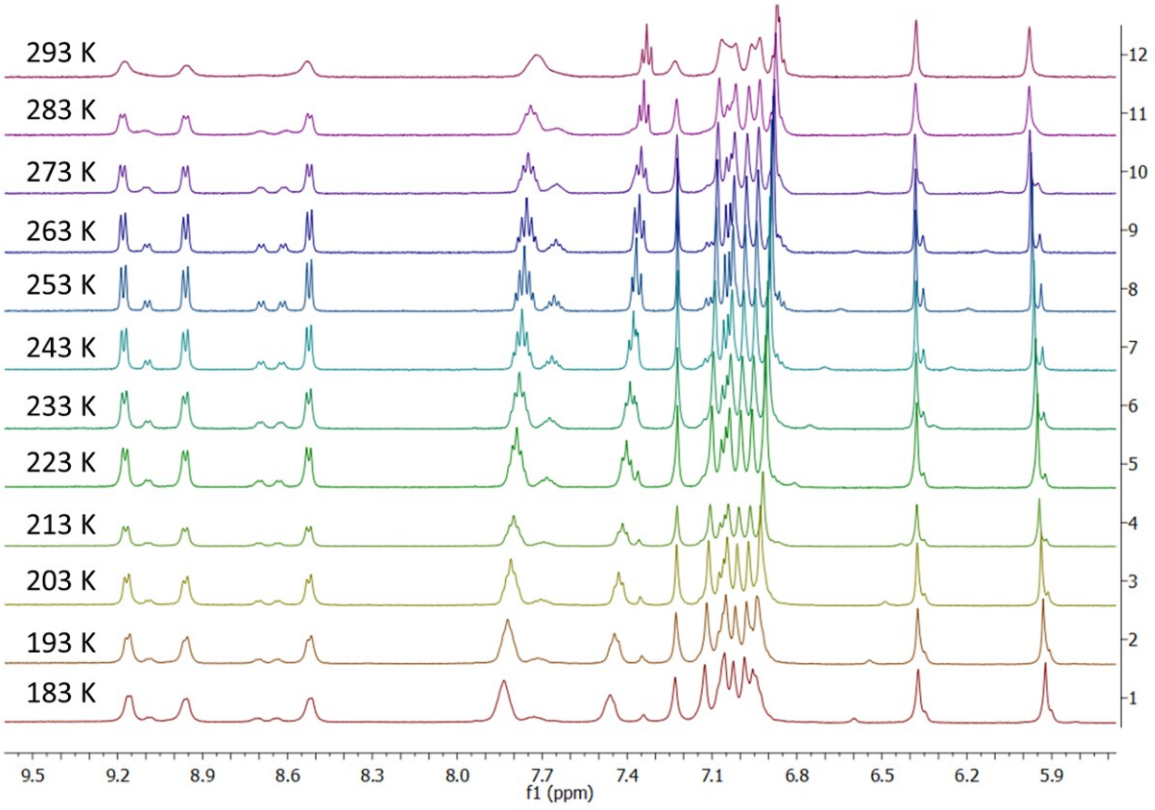


Figure S14. VT ^{1}H NMR spectra (region of aromatic protons) of **2** recorded in THF-d_8.

4. Variable-temperature EPR measurements of 2

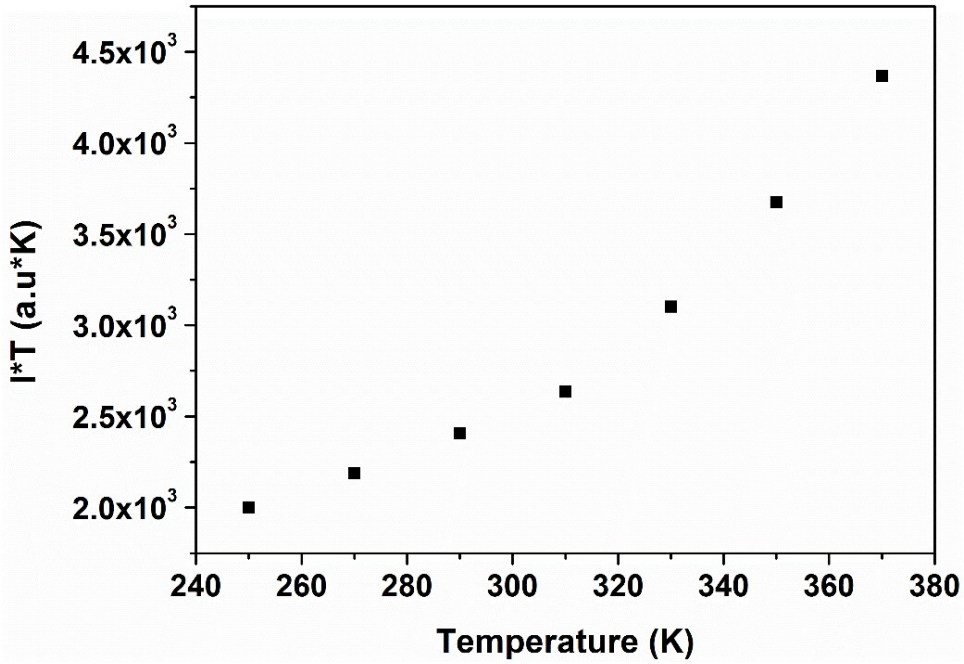


Figure S15. The change of *I***T* with temperature *T* for **2**. *I* is the integrated ESR intensity and *T* is temperature.

5. Time-dependent UV/Vis spectra of 1 and 2

During the stability test, the solution of **1** and **2** in CH_2Cl_2 was exposed to ambient air and sun light conditions. There was not significant change of the absorption curves of both molecules within 10 days under ambient conditions (Figure S16). For compound **1**, the main absorption peaks did not change with the time going on. And, the half-life time ($t_{1/2}$) of **2** was estimated as 91 days under ambient air and sun light condition by plotting the absorption intensity at the 842 nm with ambient light irradiation time according to the linear regression and extrapolation to % change = 0.50 (Figure S17).

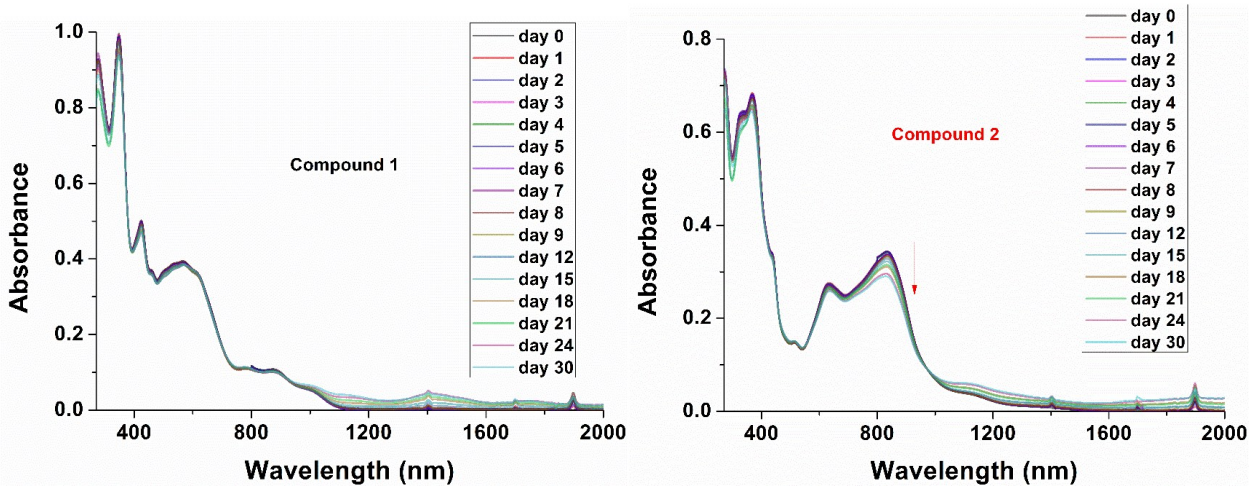


Figure S16. Absorption spectral changes under ambient air and light irradiation for **1** (a) and **2** (b) in CH_2Cl_2.

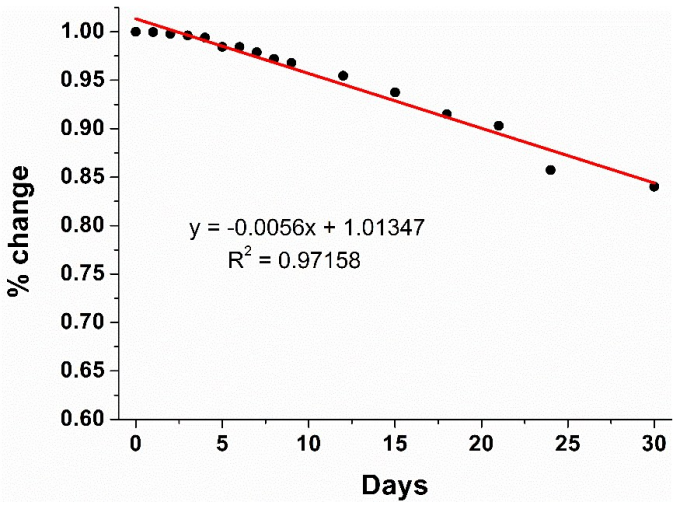


Figure S17. Changes of optical density of **2** at the absorption maximum (842 nm) as a function of ambient light irradiation time.

6. X-ray crystallographic analysis of 2 and 9

Accession codes: The X-ray crystallographic coordinates for structures reported in this article have been deposited at the Cambridge Crystallographic Data Centre (CCDC), under deposition number CCDC 1829452 (for **2**) and CCDC 1870938 (for **9**). These data can be obtained free of charge from CCDC via http://www.ccdc.cam.ac.uk/data_request/cif

Table S1. Summary of crystal data and reflection collection parameters for **2** and **9**.

	2	**9**
Empirical formula	$C_{108}H_{86}$	$C_{108}H_{90}$
Formula weight	1383.76	1387.79
Crystal size, mm	0.175 × 0.151 × 0.026	0.13 × 0.05 × 0.04
Crystal system	monoclinic	momoclinic
space group	$P2_1/n$	C2/c
a, Å	14.1458(6)	31.3411(8)
b, Å	13.4627(4)	28.1487 (6)
c, Å	22.3724(6)	24.3410 (7)
α, deg	90	90
β, deg	107.134(4)	107.002 (3)
γ, deg	90	90
V, Å^3	4071.5(2)	205535.4 (10)
Z	2	8
$D_{calcd.}$, g cm^{-3}	1.129	0.898
F_{000}	1468.0	5904.0
Temperature, K	100	100
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
μ, mm^{-1}	0.480	0.381
2Θ range for data collection/°	6.628 to 153.134	7.34 to 125
Index ranges	-17 ≤ h ≤ 17, -15 ≤ k ≤ 16, -22 ≤ l ≤ 28	-36 ≤ h ≤ 35, -29 ≤ k ≤ 32, -25 ≤ l ≤ 28
no. of collected reflections	23305	51204
no. of unique ref.(R_{int})	8423(0.0281)	16287(0.0347)
Data/restraints/parameters	8423/0/496	16287/0/843
R_1, wR_2 [obs I>2σ (I)]	0.0618, 0.1698	0.1246, 0.2951
R_1, wR_2 (all data)	0.0839, 0.1881	0.1683,0.3349
residual peak/hole, e. Å^{-3}	0.30/-0.27	0.53/-0.52
Goodness-of-fit on F^2	1.039	0.854

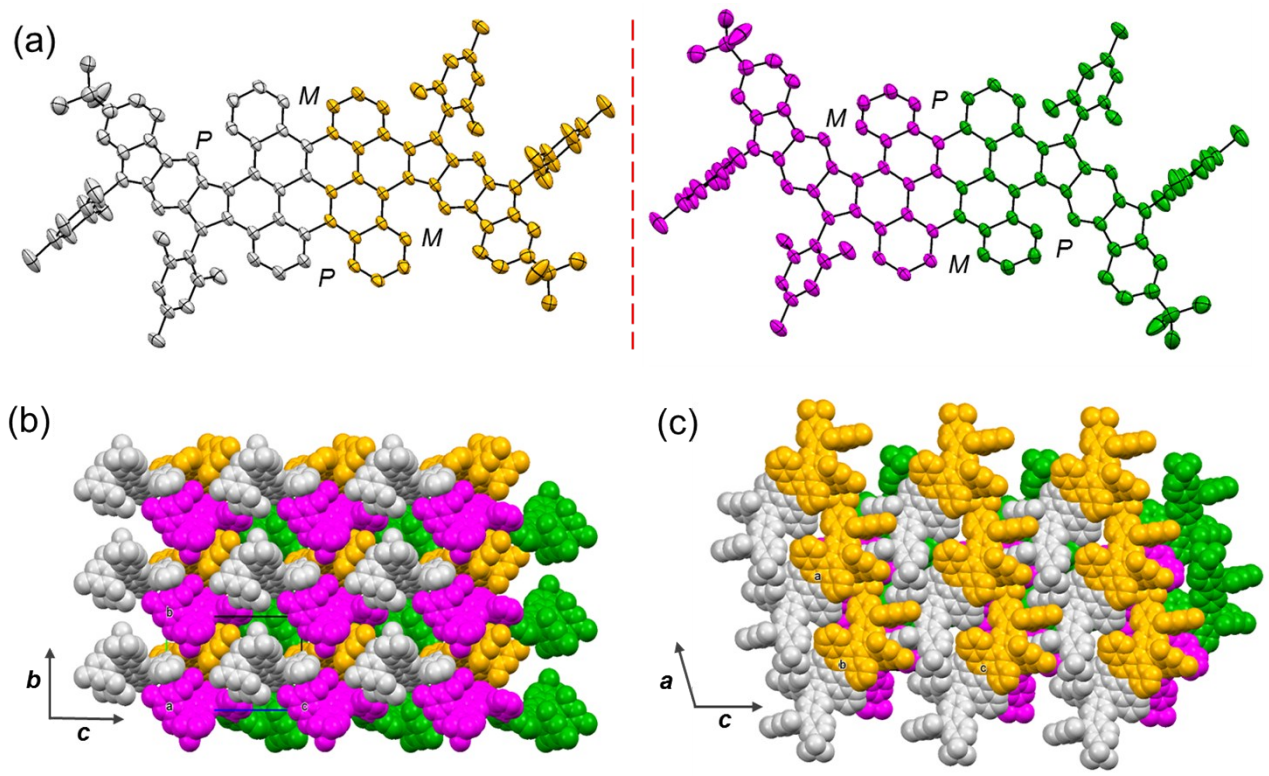


Figure S18. (a) Top views of the enantiomers of **2** and (b,c) the packing structure of **2**. Hydrogen atoms have been omitted for clarity.

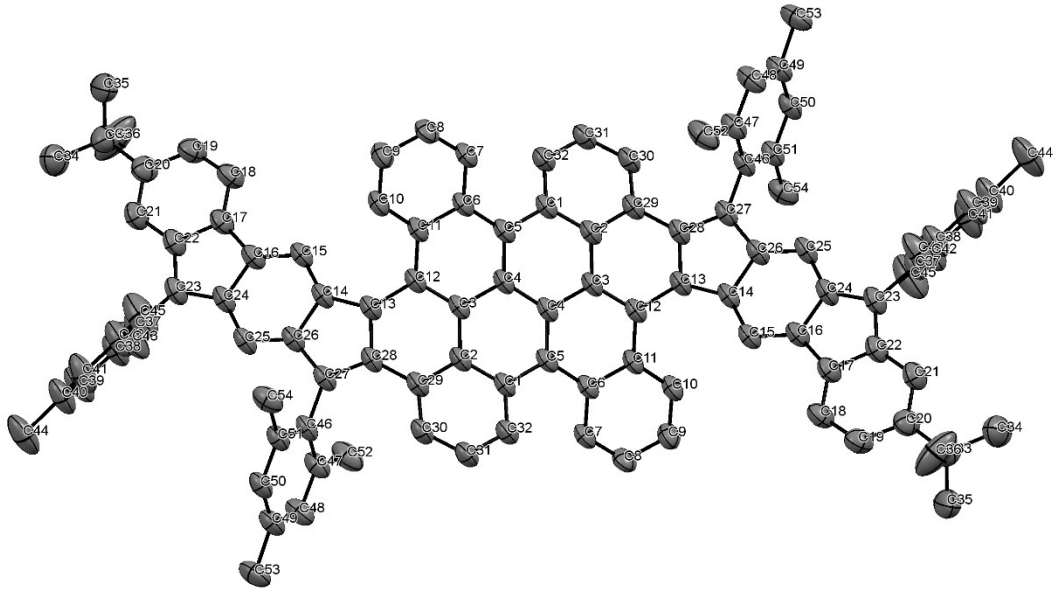


Figure S19. ORTEP drawing of **2** with 50% probability.

Table S2. Bond lengths for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.415(3)	C22	C23	1.456(3)
C1	C5[1]	1.461(2)	C23	C24	1.405(3)
C1	C32	1.401(3)	C23	C37	1.485(3)

C2	C3	1.448(3)	C24	C25	1.409(3)
C2	C29	1.428(2)	C25	C26	1.370(3)
C3	C4	1.440(2)	C26	C27	1.452(3)
C3	C12	1.408(3)	C27	C28	1.390(2)
C4	C4[1]	1.449(4)	C27	C46	1.481(3)
C4	C5	1.401(3)	C28	C29	1.448(3)
C5	C1[1]	1.461(2)	C29	C30	1.390(3)
C5	C6	1.443(3)	C30	C31	1.381(3)
C6	C7	1.423(3)	C31	C32	1.384(3)
C6	C11	1.436(2)	C33	C34	1.536(4)
C7	C8	1.367(3)	C33	C35	1.506(4)
C8	C9	1.399(3)	C33	C36	1.522(4)
C9	C10	1.366(3)	C37	C38	1.399(3)
C10	C11	1.414(3)	C37	C42	1.410(3)
C11	C12	1.434(3)	C38	C39	1.395(3)
C12	C13	1.444(2)	C38	C43	1.501(4)
C13	C14	1.412(3)	C39	C40	1.386(4)
C13	C28	1.459(3)	C40	C41	1.376(4)
C14	C15	1.415(3)	C40	C44	1.516(3)
C14	C26	1.455(2)	C41	C42	1.394(4)
C15	C16	1.371(3)	C42	C45	1.512(4)
C16	C17	1.459(3)	C46	C47	1.392(3)
C16	C24	1.447(3)	C46	C51	1.406(3)
C17	C18	1.381(3)	C47	C48	1.398(3)
C17	C22	1.425(3)	C47	C52	1.509(3)
C18	C19	1.387(4)	C48	C49	1.382(3)
C19	C20	1.407(4)	C49	C50	1.376(3)
C20	C21	1.404(3)	C49	C53	1.512(3)
C20	C33	1.534(4)	C50	C51	1.398(3)
C21	C22	1.403(3)	C51	C54	1.498(3)

[1]2-X,1-Y,2-Z

Table S3. Bond angles for **2**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C2	C1	C5[1]	119.27(18)	C23	C24	C16	109.39(19)
C32	C1	C2	118.27(18)	C23	C24	C25	130.31(19)
C32	C1	C5[1]	122.35(19)	C25	C24	C16	120.28(18)
C1	C2	C3	120.33(17)	C26	C25	C24	118.05(18)
C1	C2	C29	119.31(18)	C25	C26	C14	122.0(2)

C29	C2	C3	120.13(18)
C4	C3	C2	118.81(18)
C12	C3	C2	121.06(16)
C12	C3	C4	120.05(18)
C3	C4	C4[1]	119.4(2)
C5	C4	C3	119.78(18)
C5	C4	C4[1]	120.7(2)
C4	C5	C1[1]	118.94(18)
C4	C5	C6	118.77(16)
C6	C5	C1[1]	122.28(18)
C7	C6	C5	123.13(17)
C7	C6	C11	117.58(18)
C11	C6	C5	119.12(18)
C8	C7	C6	121.71(18)
C7	C8	C9	120.5(2)
C10	C9	C8	119.6(2)
C9	C10	C11	122.10(18)
C10	C11	C6	118.39(18)
C10	C11	C12	122.01(17)
C12	C11	C6	119.33(18)
C3	C12	C11	118.72(16)
C3	C12	C13	117.42(18)
C11	C12	C13	123.75(18)
C12	C13	C28	118.64(18)
C14	C13	C12	132.61(19)
C14	C13	C28	108.61(16)
C13	C14	C15	133.82(17)
C13	C14	C26	106.22(18)
C15	C14	C26	119.36(17)
C16	C15	C14	118.49(18)
C15	C16	C17	131.50(19)
C15	C16	C24	121.6(2)
C24	C16	C17	106.88(18)
C18	C17	C16	132.3(2)
C18	C17	C22	120.1(2)
C22	C17	C16	107.58(19)
C17	C18	C19	119.1(2)
C18	C19	C20	123.1(2)
C19	C20	C33	119.6(2)
C21	C20	C19	117.3(2)
C25	C26	C27	128.88(18)
C27	C26	C14	108.86(17)
C26	C27	C46	122.58(17)
C28	C27	C26	107.10(17)
C28	C27	C46	130.2(2)
C27	C28	C13	108.98(18)
C27	C28	C29	130.0(2)
C29	C28	C13	120.52(16)
C2	C29	C28	116.78(18)
C30	C29	C2	119.50(19)
C30	C29	C28	123.63(18)
C31	C30	C29	120.31(19)
C30	C31	C32	120.5(2)
C31	C32	C1	121.2(2)
C20	C33	C34	111.6(2)
C35	C33	C20	110.8(3)
C35	C33	C34	106.4(3)
C35	C33	C36	109.8(3)
C36	C33	C20	108.8(2)
C36	C33	C34	109.4(3)
C38	C37	C23	121.3(2)
C38	C37	C42	118.8(2)
C42	C37	C23	119.7(2)
C37	C38	C43	121.6(2)
C39	C38	C37	119.2(2)
C39	C38	C43	119.2(2)
C40	C39	C38	122.3(3)
C39	C40	C44	122.2(3)
C41	C40	C39	117.9(2)
C41	C40	C44	119.9(3)
C40	C41	C42	121.9(3)
C37	C42	C45	121.5(2)
C41	C42	C37	119.8(2)
C41	C42	C45	118.7(3)
C47	C46	C27	120.52(18)
C47	C46	C51	119.94(19)
C51	C46	C27	119.53(19)
C46	C47	C48	119.1(2)
C46	C47	C52	121.8(2)
C48	C47	C52	119.0(2)

C21	C20	C33	123.1(2)		C49	C48	C47	121.9(2)	
C22	C21	C20	120.8(2)		C48	C49	C53	120.3(2)	
C17	C22	C23	108.48(19)		C50	C49	C48	118.3(2)	
C21	C22	C17	119.6(2)		C50	C49	C53	121.4(2)	
C21	C22	C23	131.9(2)		C49	C50	C51	122.09(19)	
C22	C23	C37	128.1(2)		C46	C51	C54	121.46(19)	
C24	C23	C22	107.65(18)		C50	C51	C46	118.7(2)	
C24	C23	C37	124.2(2)		C50	C51	C54	119.81(19)	

[1]2-X,1-Y,2-Z

Table S4. Torsion angles for **2**.

A	**B**	**C**	**D**	**Angle/˚**		**A**	**B**	**C**	**D**	**Angle/˚**
C1	C2	C3	C4	-1.6(3)		C19	C20	C21	C22	0.1(4)
C1	C2	C3	C12	-178.48(17)		C19	C20	C33	C34	-169.0(3)
C1	C2	C29	C28	-166.96(17)		C19	C20	C33	C35	-50.7(4)
C1	C2	C29	C30	9.7(3)		C19	C20	C33	C36	70.1(4)
C1[1]	**C5**	**C6**	**C7**	**-22.1(3)**		C20	C21	C22	C17	1.0(4)
C1[1]	C5	C6	C11	162.84(17)		C20	C21	C22	C23	-179.2(2)
C2	C1	C32	C31	4.3(3)		C21	C20	C33	C34	14.1(4)
C2	C3	C4	C4[1]	9.5(3)		C21	C20	C33	C35	132.4(3)
C2	C3	C4	C5	-173.84(17)		C21	C20	C33	C36	-106.8(4)
C2	C3	C12	C11	159.11(17)		C21	C22	C23	C24	-179.8(2)
C2	C3	C12	C13	-17.1(3)		C21	C22	C23	C37	-0.8(4)
C2	C29	C30	C31	-2.8(3)		C22	C17	C18	C19	0.9(4)
C3	C2	C29	C28	18.5(3)		C22	C23	C24	C16	0.9(2)
C3	C2	C29	C30	-164.85(18)		C22	C23	C24	C25	-177.8(2)
C3	C4	C5	C1[1]	-166.19(17)		C22	C23	C37	C38	71.6(4)
C3	C4	C5	C6	15.1(3)		C22	C23	C37	C42	-113.9(3)
C3	C12	C13	C14	-152.2(2)		C23	C24	C25	C26	-179.5(2)
C3	C12	C13	C28	23.0(3)		C23	C37	C38	C39	177.1(3)
C4	C3	C12	C11	-17.7(3)		C23	C37	C38	C43	-2.9(4)
C4	C3	C12	C13	166.10(16)		C23	C37	C42	C41	-177.2(3)
C4[1]	C4	C5	C1[1]	10.4(3)		C23	C37	C42	C45	3.5(5)
C4[1]	C4	C5	C6	-168.3(2)		C24	C16	C17	C18	-178.0(2)
C4	C5	C6	C7	156.58(19)		C24	C16	C17	C22	1.4(2)
C4	C5	C6	C11	-18.5(3)		C24	C23	C37	C38	-109.5(3)
C5[1]	C1	C2	C3	-12.1(3)		C24	C23	C37	C42	65.0(4)
C5[1]	C1	C2	C29	173.34(17)		C24	C25	C26	C14	1.7(3)
C5[1]	C1	C32	C31	-179.45(19)		C24	C25	C26	C27	-171.90(19)

C5	C6	C7	C8	-179.3(2)	C25	C26	C27	C28	173.2(2)
C5	C6	C11	C10	178.01(17)	C25	C26	C27	C46	-2.6(3)
C5	C6	C11	C12	3.9(3)	C26	C14	C15	C16	3.2(3)
C6	C7	C8	C9	2.0(3)	C26	C27	C28	C13	3.7(2)
C6	C11	C12	C3	14.0(3)	C26	C27	C28	C29	-168.26(19)
C6	C11	C12	C13	-169.98(17)	C26	C27	C46	C47	104.5(2)
C7	C6	C11	C10	2.7(3)	C26	C27	C46	C51	-74.1(3)
C7	C6	C11	C12	-171.45(18)	C27	C28	C29	C2	158.95(19)
C7	C8	C9	C10	1.8(4)	C27	C28	C29	C30	-17.5(3)
C8	C9	C10	C11	-3.2(3)	C27	C46	C47	C48	-179.9(2)
C9	C10	C11	C6	0.9(3)	C27	C46	C47	C52	1.1(3)
C9	C10	C11	C12	174.9(2)	C27	C46	C51	C50	178.94(19)
C10	C11	C12	C3	-159.85(18)	C27	C46	C51	C54	-3.7(3)
C10	C11	C12	C13	16.1(3)	C28	C13	C14	C15	-166.5(2)
C11	C6	C7	C8	-4.2(3)	C28	C13	C14	C26	4.2(2)
C11	**C12**	**C13**	**C14**	**31.8(3)**	C28	C27	C46	C47	-70.2(3)
C11	C12	C13	C28	-152.99(18)	C28	C27	C46	C51	111.2(3)
C12	C3	C4	C4[1]	-173.6(2)	C28	C29	C30	C31	173.6(2)
C12	C3	C4	C5	3.0(3)	C29	C2	C3	C4	172.82(16)
C12	C13	C14	C15	9.1(4)	C29	C2	C3	C12	-4.0(3)
C12	C13	C14	C26	179.8(2)	C29	C30	C31	C32	-3.3(3)
C12	C13	C28	C27	178.67(17)	C30	C31	C32	C1	2.6(3)
C12	C13	C28	C29	-8.5(3)	C32	C1	C2	C3	164.24(17)
C13	C14	C15	C16	173.0(2)	C32	C1	C2	C29	-10.3(3)
C13	C14	C26	C25	-176.74(19)	C33	C20	C21	C22	177.1(2)
C13	C14	C26	C27	-2.0(2)	C37	C23	C24	C16	-178.2(2)
C13	C28	C29	C2	-12.2(3)	C37	C23	C24	C25	3.2(4)
C13	C28	C29	C30	171.32(19)	C37	C38	C39	C40	-0.9(5)
C14	C13	C28	C27	-5.1(2)	C38	C37	C42	C41	-2.6(5)
C14	C13	C28	C29	167.77(17)	C38	C37	C42	C45	178.1(3)
C14	C15	C16	C17	179.7(2)	C38	C39	C40	C41	-0.6(6)
C14	C15	C16	C24	0.4(3)	C38	C39	C40	C44	-178.4(3)
C14	C26	C27	C28	-1.1(2)	C39	C40	C41	C42	0.5(6)
C14	C26	C27	C46	-176.84(17)	C40	C41	C42	C37	1.1(6)
C15	C14	C26	C25	-4.4(3)	C40	C41	C42	C45	-179.6(4)
C15	C14	C26	C27	170.30(17)	C42	C37	C38	C39	2.5(4)
C15	C16	C17	C18	2.5(4)	C42	C37	C38	C43	-177.5(3)
C15	C16	C17	C22	-178.0(2)	C43	C38	C39	C40	179.1(3)
C15	C16	C24	C23	178.0(2)	C44	C40	C41	C42	178.3(4)
C15	C16	C24	C25	-3.1(3)	C46	C27	C28	C13	179.01(19)

C16	C17	C18	C19	-179.6(2)	C46	C27	C28	C29	7.1(3)
C16	C17	C22	C21	178.9(2)	C46	C47	C48	C49	0.5(4)
C16	C17	C22	C23	-0.9(2)	C47	C46	C51	C50	0.3(3)
C16	C24	C25	C26	2.0(3)	C47	C46	C51	C54	177.7(2)
C17	C16	C24	C23	-1.4(2)	C47	C48	C49	C50	1.3(4)
C17	C16	C24	C25	177.37(19)	C47	C48	C49	C53	-178.3(3)
C17	C18	C19	C20	0.2(4)	C48	C49	C50	C51	-2.3(4)
C17	C22	C23	C24	0.0(3)	C49	C50	C51	C46	1.5(3)
C17	C22	C23	C37	179.0(2)	C49	C50	C51	C54	-175.9(2)
C18	C17	C22	C21	-1.5(3)	C51	C46	C47	C48	-1.3(3)
C18	C17	C22	C23	178.6(2)	C51	C46	C47	C52	179.7(2)
C18	C19	C20	C21	-0.8(4)	C52	C47	C48	C49	179.6(3)
C18	C19	C20	C33	-177.9(2)	C53	C49	C50	C51	177.3(2)

[1]2-X,1-Y,2-Z

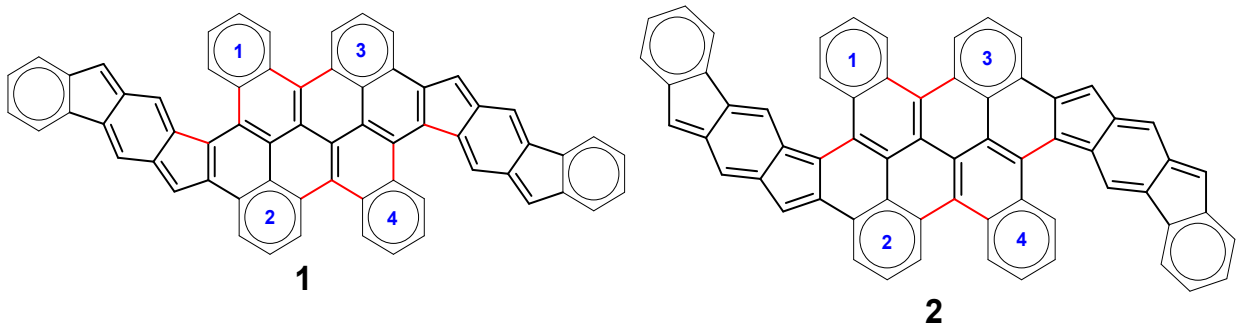


Figure S20. The resonance structures of **1** and **2**.

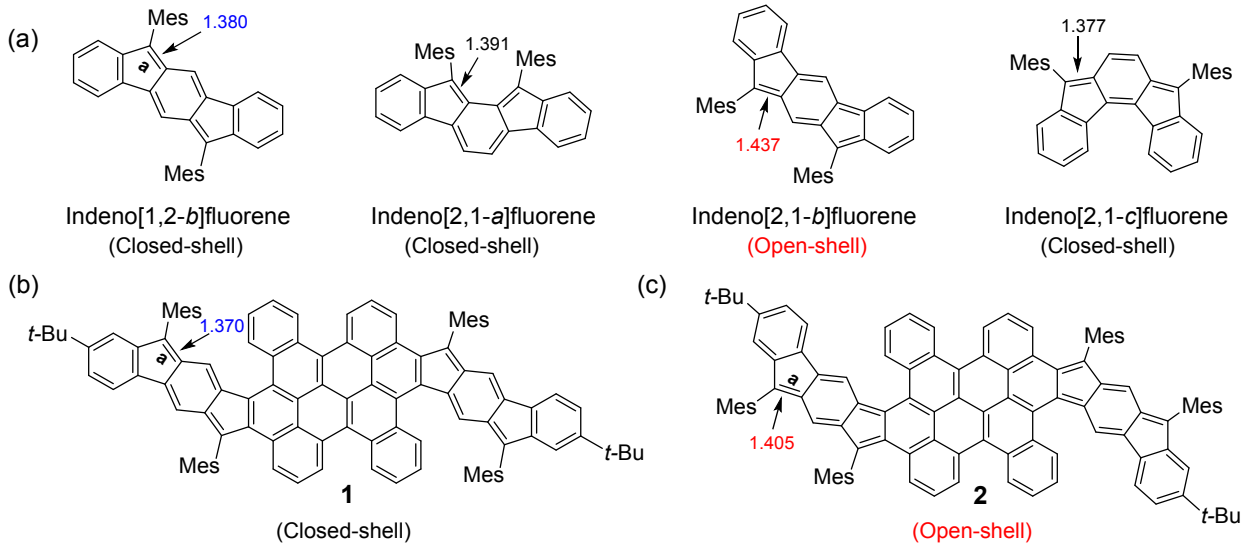


Figure S21. Comparison of the length of the most critical bond *a* of (a) the indenofluorene isomers [a], (b) compound **1** (Calculated at UCAM-B3LYP/6-311G** level) and (c) compound **2 (**from the single crystal structure). [a] data from Nat. Chem. 2016, 8, 753-759.

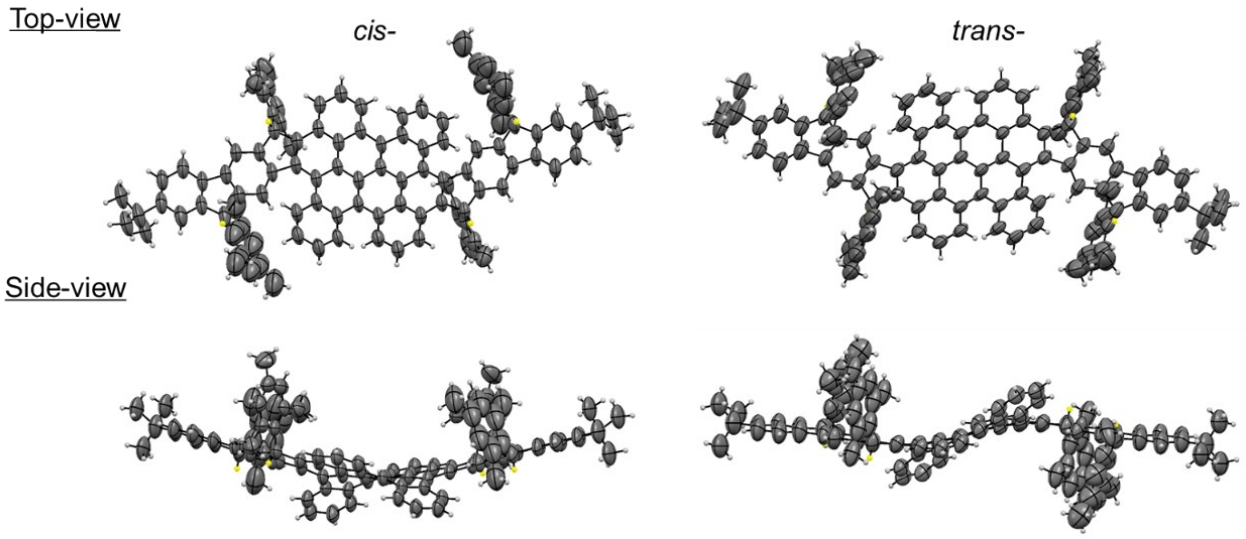


Figure S22. The *cis-trans* conformation in the crystal structure of tetrahydro-precursor **9**. The tertiary hydrogen atoms are colored yellow for a better visualization.

7. DFT calculations

Density functional theory (DFT) calculations were performed at the UCAM-B3LYP/6-311G** level of theory as implemented in Gaussian09 for structure relaxation as well as calculation of the singlet-triplet energy gap $\Delta E_{S\text{-}T}$.[4,5] NICS values were calculated at the same level of theory using the standard GIAO procedure (NMR pop=NCSall).[6] The diradical character y_0 and the tetraradical character y_1 are evaluated from CASSCF(4,4)/6-31G** calculations by $y_0 = n_{LUNO}$ and $y_1 = n_{LUNO+1}$ with n_{LUNO} the occupation of the lowest unoccupied natural orbital and n_{LUNO+1} the occupation number of the unoccupied natural orbital.[7] AICD plot was calculated by using the method developed by Herges based on the optimized ground-state geometries at a UB3LYP/6-31G* level of theory.[8]

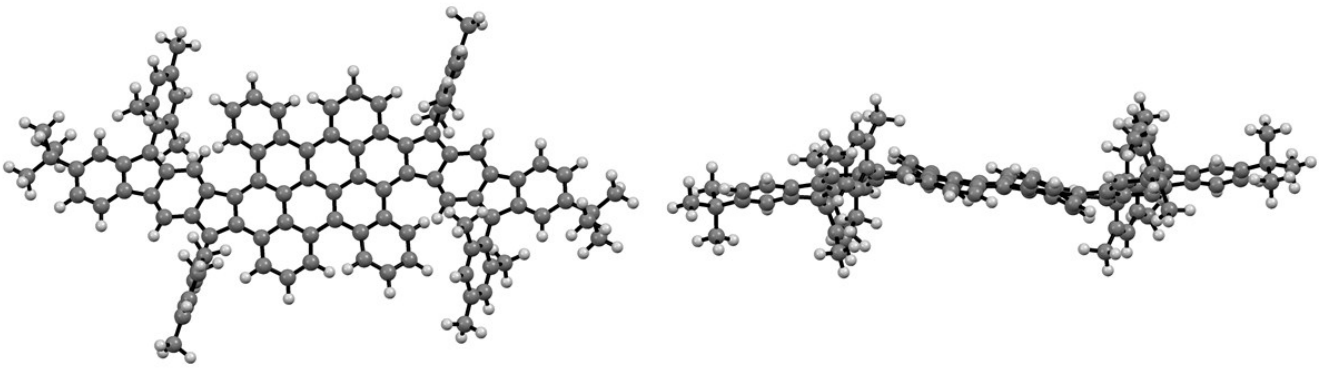


Figure S23. The optimized structure (UB3LYP/6-31G*) of compound **1** in the ground state.

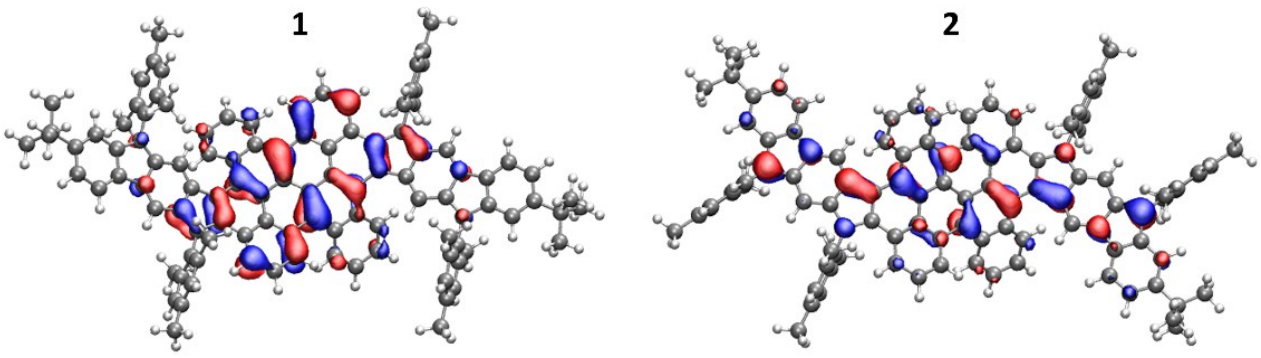


Figure S24. HOMO orbitals of compounds **1** and **2** in the closed-shell singlet state.

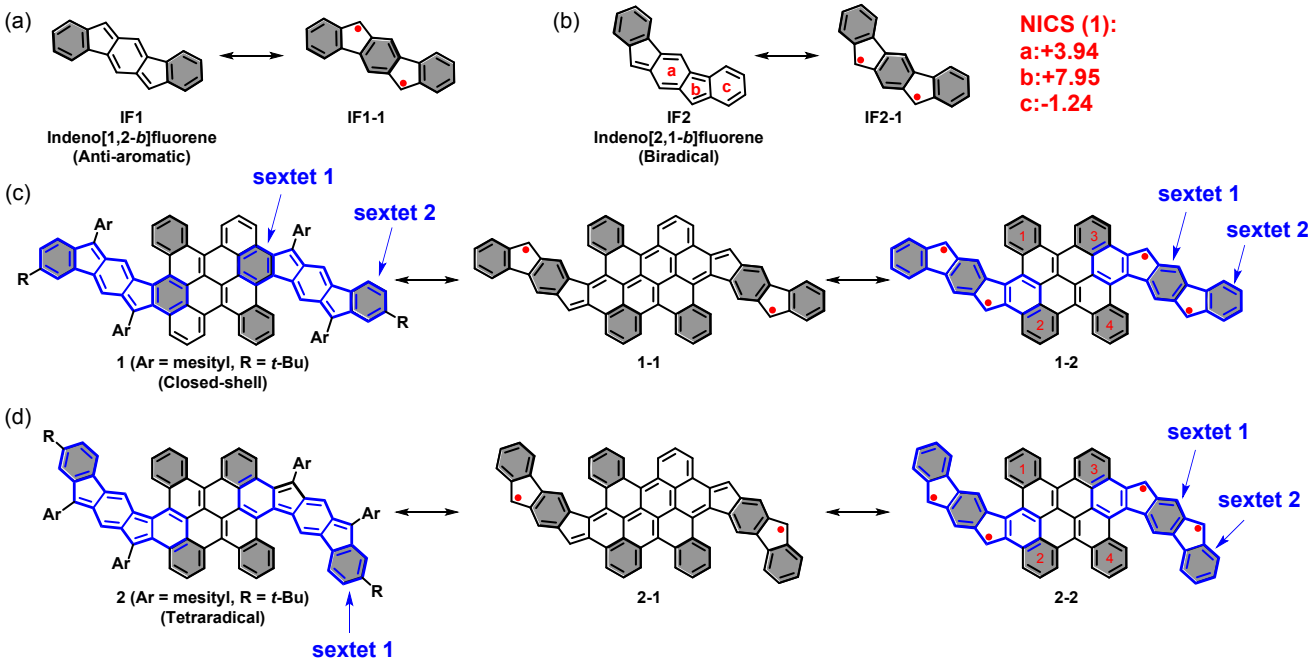


Figure S25. Resonance structures of the studied indeno[1,2-*b*]fluorene [9] (a), indeno[2,1-*b*]fluorene[10] (b) (NICS (1) values are from the SI of *J. Org. Chem.*, **2017**, *82*, 1380) and the π-extended stable wavy-shaped PHs **1** (c) and **2** (d) reported in this work. The flanked indeno[1,2-*b*]fluorene and indeno[2,1-*b*]fluorene in **1** and **2** are respectively highlighted by blue color.

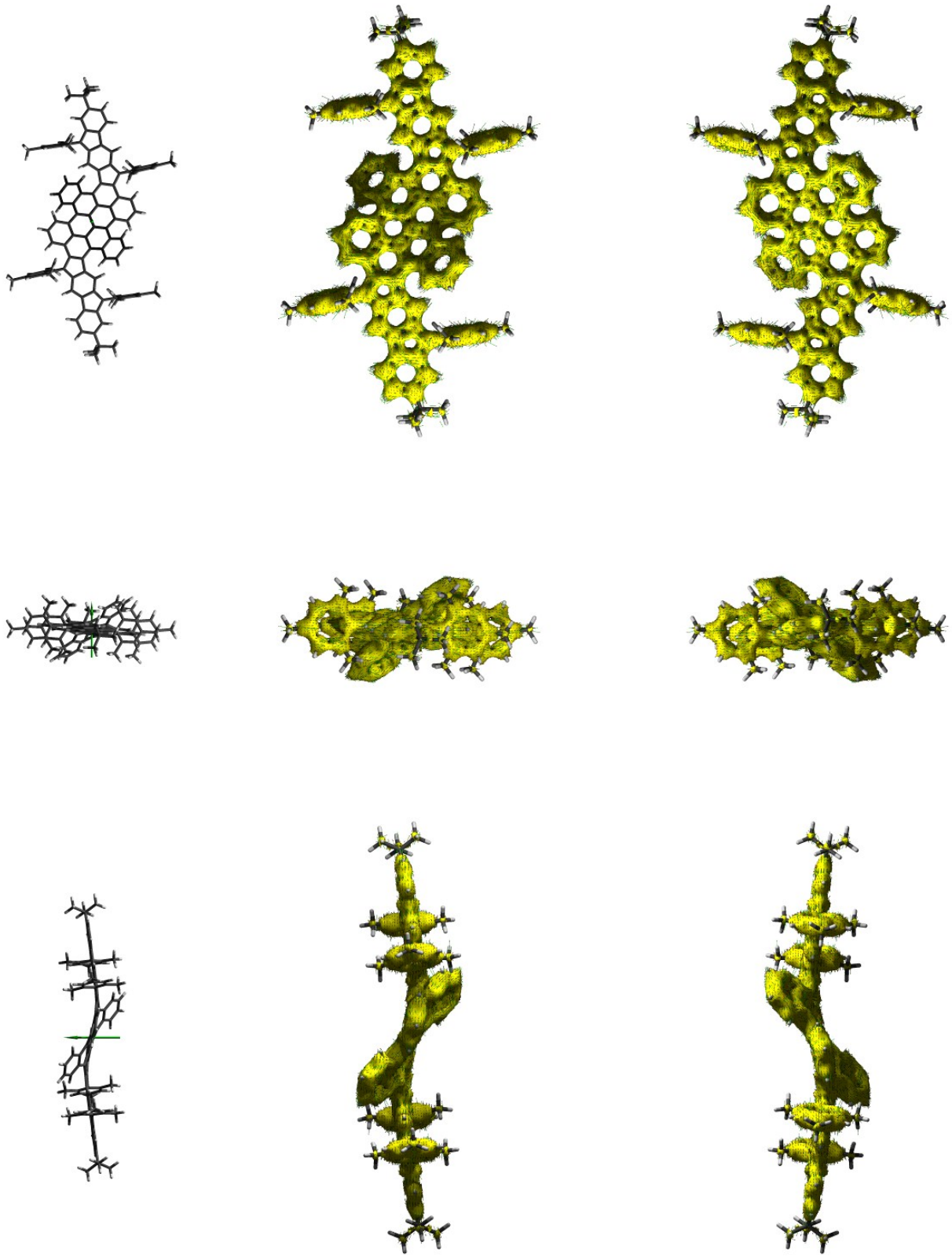


Figure S26. ACID plots of **1** viewed from different angles. The green arrow indicates the magnetic field. Isovalue is 0.05.

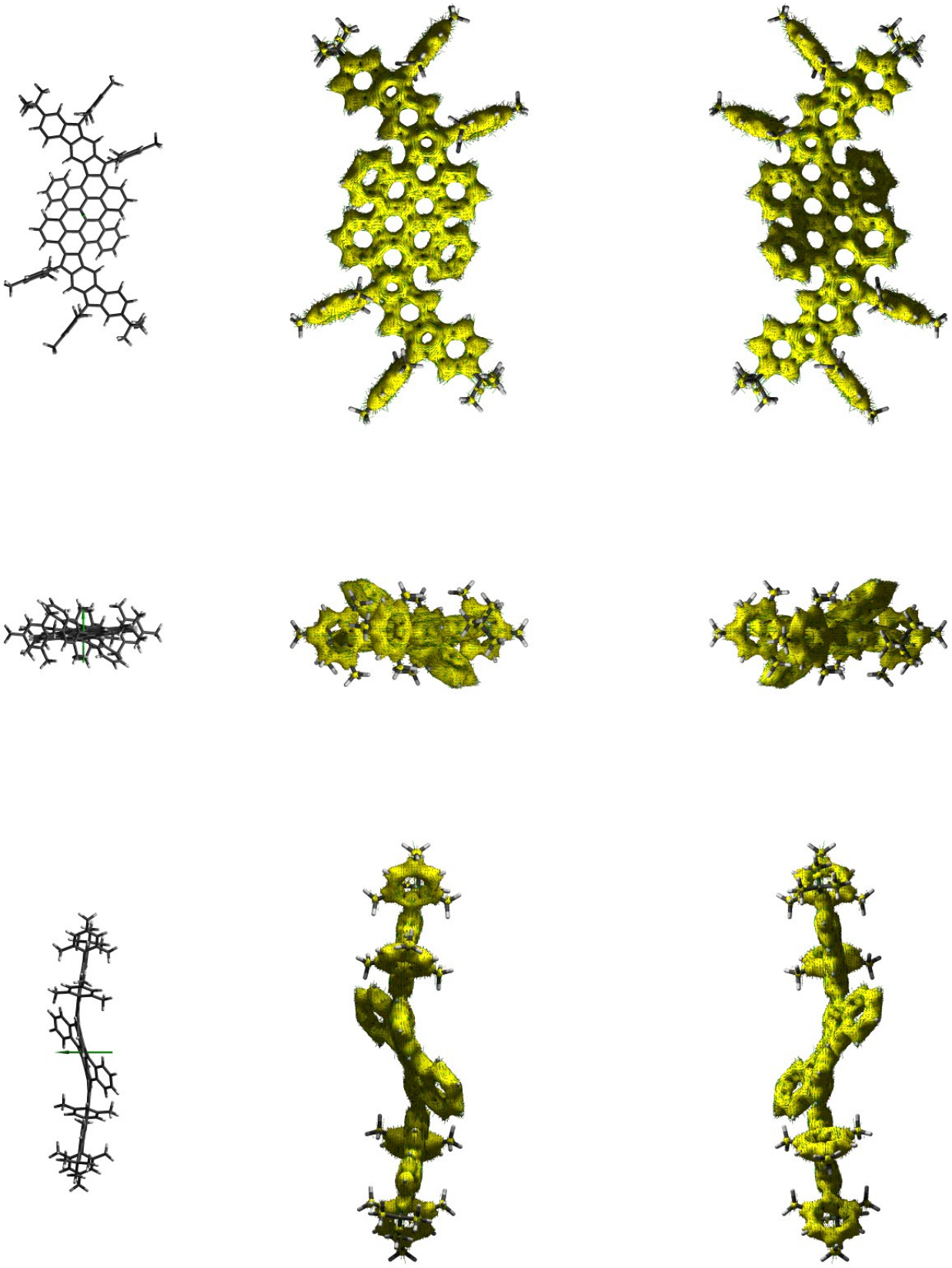


Figure S27. ACID plots of **2** viewed from different angles. The green arrow indicates the magnetic field. Isovalue is 0.05.

For transition state (TS) calculation all the structure were optimized in gas phase by using B3LYP level of density functional theory with the 6-31G* basis. To confirm the accuracy of the transition state we did frequency calculation. The Gibbs free energies of reaction ($\Delta_r G^\circ$) at room temperature (298 K) can be calculated by the following equations [11]

$$H\mathrm{corr} = E\mathrm{tot} + kBT$$

$$G\mathrm{corr} = Hc\mathrm{orr} - TS\mathrm{tot}$$

$$\Delta rG^\circ(T) = \sum(\varepsilon\mathrm{o} + Gcorr)\mathrm{products} - \sum(\varepsilon\mathrm{o} + Gcorr)\mathrm{reactants}$$

where H_{corr} is the thermal correction to Enthalpy; E_{tot} is the correction to the internal thermal energy; k_B is the Boltzmann constant; T is the temperature; G_{corr} is the thermal correction to Gibbs free energy (thermal Free Energies); S_{tot} is the correction to the internal Entropy; ε_o is the total electronic energy. In our case, the product is the transition state and the reactant is the staring state.

Initiated by the dynamic process observed in the VT ^{1}H NMR measurements, the isomerization process in the quadruple helicenes **1** and **2** were evaluated. DFT calculation on the relative energies of the inversion of [4]helicene and [7]helicene substructures as well as the transition state (TS) were performed at the B3LYP/6-31G+ (d) level. From the DTF calculations, it is estimated that the transition state of [7]helicene subunitsin **1** and **2** (Figure S29, **Δ***G*‡ = 17.4 kcal/mol for TS**-** PH**1-**B and **Δ***G*‡ =19.8 kcal/mol for TS**-** PH**2-**B) hold the larger inversion barrier than that of the [4]helicene subunits in **1** and **2** (Figure S28, **Δ***G*‡ = 12.1 kcal/mol for TS**-** PH**1-**A and **Δ***G*‡ = 12.8 kcal/mol for TS**-** PH**2-**A). Therefore, we could observe their thermodynamic inversion process at the low temperature NMR measurements (Figure S11 and S12). In addition, the inversion of single helical substructures in quadruple helicenes **1** and **2** as well as the transition state (TS) was also performed at the B3LYP/6-31G* level for the comparison (Figure S30). As expected, the inversion energy barrier of the helical substructures ([4]helicene or [7]helicene) in **1** and **2** are higher than that of the single [4]helicenes and [7]helicene (TS**-** PH**2-**A: **Δ***G*‡ = 12.8 kcal/mol > TS**-** PH**1-**A: **Δ***G*‡ = 12.1 kcal/mol > TS**-** [4]helicene: **Δ***G*‡ = 3.8 kcal/mol; TS**-** PH**1-**B: **Δ***G*‡ = 17.4 kcal/mol > TS**-** PH**1**-[7]helicene: **Δ***G*‡ = 12.7 kcal/mol; TS**-** PH**2-**B: **Δ***G*‡ = 19.8 kcal/mol > TS**-** PH**2**-[7]helicene: **Δ***G*‡ = 12.9 kcal/mol), which reflects the presence of additional repulsion from the neighboring helicene subunit at the transition state. Due to the lower isomerization barriers among the isomers, we could only observe them at low temperatures. Hence, it is difficult to separate them by chiral HPLC.

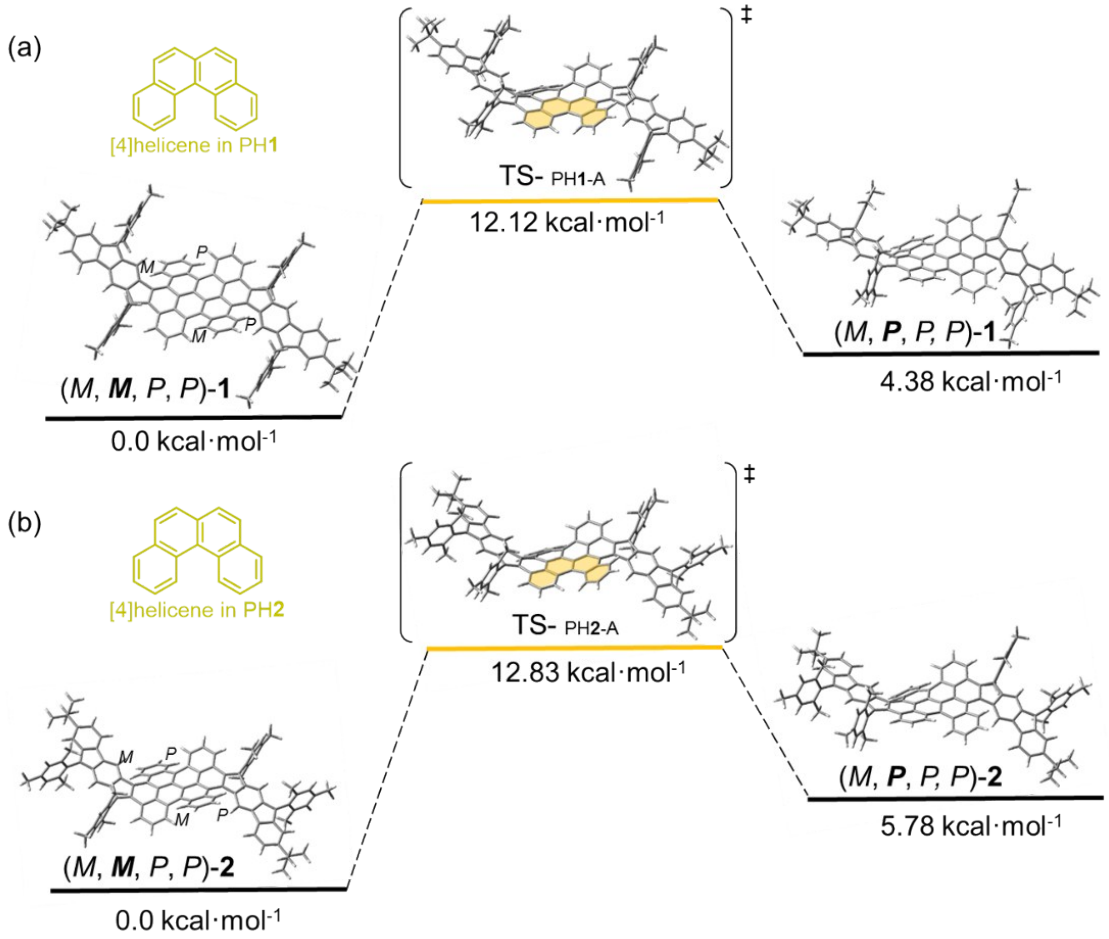


Figure S28. Isomerization between (*M*, *M*, *P*, *P*)-isomer and (*M*, *P*, *P*, *P*)-isomer in PH**1** (a) and PH**2** (b)-inversion of [4]helicene subunit.

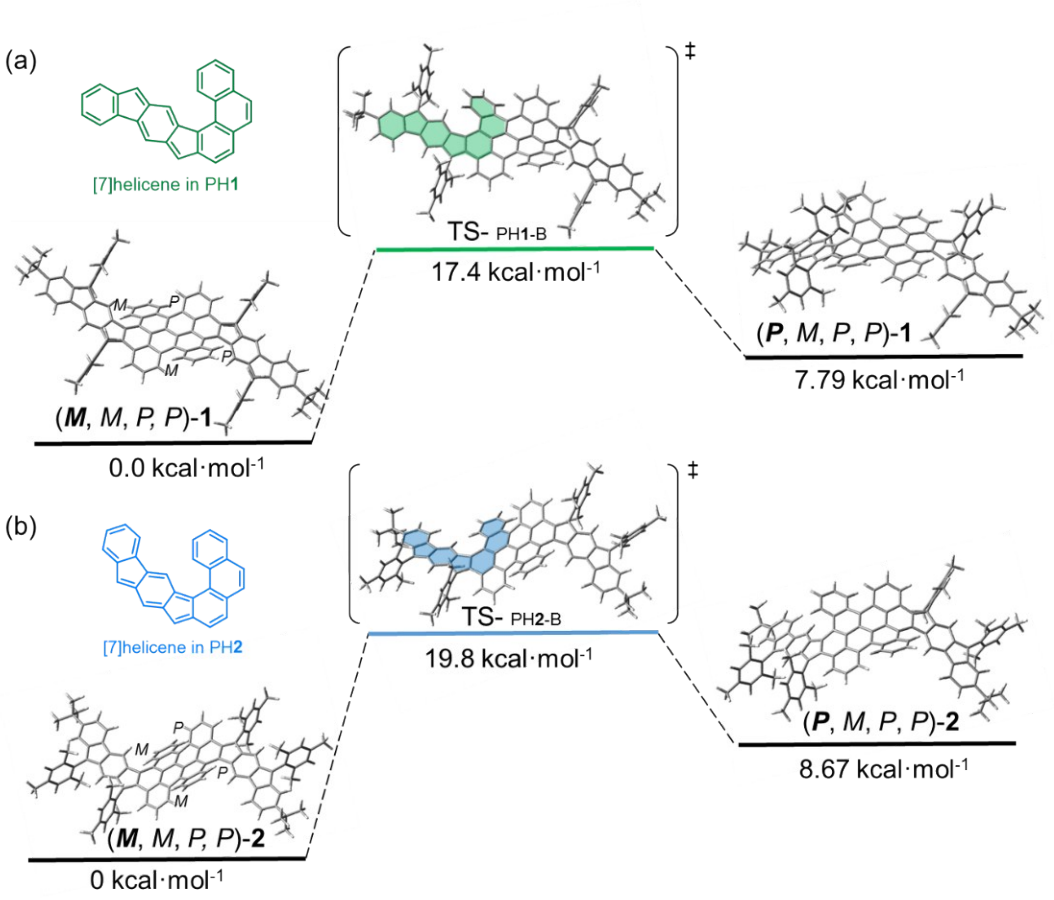


Figure S29. Isomerization between (*M*, *M*, *P*, *P*)-isomer and (***P***, *M*, *P*, *P*)-isomer in PH**1** (a) and PH**2** (b)-inversion of [7]helicene subunit.

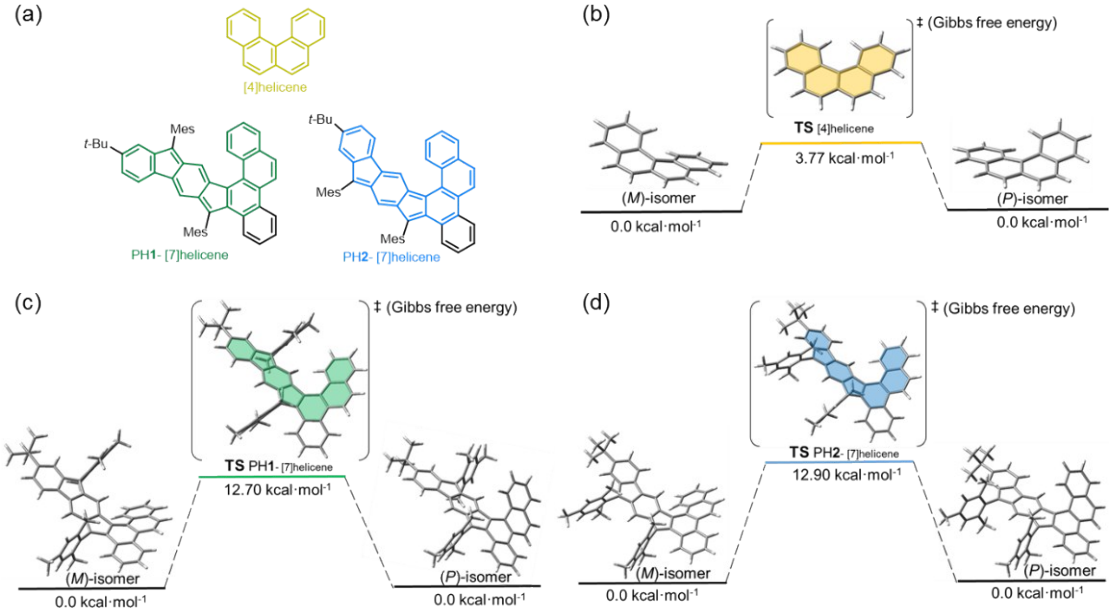


Figure S30. (a) The single helical substructures in quadruple helicenes **1** and **2**. Racemization process of the subunits of (b) [4]helicene, (c) [7]helicene in PH**1** and (d) [7]helicene in PH**2**.

Table S5. Energy and Cartesian coordinates of optimized species

(*M*, *M*, *P*, *P*)-**1**

Sum of electronic and thermal Free Energies: -4166.044659 a.u.

C	3.08281	-1.17575	1.37316
C	1.75457	0.63936	0.37952
C	3.03358	0.13352	0.75059
C	1.9504	-2.04554	1.27811
C	-4.15081	-1.0063	-0.61415
C	-1.75374	-0.63897	-0.38152
C	-1.56237	-2.04505	-0.18409
C	0.63332	-0.25692	0.24425
C	-3.03289	-0.13315	-0.75213
C	1.56332	2.04541	0.18188
C	-5.60633	-0.757	-0.51782
C	0.78745	-1.62462	0.51987
C	1.94408	-3.2283	2.06854
H	1.0511	-3.83541	2.08789
C	-0.26214	-2.55597	0.12089
C	4.15156	1.00657	0.61294
C	4.14868	-1.53883	2.23606
H	4.96503	-0.84484	2.36989
C	-3.08239	1.17625	-1.3744
C	-0.03308	-3.93258	-0.03876
H	0.97588	-4.31321	0.03559
C	-0.63247	0.25732	-0.24644
C	-0.7866	1.62503	-0.52205
C	-2.64806	-2.96137	-0.39012
C	-1.94986	2.04597	-1.27984
C	-6.24737	-2.07897	-0.44508
C	3.96306	2.40175	0.49776
C	2.64906	2.96169	0.38806
C	-3.96212	-2.40147	-0.49917
C	-4.1488	1.53958	-2.23653
H	-4.96525	0.84566	-2.36999
C	0.26312	2.55637	-0.12328
C	-6.34536	0.37798	-0.32488
H	-5.89443	1.36249	-0.30154
C	4.13173	-2.71831	2.95122
H	4.9545	-2.9617	3.6132
C	2.38412	4.346	0.4417
H	3.20252	5.03117	0.6059
C	-4.13227	2.71921	-2.95144
H	-4.95552	2.96286	-3.61273
C	0.03418	3.93302	0.03621
H	-0.97475	4.31372	-0.03814
C	3.01306	-3.56866	2.87143
C	-5.5394	-4.5181	-0.33244
C	5.85412	6.50032	-1.02365
H	5.89143	6.96991	-2.00183
C	6.06248	7.27776	0.12166
C	5.59321	5.12966	-0.93918
C	-1.94392	3.22878	-2.0702
H	-1.05086	3.83576	-2.09011
C	5.54068	4.5182	0.33208
C	5.60709	0.75711	0.51758
C	5.26809	3.06152	0.44102
C	-5.74895	-5.28473	-1.49703
C	-5.26701	-3.06139	-0.44145
C	-7.6657	-2.20444	-0.29156
H	-8.1096	-3.19368	-0.26109
C	5.74907	5.28504	1.49674
C	1.08318	4.81069	0.32127
H	0.87618	5.86781	0.44059
C	6.24837	2.07898	0.44551
C	6.00418	6.6558	1.37258
H	6.15765	7.24659	2.27019
C	-1.08205	-4.81028	-0.32387
H	-0.875	-5.86737	-0.44336
C	-3.01341	3.56937	-2.87233
C	-6.06085	-7.27773	-0.12201
C	-2.38304	-4.34566	-0.44404
H	-3.20141	-5.03086	-0.6082
C	-6.00387	-6.65553	-1.37287
H	-6.15826	-7.24615	-2.27043
C	6.34599	-0.37796	0.32477
H	5.89486	-1.36235	0.30067
C	-5.5906	-5.12981	0.93876
C	-5.85136	-6.50049	1.02324
H	-5.88767	-6.97027	2.00137
C	7.66689	2.20417	0.29337
H	8.11103	3.19333	0.26342
C	5.34929	4.3096	-2.19367
H	4.33838	3.88574	-2.18525
H	6.05585	3.47518	-2.25754
H	5.45831	4.93182	-3.08697
C	6.36693	8.76111	0.00141
H	7.41665	8.91819	-0.27837
H	6.19	9.27561	0.95105
H	5.74136	9.2289	-0.76661
C	-5.67569	-4.63436	-2.86805
H	-6.42972	-3.84589	-2.96661
H	-5.84064	-5.37674	-3.65459
H	-4.69473	-4.17104	-3.02583
C	5.67431	4.63494	2.86781
H	4.69303	4.17201	3.02476
H	5.83879	5.37741	3.65436
H	6.42797	3.84623	2.96722
C	-6.365	-8.76113	-0.00168
H	-7.41377	-8.91834	0.28155
H	-5.73685	-9.22945	0.76392
H	-6.1913	-9.27504	-0.95223
C	-5.34545	-4.30996	2.19315
H	-4.33456	-3.88606	2.18377
H	-5.45352	-4.93234	3.08645
H	-6.05198	-3.47558	2.25788
C	8.72485	-1.23826	-0.03702
C	7.7629	-0.25483	0.15649
C	8.40807	1.06712	0.16531
C	-8.72416	1.2378	0.03857
C	-7.76209	0.25458	-0.15519
C	-8.40698	-1.06755	-0.16286
C	-9.84496	-0.82919	0.02791
C	-10.03097	0.57962	0.14998
C	-11.30164	1.12583	0.33345
C	-12.42075	0.28001	0.40626
C	-12.21819	-1.11015	0.28674
C	-10.94847	-1.67011	0.09762
H	-11.40631	2.19957	0.4138
H	-10.83887	-2.74522	0.00722
C	9.8462	0.82843	-0.02403
C	10.03198	-0.58038	-0.14662
C	11.30281	-1.12683	-0.3283
C	12.42224	-0.28128	-0.39918
C	12.21989	1.10888	-0.27933
C	10.95005	1.66908	-0.09171
H	11.40738	-2.20059	-0.40855

H	10.84062 2.74416 -0.00078	H	13.07387 1.77393 -0.33144
C	-8.13701 5.48608 0.33247	C	-13.85067 0.82173 0.60824
C	-8.24339 4.69632 1.4819	H	-13.07193 -1.77539 0.34046
C	-8.42895 3.31261 1.40387	C	13.8819 -2.36566 -0.70956
C	-8.50684 2.70105 0.1343	H	14.91766 -2.6949 -0.84867
C	-8.40567 3.48255 -1.03588	H	13.49367 -2.83585 0.20073
C	-8.22383 4.86414 -0.91737	H	13.295 -2.71332 -1.56699
H	-8.18058 5.16469 2.45917	C	14.73272 -0.40738 0.61036
C	8.1278 -5.48462 -0.33908	H	15.75496 -0.77945 0.47256
C	8.20605 -4.8646 0.91094	H	14.77292 0.68154 0.71443
C	8.3923 -3.48277 1.03259	H	14.3266 -0.82863 1.53634
C	8.50623 -2.70112 -0.13502	C	14.44744 -0.23232 -1.90597
C	8.4368 -3.31178 -1.40684	H	15.4676 -0.60668 -2.0534
C	8.24695 -4.69361 -1.48783	H	13.83703 -0.52603 -2.76673
H	8.12503 -5.46638 1.8107	H	14.48341 0.86091 -1.86488
H	2.96776 -4.4648 3.47924	C	-13.88052 2.36411 0.71797
H	-2.96837 4.46556 -3.4801	H	-14.91616 2.69315 0.85844
C	8.54703 -2.47243 -2.6683	H	-13.29247 2.7123 1.5744
H	8.51421 -3.10952 -3.55709	H	-13.49373 2.83404 -0.19308
H	7.72308 -1.75193 -2.72559	C	-14.44371 0.23111 1.91609
H	9.48255 -1.90257 -2.6786	H	-15.46379 0.60517 2.06483
C	7.89619 -6.98124 -0.45558	H	-14.47934 -0.86215 1.87553
H	8.11328 -7.48608 0.49085	H	-13.83216 0.52542 2.77583
H	6.85132 -7.18925 -0.71932	C	-14.73276 0.40507 -0.59989
H	8.53238 -7.41747 -1.23352	H	-15.75489 0.77695 -0.46073
H	8.18971 -5.16071 -2.46624	H	-14.32812 0.82606 -1.52664
C	8.47335 -2.83753 2.40603	H	-14.77285 -0.68389 -0.70347
H	9.35046 -2.18617 2.48161		
H	7.58774 -2.22019 2.59713	TS- PH1-A	
H	8.53554 -3.60283 3.18564	Sum of electronic and thermal Free Energies= -4166.025350	
C	-8.49736 2.83442 -2.40724	a.u.	
H	-8.5565 3.5981 -3.18865	C	-3.04607 -0.84889 1.54555
H	-7.61786 2.20905 -2.60005	C	-1.76649 0.97386 0.49921
H	-9.38022 2.19013 -2.47751	C	-3.03639 0.42911 0.86606
C	-8.52766 2.47512 2.66751	C	-1.91443 -1.70315 1.41567
H	-9.4618 1.90314 2.68569	C	4.09845 -0.80815 -0.66752
H	-7.7016 1.7567 2.72	C	1.7301 -0.31349 -0.28678
H	-8.48986 3.11375 3.555	C	1.4772 -1.7286 -0.23129
C	-7.9054 6.98346 0.43805	C	-0.62833 0.10605 0.36189
H	-8.31605 7.37906 1.37258	C	3.02193 0.13456 -0.65624
H	-6.83104 7.20831 0.41949	C	-1.62247 2.36548 0.21615
H	-8.37472 7.51314 -0.39753	C	5.57144 -0.65705 -0.56177
H	-8.15378 5.46549 -1.81852	C	-0.79294 -1.26799 0.60962
C	13.8523 -0.82331 -0.59924	C	-1.86267 -2.88522 2.2038
H	-0.96994 -3.49353 2.17251		
C	0.1847 -2.21219 0.11096		
C	-4.19664 1.20555 0.6236		
C	-4.07099 -1.20233 2.45835		
H	-4.88817 -0.51269 2.61445		
C	3.17828 1.51516 -1.02866		
C	-0.12876 -3.56244 -0.11882		
H	-1.14755 -3.89768 0.01733		
C	0.65518 0.64137 -0.07882		
C	0.86383 2.04371 -0.20281		
C	2.49384 -2.67868 -0.58593		
C	2.19095 2.49375 -0.66616		
C	6.13053 -2.01576 -0.65153		
C	-4.08004 2.5798 0.33658		
C	-2.79677 3.20444 0.23358		
C	3.83283 -2.19058 -0.70627		
C	4.28547 1.8856 -1.83846		
H	4.90612 1.096 -2.23536		
C	-0.31497 2.93919 -0.01229		
C	6.38689 0.3971 -0.25278		
H	6.00509 1.40151 -0.12487		
C	-4.0095 -2.37365 3.18625		
H	-4.79744 -2.61613 3.88951		
C	-2.66943 4.6001 0.11812		
H	-3.55542 5.21593 0.13302		
C	4.57194 3.19876 -2.12533		
H	5.41393 3.46004 -2.75451		
C	-0.27722 4.34421 -0.06808		
H	0.64172 4.87247 -0.1677		
C	-2.89296 -3.22242 3.05811		
C	5.28433 -4.40261 -0.84344		
C	-6.48618 6.7528 0.55817		
H	-6.74681 7.43369 1.3623		
C	-6.51278 7.20727 -0.76325		
C	-6.12888 5.43578 0.87212		
C	2.62033 3.84667 -0.85784		
H	2.08347 4.66357 -0.42876		
C	-5.78345 4.55219 -0.17014		
C	-5.63205 0.85383 0.51839		
C	-5.41693 3.14546 0.14112		
C	5.37008 -5.18241 0.32783		
C	5.09496 -2.93175 -0.74958		
C	7.5397 -2.24935 -0.53441		
H	7.91744 -3.26164 -0.63017		

C	-5.80222 4.99446 -1.51133	H	6.06292 -3.41376 -3.40376
C	-1.41317 5.15181 0.00134	C	-8.62025 -1.37354 0.17383
H	-1.29354 6.22774 -0.05305	C	-7.71811 -0.32006 0.24724
C	-6.33951 2.11282 0.24209	C	-8.43017 0.94997 0.03851
C	-6.16702 6.3149 -1.78594	C	8.81841 1.05539 0.17365
H	-6.17933 6.65404 -2.81735	C	7.79344 0.16326 -0.1122
C	0.84669 -4.46032 -0.55244	C	8.35254 -1.18696 -0.27797
H	0.58118 -5.49504 -0.73455	C	9.80401 -1.06431 -0.07844
C	3.76267 4.19111 -1.54926	C	10.08158 0.30716 0.1966
C	5.65953 -7.18747 -1.03501	C	11.38502 0.74615 0.43035
C	2.1545 -4.03874 -0.73982	C	12.44641 -0.17423 0.39986
H	2.92554 -4.74018 -1.02157	C	12.15318 -1.52588 0.12823
C	5.55683 -6.5649 0.21254	C	10.84924 -1.97801 -0.11149
H	5.61767 -7.16492 1.11504	H	11.56024 1.79463 0.63124
C	-6.30384 -0.33661 0.47571	H	10.66883 -3.02713 -0.31838
H	-5.80265 -1.28621 0.61341	C	-9.84443 0.60518 -0.16281
C	5.38503 -5.01403 -2.11201	C	-9.95342 -0.81465 -0.07864
C	5.56835 -6.39771 -2.18758	C	-11.18534 -1.45277 -0.22838
H	5.64109 -6.86721 -3.16385	C	-12.34085 -0.69104 -0.46967
C	-7.75508 2.1341 0.0264	C	-12.21409 0.71085 -0.55054
H	-8.24803 3.08236 -0.15878	C	-10.98419 1.36322 -0.39925
C	-6.08986 4.97079 2.31793	H	-11.2319 -2.53118 -0.15584
H	-5.08342 4.62932 2.58754	H	-10.93258 2.44431 -0.46773
H	-6.77444 4.1306 2.47651	C	8.51417 5.28205 0.89285
H	-6.37266 5.78554 2.9911	C	8.63122 4.78722 -0.40845
C	-6.91083 8.6356 -1.09319	C	8.7244 3.41395 -0.66393
H	-7.08225 9.21441 -0.18054	C	8.69984 2.51286 0.41891
H	-7.83275 8.65433 -1.68733	C	8.58856 2.99491 1.74171
H	-6.12686 9.13516 -1.67454	C	8.49535 4.37199 1.95697
C	5.2347 -4.53178 1.69314	H	8.65373 5.48095 -1.24304
H	6.00101 -3.76266 1.83725	C	-7.79994 -5.57404 0.57304
H	5.33347 -5.27865 2.48646	C	-7.81941 -4.96604 -0.68642
H	4.25666 -4.04629 1.79064	C	-8.07887 -3.59983 -0.83463
C	-5.41048 4.0492 -2.63284	C	-8.32397 -2.81946 0.31479
H	-4.37309 3.71717 -2.50936	C	-8.31457 -3.417 1.59255
H	-5.50397 4.5447 -3.60374	C	-8.053 -4.78645 1.70102
H	-6.04533 3.15666 -2.63059	H	-7.63037 -5.56524 -1.57167
C	5.8867 -8.68547 -1.14382	H	-2.81955 -4.11628 3.66644
H	6.93862 -8.90026 -1.37201	H	4.01923 5.2385 -1.65814
H	5.27482 -9.11811 -1.94294	C	-8.58857 -2.58384 2.83335
H	5.6347 -9.18894 -0.20536	H	-8.65488 -3.22402 3.71829
C	5.27848 -4.17793 -3.37577	H	-7.78959 -1.85066 2.99343
H	4.31367 -3.659 -3.41829	H	-9.52691 -2.02799 2.73043
H	5.37289 -4.80997 -4.2638	C	-7.48456 -7.05305 0.71585
H	-7.78266 -7.60608 -0.18071		
H	-6.40714 -7.2038 0.86275		
H	-8.00532 -7.48423 1.57716		
H	-8.05101 -5.24624 2.6845		
C	-8.0879 -2.95987 -2.21231		
H	-9.03748 -2.44563 -2.39708		
H	-7.28897 -2.21455 -2.29773		
H	-7.94166 -3.71688 -2.98851		
C	8.55844 2.02445 2.90997		
H	8.52933 2.56701 3.85946		
H	7.67655 1.37633 2.85208		
H	9.44259 1.37749 2.90172		
C	8.8459 2.90287 -2.08982		
H	9.68933 2.21093 -2.18719		
H	7.94022 2.35982 -2.38481		
H	8.99301 3.73524 -2.78476		
C	8.4089 6.77418 1.15762		
H	9.22063 7.11261 1.81261		
H	8.46418 7.34153 0.22361		
H	7.45831 7.01519 1.64862		
H	8.40658 4.74141 2.97409		
C	-13.72993 -1.33522 -0.65089		
H	-13.0966 1.31168 -0.73624		
C	13.90889 0.24379 0.65342		
H	12.96191 -2.24671 0.10283		
C	-13.68053 -2.87627 -0.52592		
H	-14.69001 -3.27908 -0.66481		
H	-13.02998 -3.31533 -1.29044		
H	-13.32294 -3.18321 0.4632		
C	-14.27916 -0.98168 -2.05957		
H	-15.27047 -1.43031 -2.19715		
H	-14.36999 0.10159 -2.18778		
H	-13.60781 -1.36654 -2.83475		
C	-14.69597 -0.79175 0.43658		
H	-15.68775 -1.24288 0.31265		
H	-14.31926 -1.03796 1.43515		
H	-14.80065 0.29552 0.36492		
C	14.04459 1.75928 0.93089		
H	15.09974 1.99794 1.10495		
H	13.69676 2.35206 0.07756		
H	13.47753 2.05231 1.82145		
C	14.76497 -0.09843 -0.5962		
H	15.80879 0.18947 -0.42293		
H	14.73489 -1.17069 -0.81451		

H	14.39073 0.44365 -1.47132	H	-4.53594 -2.65234 3.64656
C	14.4555 -0.52532 1.8865	C	-2.75759 4.39653 -1.05768
H	15.49703 -0.2374 2.07342	H	-3.64639 5.00573 -1.1175
H	13.85982 -0.28868 2.77466	C	4.64014 3.64792 -1.47217
H	14.42024 -1.60731 1.72458	H	5.57522 4.07455 -1.81513
		C	-0.40229 4.06093 -1.49218
(*M*, *P*, *P*, *P*)-**1**		H	0.50466 4.40957 -1.96175
Sum of electronic and thermal Free Energies= -4166.037685		C	-2.74214 -3.29977 2.62344
a.u		C	5.42819 -4.23119 -1.38331
C	-2.95599 -0.88205 1.18451	C	-6.2921 6.74912 0.00632
C	-1.76739 0.93051 0.03041	H	-6.32246 7.52565 0.76465
C	-3.00377 0.39955 0.50182	C	-6.64969 7.05907 -1.31189
C	-1.85214 -1.75901 0.9488	C	-5.89693 5.45972 0.37114
C	4.18657 -0.67871 -0.90155	C	2.39643 3.94271 -0.64227
C	1.79016 -0.27026 -0.66165	H	1.61809 4.57798 -0.24471
C	1.55997 -1.68725 -0.68449	C	-5.85624 4.44802 -0.61356
C	-0.63073 0.05963 -0.141	C	-5.62588 0.82458 0.38156
C	3.09698 0.25466 -0.88701	C	-5.45529 3.06735 -0.23485
C	-1.67506 2.28303 -0.42434	C	5.51449 -5.11343 -0.28752
C	5.64991 -0.53993 -0.67575	C	5.21263 -2.77865 -1.15362
C	-0.76014 -1.31185 0.10842	C	7.63058 -2.12088 -0.71793
C	-1.77665 -2.96653 1.69463	H	8.02357 -3.10981 -0.9284
H	-0.90874 -3.5988 1.57357	C	-6.21445 4.74107 -1.9451
C	0.26199 -2.21278 -0.40219	C	-1.55723 4.84348 -1.57969
C	-4.18307 1.17224 0.31554	H	-1.51093 5.8057 -2.07643
C	-3.89718 -1.22665 2.18447	C	-6.35899 2.06127 0.07104
H	-4.67169 -0.51529 2.43309	C	-6.60518 6.04539 -2.27274
C	3.24189 1.68657 -1.04911	H	-6.87641 6.27122 -3.29917
C	-0.00397 -3.56047 -0.687	C	1.0076 -4.40959 -1.14222
H	-1.01394 -3.93308 -0.58207	H	0.77544 -5.44278 -1.37275
C	0.65234 0.60932 -0.54123	C	3.62794 4.47944 -0.94857
C	0.79649 1.99593 -0.70068	C	5.86145 -6.97874 -1.82418
C	2.61002 -2.5879 -1.05737	C	2.30628 -3.9467 -1.28947
C	2.12712 2.55133 -0.80439	H	3.09807 -4.61547 -1.59126
C	6.23068 -1.87451 -0.8997	C	5.72943 -6.47598 -0.5268
C	-4.10404 2.51328 -0.13008	H	5.79008 -7.15538 0.31749
C	-2.85293 3.10047 -0.5041	C	-6.30495 -0.35797 0.49599
C	3.94004 -2.0571 -1.09586	H	-5.79872 -1.30175 0.64977
C	4.44902 2.28319 -1.50458	C	5.55931 -4.72082 -2.70128
H	5.22814 1.64107 -1.88559	C	5.77236 -6.0875 -2.9009
C	-0.41212 2.81413 -0.84853	H	5.86945 -6.46356 -3.91486
C	6.42773 0.45019 -0.13816	C	-7.7901 2.0844 0.01524
H	6.02637 1.41809 0.13106	H	-8.29607 3.0227 -0.18495
C	-3.8086 -2.4178 2.87844	C	-5.50577 5.14649 1.8048
H	-4.46208 4.81532 1.85786
H	-6.12744 4.34009 2.20896
H	-5.62251 6.03138 2.43747
C	-7.07409 8.47043 -1.68051
H	-7.95136 8.77782 -1.09866
H	-7.32828 8.53678 -2.74265
H	-6.26821 9.18567 -1.47605
C	5.34775 -4.59518 1.13024
H	6.10506 -3.83853 1.36168
H	5.43747 -5.41315 1.85127
H	4.36424 -4.12712 1.25352
C	-6.14807 3.6651 -3.01514
H	-5.12845 3.27162 -3.102
H	-6.44812 4.07077 -3.98593
H	-6.80549 2.82483 -2.76768
C	6.10762 -8.4576 -2.06941
H	7.12315 -8.62356 -2.45033
H	5.40282 -8.85435 -2.80915
H	5.99421 -9.03114 -1.14446
C	5.45562 -3.77191 -3.88267
H	4.48447 -3.26347 -3.88785
H	5.56842 -4.3167 -4.82471
H	6.23017 -2.99888 -3.82921
C	-8.64303 -1.38914 0.53079
C	-7.73568 -0.34393 0.41654
C	-8.46387 0.91341 0.19075
C	8.81044 1.04566 0.55861
C	7.82264 0.20028 0.0716
C	8.41215 -1.1063 -0.25371
C	9.84381 -1.00789 0.06487
C	10.07997 0.30911 0.55979
C	11.35576 0.71324 0.95423
C	12.4309 -0.18643 0.86368
C	12.17956 -1.48375 0.37201
C	10.90336 -1.90141 -0.02611
H	11.49773 1.71865 1.32754
H	10.75465 -2.90895 -0.39854
C	-9.89283 0.57111 0.17885
C	-9.99547 -0.83585 0.38849
C	-11.23857 -1.4678 0.43676
C	-12.41183 -0.71268 0.27148
C	-12.29073 0.67599 0.06028
C	-11.04939 1.3225 0.01449
H	-11.28026 -2.53589 0.60374

H	-11.00216 2.39391 -0.14656	H	-13.18695 1.2709 -0.07013
C	8.37119 5.12389 1.84261	C	13.86483 0.1978 1.28131
C	8.72373 4.82508 0.52377	H	12.99969 -2.18842 0.29717
C	8.86743 3.50292 0.08685	C	-13.75885 -2.87323 0.57433
C	8.64836 2.45185 1.00008	H	-14.77966 -3.2708 0.59711
C	8.29865 2.73486 2.3382	H	-13.20804 -3.3929 -0.21747
C	8.16499 4.06717 2.73757	H	-13.28589 -3.09206 1.53818
H	8.89382 5.63429 -0.17954	C	-14.52234 -1.11788 -1.05087
C	-7.80566 -5.5553 1.17824	H	-15.52552 -1.56035 -1.03088
C	-8.00334 -5.05748 -0.11539	H	-14.6202 -0.04936 -1.2675
C	-8.2709 -3.70558 -0.34428	H	-13.94808 -1.5836 -1.85901
C	-8.3393 -2.82275 0.75598	C	-14.64662 -0.69493 1.44858
C	-8.14671 -3.307 2.06534	H	-15.64939 -1.13782 1.47898
C	-7.88283 -4.66857 2.25527	H	-14.15998 -0.85872 2.41607
H	-7.94793 -5.73434 -0.96253	H	-14.75083 0.38338 1.292
H	-2.64896 -4.21658 3.19373	C	13.95456 1.65546 1.79004
H	3.81258 5.53703 -0.80169	H	14.99094 1.87305 2.07137
C	-8.22732 -2.36557 3.2555	H	13.65532 2.36671 1.01215
H	-8.16977 -2.92671 4.19317	H	13.32222 1.80706 2.67178
H	-7.40633 -1.6396 3.23333	C	14.81248 0.05224 0.05997
H	-9.16478 -1.79899 3.24244	H	15.83594 0.31943 0.34934
C	-7.50471 -7.02831 1.39634	H	14.8174 -0.9755 -0.31638
H	-8.25544 -7.65813 0.90501	H	14.49087 0.71575 -0.74999
H	-6.52338 -7.28827 0.98043	C	14.33689 -0.74344 2.42261
H	-7.49766 -7.27211 2.46306	H	15.35904 -0.48234 2.72207
H	-7.73891 -5.04175 3.26439	H	13.67894 -0.64372 3.2926
C	-8.47142 -3.18526 -1.75739	H	14.32823 -1.78951 2.1005
H	-9.43728 -2.67701 -1.85227		
H	-7.69177 -2.45982 -2.0164	TS- PH1-B	
H	-8.43487 -4.00741 -2.47824	Sum of electronic and thermal Free Energies= -4166.016919	
C	8.07302 1.60472 3.32821	a.u.	
H	7.90216 2.00321 4.33262	C	3.2878 -0.7975 1.8654
H	7.20332 1.00313 3.04088	C	1.93327 0.98144 0.84019
H	8.94001 0.93554 3.35823	C	3.22457 0.43644 1.10559
C	9.24656 3.20255 -1.35353	C	2.11698 -1.60793 1.97461
H	10.13135 2.55812 -1.39734	C	-4.15234 -0.59853 0.34732
H	8.43369 2.67651 -1.8678	C	-1.71116 -0.18968 0.59017
H	9.46019 4.12834 -1.89625	C	-1.48063 -1.59933 0.70824
C	8.20604 6.56219 2.30283	C	0.76069 0.14648 0.93261
H	8.51339 7.26141 1.51925	C	-3.04434 0.34282 0.43939
H	7.15863 6.77006 2.55433	C	1.79112 2.36478 0.50979
H	8.81107 6.75907 3.1955	C	-5.65437 -0.50682 0.12446
H	7.89659 4.28417 3.76698	C	0.90349 -1.19621 1.29888
C	-13.81558 -1.34999 0.31217	C	2.13792 -2.71205 2.86957
H	1.22608 -3.27023 3.02808		
C	-0.17515 -2.11711 0.99621		
C	4.35776 1.20676 0.7212		
C	4.42169 -1.13149 2.64879		
H	5.27928 -0.47506 2.62619		
C	-3.13298 1.7768 0.17375		
C	0.05745 -3.49472 0.87618		
H	1.06659 -3.86903 0.9716		
C	-0.54602 0.67854 0.58035		
C	-0.66619 2.03079 0.23348		
C	-2.54373 -2.51929 0.46153		
C	-1.95955 2.51803 -0.17495		
C	-6.0954 -1.87396 -0.2282		
C	4.22753 2.58549 0.4432		
C	2.94388 3.21906 0.45084		
C	-3.85092 -1.98877 0.24695		
C	-4.34041 2.51321 0.18127		
H	-5.16728 2.10128 0.71114		
C	0.48474 2.92713 0.36267		
C	-6.65471 0.42057 0.28671		
H	-6.52254 1.41491 0.66767		
C	4.425 -2.23506 3.47796		
H	5.30035 -2.45915 4.07624		
C	2.76661 4.61668 0.39761		
H	3.63559 5.25666 0.35546		
C	-4.46496 3.76379 -0.38734		
H	-5.41593 4.28221 -0.34508		
C	0.36421 4.32572 0.4402		
H	-0.61587 4.77011 0.52021		
C	3.26904 -3.03015 3.59356		
C	-5.17871 -4.20472 -0.4039		
C	6.0474 6.30259 -1.88669		
H	5.94918 6.63288 -2.9163		
C	6.46939 7.21184 -0.90906		
C	5.74281 4.97643 -1.56818		
C	-2.12331 3.73118 -0.90418		
H	-1.25175 4.17224 -1.36683		
C	5.86608 4.54632 -0.22889		
C	5.77388 0.84809 0.48181		
C	5.5432 3.14024 0.12612		
C	-4.93071 -4.69912 -1.70032		
C	-5.03568 -2.74828 -0.12972		
C	-7.45335 -2.21107 -0.54008		
H	-7.67947 -3.23327 -0.82244		

C	6.29284	5.4465	0.7682	H	-6.63694	-3.79149	2.01797	H	7.76078	-7.43315	1.4347
C	1.4901	5.15288	0.45517	C	8.69226	-1.40903	-0.15082	H	6.51232	-7.29202	0.18253
H	1.35874	6.22732	0.50953	C	7.81203	-0.34662	0.01177	H	8.18126	-7.67952	-0.27244
C	6.46418	2.10162	0.14105	C	8.51431	0.91722	-0.25849	H	7.63643	-5.59516	-1.86547
C	6.58495	6.76872	0.41158	C	-9.12914	0.92292	0.00743	C	8.72041	-2.62127	2.5164
H	6.90661	7.46336	1.18112	C	-8.01361	0.0971	-0.02599	H	9.63364	-2.03296	2.37699
C	-0.98483	-4.37808	0.59642	C	-8.40259	-1.24177	-0.45931	H	7.90541	-1.91822	2.7243
H	-0.78247	-5.43924	0.51058	C	-9.85156	-1.20184	-0.69693	H	8.84929	-3.26908	3.38881
C	-3.35579	4.33397	-1.04053	C	-10.28945	0.1276	-0.41491	C	-8.22337	2.93371	-1.92668
C	-5.5091	-6.94832	-0.94679	C	-11.6273	0.49201	-0.57275	H	-8.17279	3.81009	-2.58012
C	-2.27303	-3.90663	0.42449	C	-12.56446	-0.46238	-1.00164	H	-7.22287	2.48772	-1.87396
H	-3.08154	-4.59186	0.23332	C	-12.11547	-1.77291	-1.26549	H	-8.89147	2.19445	-2.3794
C	-5.09901	-6.06595	-1.95048	C	-10.77472	-2.14911	-1.12124	C	-10.06761	1.7011	2.65853
H	-4.90345	-6.44639	-2.94806	H	-11.92453	1.51177	-0.36678	H	-10.87603	1.08745	2.24687
C	6.42495	-0.34959	0.36947	H	-10.46997	-3.16594	-1.34289	H	-9.24124	1.02685	2.91179
H	5.92635	-1.29456	0.54594	C	9.90025	0.5593	-0.59157	H	-10.42181	2.17806	3.57715
C	-5.59755	-5.07965	0.62212	C	10.00221	-0.86167	-0.5235	C	-9.20228	6.55043	1.48768
C	-5.7527	-6.43894	0.3347	C	11.20927	-1.51093	-0.78561	H	-10.1849	6.84167	1.87628
H	-6.06721	-7.11239	1.12621	C	12.34521	-0.75932	-1.12922	H	-8.45952	6.74646	2.27104
C	7.85315	2.10832	-0.2071	C	12.22541	0.64413	-1.19362	H	-8.96912	7.18931	0.63045
H	8.33673	3.05138	-0.43823	C	11.02124	1.30759	-0.92769	H	-8.41849	5.43276	-0.88489
C	5.26962	4.01195	-2.64119	H	11.25201	-2.58982	-0.71794	C	13.70667	-1.41581	-1.43597
H	4.25784	3.65422	-2.41813	H	10.97459	2.38948	-0.98592	H	13.09339	1.23734	-1.45648
H	5.92515	3.13599	-2.69376	C	-9.18943	5.08413	1.09129	C	-14.05617	-0.12371	-1.1975
H	5.25795	4.50123	-3.61968	C	-9.62361	4.10338	1.99147	H	-12.82801	-2.51941	-1.5967
C	6.80685	8.64415	-1.28635	C	-9.61418	2.74766	1.65483	C	13.65208	-2.95693	-1.3182
H	7.7449	8.68386	-1.85445	C	-9.15149	2.35763	0.3775	H	14.64075	-3.36834	-1.55047
H	6.92449	9.26687	-0.39417	C	-8.71329	3.33221	-0.54367	H	13.38223	-3.26829	-0.30301
H	6.01841	9.08099	-1.90968	C	-8.74095	4.68219	-0.16979	H	12.93061	-3.38316	-2.0241
C	-4.46304	-3.76356	-2.80082	H	-9.97481	4.39955	2.97521	C	14.76836	-0.89051	-0.43202
H	-5.18275	-2.95248	-2.95508	C	7.86674	-5.60615	0.2752	H	15.74247	-1.34594	-0.64721
H	-4.33947	-4.30773	-3.74183	C	8.15004	-4.81974	1.39463	H	14.87332	0.19693	-0.50044
H	-3.50304	-3.30639	-2.53409	C	8.41408	-3.4497	1.27978	H	14.47872	-1.1463	0.59286
C	6.41142	4.99281	2.21338	C	8.39499	-2.85306	0.00317	C	14.13534	-1.05629	-2.88432
H	5.4511	4.61299	2.58133	C	8.11647	-3.6341	-1.14075	H	15.10774	-1.5112	-3.10818
H	6.72518	5.82391	2.85195	C	7.85492	-4.99743	-0.98576	H	13.39753	-1.43125	-3.60182
H	7.14215	4.18229	2.30928	H	8.16999	-5.27907	2.37783	H	14.22309	0.02714	-3.01303
C	-5.70385	-8.42676	-1.23669	H	3.25056	-3.86295	4.28677	C	-14.3688	1.35527	-0.87096
H	-6.77159	-8.67921	-1.25965	H	-3.45915	5.24895	-1.61148	H	-15.43768	1.53782	-1.02822
H	-5.22995	-9.04319	-0.46447	C	8.08229	-2.99241	-2.51728	H	-14.13244	1.58958	0.17293
H	-5.27105	-8.69552	-2.20511	H	7.90049	-3.74703	-3.28827	H	-13.80701	2.03303	-1.52328
C	-5.8474	-4.55065	2.02355	H	7.28761	-2.23959	-2.57229	C	-14.91329	-1.01875	-0.26201
H	-4.94223	-4.08082	2.42617	H	9.02894	-2.4867	-2.73653	H	-15.97744	-0.79663	-0.40647
H	-6.14578	-5.36263	2.69324	C	7.56509	-7.08835	0.41477	H	-14.75033	-2.08026	-0.47345

H	-14.65325	-0.83086	0.78531	H	-15.51376	-0.15698	-2.82365	H	-14.28369	-1.43319	-2.94951
C	-14.45172	-0.3868	-2.67586	H	-13.85795	0.24538	-3.34479				

(*P*, *M*, *P*, *P*)-**1**

Sum of electronic and thermal Free Energies = -4166.032248 a.u.

C	-3.34674	-1.25101	-2.03218	H	5.68577	3.801	-2.12265	H	-5.12077	3.63694	2.00272
C	-1.86083	0.65299	-1.58673	C	-0.30435	3.94438	-2.27604	H	-4.3437	5.17083	2.46222
C	-3.17113	0.09584	-1.5223	H	0.63207	4.32465	-2.65354	C	-6.40143	8.70916	-0.41145
C	-2.19795	-2.07909	-2.22521	C	-3.59077	-3.70283	-3.4096	H	-7.02871	8.935	0.45919
C	4.16381	-0.87853	-1.13409	C	5.48616	-4.41625	-0.71778	H	-6.91774	9.06804	-1.30693
C	1.76436	-0.52632	-1.52834	C	-5.49202	6.54856	0.54923	H	-5.46632	9.27265	-0.3068
C	1.55044	-1.94439	-1.46802	H	-5.20289	7.10289	1.43697	C	4.99804	-4.34761	1.77687
C	-0.71093	-0.20974	-1.69294	C	-6.12485	7.21834	-0.50539	H	5.69613	-3.53313	1.99746
C	3.08849	0.00826	-1.46152	C	-5.22016	5.17946	0.48685	H	4.97194	-5.02843	2.63295
C	-1.68169	2.07128	-1.5947	C	2.40603	3.68296	-1.26431	H	4.00288	-3.90449	1.65326
C	5.54973	-0.65431	-0.62677	H	1.60699	4.31807	-0.91268	C	-6.63034	4.34376	-2.98643
C	-0.89284	-1.59486	-1.81131	C	-5.59579	4.45661	-0.66674	H	-5.75194	3.87466	-3.44503
C	-2.35514	-3.2894	-2.95386	C	-5.57967	0.69019	-0.56925	H	-7.09073	5.01246	-3.71983
H	-1.47467	-3.86067	-3.21017	C	-5.31828	2.99966	-0.7503	H	-7.34026	3.54475	-2.74671
C	0.22735	-2.48726	-1.55997	C	5.40987	-5.09109	0.51792	C	6.35323	-8.66001	-0.5231
C	-4.23043	0.9553	-1.11556	C	5.21327	-2.95608	-0.78747	H	7.42759	-8.83442	-0.66264
C	-4.5972	-1.69281	-2.53482	C	7.4896	-2.16183	0.00826	H	5.81966	-9.20822	-1.30784
H	-5.45101	-1.03692	-2.45016	H	7.90917	-3.16114	0.05205	H	6.06478	-9.07868	0.44589
C	3.25768	1.435	-1.64046	C	-6.23782	5.11284	-1.73632	C	5.91423	-4.39618	-3.22275
C	0.03892	-3.8561	-1.30651	C	-1.43149	4.77096	-2.30007	H	4.94471	-3.95258	-3.47702
H	-0.96519	-4.24462	-1.22267	H	-1.3341	5.79016	-2.65571	H	6.20033	-5.08806	-4.02052
C	0.62403	0.36004	-1.61277	C	-6.21375	2.00444	-0.38178	H	6.64774	-3.58327	-3.18324
C	0.79411	1.75849	-1.62021	C	-6.49014	6.48699	-1.63895	C	-8.33611	-1.3165	0.97503
C	2.65727	-2.8419	-1.29616	H	-6.98017	6.99256	-2.46506	C	-7.49979	-0.33103	0.46566
C	2.13086	2.304	-1.51052	C	1.12335	-4.71469	-1.12903	C	-8.15327	0.9805	0.59499
C	6.15709	-1.98843	-0.49067	H	0.9485	-5.76888	-0.94836	C	8.41461	1.20968	0.90741
C	-4.07153	2.35804	-1.16429	C	3.66988	4.20729	-1.43071	C	7.53572	0.26259	0.40014
C	-2.82097	2.94324	-1.54361	C	6.03881	-7.17521	-0.58814	C	8.16843	-1.06273	0.43815
C	3.96172	-2.27781	-1.13297	C	2.41804	-4.22747	-1.1668	C	9.50808	-0.86945	1.01091
C	4.5125	2.01661	-1.96182	H	3.25849	-4.89154	-1.04071	C	9.6524	0.52108	1.29493
H	5.31803	1.36368	-2.26533	C	5.68603	-6.46297	0.56157	C	10.82886	1.02438	1.85101
C	-0.37793	2.61897	-1.81297	H	5.61943	-6.98316	1.5119	C	11.89246	0.15257	2.13892
C	6.21361	0.43291	-0.1255	C	-6.19589	-0.4442	-0.11675	C	11.73258	-1.21798	1.85047
H	5.77795	1.42156	-0.1167	H	-5.73242	-1.42052	-0.18986	C	10.55714	-1.73513	1.29154
C	-4.7267	-2.90332	-3.1852	C	5.84036	-5.11978	-1.88974	H	10.90494	2.08438	2.05359
H	-5.69175	-3.20939	-3.57147	C	6.11032	-6.48838	-1.80631	H	10.47704	-2.79665	1.08462
C	-2.66431	4.3054	-1.87126	H	6.37991	-7.02838	-2.70884	C	-9.45988	0.73367	1.22077
H	-3.52333	4.95912	-1.83351	C	-7.52149	2.11856	0.18946	C	-9.56495	-0.67038	1.44959
C	4.71684	3.37842	-1.88545	H	-7.96722	3.10139	0.29947	C	-10.70095	-1.22124	2.044
				C	-4.51972	4.47584	1.63583	C	-11.76416	-0.38531	2.42359
				H	-3.5548	4.07227	1.30793	C	-11.64403	0.99968	2.18779

C	-10.50867 1.56465 1.59377	H	6.99562 4.99416 3.20808
H	-10.74409 -2.29004 2.20625	C	-13.04529 -0.92934 3.08764
H	-10.45811 2.63591 1.43275	H	-12.4559 1.6571 2.47598
C	7.77423 5.44605 1.25266	C	13.21744 0.64364 2.75735
C	8.33095 4.89993 0.09272	H	12.54476 -1.90206 2.06684
C	8.54454 3.52246 -0.03745	C	-13.00489 -2.46516 3.26548
C	8.18588 2.66993 1.0264	H	-13.93575 -2.79458 3.74063
C	7.62679 3.20432 2.20715	H	-12.9164 -2.97424 2.29931
C	7.42845 4.58443 2.30058	H	-12.16905 -2.76941 3.90514
H	8.6104 5.55656 -0.72539	C	-14.27215 -0.57669 2.20342
C	-7.60449 -5.54707 1.17756	H	-15.18966 -0.95167 2.67268
C	-8.3099 -4.99397 0.10409	H	-14.36828 0.50611 2.07486
C	-8.55111 -3.61907 0.01923	H	-14.16991 -1.03521 1.21396
C	-8.07013 -2.77341 1.04086	C	-13.21049 -0.283 4.48961
C	-7.36351 -3.31454 2.13541	H	-14.1226 -0.6596 4.9679
C	-7.14164 -4.69439 2.1853	H	-12.35224 -0.52996 5.12373
H	-8.68112 -5.64385 -0.68226	H	-13.28371 0.80662 4.41571
H	-3.67628 -4.61876 -3.98254	C	13.21601 2.16995 3.00715
H	3.85515 5.25487 -1.22511	H	14.17656 2.46128 3.44671
C	-6.85886 -2.41171 3.24848	H	13.08665 2.72505 2.07142
H	-6.41951 -3.00669 4.05466	H	12.42076 2.45714 3.70386
H	-6.09695 -1.7184 2.87473	C	14.38895 0.31202 1.79381
H	-7.67623 -1.81015 3.66141	H	15.33684 0.64761 2.23141
C	-7.3236 -7.03869 1.2366	H	14.45609 -0.76471 1.60882
H	-8.08565 -7.60364 0.69018	H	14.24494 0.81969 0.83397
H	-6.34801 -7.26404 0.78651	C	13.44382 -0.06933 4.11814
H	-7.30619 -7.39401 2.27219	H	14.38729 0.26924 4.56286
H	-6.60087 -5.11033 3.02972	H	12.62579 0.16324 4.80838
C	-9.31268 -3.04013 -1.16111	H	13.4916 -1.15551 3.99193
H	-10.18393 -2.46917 -0.82177		
H	-8.67634 -2.35622 -1.73454	(*M*, *M*, *P*, *P*)-**2**	
H	-9.65436 -3.83839 -1.82682	Sum of electronic and thermal Free Energies = -4166.030491	
C	7.24072 2.28679 3.35472	a.u.	
H	6.90263 2.87022 4.21619	C	0.57696 -2.48579 0.12773
H	6.43294 1.60957 3.05491	C	1.78637 -1.85909 -0.19084
H	8.09157 1.66814 3.66087	C	1.81407 -0.4078 -0.38411
C	9.1501 2.95173 -1.30885	C	0.59539 0.32943 -0.25795
H	10.02437 2.33298 -1.07924	C	0.56669 1.67631 -0.56427
H	8.42769 2.31453 -1.8323	C	1.64111 2.22365 -1.34048
H	9.45749 3.75634 -1.9837	C	1.48541 3.39643 -2.13106
C	7.55918 6.94394 1.38802	H	0.54188 3.8952 -2.13471
H	7.76519 7.45566 0.44298	C	2.48022 3.84426 -2.93766
H	6.52636 7.16519 1.68123	H	2.32732 4.71424 -3.54469
H	8.22298 7.36352 2.15416	C	3.69205 3.13342 -3.02652
H	4.45948 3.46849 -3.69543		
C	3.86268 1.99228 -2.31335		
H	4.75004 1.41323 -2.44111		
C	2.85101 1.50495 -1.44271		
C	2.96828 0.2314 -0.80075		
C	4.22646 -0.48434 -0.66086		
C	5.51301 -0.06734 -0.50191		
C	6.12326 1.23399 -0.31715		
H	5.51071 2.11127 -0.30331		
C	7.44665 1.29992 -0.15247		
C	8.36533 2.43564 0.05175		
C	8.17356 3.79526 0.131		
H	7.19433 4.22376 0.04404		
C	9.27563 4.6172 0.32883		
H	9.1139 5.67431 0.39071		
C	10.57009 4.11445 0.44859		
C	10.7512 2.73414 0.36514		
H	11.72268 2.2959 0.45086		
C	9.66022 1.91399 0.16931		
C	9.58678 0.43949 0.0523		
C	8.29608 0.09403 -0.13611		
C	7.68682 -1.20823 -0.26682		
H	8.29323 -2.09164 -0.21709		
C	6.35844 -1.26948 -0.42671		
C	5.46823 -2.4342 -0.49487		
C	4.20436 -1.96599 -0.59609		
C	2.91897 -2.64808 -0.49197		
C	2.78695 -4.01956 -0.61348		
H	3.64163 -4.61193 -0.85614		
C	1.54907 -4.61748 -0.44641		
H	1.44066 -5.67143 -0.60704		
C	0.46223 -3.86661 -0.07121		
H	-0.49171 -4.33501 0.03701		
C	11.74152 5.08677 0.66675		
C	13.0957 4.35651 0.77571		
H	13.10898 3.67109 1.61548		
H	13.88128 5.0882 0.92809		
H	13.3221 3.80575 -0.13019		
C	11.82347 6.06869 -0.52488		
H	11.9806 5.52554 -1.44973		
H	12.65099 6.7563 -0.38246		
H	10.91494 6.64991 -0.62149		
C	11.51763 5.87512 1.97794		
H	10.60177 6.45167 1.94123		

H	12.34234 6.56088 2.1437	C	-1.81407 0.4078 0.38413	H	-13.10896 -3.6711 -1.61557
H	11.45866 5.19528 2.82015	C	-0.59539 -0.32943 0.25797	H	-13.88127 -5.0882 -0.92816
C	10.7633 -0.46061 0.14556	C	-0.5667 -1.67631 0.56429	H	-13.32211 -3.80573 0.1301
C	11.1639 -0.95254 1.38568	C	-1.64111 -2.22365 1.3405	C	-11.82349 -6.06868 0.52484
C	12.27655 -1.77888 1.45669	C	-1.48541 -3.39644 2.13108	H	-11.98063 -5.52552 1.44969
H	12.58436 -2.1585 2.41181	H	-0.54189 -3.89521 2.13473	H	-12.651 -6.75629 0.38241
C	12.99371 -2.11957 0.32454	C	-2.48022 -3.84426 2.93767	H	-10.91496 -6.6499 0.62147
C	12.58448 -1.61531 -0.90096	H	-2.32733 -4.71424 3.5447	C	-11.5176 -5.87513 -1.97798
H	13.13607 -1.86942 -1.78619	C	-3.69205 -3.13342 3.02653	H	-10.60174 -6.45168 -1.94125
C	11.47971 -0.78923 -1.0078	H	-4.45948 -3.4685 3.69544	H	-12.34231 -6.56089 -2.14374
C	10.39382 -0.5967 2.64537	C	-3.86269 -1.99229 2.31337	H	-11.45861 -5.1953 -2.82019
H	10.29605 0.47751 2.74771	H	-4.75005 -1.41324 2.44112	C	-10.76329 0.46061 -0.14558
H	10.90034 -0.9813 3.52146	C	-2.85101 -1.50495 1.44273	C	-11.16389 0.95254 -1.38571
H	9.39517 -1.01727 2.61526	C	-2.96829 -0.2314 0.80077	C	-12.27654 1.77888 -1.45673
C	14.20275 -3.0324 0.40668	C	-4.22646 0.48434 0.66088	H	-12.58435 2.15849 -2.41185
H	14.45955 -3.24707 1.43636	C	-5.51302 0.06734 0.50193	C	-12.99371 2.11957 -0.32458
H	15.06304 -2.57432 -0.069	C	-6.12326 -1.234 0.31716	C	-12.58449 1.6153 0.90092
H	14.00216 -3.97368 -0.09477	H	-5.51071 -2.11127 0.30332	H	-13.13609 1.86941 1.78614
C	11.05096 -0.25141 -2.36166	C	-7.44665 -1.29992 0.15246	C	-11.47972 0.78923 1.00777
H	10.07785 -0.64108 -2.63755	C	-8.36533 -2.43564 -0.05176	C	-10.3938 0.5967 -2.64539
H	11.76305 -0.53567 -3.12597	C	-8.17355 -3.79526 -0.131	H	-10.29603 -0.47751 -2.74773
H	10.97958 0.82972 -2.34226	H	-7.19432 -4.22376 -0.04404	H	-10.90031 0.98131 -3.52148
C	5.96625 -3.82884 -0.37929	C	-9.27562 -4.6172 -0.32885	H	-9.39515 1.01726 -2.61527
C	6.07323 -4.43107 0.87353	H	-9.11389 -5.67431 -0.39073	C	-14.20273 3.03243 -0.40673
C	6.55531 -5.72894 0.96257	C	-10.57009 -4.11445 -0.44862	H	-14.45983 3.24668 -1.43643
H	6.63384 -6.19163 1.92762	C	-10.7512 -2.73414 -0.36518	H	-15.06289 2.5746 0.0694
C	6.9339 -6.43637 -0.1645	H	-11.72267 -2.2959 -0.45091	H	-14.00192 3.9739 0.09426
C	6.82294 -5.82359 -1.40302	C	-9.66022 -1.91399 -0.16933	C	-11.05098 0.2514 2.36163
H	7.11189 -6.3621 -2.28563	C	-9.58677 -0.43949 -0.05232	H	-10.07787 0.64106 2.63753
C	6.34712 -4.52893 -1.52653	C	-8.29608 -0.09403 0.1361	H	-11.76307 0.53567 3.12594
C	5.64893 -3.68599 2.12594	C	-7.68682 1.20823 0.26681	H	-10.97961 -0.82973 2.34223
H	6.16816 -2.73873 2.2051	H	-8.29323 2.09164 0.21708	C	-5.96625 3.82884 0.37932
H	5.86461 -4.27334 3.00971	C	-6.35844 1.26948 0.42671	C	-6.07322 4.43108 -0.8735
H	4.58533 -3.4792 2.10104	C	-5.46823 2.4342 0.4949	C	-6.5553 5.72895 -0.96253
C	7.48262 -7.84656 -0.054	C	-4.20437 1.96599 0.59611	H	-6.63382 6.19165 -1.92758
H	7.07705 -8.48198 -0.83298	C	-2.91897 2.64808 0.49199	C	-6.93391 6.43637 0.16454
H	7.23674 -8.28606 0.90476	C	-2.78695 4.01956 0.6135	C	-6.82295 5.82359 1.40305
H	8.56366 -7.83972 -0.1543	H	-3.64164 4.61193 0.85616	H	-7.11191 6.36209 2.28566
C	6.22709 -3.8855 -2.89681	C	-1.54908 4.61748 0.44643	C	-6.34713 4.52892 1.52657
H	5.19477 -3.63649 -3.11455	H	-1.44066 5.67143 0.60707	C	-5.6489 3.68601 2.12591
H	6.58828 -4.55719 -3.66544	C	-0.46223 3.86661 0.07124	H	-6.16814 2.73875 2.20508
H	6.80218 -2.96839 -2.9425	H	0.49171 4.33501 -0.03698	H	-5.86457 4.27337 3.00968
C	-0.57696 2.48579 -0.12771	C	-11.74151 -5.08677 -0.66679	H	-4.58531 3.47922 2.10099
C	-1.78637 1.85909 0.19086	C	-13.09569 -4.35651 -0.77579	C	-7.48263 7.84657 0.05404

H	-7.07709 8.48197 0.83305	H	8.45956 -1.98742 -0.1
H	-7.2367 8.28609 -0.9047	C	6.46782 -1.30689 0.33937
H	-8.56367 7.83972 0.1543	C	5.6573 -2.51563 0.23537
C	-6.22712 3.88548 2.89684	C	4.33332 -2.14198 0.43457
H	-5.1948 3.63647 3.11459	C	3.11029 -2.91272 0.32814
H	-6.58831 4.55717 3.66547	C	3.15208 -4.30467 0.22897
H	-6.8022 2.96837 2.94251	H	4.10433 -4.8117 0.27121
		C	1.9692 -5.00941 0.07639
TS-PH2-A		H	1.98419 -6.09165 0.0203
Sum of electronic and thermal Free Energies= -4166.010037		C	0.75716 -4.34491 -0.02549
a.u.		H	-0.09162 -4.97249 -0.15853
C	0.6304 -2.93669 0.04064	C	11.54112 5.44412 0.07314
C	1.85389 -2.21826 0.28163	C	12.92923 4.82518 -0.21321
C	1.82566 -0.80496 0.57574	H	13.22312 4.12767 0.57905
C	0.59079 -0.09344 0.43929	H	13.67614 5.62574 -0.25738
C	0.57642 1.29232 0.70862	H	12.93798 4.29641 -1.17283
C	1.61252 1.85122 1.54007	C	11.20905 6.43951 -1.07148
C	1.40325 3.01613 2.33058	H	11.15374 5.91001 -2.02872
H	0.4439 3.51201 2.28315	H	11.98991 7.20678 -1.13759
C	2.36879 3.46742 3.20524	H	10.25028 6.93803 -0.89651
H	2.17718 4.33979 3.81892	C	11.62128 6.20904 1.42199
C	3.57958 2.7578 3.34953	H	10.67053 6.69887 1.65511
H	4.31617 3.08678 4.07318	H	12.40216 6.97723 1.36944
C	3.80099 1.61175 2.61443	H	11.86243 5.51684 2.23589
H	4.69646 1.02775 2.77446	C	10.85564 -0.18877 -0.30523
C	2.83951 1.14001 1.68287	C	11.65025 -0.66067 0.75891
C	3.00204 -0.11099 0.98323	C	12.78856 -1.42265 0.47177
C	4.27218 -0.70827 0.73329	H	13.40049 -1.78486 1.29184
C	5.58703 -0.18093 0.63413	C	13.15337 -1.7244 -0.84312
C	6.11728 1.13963 0.63051	C	12.35467 -1.24358 -1.88754
H	5.46552 1.98846 0.79412	H	12.62819 -1.4652 -2.91468
C	7.46209 1.31463 0.41443	C	11.21124 -0.47918 -1.64046
C	8.30447 2.51182 0.36196	C	11.27361 -0.34702 2.19694
C	8.04599 3.86948 0.52039	H	11.18946 0.73464 2.34997
H	7.04191 4.22646 0.72141	H	12.0266 -0.74123 2.8859
C	9.10364 4.77872 0.41855	H	10.30377 -0.79047 2.44946
H	8.88947 5.83364 0.54569	C	14.38221 -2.56666 -1.14034
C	10.43347 4.37502 0.15945	H	14.99346 -2.69685 -0.24206
C	10.69267 3.00828 -0.00248	H	15.00138 -2.09669 -1.9129
H	11.69292 2.6481 -0.20331	H	14.09139 -3.56135 -1.50105
C	9.64563 2.08427 0.09781	C	10.36013 0.03423 -2.78935
C	9.65654 0.63511 -0.02228	H	9.35145 -0.39208 -2.74693
C	8.34519 0.17664 0.17063	H	10.81043 -0.23294 -3.74998
C	7.81725 -1.14174 0.12216	H	10.25743 1.12397 -2.74034
C	6.23445 -3.84436 -0.08964		
C	6.74235 -4.66006 0.94208		
C	7.29972 -5.90312 0.61791		
H	7.68725 -6.53094 1.41409		
C	7.36898 -6.34964 -0.70441		
C	6.86606 -5.52406 -1.71772		
H	6.91598 -5.85568 -2.75051		
C	6.30031 -4.27876 -1.43235		
C	6.66683 -4.20284 2.38883		
H	7.2047 -3.25855 2.52743		
H	7.1031 -4.95497 3.05308		
H	5.62597 -4.03343 2.68797		
C	7.97737 -7.69934 -1.04537		
H	7.24674 -8.33878 -1.55536		
H	8.31165 -8.21671 -0.14101		
H	8.84118 -7.57995 -1.7105		
C	5.74432 -3.40805 -2.54492		
H	4.66069 -3.28744 -2.43207		
H	5.94469 -3.85787 -3.52204		
H	6.19195 -2.40874 -2.51791		
C	-0.49236 2.11352 0.18542		
C	-1.71191 1.49178 -0.17152		
C	-1.7994 0.03919 -0.2155		
C	-0.61671 -0.77307 -0.01787		
C	-0.64857 -2.19513 -0.15692		
C	-1.90648 -2.80023 -0.6229		
C	-2.17415 -4.19533 -0.82304		
H	-1.54437 -4.94648 -0.40051		
C	-3.26849 -4.66755 -1.51359		
H	-3.39651 -5.73727 -1.63318		
C	-4.19719 -3.77404 -2.07664		
H	-5.00134 -4.12923 -2.70939		
C	-4.075 -2.44093 -1.7739		
H	-4.79345 -1.72767 -2.15049		
C	-3.0105 -1.94476 -0.96889		
C	-3.01945 -0.56303 -0.58475		
C	-4.21959 0.23461 -0.58184		
C	-5.59227 -0.08689 -0.45015		
C	-6.29351 -1.28298 -0.11411		
H	-5.75014 -2.20783 0.02854		
C	-7.65607 -1.23508 0.02606		
C	-8.65098 -2.26121 0.35834		
C	-8.56251 -3.61829 0.64673		
H	-7.60432 -4.12591 0.65628		

C	-9.73382 -4.32999 0.93037	H	-10.3529 0.1535 -2.78285	H	4.05898 3.10659 3.78307
H	-9.65181 -5.38722 1.15524	C	-14.06392 3.68178 -0.2634	C	3.63305 1.64085 2.28547
C	-11.00988 -3.72445 0.93668	H	-14.93015 3.27663 -0.79737	H	4.48517 1.02574 2.53824
C	-11.0958 -2.35472 0.65124	H	-14.38887 3.99666 0.73318	C	2.75544 1.19618 1.26435
H	-12.04798 -1.84084 0.65159	H	-13.72103 4.57292 -0.80499	C	2.96946 -0.05336 0.56291
C	-9.93478 -1.63065 0.3626	C	-10.28113 1.52895 2.33375	C	4.2549 -0.65377 0.37326
C	-9.7608 -0.21833 0.04568	H	-9.24928 1.8499 2.15099	C	5.58046 -0.14427 0.45701
C	-8.39541 0.01283 -0.15641	H	-10.70521 2.1618 3.11897	C	6.1269 1.16106 0.61781
C	-7.70362 1.21944 -0.45391	H	-10.24384 0.49595 2.69652	H	5.47349 2.01176 0.75784
H	-8.24399 2.15417 -0.56035	C	-5.77821 3.68183 -0.84648	C	7.48989 1.32322 0.58148
C	-6.33497 1.16744 -0.57398	C	-5.95934 4.26252 -2.12017	C	8.34528 2.50449 0.72038
C	-5.37881 2.25659 -0.73569	C	-6.34228 5.60464 -2.21041	C	8.08381 3.85336 0.93796
C	-4.1099 1.69667 -0.68862	H	-6.47574 6.0502 -3.19139	H	7.0663 4.21542 1.03626
C	-2.8089 2.31822 -0.57268	C	-6.55592 6.38178 -1.06649	C	9.15565 4.74737 1.02648
C	-2.61413 3.69377 -0.7527	C	-6.37419 5.79044 0.18781	H	8.9387 5.7965 1.19121
H	-3.44865 4.30237 -1.06995	H	-6.53134 6.38249 1.08414	C	10.50304 4.33573 0.90947
C	-1.3619 4.26849 -0.53268	C	-5.98977 4.45135 0.31713	C	10.76575 2.97679 0.69575
H	-1.21016 5.32277 -0.73142	C	-5.7224 3.44166 -3.37617	H	11.77949 2.60976 0.60461
C	-0.31617 3.4956 -0.05244	H	-6.36185 2.55208 -3.3856	C	9.70423 2.06935 0.59766
H	0.65788 3.93586 0.10862	H	-5.93567 4.03595 -4.26976	C	9.71442 0.6323 0.37481
C	-12.25055 -4.58162 1.25834	H	-4.6826 3.09835 -3.42506	C	8.38328 0.18899 0.36556
C	-13.55979 -3.76102 1.19139	C	-7.0041 7.82826 -1.18605	C	7.84829 -1.10612 0.13565
H	-13.71345 -3.34175 0.19078	H	-6.691 8.40952 -0.31276	H	8.50167 -1.94531 -0.07865
H	-14.40629 -4.41786 1.42073	H	-6.5838 8.29676 -2.08213	C	6.47953 -1.25611 0.16368
H	-13.55434 -2.94446 1.92186	H	-8.09808 7.88741 -1.25646	C	5.67872 -2.42897 -0.16029
C	-12.11435 -5.16235 2.69186	C	-5.77596 3.83892 1.69023	C	4.34267 -2.05558 -0.07838
H	-12.05633 -4.35036 3.42473	H	-4.73749 3.50836 1.80578	C	3.14438 -2.77744 -0.46234
H	-12.98483 -5.78702 2.9258	H	-6.00052 4.56735 2.47522	C	3.19928 -4.07221 -0.99874
H	-11.21304 -5.77662 2.7847	H	-6.41762 2.96213 1.83042	H	4.15138 -4.57918 -1.04613
C	-12.35543 -5.74267 0.23282			C	2.0579 -4.65907 -1.53761
H	-11.467 -6.38139 0.26408	(*M*, *P*, *P*, *P*)-**2**		H	2.13112 -5.61869 -2.03584
H	-13.23248 -6.36048 0.45986	Sum of electronic and thermal Free Energies= -4166.021275		C	0.83183 -4.01226 -1.46627
H	-12.45909 -5.34365 -0.78202	a.u		H	-0.02801 -4.45073 -1.94859
C	-10.85302 0.77924 -0.03151	C	0.70105 -2.76394 -0.81888	C	11.62408 5.38931 1.01334
C	-11.64366 0.86452 -1.19835	C	1.89017 -2.09601 -0.39668	C	13.03028 4.76 0.87742
C	-12.67894 1.80197 -1.25022	C	1.82096 -0.72689 0.06618	H	13.21643 4.02982 1.67292
H	-13.28464 1.86822 -2.14876	C	0.58794 -0.00926 -0.09978	H	13.7855 5.5501 0.95469
C	-12.95024 2.65286 -0.17273	C	0.54336 1.37052 0.16532	H	13.15139 4.26595 -0.09302
C	-12.16137 2.54959 0.97675	C	1.5564 1.93803 1.02008	C	11.44908 6.43555 -0.12056
H	-12.36699 3.1956 1.82444	C	1.3259 3.12466 1.77084	H	11.5133 5.94765 -1.09904
C	-11.11367 1.62636 1.06601	H	0.39156 3.65142 1.63724	H	12.23747 7.19482 -0.05248
C	-11.35754 -0.03643 -2.38773	C	2.22678 3.55744 2.72083	H	10.47898 6.93733 -0.04744
H	-11.40184 -1.09215 -2.09901	H	2.01533 4.44894 3.29958	C	11.54222 6.0981 2.39249
H	-12.08445 0.13962 -3.18617	C	3.3855 2.8014 2.99074	H	10.57693 6.59732 2.52409

H	12.33412 6.85267 2.4712	C	-1.8587 0.02732 -0.59882	H	-13.66693 -3.3348 1.24111
H	11.66813 5.36977 3.20076	C	-0.62353 -0.70336 -0.50127	H	-14.23158 -4.22029 2.67173
C	10.92948 -0.19523 0.1899	C	-0.59744 -2.10171 -0.67098	H	-13.35833 -2.68913 2.87396
C	11.47564 -0.89942 1.28584	C	-1.84713 -2.81373 -0.77323	C	-11.82929 -4.77808 3.8234
C	12.63082 -1.66155 1.09529	C	-1.95073 -4.23139 -0.63108	H	-11.70818 -3.87112 4.42552
H	13.05259 -2.1985 1.93955	H	-1.10294 -4.7769 -0.24274	H	-12.67243 -5.35558 4.22121
C	13.25599 -1.744 -0.1549	C	-3.10976 -4.90345 -0.94701	H	-10.92093 -5.3812 3.92103
C	12.70258 -1.03964 -1.2272	H	-3.16629 -5.97844 -0.82237	C	-12.2757 -5.70091 1.5023
H	13.17574 -1.09417 -2.20254	C	-4.2177 -4.18744 -1.45363	H	-11.37762 -6.32547 1.54274
C	11.54816 -0.26276 -1.07517	H	-5.09068 -4.71729 -1.81632	H	-13.11882 -6.28353 1.89259
C	10.82191 -0.81899 2.65519	C	-4.19555 -2.81074 -1.45226	H	-12.47614 -5.45005 0.45509
H	10.70845 0.22417 2.97042	H	-5.05022 -2.25559 -1.80941	C	-10.88947 0.71613 0.18356
H	11.42576 -1.34675 3.39937	C	-3.06128 -2.08354 -0.99147	C	-11.5984 0.81449 -1.03123
H	9.82213 -1.26695 2.63756	C	-3.08593 -0.65275 -0.80681	C	-12.65368 1.72793 -1.12973
C	14.50707 -2.58707 -0.33277	C	-4.29823 0.13175 -0.77959	H	-13.20184 1.80034 -2.06382
H	15.28952 -2.27743 0.37015	C	-5.65484 -0.17662 -0.5074	C	-13.01864 2.5425 -0.05371
H	14.90201 -2.49099 -1.34868	C	-6.31458 -1.3118 0.05307	C	-12.30768 2.42641 1.1462
H	14.29057 -3.64662 -0.14929	H	-5.74881 -2.19819 0.30744	H	-12.58308 3.04802 1.99265
C	10.95655 0.47987 -2.26122	C	-7.66513 -1.25343 0.28054	C	-11.24831 1.52489 1.28343
H	9.95673 0.09713 -2.49692	C	-8.61448 -2.22543 0.83304	C	-11.22443 -0.0635 -2.21346
H	11.59122 0.36073 -3.14435	C	-8.48426 -3.52849 1.30076	H	-11.22319 -1.12102 -1.92704
H	10.85508 1.54826 -2.04249	H	-7.52089 -4.02647 1.30554	H	-11.93331 0.07682 -3.03489
C	6.28384 -3.7292 -0.54649	C	-9.61881 -4.19666 1.77459	H	-10.21927 0.17949 -2.57634
C	6.54818 -4.70206 0.43946	H	-9.50339 -5.2099 2.14185	C	-14.1475 3.55008 -0.18723
C	7.13747 -5.91397 0.06132	C	-10.90003 -3.60195 1.79409	H	-14.81077 3.28737 -1.01726
H	7.33667 -6.66295 0.82139	C	-11.02996 -2.29008 1.31824	H	-14.74374 3.59563 0.73048
C	7.47241 -6.17978 -1.26981	H	-11.98925 -1.78976 1.3094	H	-13.74664 4.55382 -0.37878
C	7.20347 -5.20312 -2.23612	C	-9.90472 -1.60709 0.8452	C	-10.48564 1.42078 2.59325
H	7.45405 -5.39613 -3.27482	C	-9.77844 -0.25549 0.31594	H	-9.43574 1.703 2.45399
C	6.61769 -3.98041 -1.89553	C	-8.43599 -0.04884 -0.02157	H	-10.92565 2.0801 3.34729
C	6.18114 -4.4418 1.89004	C	-7.78008 1.11308 -0.51366	H	-10.50106 0.39322 2.97289
H	6.67001 -3.53287 2.25763	H	-8.3345 2.02933 -0.68734	C	-5.92504 3.52613 -1.28024
H	6.4849 -5.28292 2.52047	C	-6.42294 1.04975 -0.72625	C	-6.2129 3.98483 -2.58248
H	5.09976 -4.29817 1.99547	C	-5.49587 2.12107 -1.06745	C	-6.62563 5.30975 -2.76393
C	8.13831 -7.48798 -1.66036	C	-4.21734 1.58278 -1.04467	H	-6.84274 5.66183 -3.76759
H	7.73545 -7.86709 -2.60593	C	-2.9294 2.24777 -1.03505	C	-6.76429 6.1859 -1.68291
H	7.98601 -8.25044 -0.89005	C	-2.77443 3.6155 -1.30231	C	-6.47648 5.71409 -0.39715
H	9.21932 -7.34663 -1.78797	H	-3.63094 4.18631 -1.6307	H	-6.57499 6.38412 0.45151
C	6.31137 -2.94458 -2.9628	C	-1.53232 4.23194 -1.14697	C	-6.0602 4.39748 -0.17753
H	5.23142 -2.76591 -3.02487	H	-1.41713 5.27887 -1.40172	C	-6.05945 3.05417 -3.77332
H	6.66569 -3.28336 -3.94097	C	-0.44773 3.51543 -0.65861	H	-6.67916 2.15921 -3.64934
H	6.78987 -1.98823 -2.72642	H	0.5157 3.99407 -0.54613	H	-6.35484 3.56004 -4.69742
C	-0.57186 2.1428 -0.35664	C	-12.09718 -4.40578 2.33992	H	-5.02005 2.72122 -3.8741
C	-1.79654 1.47834 -0.63293	C	-13.41794 -3.60376 2.27364	C	-7.2435 7.61205 -1.89293

H	-6.72828	8.30307	-1.21712	C	-5.72446	3.91625	1.22298	H	-6.31287	3.03	1.48294
H	-7.06452	7.93817	-2.92237	H	-4.66577	3.63981	1.28838				
H	-8.32069	7.68907	-1.696	H	-5.92645	4.70122	1.95799	TS-PH**2**-B			
Sum of electronic and thermal Free Energies= -4165.998926 a.u.											
C	-0.81661	-2.74294	0.56209	C	-1.995	-4.74777	1.29209	H	-7.11696	-6.37088	-1.15683
C	-2.02183	-2.00612	0.69046	H	-1.97126	-5.78813	1.59422	C	-7.46115	-6.31245	0.96741
C	-1.96912	-0.56025	0.68572	C	-0.81512	-4.10394	0.94585	C	-7.33452	-5.53476	2.12176
C	-0.69599	0.09931	0.55231	H	0.1235	-4.63591	0.99916	H	-7.66753	-5.93503	3.07418
C	-0.63867	1.49849	0.64915	C	-11.61646	5.21148	-1.85853	C	-6.79001	-4.24559	2.07891
C	-1.74056	2.20369	1.26389	C	-13.00913	4.54429	-1.94201	C	-5.99402	-3.9441	-1.66272
C	-1.56895	3.46178	1.90697	H	-13.01582	3.72938	-2.67432	H	-6.47811	-2.98702	-1.88504
H	-0.58445	3.90622	1.92627	H	-13.74581	5.29176	-2.25708	H	-6.21333	-4.64624	-2.47276
C	-2.60806	4.07762	2.57162	H	-13.31834	4.14925	-0.96791	H	-4.91271	-3.7673	-1.63655
H	-2.44259	5.02294	3.07501	C	-11.70064	6.38088	-0.84053	C	-8.06892	-7.70368	1.02269
C	-3.86598	3.44704	2.65277	H	-11.95633	6.00025	0.15423	H	-9.03178	-7.72665	0.49727
H	-4.67005	3.91106	3.21183	H	-12.47348	7.0926	-1.15472	H	-8.239	-8.01507	2.05778
C	-4.05355	2.20747	2.079	H	-10.74783	6.9154	-0.7716	H	-7.409	-8.43823	0.54661
H	-4.99077	1.68763	2.21356	C	-11.26121	5.76851	-3.2638	C	-6.65374	-3.42342	3.34906
C	-3.01273	1.55799	1.36277	H	-10.29558	6.28396	-3.25247	H	-5.6	-3.20547	3.5587
C	-3.15037	0.1988	0.89164	H	-12.02968	6.48071	-3.5877	H	-7.07437	-3.96248	4.20328
C	-4.41221	-0.46804	0.74717	H	-11.20868	4.95174	-3.99164	H	-7.17295	-2.46399	3.24914
C	-5.71971	-0.00086	0.47778	C	-10.97838	-0.26457	-0.44795	C	0.5547	2.17498	0.18967
C	-6.24114	1.26494	0.08275	C	-11.22428	-1.10202	-1.55632	C	1.76796	1.43966	0.03881
H	-5.58228	2.12016	-0.00473	C	-12.37589	-1.89673	-1.56458	C	1.78372	-0.0089	0.04297
C	-7.58121	1.37266	-0.18879	H	-12.56898	-2.53437	-2.42157	C	0.50363	-0.66444	0.22758
C	-8.41586	2.50241	-0.60853	C	-13.28343	-1.88183	-0.50125	C	0.39498	-2.05968	0.1205
C	-8.14538	3.83991	-0.87631	C	-13.02529	-1.04202	0.58788	C	1.50137	-2.78447	-0.42647
H	-7.13973	4.23515	-0.78503	H	-13.722	-1.01789	1.42013	C	1.31676	-4.0734	-1.00773
C	-9.19312	4.67832	-1.27149	C	-11.88802	-0.23092	0.6319	H	0.30599	-4.42562	-1.15562
H	-8.97065	5.71836	-1.47931	C	-10.2645	-1.12874	-2.73447	C	2.38032	-4.84757	-1.40979
C	-10.52237	4.22067	-1.41212	H	-10.07077	-0.1148	-3.10096	H	2.21578	-5.81392	-1.87076
C	-10.79276	2.87203	-1.14372	H	-10.68032	-1.72446	-3.55251	C	3.68421	-4.36201	-1.19885
H	-11.79255	2.47084	-1.24425	H	-9.3005	-1.56312	-2.4462	H	4.54469	-4.98319	-1.41952
C	-9.75667	2.02122	-0.74311	C	-14.51085	-2.77655	-0.51294	C	3.86593	-3.07467	-0.74473
C	-9.77612	0.60054	-0.42047	H	-15.36694	-2.27495	-0.04929	H	4.8517	-2.72367	-0.58195
C	-8.4704	0.21593	-0.08967	H	-14.3179	-3.70073	0.04714	C	2.80606	-2.19221	-0.43934
C	-7.9515	-1.06121	0.2609	H	-14.78491	-3.05308	-1.53592	C	2.99574	-0.76532	-0.19527
H	-8.60203	-1.92829	0.30505	C	-11.62045	0.65799	1.83455	C	4.28362	-0.04422	-0.24572
C	-6.60384	-1.16425	0.5162	H	-10.68112	0.37389	2.32269	C	5.7178	-0.34988	-0.29295
C	-5.79387	-2.35065	0.77715	H	-12.43173	0.57198	2.56357	C	6.59499	-1.45415	-0.56795
C	-4.4732	-1.93532	0.87115	H	-11.5288	1.70716	1.53357	H	6.25084	-2.40836	-0.92277
C	-3.24425	-2.69696	0.96051	C	-6.35503	-3.72349	0.8436	C	7.96132	-1.32752	-0.48134
C	-3.21226	-4.06666	1.24978	C	-6.47532	-4.49637	-0.33259	C	9.0388	-2.28992	-0.72598
H	-4.1387	-4.58061	1.46349	C	-7.02591	-5.77818	-0.25157	C	9.06234	-3.63134	-1.09502

H	8.14265 -4.18134 -1.26271	H	11.45605 -1.16374 2.1149	C	-4.31615 -3.51878 -3.3161
C	10.29443 -4.27243 -1.25222	H	11.91935 0.02995 3.3499	H	-5.24362 -3.94968 -3.67455
H	10.2983 -5.31727 -1.54017	C	13.98034 3.87364 0.91277	C	-4.33111 -2.31299 -2.64747
C	11.52915 -3.61143 -1.05406	H	14.23982 4.41952 0.00061	H	-5.26231 -1.78168 -2.51499
C	11.50676 -2.26255 -0.68221	H	13.59621 4.59577 1.64415	C	-3.13175 -1.70498 -2.18935
H	12.42345 -1.70944 -0.52603	H	14.89668 3.43454 1.32359	C	-3.1225 -0.35428 -1.67529
C	10.28095 -1.60573 -0.51184	C	10.64646 1.71702 -2.23718	C	-4.29189 0.34736 -1.2358
C	9.99591 -0.22933 -0.14662	H	9.60144 2.04058 -2.16388	C	-5.50616 -0.07723 -0.64949
C	8.59894 -0.0769 -0.1291	H	11.15988 2.37707 -2.94287	C	-5.95602 -1.32915 -0.13947
C	7.78412 1.05335 0.08583	H	10.64651 0.69931 -2.64105	H	-5.32477 -2.20616 -0.21846
H	8.21589 2.02011 0.32173	C	5.86902 3.40084 0.26102	C	-7.19184 -1.39599 0.45219
C	6.41774 0.91682 -0.03796	C	5.74197 3.97022 1.54837	C	-7.9393 -2.5023 1.05817
C	5.46446 1.9898 0.03288	C	6.15567 5.28838 1.7538	C	-7.66539 -3.85352 1.24012
C	4.20721 1.43662 -0.12916	H	6.05866 5.72203 2.7445	H	-6.72804 -4.28344 0.90476
C	2.96485 2.16318 -0.18603	C	6.6895 6.06035 0.71427	C	-8.61926 -4.66156 1.86844
C	2.91779 3.53879 -0.46217	C	6.80753 5.4832 -0.55244	H	-8.39226 -5.71236 2.0072
H	3.83493 4.06776 -0.66709	H	7.2145 6.06983 -1.37021	C	-9.85919 -4.16099 2.32457
C	1.69737 4.20611 -0.50956	C	6.41337 4.16117 -0.79515	C	-10.13501 -2.79977 2.13764
H	1.66195 5.24779 -0.80549	C	5.15352 3.16108 2.69031	H	-11.07167 -2.36808 2.46519
C	0.53012 3.53957 -0.16829	H	5.67907 2.20676 2.80264	C	-9.18905 -1.97729 1.5166
H	-0.41905 4.0548 -0.20472	H	5.22535 3.71596 3.63057	C	-9.23526 -0.55312 1.21443
C	12.84184 -4.39527 -1.25399	H	4.09851 2.93643 2.49718	C	-8.0365 -0.20829 0.57799
C	14.08992 -3.51464 -1.01156	C	7.14038 7.48797 0.97062	C	-7.57156 1.05707 0.12289
H	14.11125 -3.13004 0.01423	H	8.02879 7.50326 1.61436	H	-8.1768 1.94739 0.25759
H	14.99044 -4.11919 -1.16752	H	7.39215 7.99279 0.03293	C	-6.33084 1.11622 -0.46724
H	14.12115 -2.66925 -1.70793	H	6.35327 8.06381 1.47097	C	-5.57387 2.27532 -0.93371
C	12.9047 -4.93372 -2.709	C	6.564 3.56563 -2.18553	C	-4.33662 1.8153 -1.35888
H	12.8758 -4.10286 -3.42204	H	5.6865 2.96954 -2.45562	C	-3.16101 2.53223 -1.81089
H	13.83505 -5.49476 -2.8584	H	6.70017 4.35626 -2.92974	C	-3.19333 3.86839 -2.22616
H	12.06293 -5.60067 -2.92086	H	7.43521 2.90061 -2.22804	H	-4.13412 4.40075 -2.22212
C	12.88692 -5.58431 -0.25653			C	-2.03039 4.47756 -2.69774
H	12.03945 -6.2603 -0.4092	(*M*, *P*, *P*, *P*)-**2**		H	-2.07862 5.47409 -3.12082
H	13.81337 -6.15374 -0.39791	Sum of electronic and thermal Free Energies = -4166.016681		C	-0.81059 3.81675 -2.63526
H	12.85403 -5.21542 0.77424	a.u.		H	0.06739 4.28689 -3.05038
C	11.00679 0.81914 0.12052	C	-0.70994 2.5138 -2.09316	C	-10.85364 -5.11915 3.01026
C	11.65959 0.86369 1.37316	C	-1.92158 1.81954 -1.82047	C	-12.16632 -4.40662 3.4118
C	12.61648 1.85438 1.60584	C	-1.90876 0.37399 -1.7609	H	-11.97635 -3.59703 4.12516
H	13.11384 1.89003 2.57036	C	-0.65998 -0.32281 -1.89198	H	-12.8362 -5.13106 3.88817
C	12.94504 2.7996 0.62659	C	-0.65443 -1.72386 -2.02935	H	-12.67677 -3.99367 2.53461
C	12.29396 2.73696 -0.60792	C	-1.88701 -2.36894 -2.43282	C	-11.20993 -6.27796 2.04039
H	12.54543 3.45679 -1.38046	C	-1.90501 -3.57782 -3.18289	H	-11.66993 -5.88135 1.12894
C	11.32664 1.76163 -0.87842	H	-0.96549 -4.01632 -3.48697	H	-11.91756 -6.96265 2.52302
C	11.30376 -0.13574 2.46077	C	-3.08864 -4.14881 -3.60199	H	-10.31856 -6.84738 1.75853
H	10.24929 -0.03819 2.74366	H	-3.07044 -5.05592 -4.19464	C	-10.20211 -5.69686 4.29593

H	-9.28109 -6.23992 4.06136	C	1.8122 -1.75292 -1.67607	C	12.33104 4.22053 3.33108
H	-10.89623 -6.38855 4.78837	C	1.83273 -0.30137 -1.71303	H	12.81729 3.82487 2.43247
H	-9.95759 -4.88783 4.99275	C	0.58951 0.41689 -1.82401	H	13.02148 4.9217 3.81275
C	-10.36644 0.34979 1.53172	C	0.56777 1.83137 -1.87297	H	12.14364 3.39421 4.02578
C	-10.4927 0.89079 2.82974	C	1.81082 2.55623 -1.77647	C	10.41059 5.51922 4.2928
C	-11.57512 1.72811 3.11431	C	1.89424 3.97241 -1.5986	H	10.16788 4.69772 4.97547
H	-11.6701 2.14531 4.11213	H	1.01012 4.51224 -1.29502	H	11.12905 6.18586 4.78482
C	-12.53505 2.03809 2.14426	C	3.07921 4.65065 -1.77494	H	9.49481 6.08514 4.09456
C	-12.39768 1.48754 0.8666	H	3.11625 5.72441 -1.633	C	11.37112 6.13827 2.02666
H	-13.13987 1.7112 0.10672	C	4.24136 3.94456 -2.16017	H	10.48049 6.72324 1.77594
C	-11.32644 0.64793 0.54244	H	5.14632 4.48052 -2.42123	H	12.09677 6.80429 2.50875
C	-9.45513 0.57931 3.89477	C	4.22639 2.56734 -2.15739	H	11.80725 5.75608 1.09747
H	-9.37184 -0.50106 4.05542	H	5.12196 2.01206 -2.39791	C	10.44017 -0.4449 1.31477
H	-9.7231 1.05525 4.84271	C	3.04669 1.83865 -1.83844	C	11.36549 -0.72681 0.28599
H	-8.46702 0.94217 3.5894	C	3.06121 0.41208 -1.62237	C	12.43155 -1.59085 0.55032
C	-13.68754 2.97224 2.47054	C	4.24892 -0.30259 -1.23456	H	13.14636 -1.80195 -0.23918
H	-14.07352 2.78258 3.47795	C	5.50005 0.10763 -0.69023	C	12.5997 -2.18333 1.80734
H	-14.50793 2.8463 1.75711	C	5.99098 1.32987 -0.14398	C	11.67624 -1.88964 2.81463
H	-13.35881 4.01863 2.42731	H	5.37239 2.21605 -0.14992	H	11.79486 -2.33943 3.79535
C	-11.20704 0.05525 -0.85171	C	7.24912 1.36266 0.40283	C	10.59764 -1.02711 2.58963
H	-10.31688 0.4379 -1.36367	C	8.02316 2.44 1.02645	C	11.21139 -0.08846 -1.08437
H	-12.0871 0.30633 -1.45127	C	7.76451 3.78457 1.27102	H	11.13775 1.0013 -0.99859
H	-11.11394 -1.03529 -0.80326	H	6.8187 4.23137 0.98482	H	12.06771 -0.33391 -1.71955
C	-6.08399 3.66766 -0.8668	C	8.7442 4.56158 1.89846	H	10.29927 -0.44089 -1.57887
C	-5.7848 4.47714 0.24944	H	8.52937 5.60712 2.0876	C	13.75221 -3.14016 2.05935
C	-6.28988 5.78091 0.30026	C	9.99594 4.03662 2.29257	H	14.68432 -2.75253 1.63357
H	-6.05796 6.40249 1.15953	C	10.25684 2.68325 2.04198	H	13.90262 -3.29803 3.13176
C	-7.08306 6.29912 -0.72842	H	11.20139 2.23416 2.31952	H	13.55131 -4.11539 1.5977
C	-7.36757 5.48429 -1.82998	C	9.2852 1.89064 1.42054	C	9.59756 -0.73766 3.69613
H	-7.9776 5.87402 -2.63919	C	9.3117 0.48083 1.06149	H	8.59733 -1.08584 3.4135
C	-6.8835 4.17491 -1.91377	C	8.08811 0.16982 0.4509	H	9.89236 -1.24119 4.62158
C	-4.91035 3.94364 1.37001	C	7.58503 -1.07139 -0.02025	H	9.52734 0.33831 3.88868
H	-5.31261 3.00462 1.76494	H	8.17564 -1.97727 0.06657	C	6.02812 -3.6392 -0.8641
H	-4.84534 4.66957 2.18612	C	6.3153 -1.09679 -0.55278	C	6.62494 -4.23433 -1.99571
H	-3.89817 3.74008 1.00235	C	5.51527 -2.24747 -0.94365	C	7.11888 -5.53962 -1.89948
C	-7.64937 7.70603 -0.64156	C	4.25717 -1.77474 -1.29715	H	7.57361 -5.99719 -2.77268
H	-7.69217 8.17372 -1.63094	C	3.02279 -2.49867 -1.52407	C	7.038 -6.26549 -0.70641
H	-7.03727 8.3357 0.01196	C	2.97661 -3.899 -1.47009	C	6.44425 -5.66031 0.4064
H	-8.6685 7.68594 -0.23404	H	3.90032 -4.44741 -1.36343	H	6.36979 -6.2129 1.33794
C	-7.19325 3.31324 -3.12626	C	1.755 -4.56708 -1.46754	C	5.94019 -4.3568 0.34815
H	-6.27009 3.02165 -3.64056	H	1.72925 -5.6419 -1.33182	C	6.71338 -3.46952 -3.3049
H	-7.82915 3.85657 -3.83161	C	0.57227 -3.8593 -1.60846	H	7.25907 -2.52917 -3.16923
H	-7.70598 2.39196 -2.82871	H	-0.37204 -4.37742 -1.53744	H	7.22679 -4.06612 -4.06493
C	0.57842 -2.45912 -1.80451	C	11.02081 4.96241 2.97808	H	5.71293 -3.21762 -3.67461

C	7.6095	-7.66986	-0.61289
H	7.06991	-8.26419	0.13165
H	7.54694	-8.18428	-1.57745
H	8.66594	-7.63598	-0.31619
C	5.27104	-3.7319	1.55955
H	4.2149	-3.52547	1.3491
H	5.32972	-4.40394	2.42101
H	5.74675	-2.78099	1.82105

(*M*)-[4]Helicene

Sum of electronic and thermal Free Energies = - 692.967716 a.u

C	-3.76516	1.23566	-0.11066
C	-3.55816	-0.06455	-0.35155
C	-2.32357	-0.59721	-0.26848
C	-1.22701	0.15611	-0.0134
C	-1.49626	1.43671	0.32424
C	-2.72076	1.98228	0.26311
C	-2.21112	-1.92682	-0.40842
C	-1.02346	-2.50609	-0.2149
C	0.07091	-1.75695	-0.00007
C	0.01625	-0.40273	-0.00002
C	1.22209	-2.41548	0.2147
C	2.35921	-1.7424	0.40827
C	2.36414	-0.40804	0.26844
C	1.21044	0.25449	0.01342
C	3.5518	0.22237	0.35156
C	3.65334	1.53505	0.11077
C	2.55216	2.19511	-0.26295
C	1.37561	1.55264	-0.32412
H	-4.77978	1.66515	-0.15049
H	-4.4395	-0.68797	-0.58253
H	-0.73479	2.11035	0.74217
H	-2.88072	3.035	0.55282
H	-3.0875	-2.57006	-0.59874
H	-0.97497	-3.60847	-0.25036
H	1.2626	-3.51819	0.25007
H	3.28458	-2.31294	0.59854
H	4.48051	-0.32801	0.58249
H	4.63005	2.04491	0.15064
H	2.62677	3.25732	-0.55257
H	0.56233	2.16276	-0.74199

TS-[4]Helicene

Sum of electronic and thermal Free Energies = -692.961736 a.u

C	3.97833	-1.43352	0.00149
C	3.79878	-0.08968	0.00214
C	2.49948	0.48749	0.0008
C	1.33487	-0.31362	-0.00075
C	1.58484	-1.72108	-0.00203
C	2.83594	-2.25691	-0.00091
C	2.41142	1.9247	0.00069
C	1.21819	2.51677	-0.00057
C	0.	1.74287	-0.00094
C	-0.00001	0.34753	-0.00109
C	-1.21819	2.51676	-0.00088
C	-2.41145	1.92471	-0.00025
C	-2.49951	0.48752	0.00007
C	-1.33489	-0.31359	-0.00079
C	-3.7988	-0.08972	0.00144
C	-3.97829	-1.43353	0.00199
C	-2.8359	-2.25695	0.00044
C	-1.58485	-1.72112	-0.00113
H	4.96861	-1.86982	0.0024
H	4.6483	0.58072	0.00356
H	0.78059	-2.4253	-0.00439
H	2.95168	-3.33306	-0.00197
H	3.32967	2.49686	0.00145
H	1.12705	3.5946	-0.00074
H	-1.12703	3.59459	-0.00075
H	-3.32968	2.49689	0.00022
H	-4.64835	0.58064	0.00203
H	-4.96857	-1.86984	0.00312
H	-2.95168	-3.3331	0.00024
H	-0.78039	-2.42512	-0.00336

(*P*)-[4]Helicene

Sum of electronic and thermal Free Energies =-692.967714 a.u

C	-3.85812	-1.51425	0.10369
C	-3.74278	-0.17213	-0.18922
C	-2.48377	0.47618	-0.18267
C	-1.28907	-0.28026	0.05691
C	-1.46032	-1.6395	0.43515
C	-2.70446	-2.24098	0.45487
C	-2.40689	1.8933	-0.34078
C	-1.21788	2.53871	-0.18816
C	0.	1.81343	0.
C	0.	0.39497	0.
C	1.21788	2.53871	0.18816
C	2.40689	1.8933	0.34078
C	2.48377	0.47618	0.18267
C	1.28907	-0.28026	-0.05691
C	3.74278	-0.17213	0.18922
C	3.85812	-1.51425	-0.10369
C	2.70446	-2.24098	-0.45487
C	1.46032	-1.6395	-0.43515
H	-4.83157	-1.99687	0.10445
H	-4.62799	0.42293	-0.40187
H	-0.60685	-2.21098	0.77461
H	-2.79125	-3.27932	0.76374
H	-3.32337	2.44866	-0.52441
H	-1.16726	3.62396	-0.23177
H	1.16726	3.62396	0.23177
H	3.32337	2.44866	0.52441
H	4.62799	0.42293	0.40187
H	4.83157	-1.99687	-0.10445
H	2.79125	-3.27932	-0.76374
H	0.60685	-2.21098	-0.77461

(*M*)-PH**1**-[7]Helicene

Sum of electronic and thermal Free Energies =-2084.787466 a.u.

C	-0.03593	4.47881	1.86917
C	-0.79721	3.39704	1.46616
C	-1.88088	3.54454	0.5657
C	-2.23053	4.87381	0.17561
C	-1.41515	5.96225	0.5691
C	-0.32427	5.77222	1.39171
C	-3.44156	5.08502	-0.54661
C	-6.95913	-0.38602	-0.56039
C	-7.30742	0.93895	-0.87728
C	-6.34841	1.93173	-0.84028
C	-5.00198	1.65704	-0.49325
C	-4.64795	0.30294	-0.1909
C	-5.65643	-0.69357	-0.22328
C	-4.01002	2.71242	-0.37225
C	-2.70942	2.42701	0.13082
C	-2.31248	1.05005	0.18398
C	-3.26553	0.01667	0.07682
C	-4.31652	4.05808	-0.74887

C	-1.22756 -1.03912 0.26171	H	-5.39818 -1.71511 0.02263
C	-0.98581 0.4029 0.22428	H	-5.25754 4.27013 -1.24214
C	0.29501 0.86528 0.07097	H	0.52033 1.92033 -0.03884
C	1.37803 -0.07312 0.04855	H	-0.36576 -3.04184 0.33858
C	1.12931 -1.50642 0.17748	H	2.11551 -4.29194 0.32214
C	-0.14639 -1.97864 0.27539	H	4.49791 -4.83773 0.1865
C	2.4357 -2.16419 0.13707	H	5.49595 -0.66232 -0.21827
C	-2.58898 -1.27673 0.18029	H	8.05468 -4.82351 -0.08209
C	2.7428 0.1532 -0.07043	H	6.4973 -5.20193 -0.82779
C	2.83994 -3.48909 0.20755	H	6.63085 -5.06234 0.93771
C	4.20722 -3.79493 0.1282	H	8.51995 -2.64334 0.98738
C	5.19241 -2.80435 -0.02362	H	7.32112 -1.34164 1.00812
C	4.77101 -1.46249 -0.09625	H	7.07928 -2.77677 2.01574
C	3.41728 -1.14411 -0.01422	H	6.74543 -3.11671 -2.30522
C	6.69491 -3.13237 -0.11324	H	8.32496 -2.84499 -1.54214
C	6.9757 -4.64393 -0.01481	H	7.12319 -1.54628 -1.58206
C	7.44553 -2.42904 1.04293	H	5.15782 3.78373 1.55237
C	7.25248 -2.62741 -1.46571	H	4.20034 3.75965 -2.6249
C	3.4264 1.46087 -0.23613	H	-4.37126 -5.02769 2.28382
C	-3.18069 -2.64336 0.16429	H	-4.00754 -5.15067 -1.98529
C	4.03767 2.08327 0.874	H	-2.34671 -2.29112 2.89949
C	4.68963 3.30726 0.69295	H	-3.7597 -3.15901 3.52513
C	4.75629 3.93268 -0.55444	H	-3.95206 -1.59834 2.70808
C	4.15128 3.2954 -1.64159	H	-3.172 -3.36033 -3.20945
C	3.48621 2.07335 -1.50786	H	-1.9035 -2.42312 -2.40058
C	-3.54981 -3.26389 1.3777	H	-3.52858 -1.7607 -2.53621
C	-4.08102 -4.5573 1.34613	H	2.94935 1.3068 2.58181
C	-4.25051 -5.25836 0.14901	H	4.49057 2.0832 2.98616
C	-3.87757 -4.6259 -1.04054	H	4.46018 0.46668 2.26142
C	-3.34309 -3.33393 -1.05676	H	3.10869 1.97424 -3.63129
C	-3.39446 -2.54261 2.69787	H	1.76568 1.38464 -2.64144
C	-2.9667 -2.68779 -2.37083	H	3.20129 0.38813 -2.84464
C	3.98355 1.45376 2.2483	H	6.16387 5.45256 0.0803
C	2.8585 1.42182 -2.72034	H	4.7164 6.09319 -0.70478
C	5.44184 5.26875 -0.72217	H	5.97461 5.32953 -1.67775
C	-4.79726 -6.66715 0.14213	H	-5.45601 -6.84622 0.99859
H	0.78261 4.32859 2.5678	H	-3.98861 -7.40876 0.19377
H	-0.58403 2.41879 1.87756	H	-5.3656 -6.87252 -0.77154
H	-1.687 6.96098 0.23505		
H	0.28726 6.61661 1.69795	TS-PH**1**-[7]Helicene	
H	-3.68853 6.09124 -0.87616	Sum of electronic and thermal Free Energies = -2084.767230	
H	-7.71333 -1.16822 -0.57569	a.u.	
H	-8.33267 1.18763 -1.1379	C	-0.24718 4.96757 -0.68804
H	-6.65465 2.94884 -1.05471	C	-0.87337 3.79492 -0.3081
C	-2.2668 3.58974 -0.40611
C	-3.02466 4.72282 -0.86162
C	-2.37014 5.9122 -1.26911
C	-0.99965 6.03934 -1.19963
C	-4.44497 4.66628 -0.87322
C	-6.71157 -0.99599 1.18171
C	-7.29144 0.28822 1.19225
C	-6.5402 1.38921 0.83456
C	-5.1781 1.26115 0.45461
C	-4.58619 -0.03087 0.48558
C	-5.38477 -1.15163 0.84032
C	-4.38051 2.3936 0.02281
C	-2.94689 2.33048 -0.05304
C	-2.33444 1.01218 0.10773
C	-3.18729 -0.12604 0.20324
C	-5.08358 3.56299 -0.40572
C	-1.1013 -1.02485 -0.15136
C	-0.93424 0.43904 0.00675
C	0.34999 0.87874 0.20363
C	1.45976 -0.01485 0.05504
C	1.26542 -1.43466 -0.23376
C	0.00121 -1.92751 -0.31462
C	2.60585 -2.02987 -0.32997
C	-2.42814 -1.35674 0.0065
C	2.81452 0.26872 0.14017
C	3.06246 -3.31259 -0.58796
C	4.44625 -3.55416 -0.61905
C	5.38854 -2.53467 -0.40361
C	4.91822 -1.23035 -0.14757
C	3.55112 -0.98042 -0.10321
C	6.90839 -2.79365 -0.44021
C	7.24747 -4.27549 -0.72458
C	7.54968 -1.92662 -1.55746
C	7.52554 -2.41152 0.9327
C	3.4221 1.59356 0.40586
C	-2.92889 -2.75617 -0.05074
C	3.97644 1.87118 1.67397
C	4.54295 3.12864 1.91068
C	4.57504 4.11458 0.92078
C	4.02552 3.8218 -0.3332
C	3.4479 2.57828 -0.60843
C	-3.49354 -3.25013 -1.24416
C	-3.94399 -4.5744 -1.28654
C	-3.84699 -5.41644 -0.17488

C	-3.28346 -4.90929 1.00224	H	-2.78823 -2.17387 2.71592
C	-2.81837 -3.59321 1.08166	H	-2.28336 -3.81972 3.16319
H	0.82745 5.05461 -0.57384	C	-3.62517 -2.35081 -2.46022
H	-0.27558 3.0292 0.12278	H	-4.28865 -1.50565 -2.2434
H	-2.98317 6.73418 -1.62357	H	-2.65125 -1.94022 -2.74794
H	-0.51228 6.95635 -1.50865	H	-4.03655 -2.90747 -3.30748
H	-5.00256 5.51961 -1.24292	C	-4.32402 -6.85706 -0.24167
H	-7.30285 -1.85999 1.4614	H	-4.96303 -7.01729 -1.11547
H	-8.32462 0.41373 1.49463	H	-3.47091 -7.5437 -0.31464
H	-6.99378 2.36952 0.88665	H	-4.89352 -7.1235 0.65565
H	-4.93163 -2.12998 0.85331		
H	-6.16349 3.53646 -0.42082	(*P*)-PH**1**-[7]Helicene	
H	0.6221 1.87228 0.51123	Sum of electronic and thermal Free Energies = -2084.787466	
H	-0.21083 -2.97839 -0.4787	a.u.	
H	2.36912 -4.12693 -0.76733	C	-0.01447 4.47621 1.81489
H	4.78541 -4.56119 -0.8197	C	0.76279 3.39877 1.43194
H	5.6121 -0.41312 0.01264	C	1.85413 3.5554 0.54051
H	8.33642 -4.39625 -0.73544	C	2.20267 4.88524 0.14848
H	6.8391 -4.93199 0.05184	C	1.37315 5.96976 0.52811
H	6.8594 -4.59159 -1.69927	C	0.27119 5.77051 1.33376
H	8.6327 -2.09724 -1.58532	C	3.42843 5.10223 -0.55172
H	7.37275 -0.86107 -1.3806	C	6.93483 -0.38631 -0.5966
H	7.12614 -2.19103 -2.53232	C	7.28998 0.94119 -0.90538
H	7.08593 -3.02229 1.72867	C	6.34075 1.94295 -0.85713
H	8.6087 -2.58219 0.91513	C	4.9938 1.67397 -0.50198
H	7.34661 -1.35714 1.16563	C	4.63684 0.31906 -0.20029
H	4.96338 3.34074 2.88857	C	5.63402 -0.68941 -0.25131
H	4.06005 4.57102 -1.11872	C	4.0019 2.73078 -0.37276
H	-4.38115 -4.95235 -2.20539	C	2.69675 2.44058 0.12222
H	-3.2077 -5.54846 1.87663	C	2.30198 1.06541 0.18736
C	3.92788 0.83187 2.78139	C	3.26058 0.03451 0.08067
H	2.88968 0.58344 3.03051	C	4.31077 4.07998 -0.74118
H	4.42095 -0.09588 2.47247	C	1.22547 -1.03982 0.27536
H	4.42121 1.20847 3.68225	C	0.96985 0.41047 0.23592
C	2.86827 2.29743 -1.98593	C	-0.30885 0.86948 0.07679
H	3.15749 1.30204 -2.33665	C	-1.38659 -0.0761 0.05657
H	1.7725 2.3356 -1.96545	C	-1.12601 -1.51832 0.18576
H	3.22154 3.04211 -2.70562	C	0.14883 -1.98619 0.28508
C	5.18546 5.47865 1.19282	C	-2.43617 -2.18426 0.1396
H	5.92175 5.73761 0.42318	C	2.58795 -1.26657 0.18863
H	4.41176 6.25653 1.19335	C	-2.75157 0.13955 -0.06586
H	5.6851 5.49635 2.16604	C	-2.8321 -3.51024 0.21005
C	-2.23515 -3.05844 2.37892	C	-4.20025 -3.82222 0.12857
H	-1.18987 -2.7601 2.2442	C	-5.18551 -2.83266 -0.02423
C	-4.77601 -1.48557 -0.09741
C	-3.42564 -1.16471 -0.01463
C	-6.68821 -3.16703 -0.1137
C	-6.96123 -4.68611 -0.01628
C	-7.43801 -2.46408 1.05044
C	-7.24513 -2.65989 -1.47176
C	-3.4457 1.44001 -0.2235
C	3.2041 -2.61937 0.17462
C	-4.01595 2.07025 0.90208
C	-4.6874 3.28599 0.73396
C	-4.80635 3.88717 -0.52266
C	-4.24043 3.24419 -1.6293
C	-3.56132 2.02916 -1.501
C	3.6294 -3.20551 1.38415
C	4.20455 -4.48128 1.3577
C	4.36155 -5.18706 0.16117
C	3.93238 -4.58985 -1.03031
C	3.35492 -3.31699 -1.04356
C	3.48301 -2.45185 2.69469
C	2.92057 -2.67794 -2.35082
C	-3.89099 1.44146 2.2796
C	-2.96755 1.34544 -2.72113
C	-5.51434 5.22124 -0.68496
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H	-0.83951 4.32688 2.50141
H	0.55963 2.42027 1.84213
H	1.6409 6.96735 0.19621
H	-0.35285 6.60679 1.62613
H	3.6722 6.1082 -0.87566
H	7.68348 -1.16918 -0.62835
H	8.31318 1.18003 -1.17136
H	6.64745 2.95685 -1.07419
H	5.35238 -1.70505 -0.01755
H	5.26016 4.29135 -1.21293
H	-0.53615 1.92197 -0.03033
H	0.3769 -3.04473 0.3474
H	-2.10438 -4.30583 0.32662
H	-4.49233 -4.86195 0.1861
H	-5.50295 -0.69099 -0.21959
H	-8.04076 -4.86074 -0.08493
H	-6.47518 -5.22945 -0.83431
H	-6.61064 -5.09158 0.93947
H	-8.51074 -2.68305 0.98894
H	-7.30441 -1.37851 1.00701

H	-7.06014 -2.82165 2.01443	C	-6.68961 1.66963 0.41802
H	-6.72826 -3.15421 -2.3014	C	-7.40949 0.52706 0.77969
H	-8.31674 -2.88194 -1.5413	C	-6.77107 -0.70503 0.82265
H	-7.10957 -1.57858 -1.57469	C	-5.46523 -3.33584 0.86741
H	-5.12652 3.76995 1.60085	C	-4.96101 -4.59439 0.6753
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H	4.5373 -4.92868 2.28899	C	1.16848 -1.3199 0.06636
H	4.05371 -5.12286 -1.96843	C	1.40028 0.10925 -0.05882
H	2.43098 -2.22243 2.89665	C	0.29781 1.00425 -0.16251
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H	3.10136 -3.35749 -3.18902	C	2.48204 -1.94405 0.19665
H	1.85529 -2.42473 -2.32685	C	2.9083 -3.25728 0.34594
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H	-6.1691 5.42392 0.16837	C	6.76734 -2.81327 0.49162
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H	-6.12123 5.23518 -1.59676	C	7.35816 -2.06838 1.71253
H	5.44672 -6.80629 1.10678	C	7.47688 -2.32733 -0.79471
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H	5.72539 -6.66847 -0.64133	C	4.26203 3.70495 0.97429
		C	4.71303 4.20936 -0.24803
(*M*)-PH**2**-[7]Helicene		C	4.51888 3.43022 -1.39225
Sum of electronic and thermal Free Energies = --2084.778337		C	3.88802 2.18394 -1.34064
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C	-1.93874 -3.84798 -1.37179	C	-2.42291 4.76015 1.06348
C	-3.01217 -3.63714 -0.46782	C	-2.36868 3.36324 1.08913
C	-3.76053 -4.78666 -0.05946	C	3.15953 1.95936 2.42193
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C	-2.61512 -1.1348 -0.10298	C	-2.35923 2.6259 -2.67597
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C	-4.66719 0.32821 0.17807	C	-2.47395 6.98959 -0.13605
C	-5.40041 -0.8423 0.52379	H	-1.93042 -7.24862 -1.57077
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C	-1.2136 -0.95783 -0.11101	H	-1.42954 -2.98967 -1.79196
C	-5.33834 1.5658 0.11818	H	-3.89913 -6.94123 -0.0931
H	-4.78676 2.45351 -0.1652		
H	-7.18198 2.63696 0.36627		
H	-8.46885 0.59389 1.01207		
H	-7.36478 -1.57839 1.06594		
H	-6.41811 -3.23358 1.37274		
H	-5.50908 -5.46441 1.02863		
H	-0.25822 -2.90371 0.17611		
H	0.45995 2.07844 -0.21423		
H	2.19497 -4.07675 0.39143		
H	4.58539 -4.56174 0.55693		
H	5.53636 -0.37297 0.1937		
H	8.14487 -4.47221 0.73312		
H	6.7004 -4.90258 -0.19053		
H	6.60966 -4.72047 1.57366		
H	8.4347 -2.26292 1.7951		
H	7.22094 -0.98484 1.63436		
H	6.8807 -2.39946 2.64189		
H	7.08371 -2.84419 -1.67769		
H	8.55442 -2.52542 -0.73624		
H	7.34423 -1.25164 -0.95078		
H	4.41198 4.29074 1.87929		
H	4.86875 3.8007 -2.35412		
H	-2.45164 5.29692 -2.27794		
H	-2.44479 5.3012 2.00787		
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H	3.56904 0.96694 2.64321		
H	4.12837 1.89834 -3.46839		
H	2.63382 1.20627 -2.81566		
H	4.16764 0.39263 -2.53407		
H	5.84374 5.84555 0.61187		
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H	6.13809 5.59108 -1.11758		
H	-1.46541 2.00026 -2.78223		
H	-2.38183 3.32905 -3.5144		
H	-3.22336 1.9576 -2.771		
H	-2.31529 3.33794 3.24802		
H	-1.49531 1.95867 2.49312		
H	-3.25418 2.01526 2.53574		
H	-2.95604 7.38249 -1.03765		
H	-1.45745 7.40469 -0.10412		
H	-3.01075 7.38279 0.73418		
TS-PH**2**-[7]Helicene			

Sum of electronic and thermal Free Energies = -2084.757787

a.u.

C	-2.94238	-6.31689	1.22679
C	-1.91111	-5.56506	0.63214
C	-2.13921	-4.26959	0.21163
C	-3.38645	-3.61913	0.34678
C	-4.44856	-4.43171	0.8822
C	-4.19288	-5.753	1.333
C	-3.64234	-2.22688	-0.04622
C	-2.63523	-1.15911	-0.23205
C	-3.15977	0.2471	-0.26742
C	-4.53924	0.5446	-0.59583
C	-5.45559	-0.52733	-0.59262
C	-5.01644	-1.83842	-0.09379
C	-1.20166	-1.03893	-0.17383
C	-4.97736	1.82702	-0.98926
C	-6.28609	2.03341	-1.40234
C	-7.18442	0.9595	-1.44938
C	-6.77135	-0.30388	-1.04781
C	-6.03777	-2.68851	0.41626
C	-5.76859	-3.92083	0.93172
C	-0.05443	-1.88469	-0.34474
C	1.21634	-1.38523	-0.2207
C	1.46568	0.01697	0.07176
C	0.36159	0.90056	0.17317
C	-0.90268	0.39182	0.00682
C	-2.13324	1.14728	-0.06708
C	2.53206	-2.0202	-0.3683
C	2.94573	-3.31383	-0.65136
C	4.31905	-3.5957	-0.72631
C	5.30281	-2.60972	-0.52436
C	4.88163	-1.29874	-0.2374
C	3.52161	-1.00448	-0.15485
C	2.8417	0.25932	0.10945
C	3.51275	1.5613	0.32807
C	-2.17139	2.62808	0.04772
C	6.81158	-2.9179	-0.60919
C	7.09225	-4.40465	-0.93031
C	7.44991	-2.0518	-1.7289
C	7.48044	-2.58207	0.75144
C	3.62247	2.48368	-0.73376
C	4.27569	3.70088	-0.51142
C	4.81769	4.02362	0.73616
C	4.70435	3.09416	1.77609
C	4.06189	1.86648	1.59266
C	-2.55634	3.22671	1.2684
C	-2.56548	4.61998	1.37115
C	-2.20612	5.43707	0.29235
C	-1.8272	4.83	-0.90752
C	-1.79677	3.43661	-1.04636
C	3.05531	2.15867	-2.10611
C	3.93472	0.88246	2.74329
C	5.4949	5.36333	0.96774
C	-2.96558	2.36615	2.4509
C	-1.3851	2.81051	-2.36825
C	-2.2225	6.94934	0.43519
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H	-5.02058	-6.31712	1.74963
H	-4.27459	2.64609	-0.98024
H	-6.60343	3.02284	-1.71021
H	-8.19621	1.10896	-1.80755
H	-7.46441	-1.13188	-1.12013
H	-7.04897	-2.30877	0.45323
H	-6.55523	-4.52842	1.36508
H	-0.1368	-2.91165	-0.65318
H	2.22586	-4.10783	-0.81801
H	4.62051	-4.60993	-0.95049
H	5.6034	-0.50516	-0.08105
H	8.17575	-4.56163	-0.97525
H	6.68427	-5.06234	-0.15465
H	6.66595	-4.68839	-1.89903
H	8.52477	-2.25988	-1.79413
H	7.31703	-0.98449	-1.52566
H	6.98755	-2.28071	-2.6951
H	7.04242	-3.19098	1.54969
H	8.55596	-2.79005	0.69932
H	7.34521	-1.52637	1.00685
H	4.36753	4.40611	-1.33152
H	5.12352	3.32857	2.74975
H	-2.86012	5.07668	2.31115
H	-1.5498	5.44979	-1.75443
H	0.50989	1.96093	0.34796
H	-3.11923	2.98505	3.34011
H	-3.89696	1.831	2.23378
H	-2.19823	1.6164	2.67087
H	-3.2007	7.29841	0.78621
H	-1.46823	7.27844	1.16064
H	-2.00852	7.43458	-0.52196
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H	-2.08866	2.02576	-2.66548
H	4.43897	1.26732	3.63462
H	2.88036	0.70826	2.987
H	4.3747	-0.08598	2.48179
H	3.36551	1.15969	-2.43026
H	1.95914	2.17293	-2.09119
H	3.39721	2.89093	-2.84367
H	6.34165	5.26154	1.65478
H	5.86202	5.78511	0.02675
H	4.78871	6.07989	1.40688

(*P*)-PH**2**-[7]Helicene

Sum of electronic and thermal Free Energies = -2084.778337

a.u.

C	-2.15966	-6.26687	1.24827
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C	-1.88528	-3.85837	1.3622
C	-2.96669	-3.66281	0.46189
C	-3.70783	-4.81876	0.05477
C	-3.25768	-6.11132	0.431
C	-3.41894	-2.34511	0.05126
C	-2.59663	-1.16046	0.11699
C	-3.23338	0.17296	0.06052
C	-4.65839	0.29342	-0.18884
C	-5.38466	-0.88241	-0.53507
C	-4.73623	-2.2077	-0.45528
C	-1.19583	-0.96909	0.13646
C	-5.32327	1.53614	-0.15901
C	-6.67118	1.63438	-0.47516
C	-7.38861	0.48522	-0.82648
C	-6.75298	-0.74956	-0.84974
C	-5.43961	-3.38309	-0.85065
C	-4.92208	-4.63672	-0.66348
C	-0.07799	-1.84269	-0.0269
C	1.18507	-1.31194	-0.04083
C	1.40678	0.12866	0.08523
C	0.2977	1.01651	0.18923
C	-0.96423	0.47583	0.19595
C	-2.25646	1.15282	0.15692
C	2.5112	-1.92491	-0.17927

C	2.94683 -3.23311 -0.33115	C	-2.30876 2.57908 -2.39197
C	4.32357 -3.4899 -0.43323	C	-2.65535 6.96084 0.12687
C	5.28703 -2.46522 -0.38778	H	-1.82992 -7.25647 1.54188
C	4.84238 -1.13923 -0.23432	H	-0.67379 -5.24449 2.44658
C	3.47907 -0.86909 -0.12959	H	-1.39104 -2.992 1.77833
C	2.77579 0.39988 0.0297	H	-3.81722 -6.97462 0.08662
C	3.4262 1.72959 0.10121	H	-4.75962 2.41896 0.10649
C	-2.38456 2.63217 0.14753	H	-7.1639 2.59914 -0.44781
C	6.79955 -2.74734 -0.49758	H	-8.4426 0.55225 -1.06964
C	7.10745 -4.25306 -0.67136	H	-7.33976 -1.62384 -1.09573
C	7.37495 -1.99106 -1.72561	H	-6.39886 -3.28487 -1.33906
C	7.50611 -2.25386 0.79396	H	-5.46265 -5.51133 -1.00873
C	3.60332 2.48889 -1.07371	H	-0.23296 -2.90666 -0.14771
C	4.2344 3.73476 -0.98822	H	0.45118 2.08939 0.23797
C	4.69065 4.24114 0.23235	H	2.24085 -4.0553 -0.3729
C	4.51126 3.47083 1.38688	H	4.64435 -4.516 -0.55173
C	3.88644 2.22131 1.34143	H	5.54869 -0.31752 -0.19659
C	-2.4764 3.33673 1.36561	H	8.19201 -4.38904 -0.74718
C	-2.5744 4.73297 1.34131	H	6.75033 -4.83311 0.18691
C	-2.57704 5.44381 0.13761	H	6.64934 -4.64846 -1.58481
C	-2.48362 4.72916 -1.06249	H	8.45248 -2.17805 -1.80734
C	-2.3853 3.33483 -1.07737	H	7.21825 -0.91177 -1.63277
C	3.12126 1.9578 -2.41322	H	6.88747 -2.33412 -2.64456
C	3.69821 1.40367 2.60792	H	7.11164 -2.784 1.6676
C	5.34741 5.60856 0.31195	H	8.58452 -2.44124 0.72517
C	-2.48978 2.58542 2.68574	H	7.351 -1.18037 0.94127
H	4.37506 4.31697 -1.8935		
H	4.86576 3.8482 2.34113		
H	-2.65057 5.2727 2.28009		
H	-2.48853 5.26727 -2.00558		
H	2.02887 1.86984 -2.42741		
H	3.42557 2.62722 -3.22329		
H	3.53341 0.96136 -2.60697		
H	4.145 1.9154 3.4655		
H	2.63319 1.24554 2.81225		
H	4.1631 0.41651 2.50735		
H	5.73613 5.91414 -0.66451		
H	4.62271 6.36513 0.63961		
H	6.17619 5.60477 1.02805		
H	-1.58841 1.97217 2.79371		
H	-2.54053 3.28474 3.52573		
H	-3.35282 1.91183 2.7389		
H	-2.2642 3.27618 -3.23421		
H	-1.42361 1.93457 -2.42029		
H	-3.18869 1.93732 -2.51591		
H	-3.02423 7.34093 1.08464		
H	-1.6639 7.39671 -0.05154		
H	-3.32479 7.31357 -0.66538		

8. OFET fabrication and measurement

Heavily doped silicon substrates with a 300 nm SiO_2 dielectric (with a capacitance of 11 nF cm^{-2}) were modified by octadecyltrichlorosilane (OTS) through thermal vapor at 150 °C. The sample (**1** or **2**) layer was spin-coated 60s at 2000 rpm from 5 mg/mL $CHCl_3$ and then annealed at 200 °C for 2 hours under glove box conditions. Source and drain gold electrodes were thermal vapor deposited at a thickness of 50 nm. The channel length and width were 50 μm and 1000 μm, respectively. A Keithley 4200-SCS was used for all standard electrical measurements in glove box under nitrogen atmosphere.

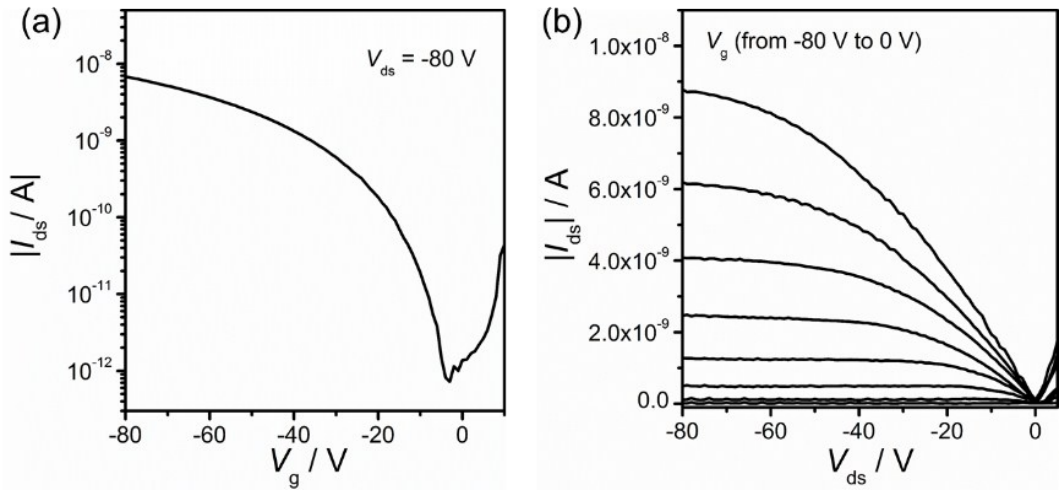
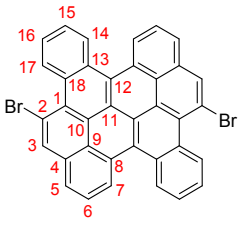


Figure S31. (a) Transfer curve and (b) output curve of transistors based on the spin-coated film of **1**.

9. NMR characterization



4

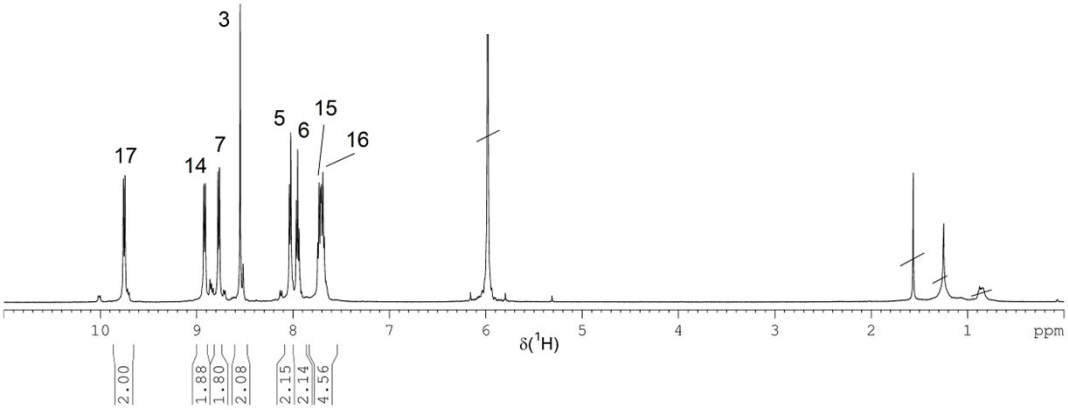


Figure S32. ^1H NMR spectrum of **4** (solvent: $C_2D_2Cl_4$, 30°C).

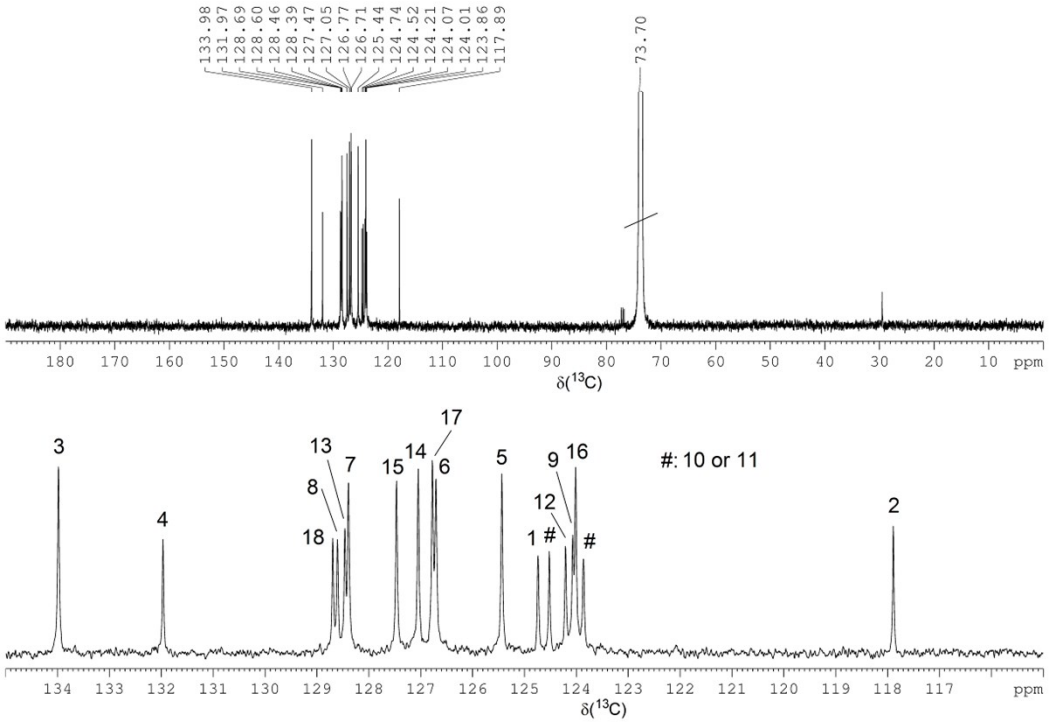


Figure S33. ^{13}C NMR spectrum of **4** (solvent: $C_2D_2Cl_4$, 30°C).

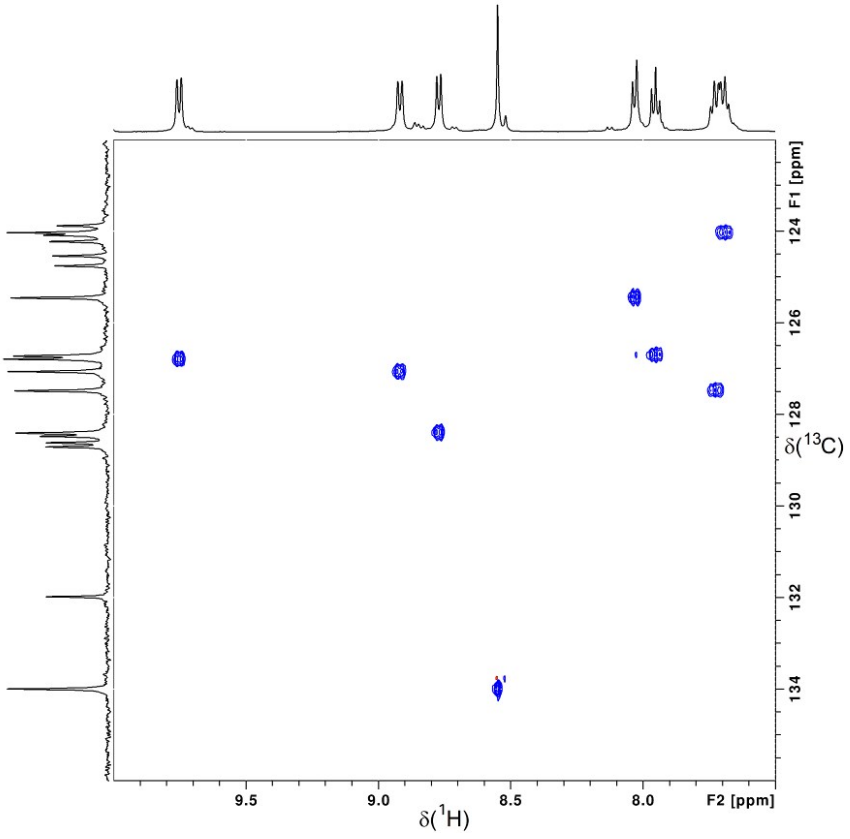


Figure S34. HSQC spectrum of **4** (solvent: $C_2D_2Cl_4$, 30°C).

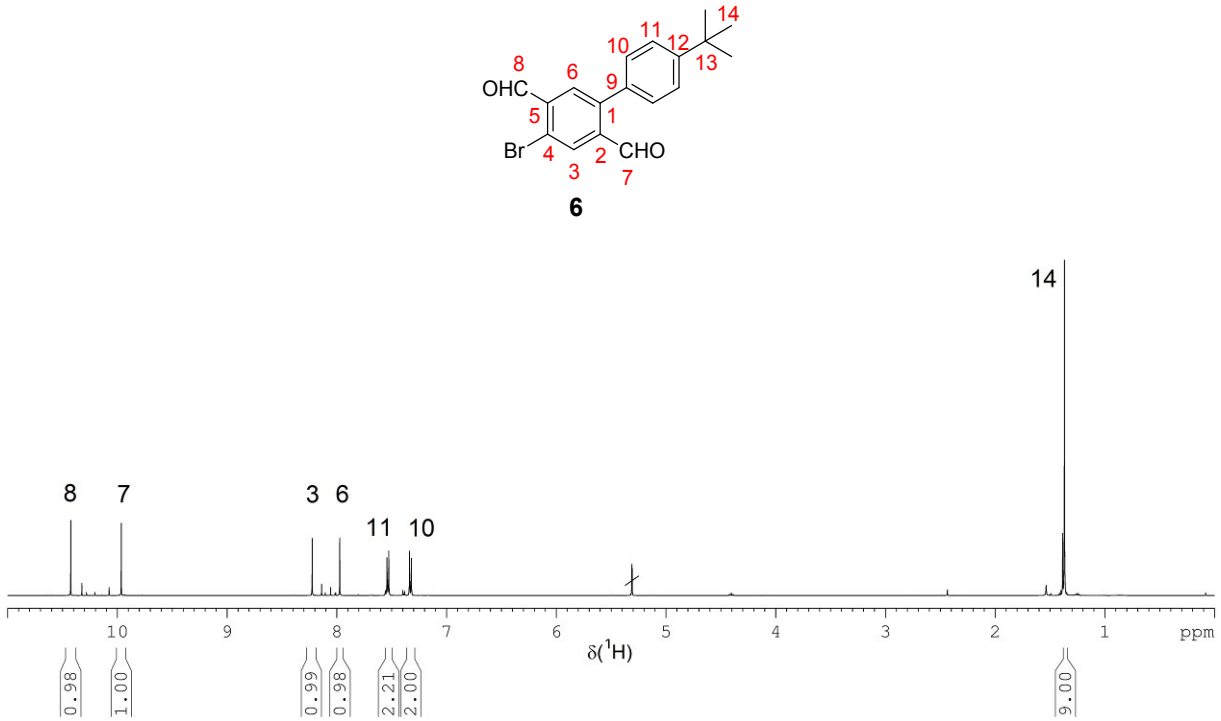


Figure S35. ^{1}H NMR spectrum of **6** (solvent: CD_2Cl_2, 30°C).

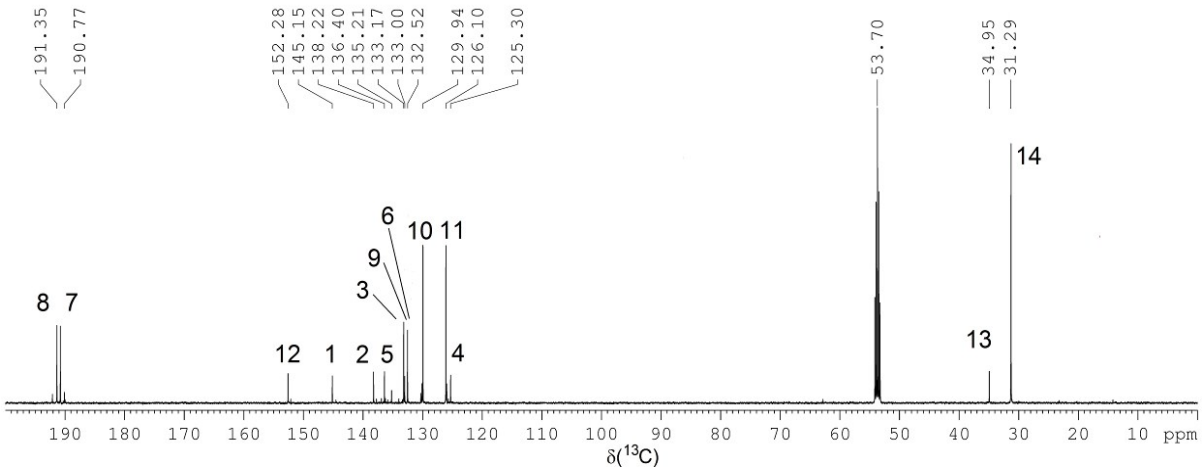


Figure S36. ^{13}C NMR spectrum of **6** (solvent: CD_2Cl_2, 30°C).

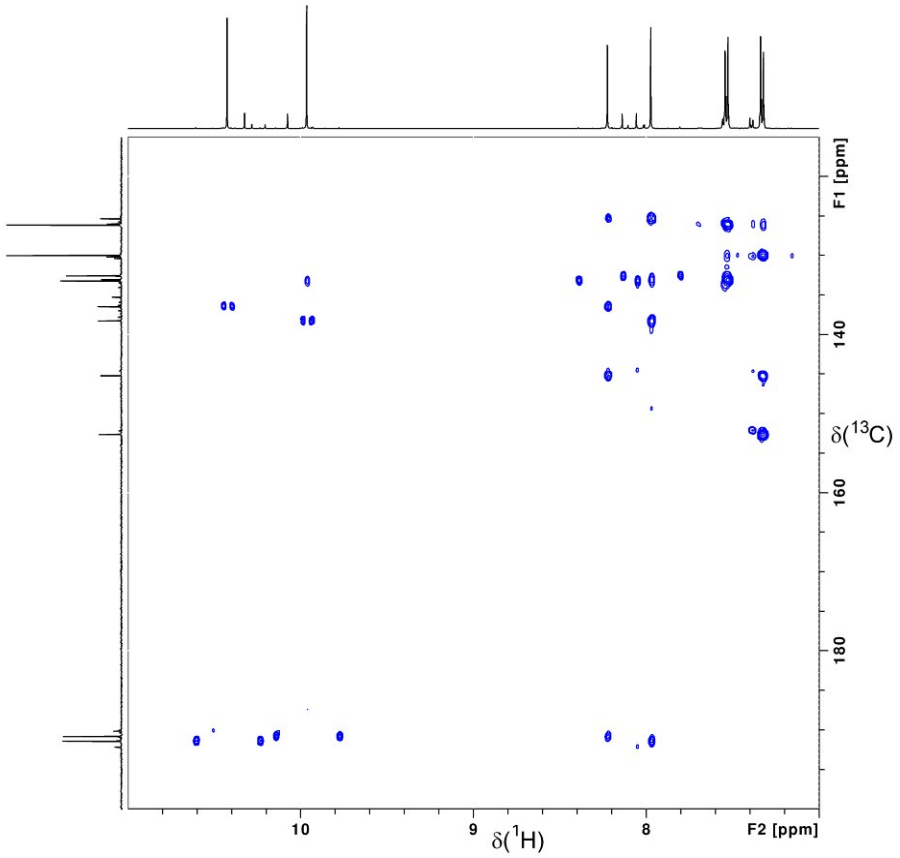
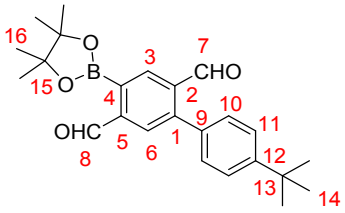


Figure S37. HMBC spectrum (region) of **6** (solvent: CD_2Cl_2, 30°C).



7

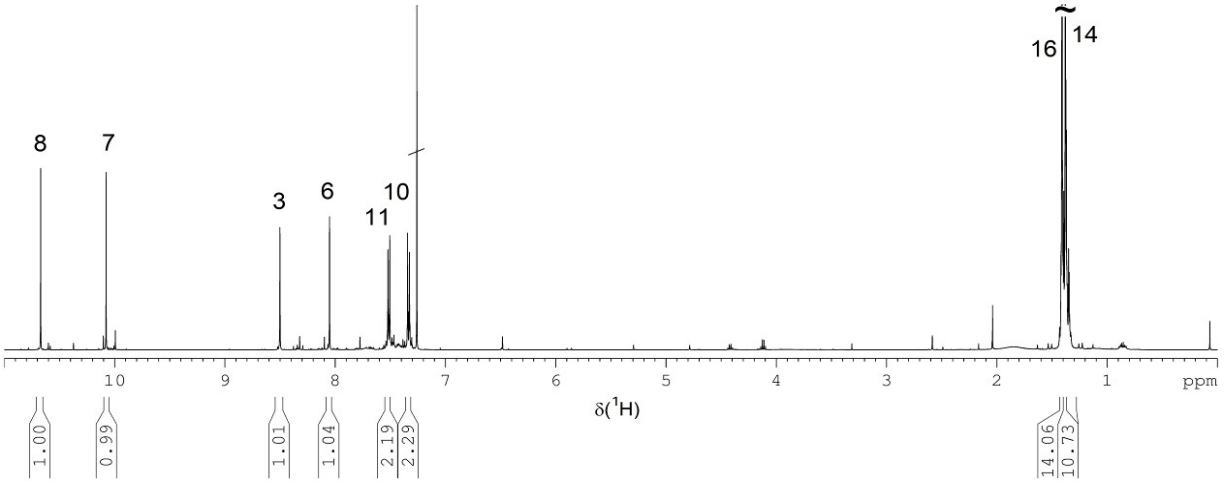


Figure S38. ^1H NMR spectrum of **7** (solvent: $CDCl_3$, 30°C).

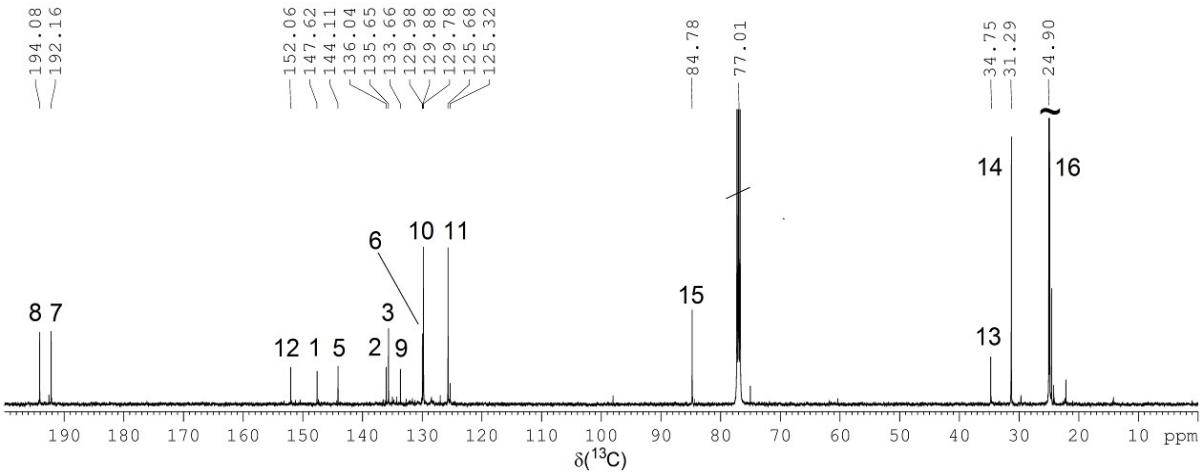
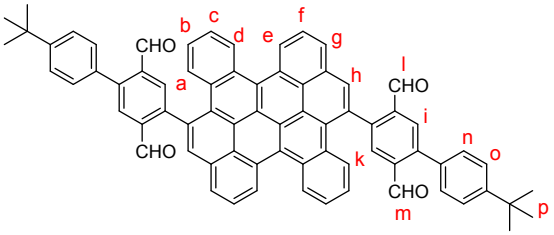


Figure S39. ^{13}C NMR spectrum of **7** (solvent: $CDCl_3$, 30°C).



8

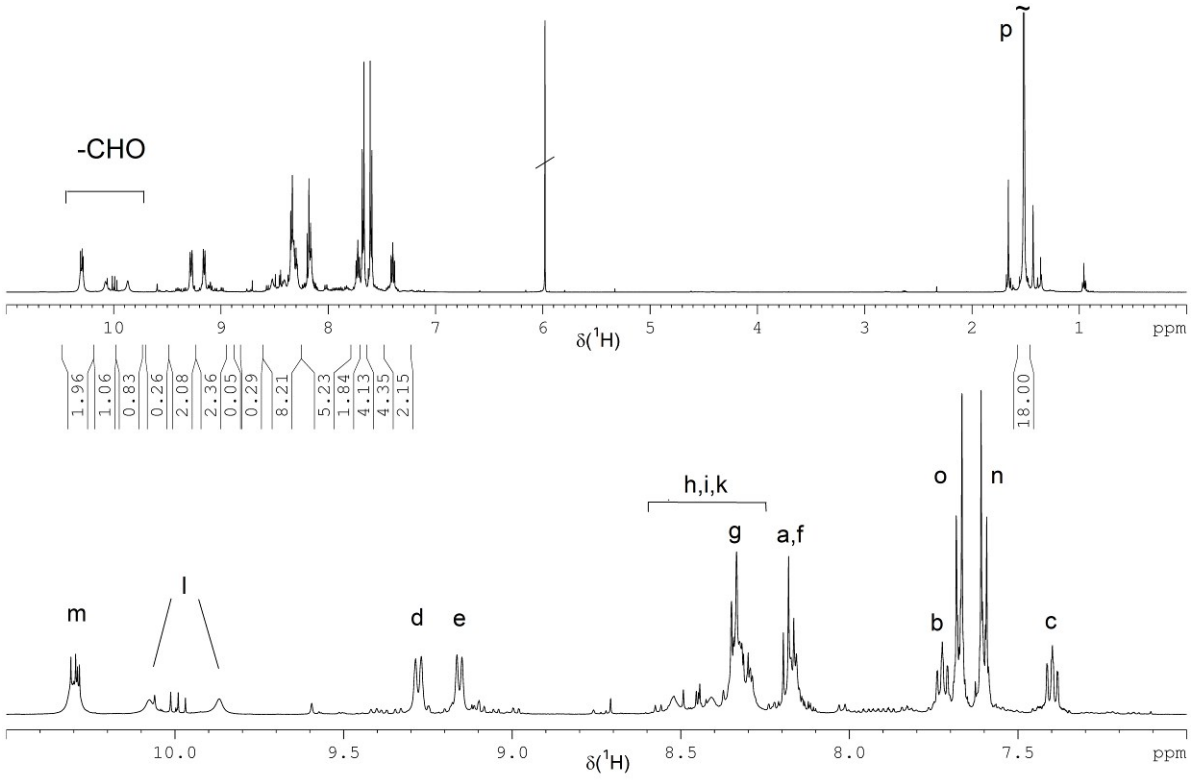


Figure S40. ^{1}H NMR spectrum of **8** (solvent: $C_2D_2Cl_4$, 120°C).

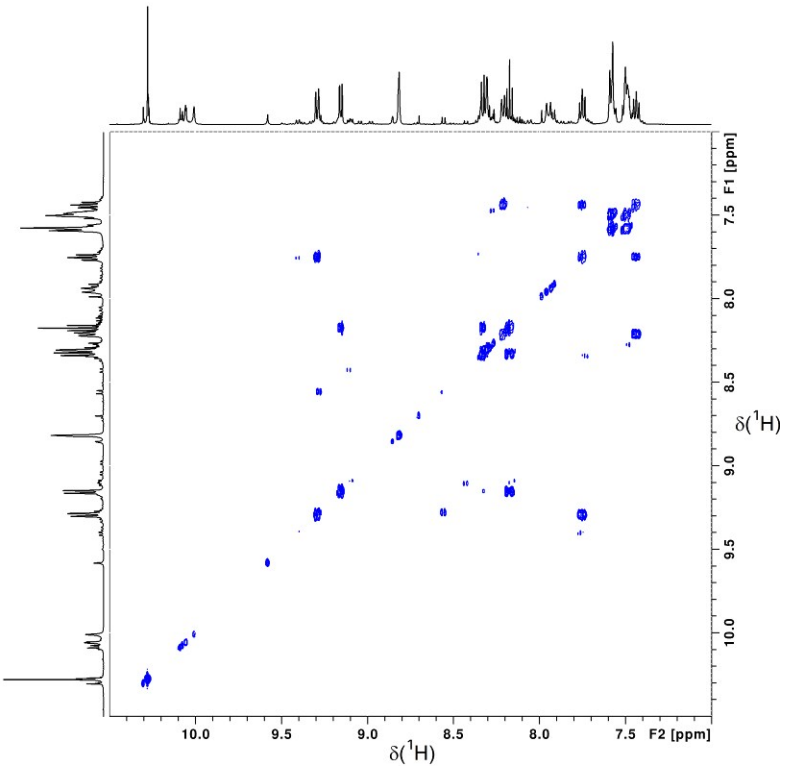


Figure S41. COSY spectrum (region) of **8** (solvent: $C_2D_2Cl_4$, 120°C).

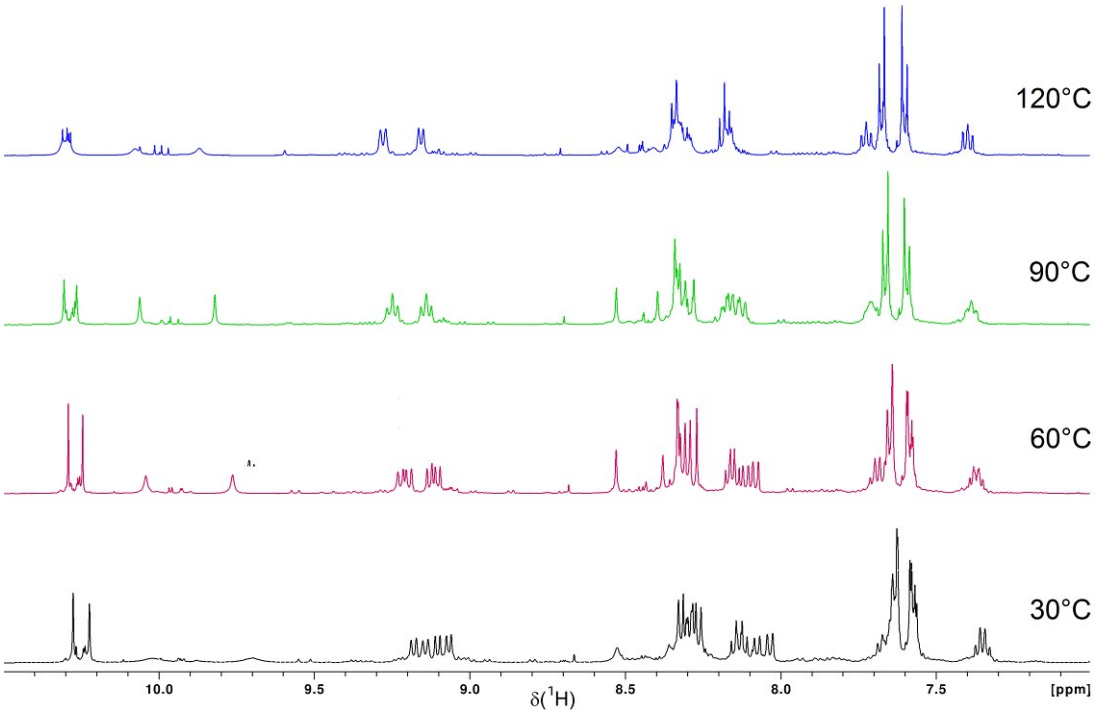


Figure S42. Variable-temperature ^{1}H NMR spectra (region) of **8** indicating dynamic processes (solvent: $C_2D_2Cl_4$).

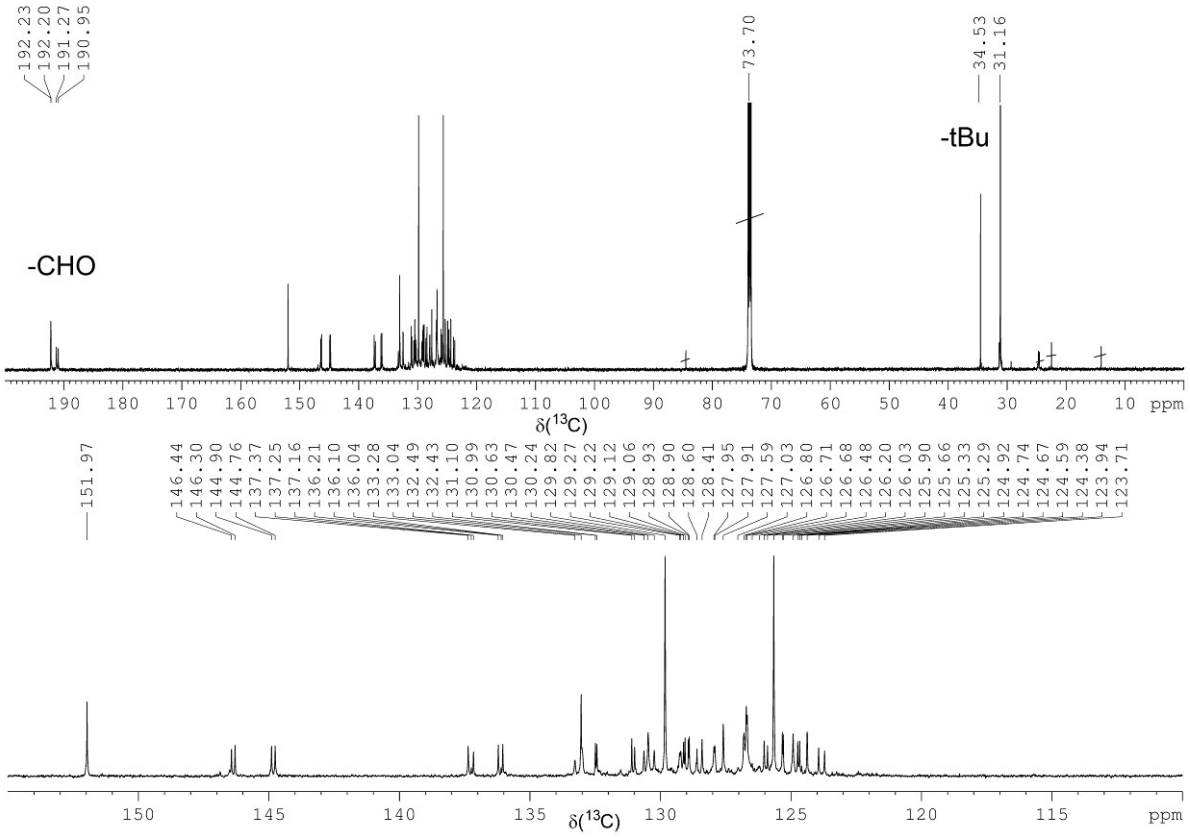
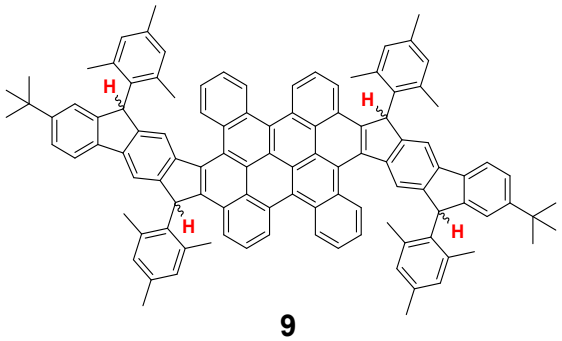


Figure S43. ^{13}C NMR spectrum of **8** (solvent: $C_2D_2Cl_4$, 30°C).



9

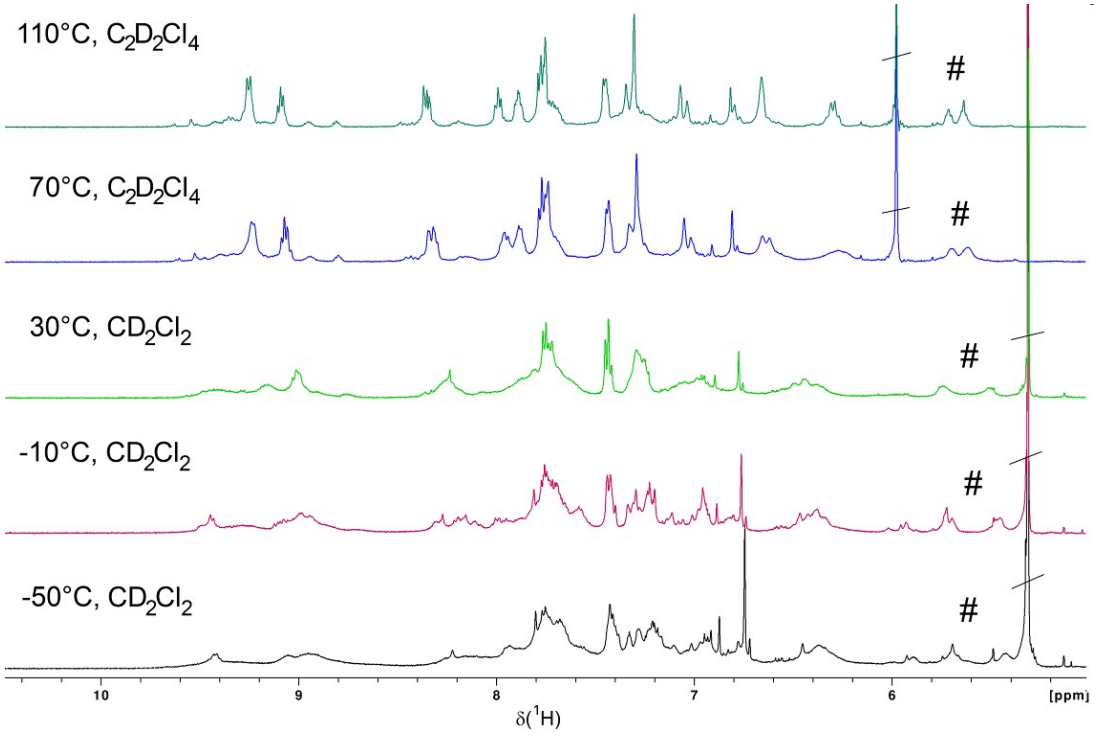


Figure S44. ^{1}H NMR spectra (region) of **9** recorded in different solvents ($C_2D_2Cl_4$, CD_2Cl_2) and at different temperatures. Note the general trend of line narrowing with increasing temperature. # marks the signal group of the aliphatic ring protons. At -50°C several signals were observed pointing to several isomers. With increasing temperature fast interconversion of isomers finally results in fewer CH signals.

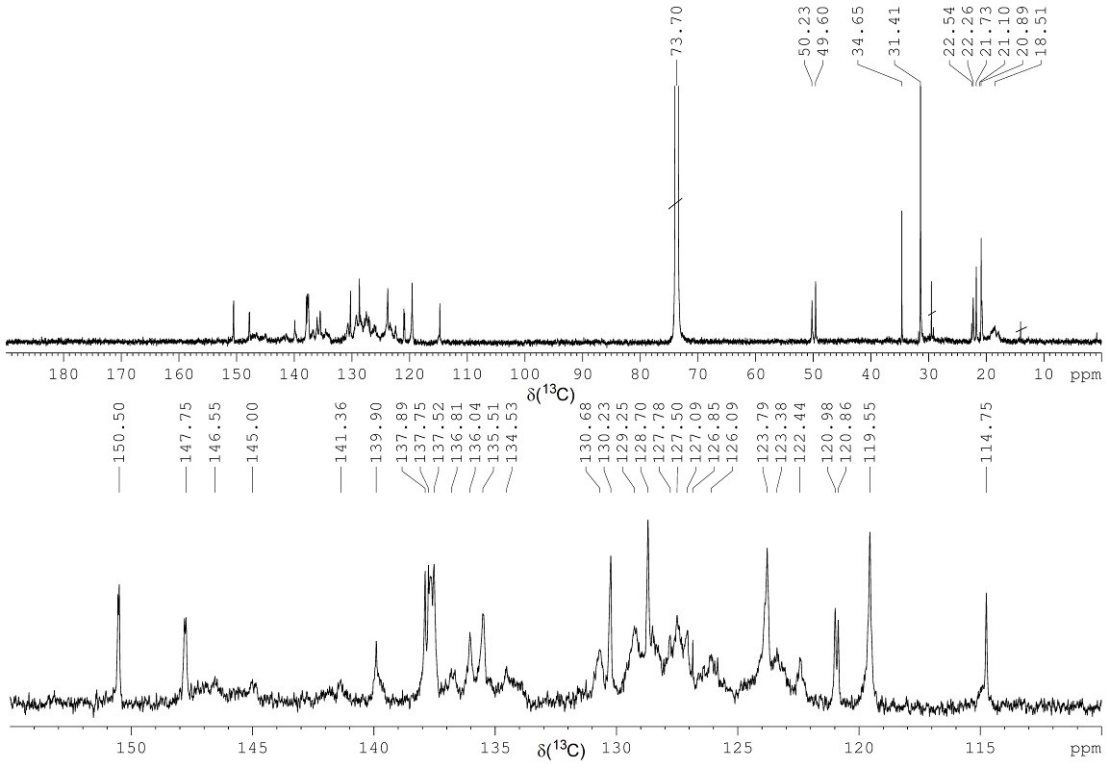
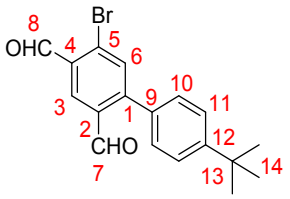


Figure S45. ^{13}C NMR spectrum of **9** (solvent: $C_2D_2Cl_4$, 30°C).



11

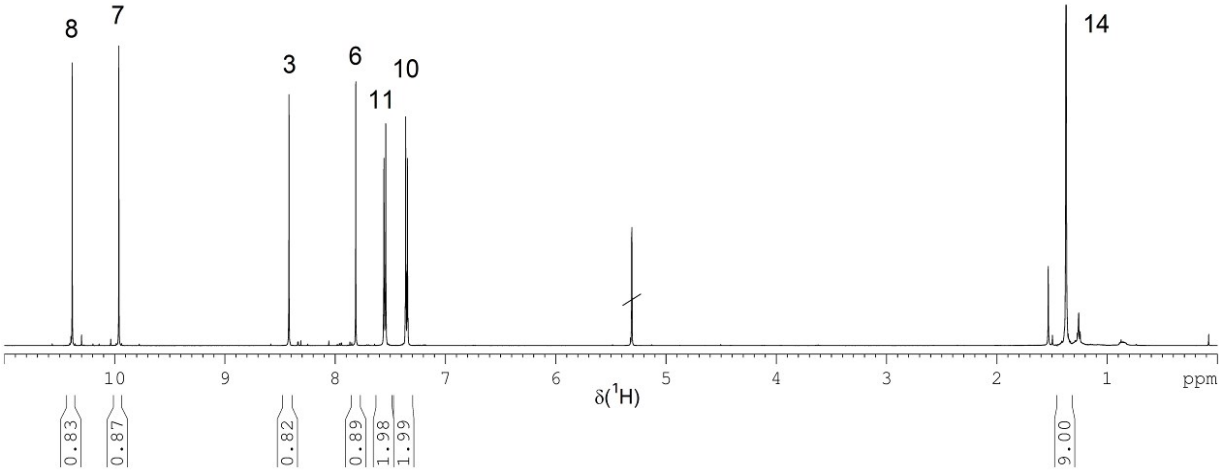


Figure S46. ^{1}H NMR spectrum of **11** (solvent: CD_2Cl_2, 30°C).

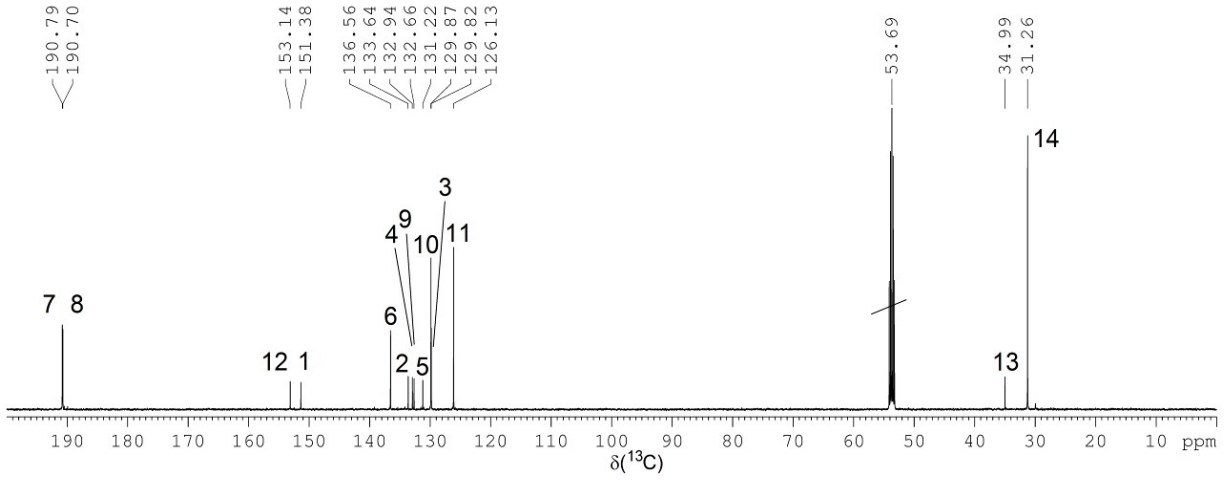


Figure S47. ^{13}C NMR spectrum of **11** (solvent: CD_2Cl_2, 30°C).

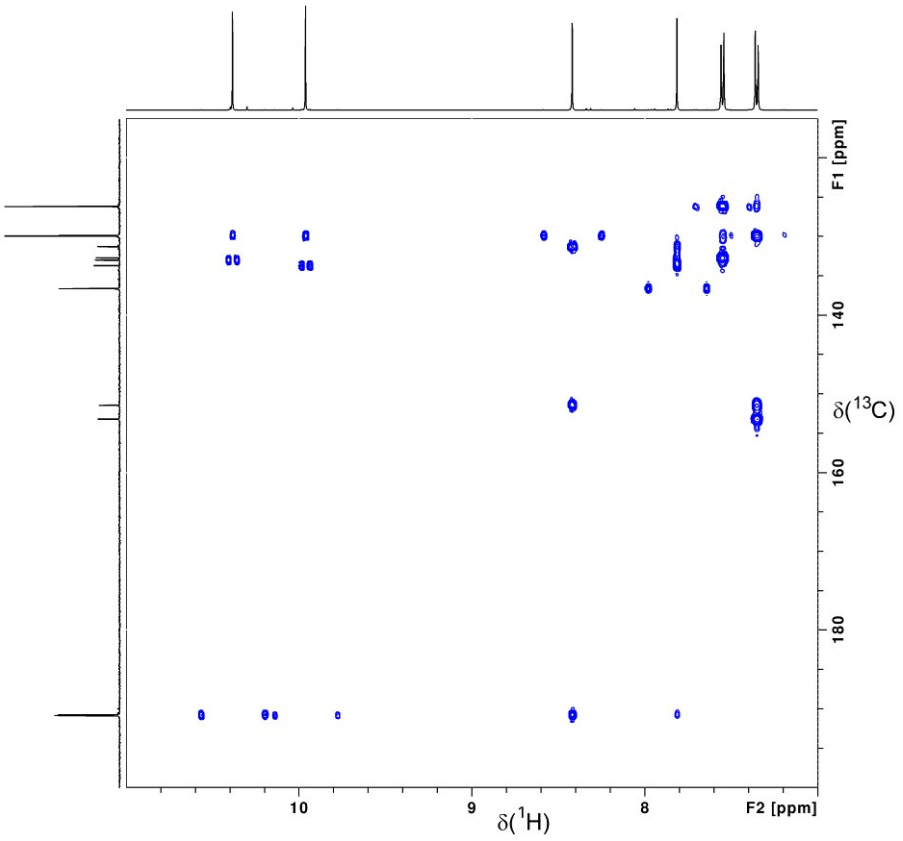
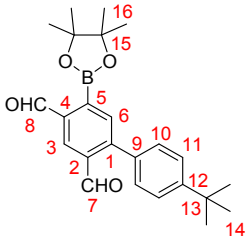


Figure S48. HMBC spectrum (region) of **11** (solvent: CD_2Cl_2, 30°C).



12

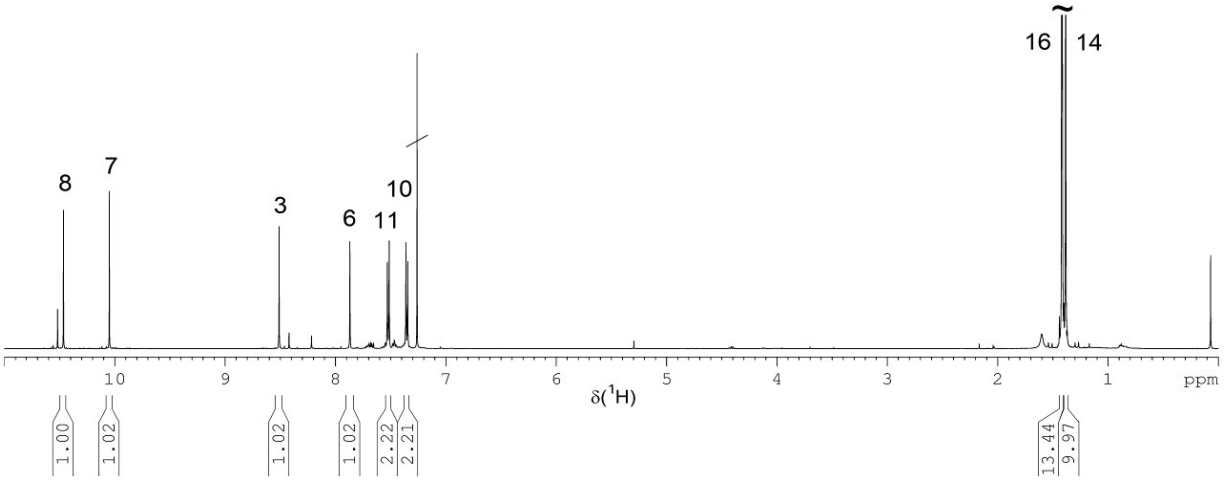


Figure S49. ^1H NMR spectrum of **12** (solvent: $CDCl_3$, 30°C).

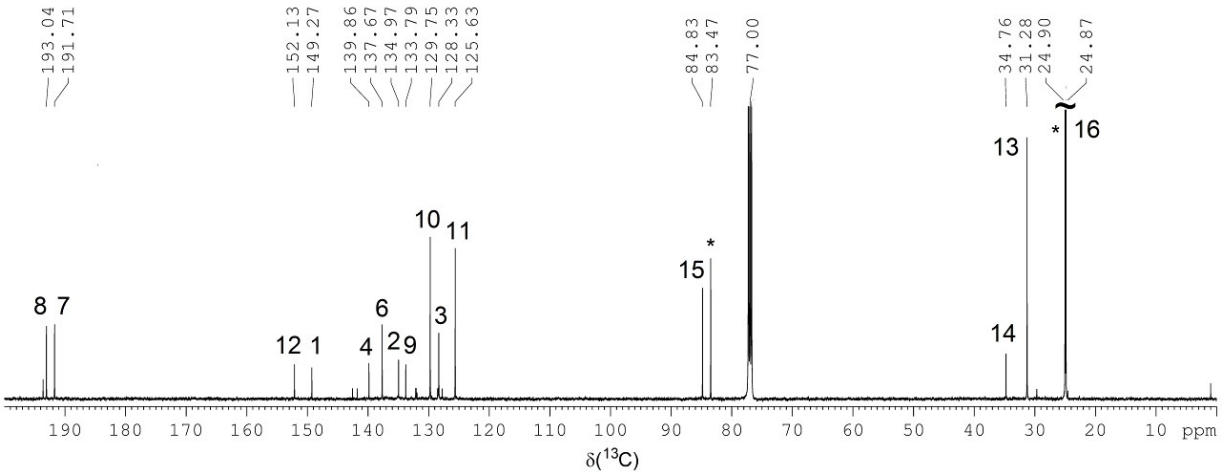
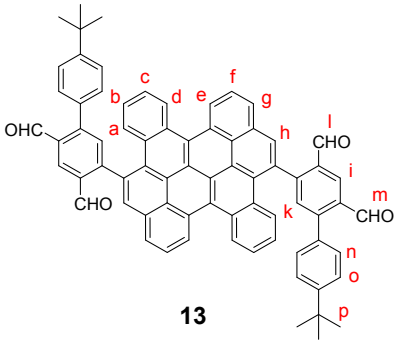


Figure S50. ^{13}C NMR spectrum of **12** (solvent: $CDCl_3$, 30°C). * marks signals of a further 4,4,5,5-tetramethyl-1,3,2-dioxaborolane derivative.



13

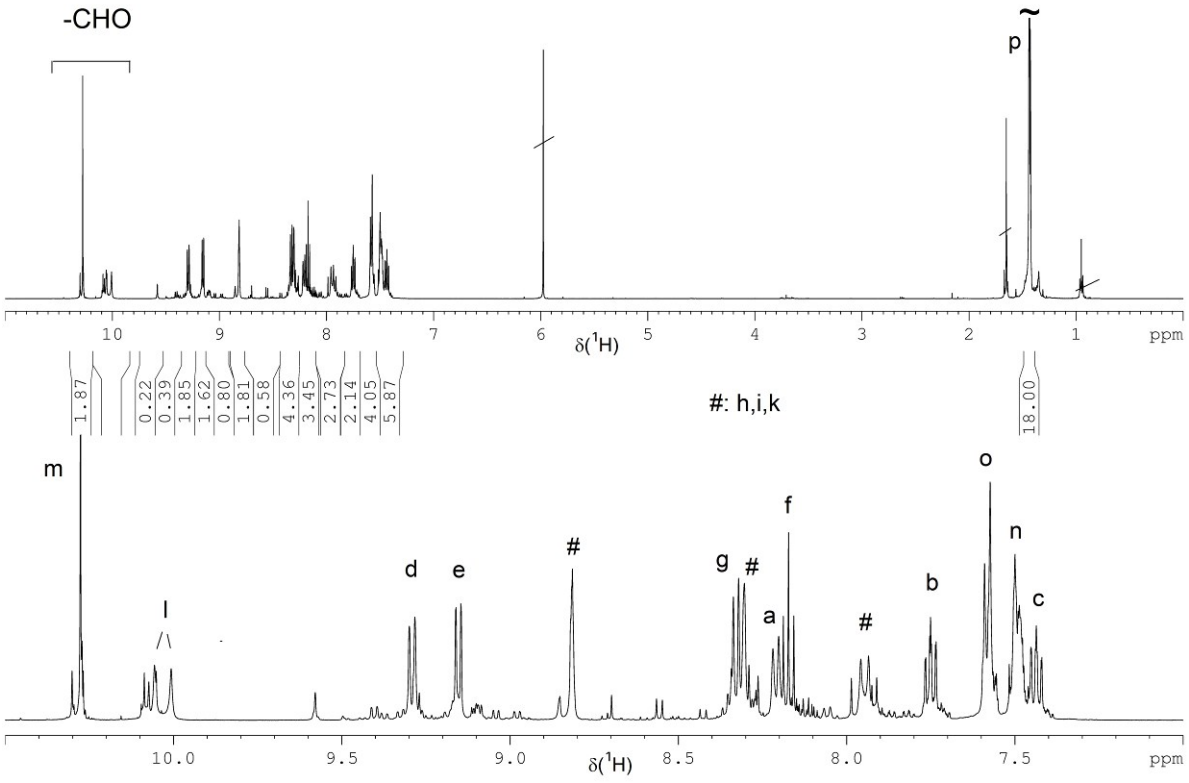


Figure S51. ^{1}H NMR spectrum of **13** (solvent: $C_2D_2Cl_4$, 120°C).

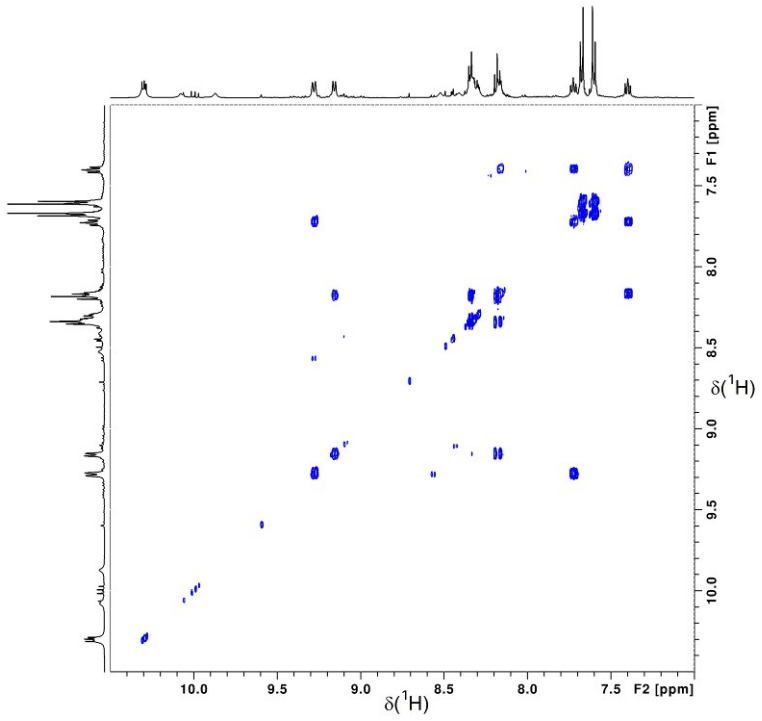


Figure S52. COSY spectrum of **13** (solvent: $C_2D_2Cl_4$, 120°C).

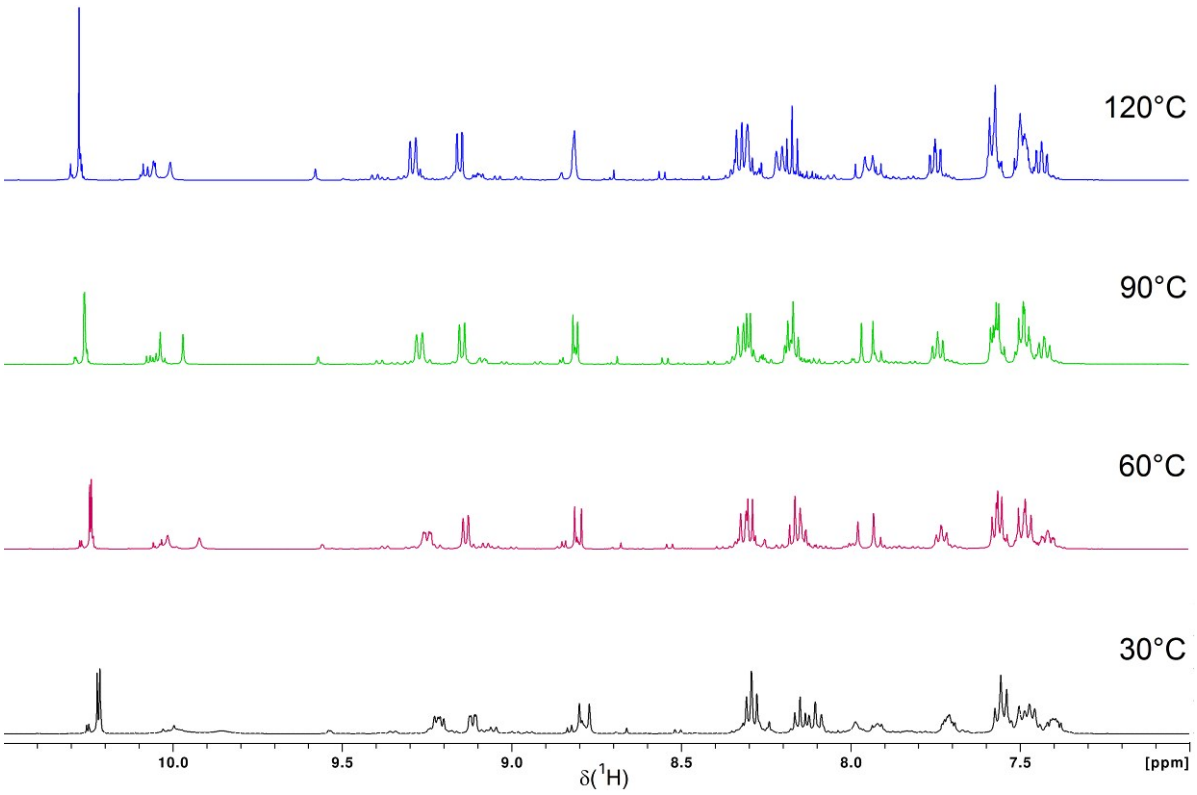


Figure S53. Variable-temperature ^{1}H NMR spectra (region) of **13** indicating dynamic processes (solvent: $C_2D_2Cl_4$).

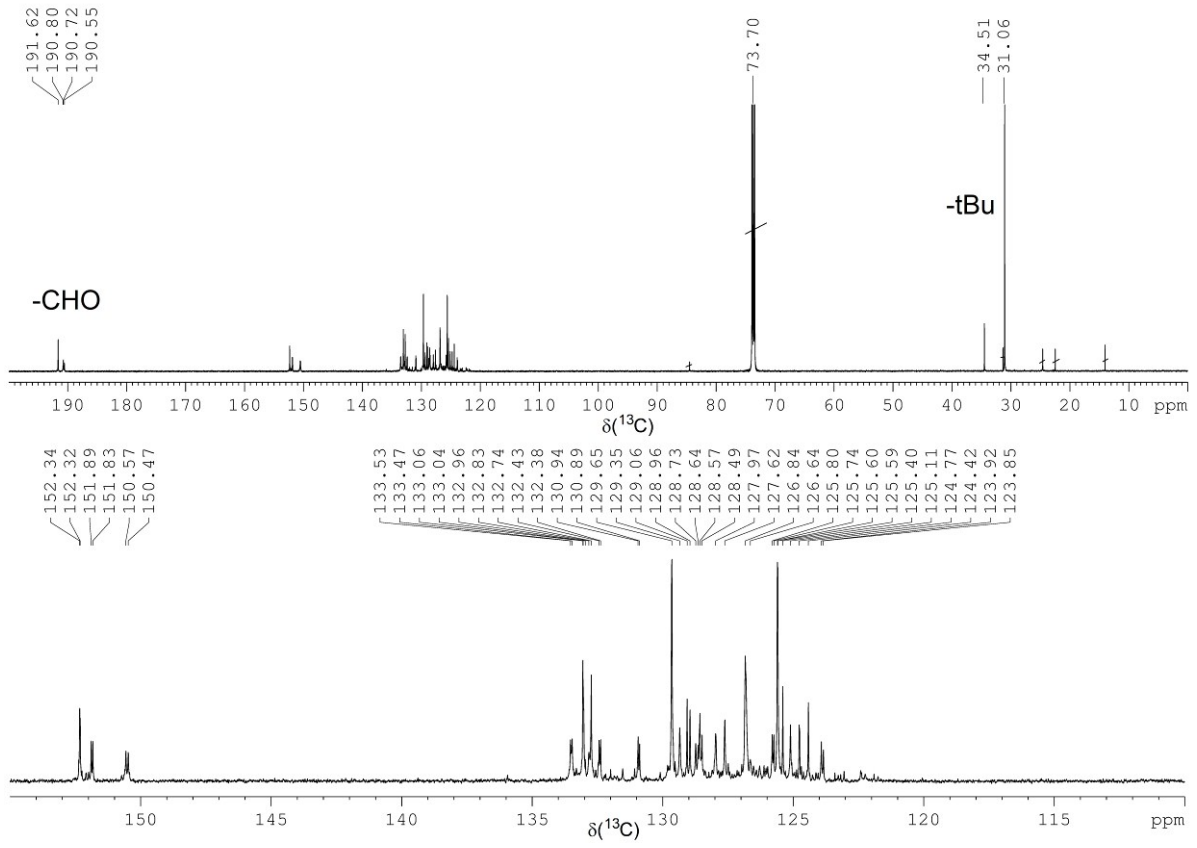
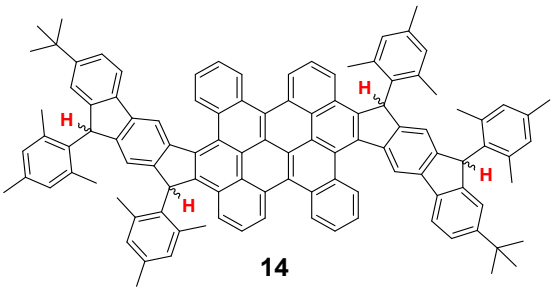


Figure S54. ^{13}C NMR spectrum of **13** (solvent: $C_2D_2Cl_4$, 30°C).



14

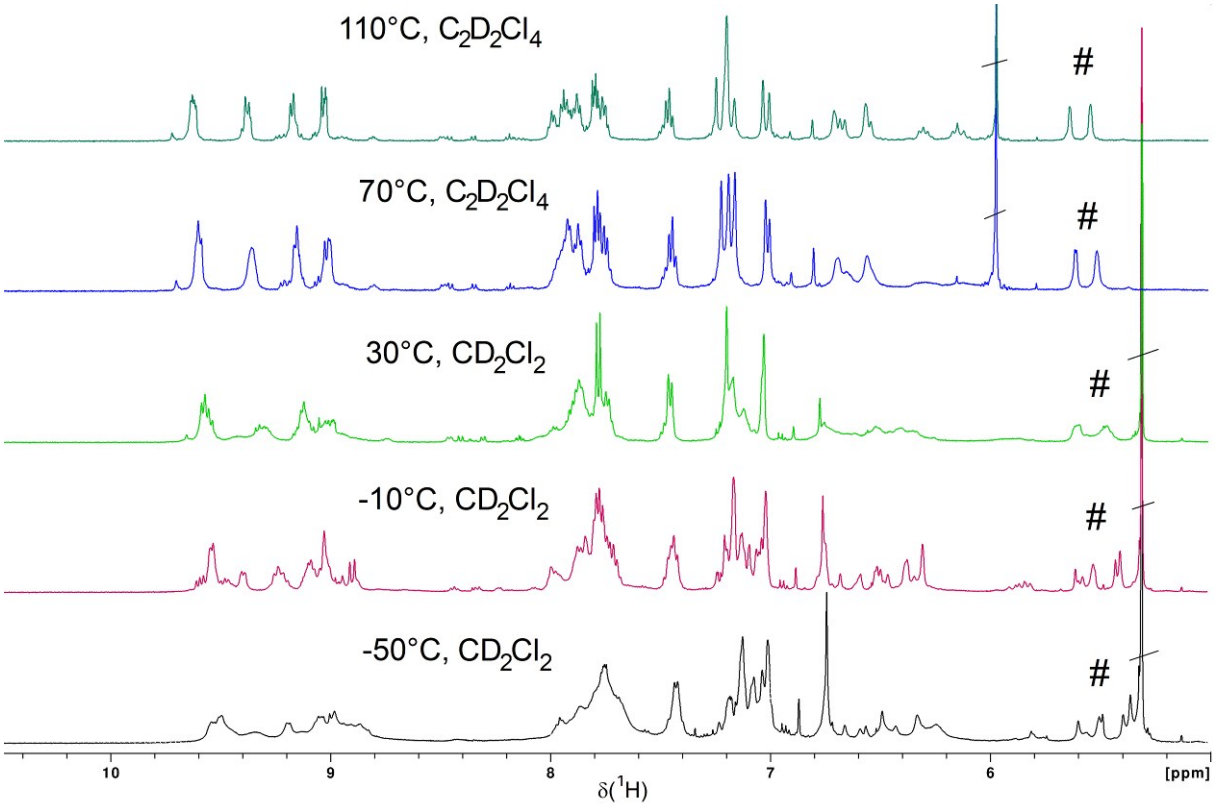


Figure S55. ^{1}H NMR spectra (region) of **14** recorded in different solvents ($C_2D_2Cl_4$, CD_2Cl_2) and at different temperatures. Note the general trend of line narrowing with increasing temperature. # marks the signal group of the aliphatic ring protons. At -50°C several signals were observed pointing to several isomers. With increasing temperature fast interconversion of isomers finally results in two CH signals.

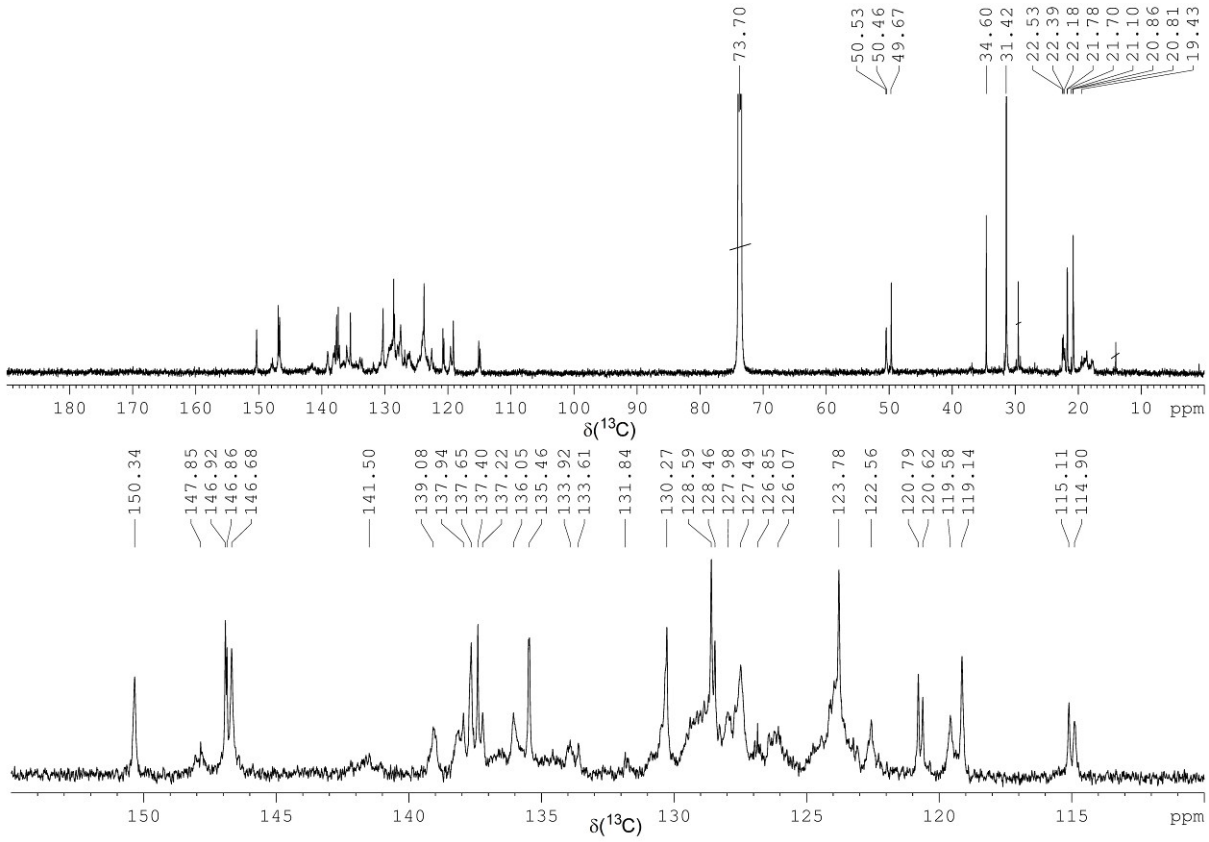


Figure S56. ^{13}C NMR spectrum of **14** (solvent: $C_2D_2Cl_4$, 30°C).

10. High resolution mass spectra (HR-MS)

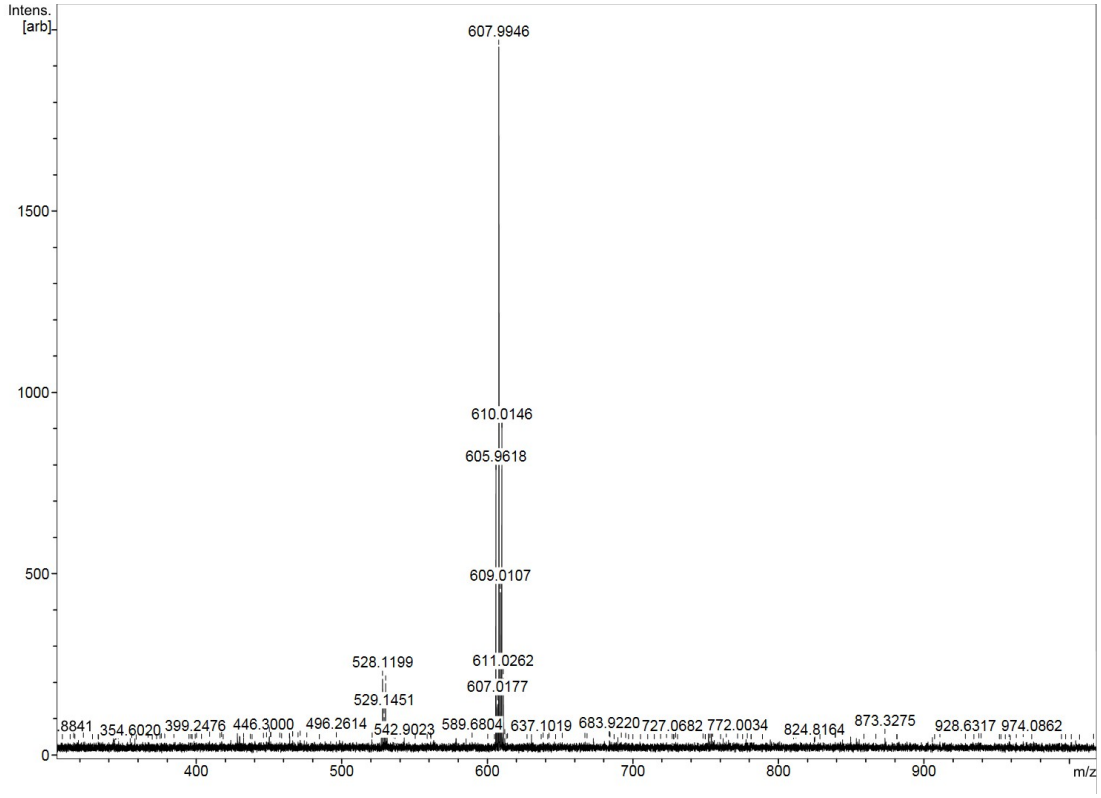


Figure S57. HR-MALDI-TOF mass spectrum of compound **4**.

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C18 H17 Br O2	97.65	-1.51	C18 H17 Br O2	1.421	344.04119	344.04067

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
345.0317	1.421	344.04067	C18 H17 Br O2	344.04119	-1.51	Find By Formula	

MS Zoomed Spectrum

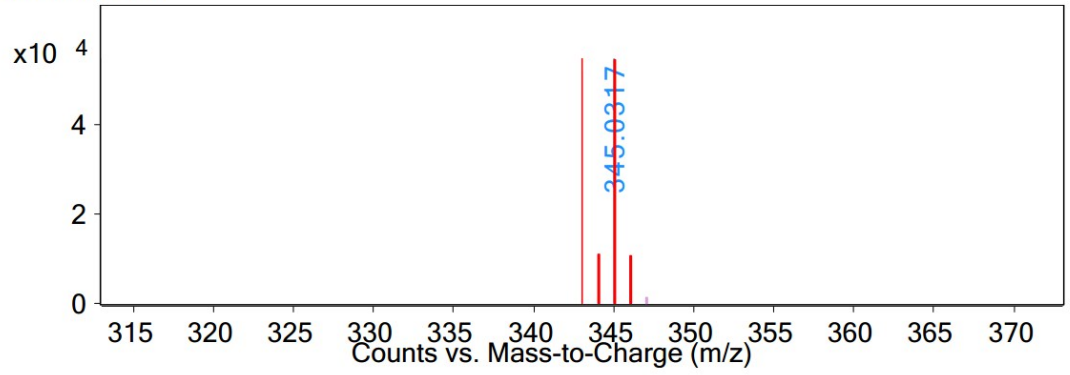


Figure S58. HR-ESI mass spectrum of compound **6**.

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H29 B O4	42.68	-0.45	C24 H29 B O4	1.587	391.21952	391.21935

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
393.2233	1.587	391.21935	C24 H29 B O4	391.21952	-0.45	Find By Formula	

MS Zoomed Spectrum

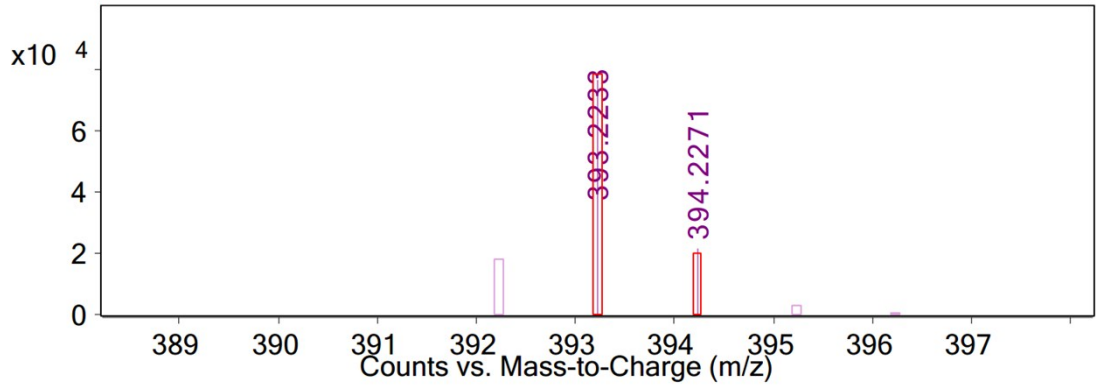


Figure S59. HR-ESI mass spectrum of compound **7**.

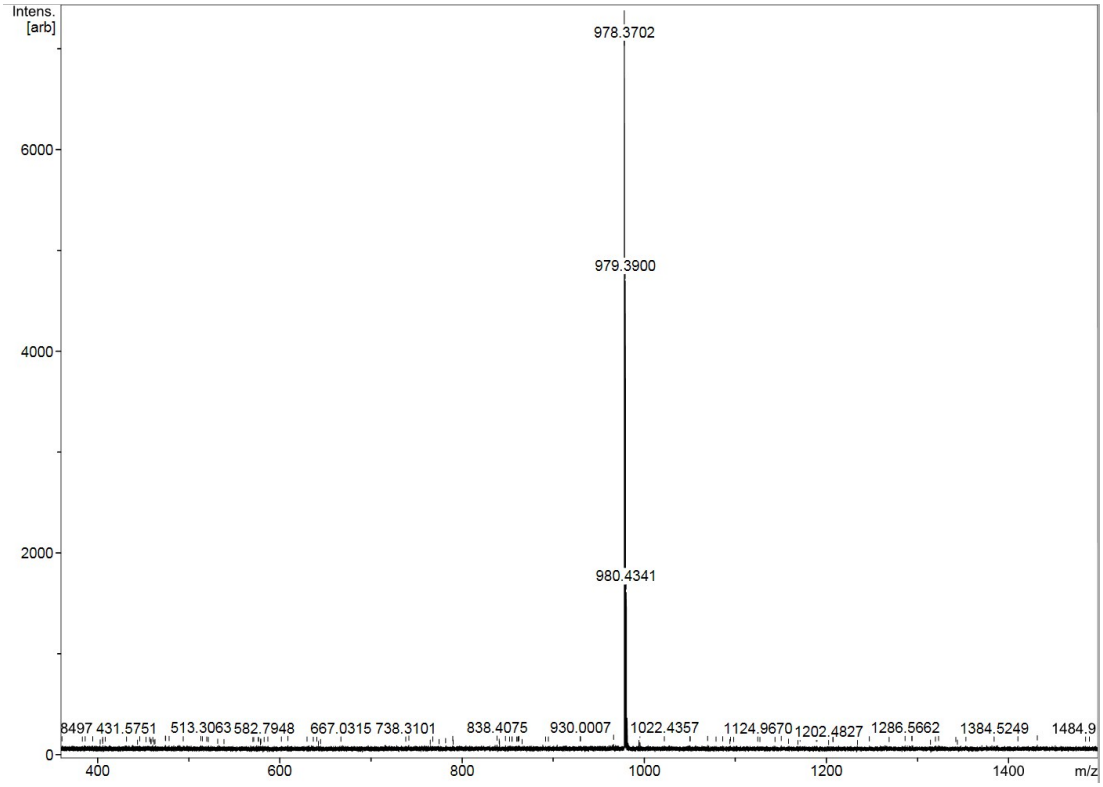


Figure S60. HR-MALDI-TOF mass spectrum of compound **8**.

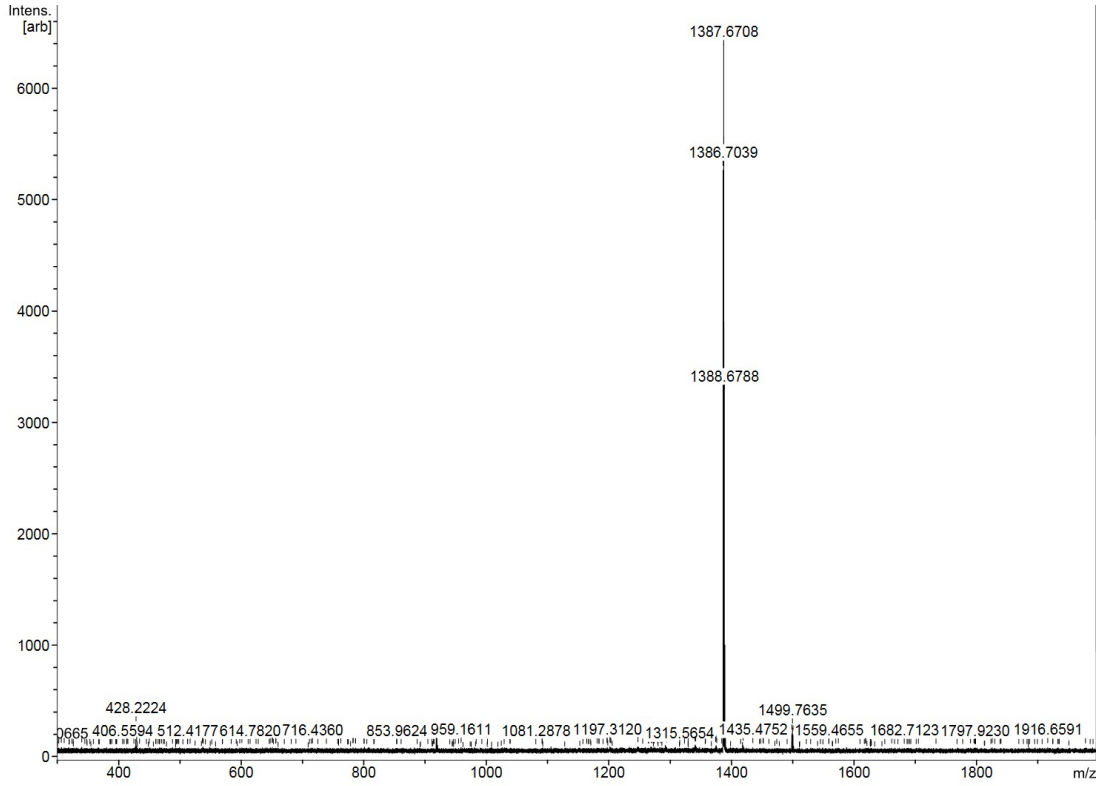


Figure S61. HR-MALDI-TOF mass spectrum of compound **9**.

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C18 H17 Br O2	96.18	-1.61	C18 H17 Br O2	2.005	344.04119	344.04064

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
369.0283	2.005	344.04064	C18 H17 Br O2	344.04119	-1.61	Find By Formula	

MS Zoomed Spectrum

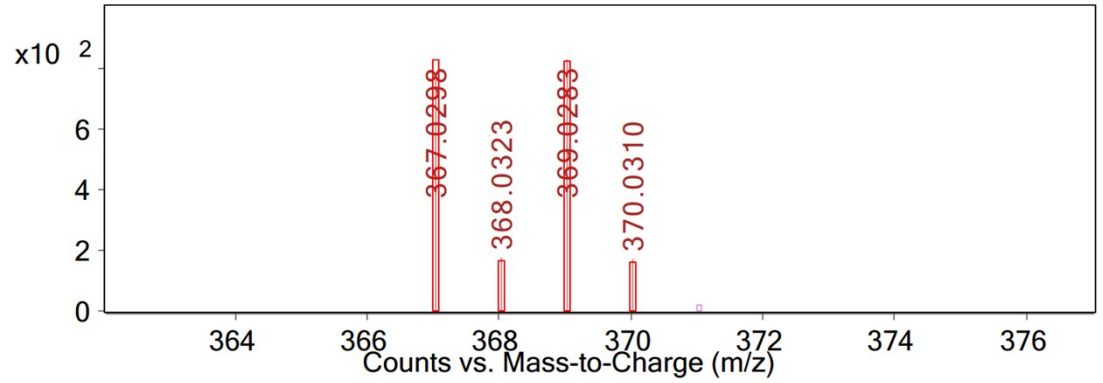


Figure S62. HR-ESI mass spectrum of compound **11**.

Compound Table

Label	Tgt Score	Mass Error (ppm)	Tgt Formula	Obs. RT	Ref. Mass	Obs. Mass
Cpd 1: C24 H29 B O4	58.87	0.67	C24 H29 B O4	1.671	391.21952	391.21978

Obs. *m/z*	Obs. RT	Obs. Mass	Tgt Formula	Tgt Mass	Tgt Mass Error (ppm)	RT Diff.	Find Cpds Algorithm
393.2237	1.671	391.21978	C24 H29 B O4	391.21952	0.67	Find By Formula	

MS Zoomed Spectrum

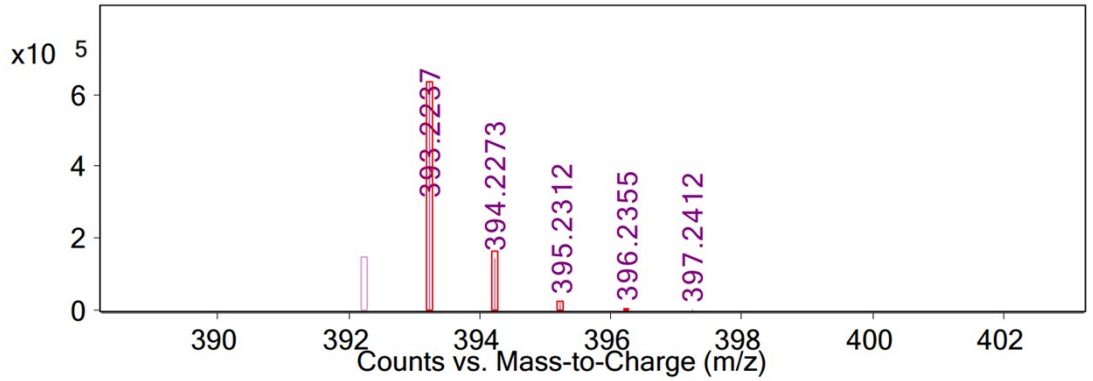


Figure S63. HR-ESI mass spectrum of compound **12**.

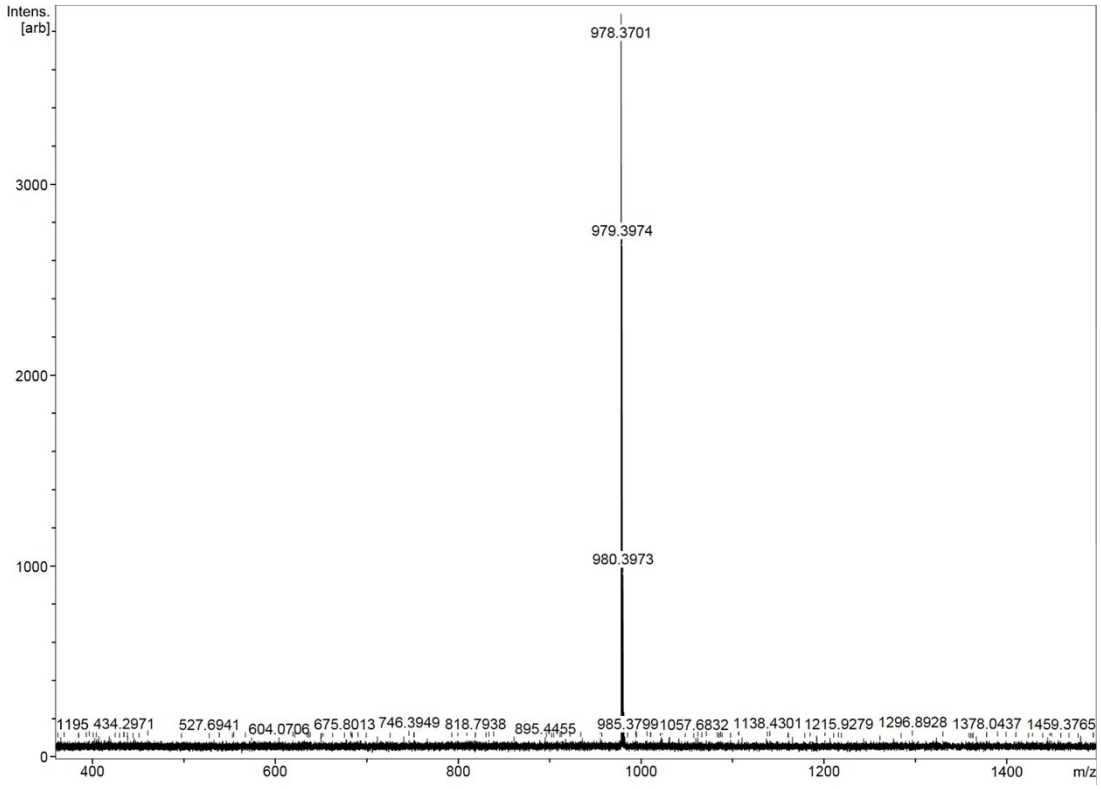


Figure S64. HR-MALDI-TOF mass spectrum of compound **13**.

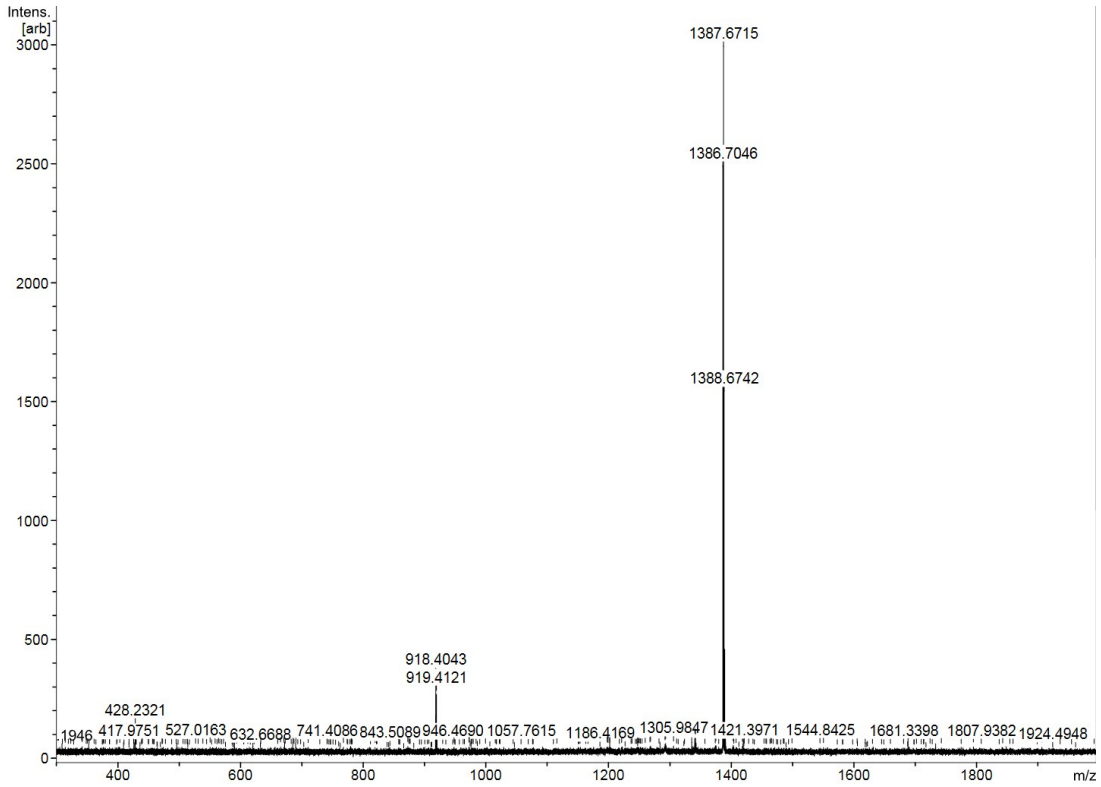


Figure S65. HR-MALDI-TOF mass spectrum of compound **14**.

11. Elemental analysis

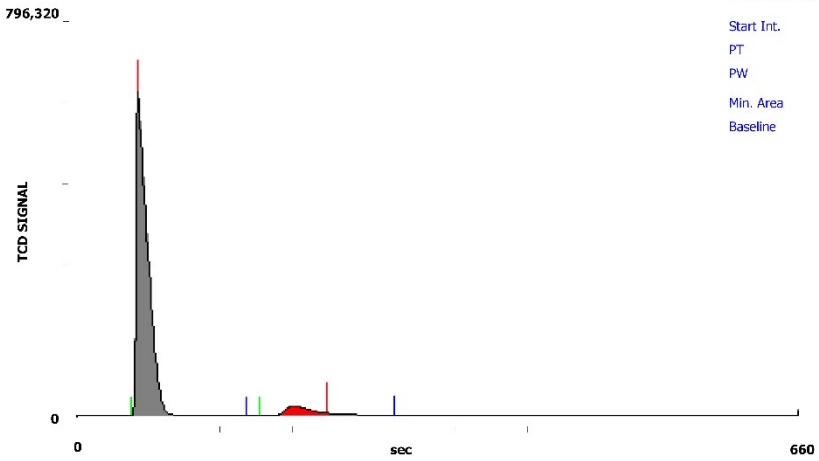
EuroEA Elemental Analyser

AutoRun name	:	180212- (805)
Date of Analysis	:	12 Feb 2018
Time of Analysis	:	09:52:30
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	T1-13-no
Sample position #	:	14
Type	:	Smp
Sample weight	:	2.036 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	57	51	156	8,696,803	92.636	70.042
Hydrogen	228	167	290	691,368	7.364	2.431
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.612535 E-07
Carbon	-	1.639756 E-07
Hydrogen	-	7.157954 E-08
Sulphur	-	4.040296 E-07
Oxygen	-	-

12 Feb 2018 16:16:20 AutoRun: 180212- (805)

Figure S66. Elemental analysis of compound **4**.

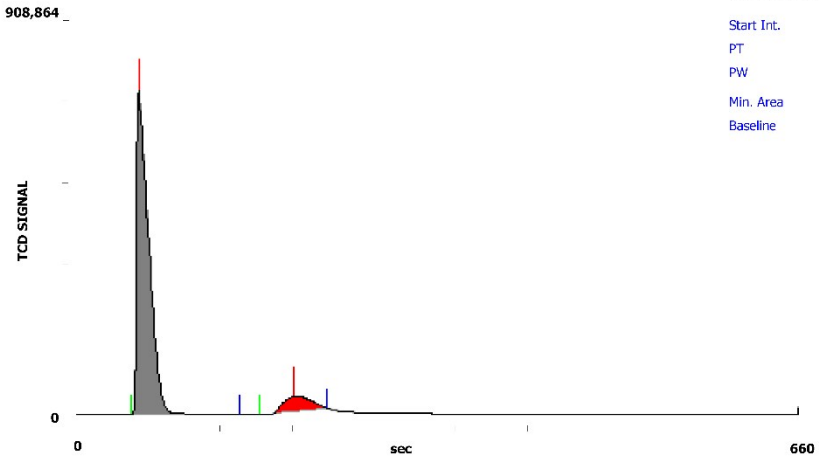
EuroEA Elemental Analyser

AutoRun name	:	180205- (800)
Date of Analysis	:	05 Feb 2018
Time of Analysis	:	09:30:55
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4A-006
Sample position #	:	17
Type	:	Smp
Sample weight	:	1.576 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	58	51	150	8,234,425	90.723	88.013
Hydrogen	198	167	229	841,981	9.277	5.452
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.672328 E-07
Carbon	-	1.684494 E-07
Hydrogen	-	1.020458 E-07
Sulphur	-	3.863342 E-07
Oxygen	-	-

05 Feb 2018 14:43:04 AutoRun: 180205- (800)

Figure S67. Elemental analysis of compound **8**.

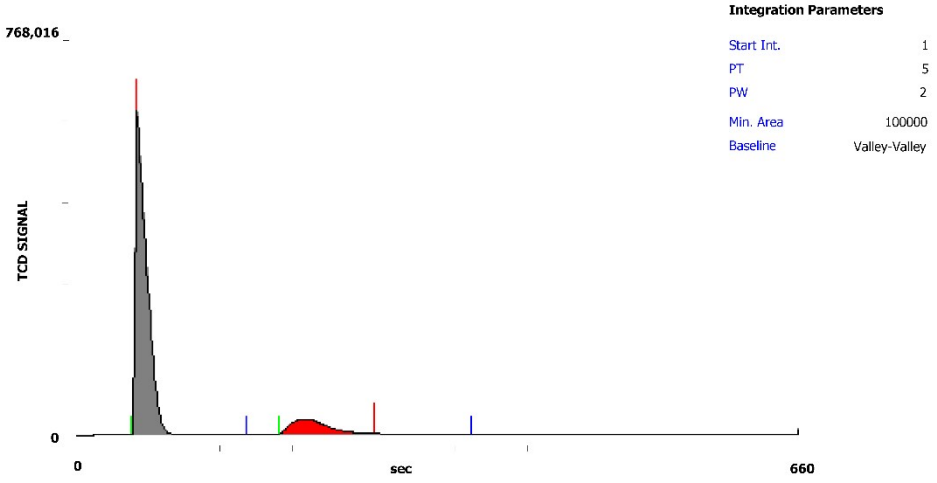
EuroEA Elemental Analyser

AutoRun name	:	180212- (805)
Date of Analysis	:	12 Feb 2018
Time of Analysis	:	09:52:30
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4A-008
Sample position #	:	11
Type	:	Smp
Sample weight	:	1.569 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	56	51	155	8,918,703	85.245	93.209
Hydrogen	272	185	360	1,543,744	14.755	6.752
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.612535 E-07
Carbon	-	1.639756 E-07
Hydrogen	-	6.862405 E-08
Sulphur	-	4.040296 E-07
Oxygen	-	-

12 Feb 2018 14:10:04 AutoRun: 180212- (805)

Figure S68. Elemental analysis of compound **9**.

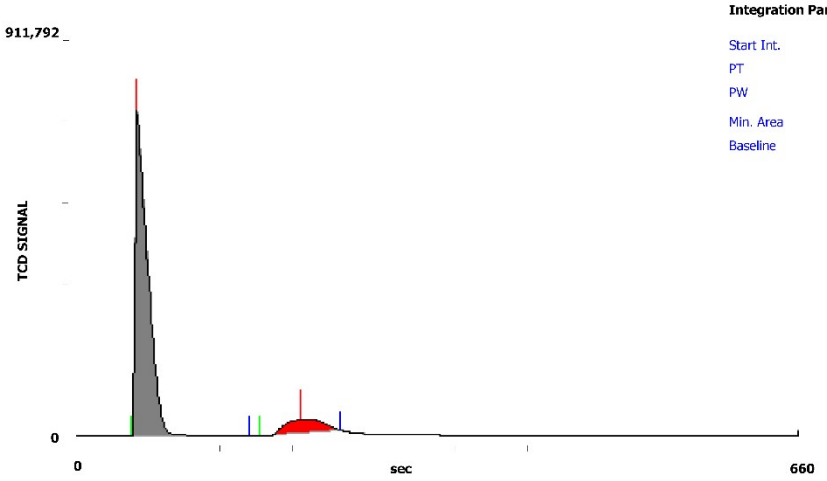
EuroEA Elemental Analyser

AutoRun name	:	180205- (800)
Date of Analysis	:	05 Feb 2018
Time of Analysis	:	09:30:55
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4A-009
Sample position #	:	15
Type	:	Smp
Sample weight	:	1.886 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results **R**

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	56	51	159	10,515,530	88.939	93.920
Hydrogen	204	167	241	1,307,759	11.061	6.043
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.672328 E-07
Carbon	-	1.684494 E-07
Hydrogen	-	8.715154 E-08
Sulphur	-	3.863342 E-07
Oxygen	-	-

05 Feb 2018 14:11:27 AutoRun: 180205- (800)

Figure S69. Elemental analysis of compound **1**.

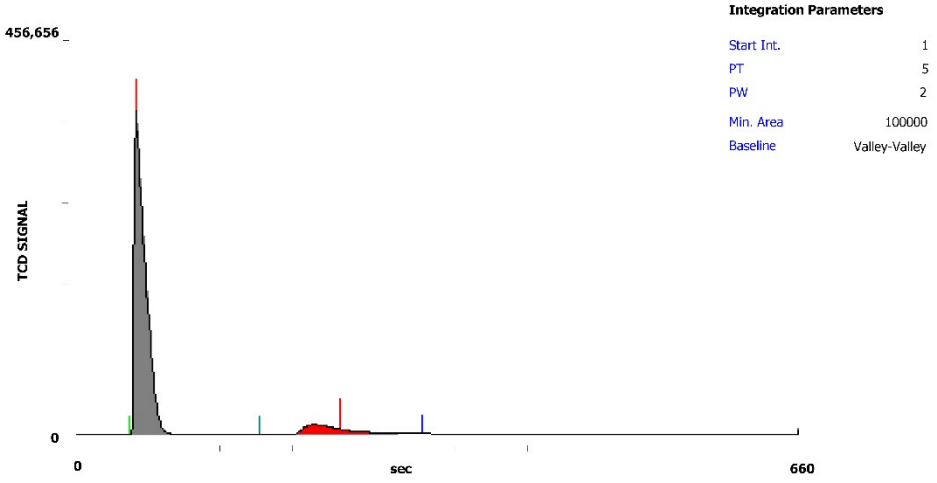
EuroEA Elemental Analyser

AutoRun name	:	180321- (822)
Date of Analysis	:	21 Mar 2018
Time of Analysis	:	11:05:46
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4-005
Sample position #	:	14
Type	:	Smp
Sample weight	:	1.680 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	55	50	167	8,821,664	89.970	88.598
Hydrogen	241	167	315	983,457	10.030	4.988
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.601519 E-07
Carbon	-	1.687254 E-07
Hydrogen	-	8.520525 E-08
Sulphur	-	3.956067 E-07
Oxygen	-	-

22 Mar 2018 10:25:49 AutoRun: 180321- (822)

Figure S70. Elemental analysis of compound **13**.

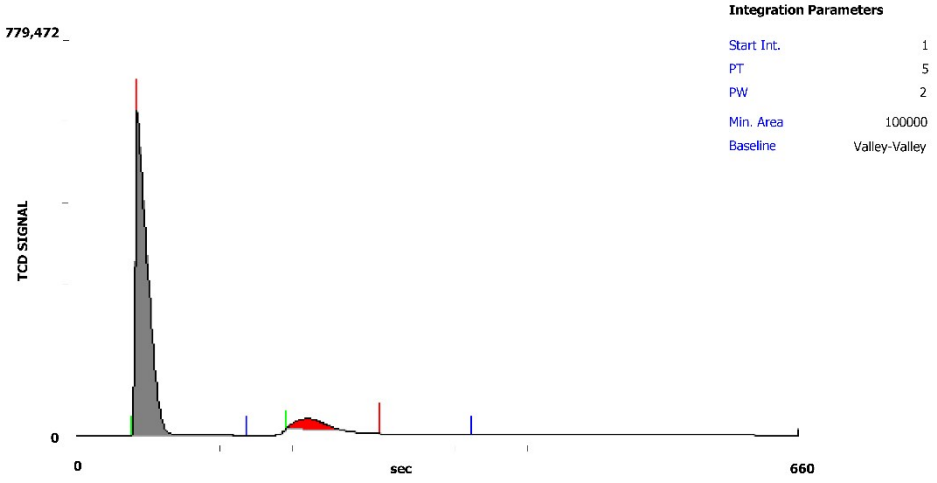
EuroEA Elemental Analyser

AutoRun name	:	180212- (805)
Date of Analysis	:	12 Feb 2018
Time of Analysis	:	09:52:30
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4-007
Sample position #	:	9
Type	:	Smp
Sample weight	:	1.668 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	56	51	156	9,509,078	92.454	93.481
Hydrogen	276	192	360	776,173	7.546	6.464
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.612535 E-07
Carbon	-	1.639756 E-07
Hydrogen	-	1.389080 E-07
Sulphur	-	4.040296 E-07
Oxygen	-	-

12 Feb 2018 13:37:40 AutoRun: 180212- (805)

Figure S71. Elemental analysis of compound **14**.

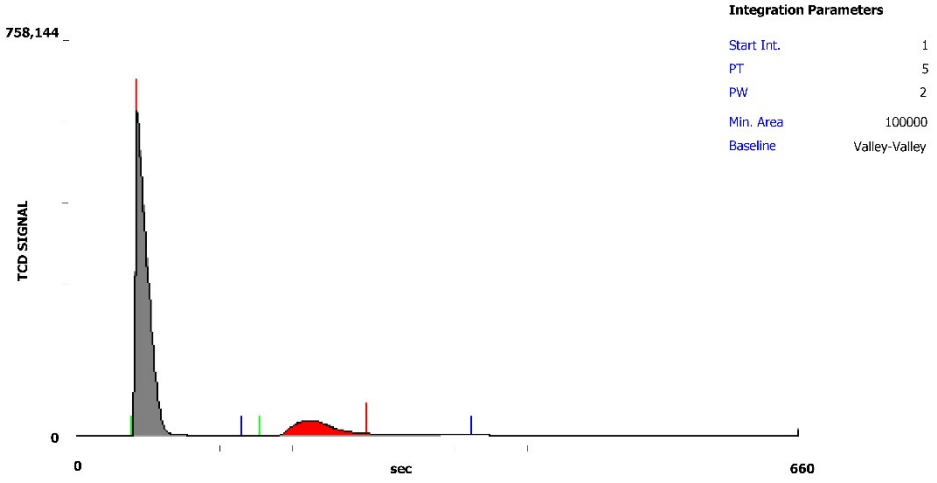
EuroEA Elemental Analyser

AutoRun name	:	180212- (805)
Date of Analysis	:	12 Feb 2018
Time of Analysis	:	09:52:30
Analysed By	:	EVR
Signed By	:	EVR
Operator Group	:	GRP1
Configuration	:	CHNS
Sample name	:	M4-008
Sample position #	:	7
Type	:	Smp
Sample weight	:	1.729 (mg)
Calibration type	:	K-Factor

Instrument Parameters

Carrier (kPa)	Purge (ml/min)	Oxygen (ml)	Delta P O2 (kPa)	Sampling Delay (s)	Run Time (s)	Front (°C)	Rear (°C)	Oven (°C)
50	100	15	25	10	660	1000	Off	70

Chromatogram



Integration Parameters

Start Int.	1
PT	5
PW	2
Min. Area	100000
Baseline	Valley-Valley

Results R

Element	*RT (s)*	*Start (s)*	*End (s)*	*Area*	*Area %*	*Element %*
Nitrogen	-	-	-	-	-	-
Carbon	56	51	151	9,873,429	85.214	93.638
Hydrogen	264	167	360	1,713,175	14.786	6.323
Sulphur	-	-	-	-	-	-
Oxygen	-	-	-	-	-	-

	K-Factor	*KFactor (Average)*
Nitrogen	-	4.612535 E-07
Carbon	-	1.639756 E-07
Hydrogen	-	6.381622 E-08
Sulphur	-	4.040296 E-07
Oxygen	-	-

12 Feb 2018 13:02:01 AutoRun: 180212- (805)

Figure S72. Elemental analysis of compound **2**.

12. References

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