Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Stereoselective Syntheses, Structures, and Properties of Extremely Distorted Chiral Nanographenes Embedding Hextuple Helicenes

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Supporting Information

Table of content

1. Syntheses

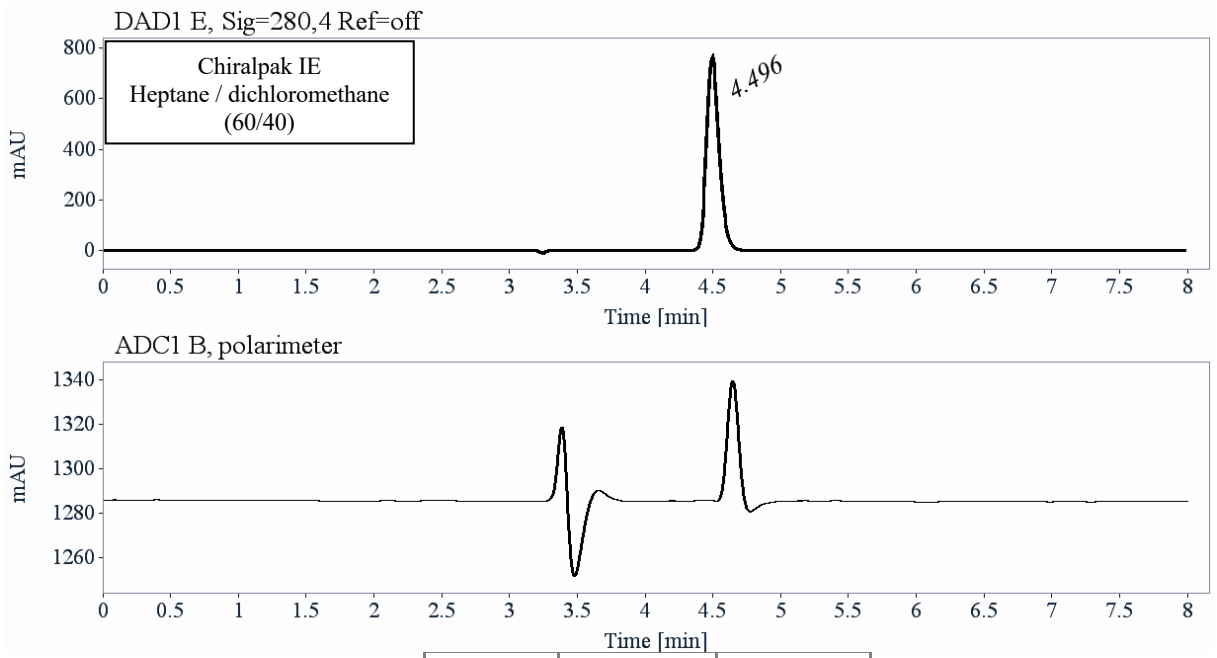
1.1. General methods. All chemicals were obtained from regular commercial sources (reagent or analytical grade) and used as received unless otherwise stated. Anhydrous THF was obtained from a solvent purification system, and other solvents were used as received (analytical, HPLC or Uvasol® grade). The reactions were monitored by TLC and/or HPLC-MS. Silica gel filtrations were performed on 40-63 µm silica gel. HPLC-MS analyses were performed with a C18 Phenomenex Luna (3µm; 100 x 2 mm) column on a Shimadzu LCMS-2020 fitted with two LC-20AD prominence pumps equipped with a DGU-20AD prominence line degasser, a SIL-20AHT prominence auto-sampler, a CTO-20A prominence column oven, a SPD-20A prominence UV/Vis detector, a FCV-20AH valve unit, a Parker NitroFloLab nitrogen generator and an APCI source. NMR data were recorded at 300 MHz, 400 MHz, 500 MHz or 600 MHz in *d1*-chloroform or *d1*-bromoform using as internal standards the residual non-deuterated solvent signal for ^{1}H NMR (δ = 7.26 ppm for $CHCl_3$ in $CDCl_3$, δ = 6.85 ppm for $CHBr_3$ in $CDBr_3$) and the deuterated solvent signal for ^{13}C NMR (δ = 77.16 ppm for $CDCl_3$). Coupling constants (*J*) are in Hertz (Hz) and the classical abbreviations are used to describe the signal multiplicities.

1.2. Experimental protocols:

*Resolution of 9,10-dibromo[7]helicene (**1**):*

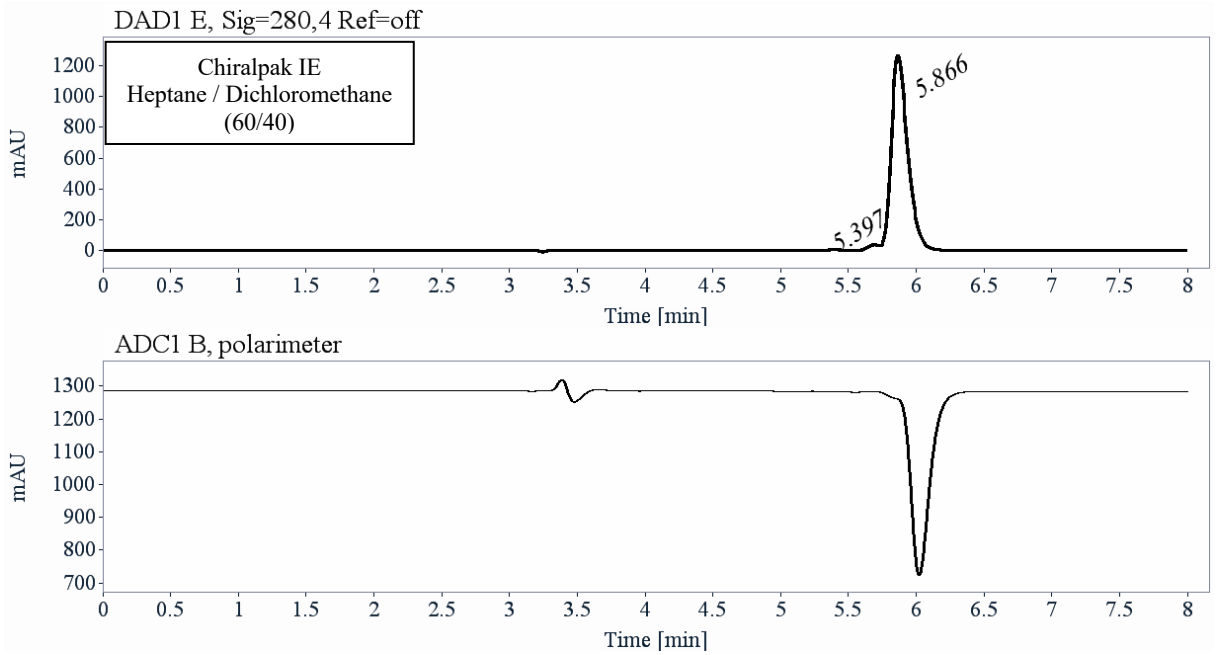
Racemic 9,10-dibromo[7]helicene (rac-**1**) containing ca. 20% of (±)-9-bromo[7]helicene was prepared by known procedures,[1] and its resolution was achieved by semi-preparative HPLC (Figures **S1-a** and **S1-b**). 175 mg of the racemic material were dissolved in 19 mL of dichloromethane and periodically injected (stacked injections, 190 times 100 µL, every 3.4 minutes) on a Chiralpak IE (250 x 10 mm) column eluted with hexane/dichloromethane (60:40) as mobile phase (flow rate = 5 mL/min) with a UV detection (310 nm), which allowed the collection of 48 mg of (+)-(*P*)-**1** (ee > 99.5%) and 56 mg of (–)-(*M*)-**1** (ee > 99.5%).

[1] V. Terrasson, M. Roy, S. Moutard, M.-P. Lafontaine, G. Pèpe, G. Félix, M. Gingras, *RSC Adv.* **2014**, *4*, 32412.



t_r [min]	Area	Area%
4.50	5017	100.00
Sum	5017	100.00

Figure S1-a. HPLC analysis of (+)-(*P*)-**1**. Conditions: Chiralpak IE (250 x 4.6 mm), heptane/dichloromethane (60:40) as mobile phase, flow rate = 1 mL/min, UV detection at 280 nm.



t_r [min]	Area	Area%
5.40	51	0.48
5.87	10679	99.52
Sum	10730	100.00

Figure S1-b. HPLC analysis of (–)-(*M*)-**1**. Conditions: Chiralpak IE (250 x 4.6 mm), heptane/dichloromethane (60:40) as mobile phase, flow rate = 1 mL/min, UV detection at 280 nm. The impurity detected at t_r = 5.40 min is (–)-(*M*)-9-bromo[7]helicene.

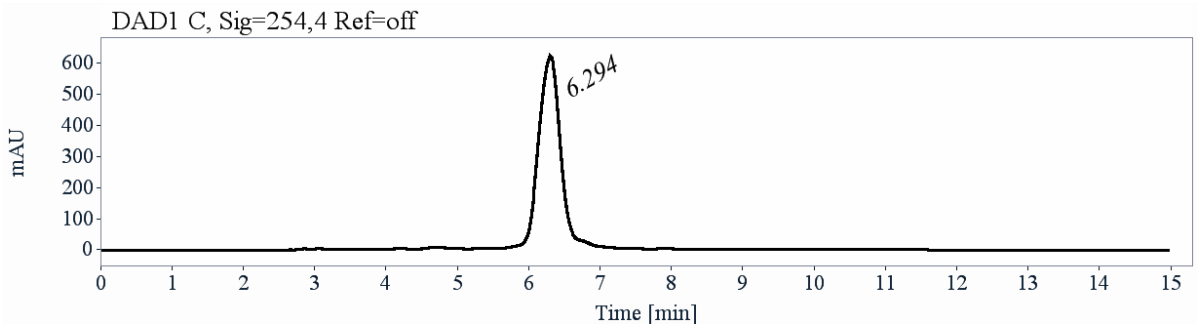
Synthesis of (+)-*(P,P,P,M,M,M)-D*$_3$-**2**:

In a glovebox, a 4-mL tubular reaction vessel was charged with enantiopure (+)-(*P*)-9,10-dibromo[7]helicene [(+)-**1**, 33.2 mg, 0.062 mmol, 1.0 equiv], 2,2'-bipyridine (25.2 mg, 0.161 mmol, 2.6 equiv), degassed *cis*-1,5-cyclooctadiene (50 μL, 0.407 mmol, 6.6 equiv), degassed dry THF (0.45 mL), and Ni(COD)$_2$ (29.3 mg, 0.106 mmol, 1.7 equiv). The reaction vessel was sealed in the glovebox and then heated under microwave irradiation for 30 min at 130°C. The crude reaction mixture was concentrated *in vacuo* and the resulting material (133.6 mg) was dissolved in 20 mL of boiling chloroform and filtrated on a short silica plug. The silica plug was washed with hot chloroform until the filtrate is colorless. Concentration of the filtrate under reduced pressure afforded 27 mg of an orange solid. Analysis of the crude material by HPLC/MS revealed the presence of a single diastereomer with the expected *m/z*. Purification by semi-preparative HPLC gave 9.0 mg (39%) of the enantiopure product (+)-(*P,P,P,M,M,M*)-*D*$_3$-**2** (Figure S2).

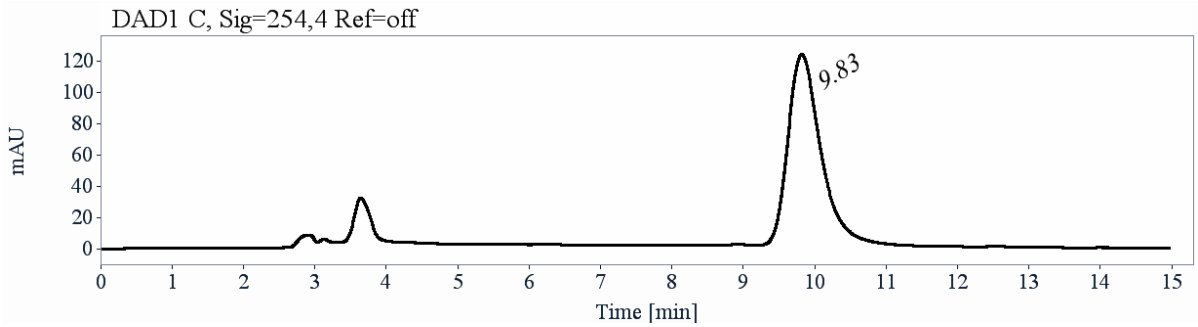
Synthesis of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**:

The same procedure with enantiopure (–)-(*M*)-9,10-dibromo[7]helicene [(–)-**1**, 11.7 mg, 0.022 mmol, 1.0 equiv], Ni(COD)$_2$ (12.1 mg, 0.044 mmol, 2.0 equiv), 2,2'-bipyridine (9.2 mg, 0.059 mmol, 2.7 equiv), degassed *cis*-1,5-cyclooctadiene (20 μL, 0.163 mmol, 7.5 equiv) and degassed dry THF (0.20 mL) afforded 3.1 mg (38%) of the product (–)-(*M,M,M,P,P,P,*)-*D*$_3$-**2** (Figure S2). Recrystallization of this material from *d1*-chloroform at –18 ºC afforded crystalline orange prisms suitable for X-ray diffraction analysis (Figure S7).

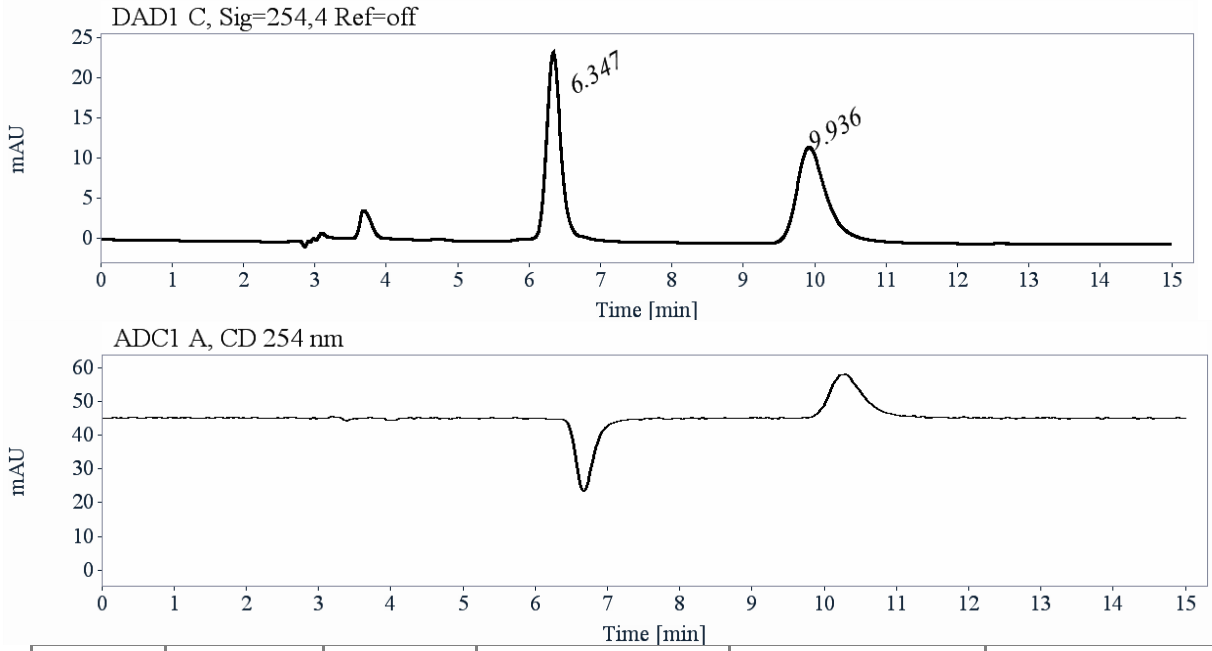
(a)



(b)



(c)



t_r [min]	Area	Area%	Capacity Factor	Enantioselectivity	Resolution (USP)
6.35	426	49.54	1.15		
9.94	433	50.46	2.37	2.06	6.50
Sum	859	100.00			

Figure S2. (a) HPLC analysis of (+)-(*P,P,P,M,M,M*)-D_3-**2**. (b) HPLC analysis of (–)-(*M,M,M,P,P,P*)-D_3-**2**. (c) HPLC analysis of (±)-D_3-**2**. (+)-(*P,P,P,M,M,M*)-D_3-**2** and (–)-(*M,M,M,P,P,P*)-D_3-**2** were mixed in equal proportions to obtain an analytical racemic mixture. Conditions: (*S,S*)-Whelk-O1 (250 x 4.6 mm), heptane/ethanol/dichloromethane (20:40:40) as mobile phase, flow rate = 1 mL/min, UV detection at 254 nm, and circular dichroism detection at 254 nm for (c).

Synthesis of rac-(*P,M,P,P,P,M*)-C_2-**2**:

Following the procedure described above with this time racemic (±)-9,10-dibromo[7]helicene (rac-**1**, 41.0 mg, 0.076 mmol, 1.0 equiv), $Ni(COD)_2$ (38.0 mg, 0.138 mmol, 1.8 equiv), 2,2'-bipyridine (45.2 mg, 0.289 mmol, 3.8 equiv), degassed *cis*-1,5-cyclooctadiene (75 µL, 0.611 mmol, 8.0 equiv) and degassed dry THF (8 mL), afforded 22.4 mg of crude product. Analysis of this material by HPLC revealed the presence of the two diastereomers C_2-**2** and D_3-**2** in a ratio 13.8:1 together with unidentified products. The crude product was then purified by semi-preparative HPLC [(*S*,*S*)-Whelk-O1 (250 x 10 mm), hexane / ethanol / dichloromethane (1:2:2) as mobile phase, flow rate = 5 mL/min, UV detection at 280 nm, stacked injections of 80 µL every 7.4 min.) to afford 4.6 mg of rac-C_2-**2** (16%, Figure S3). The actual yield of rac-C_2-**2** was estimated around 25% but its isolation by semi-preparative HPLC was complicated by the presence of both enantiomers in the sample. Recrystallization of rac-C_2-**2** from hexane / chloroform at –18 ºC afforded crystalline orange prisms suitable for X-ray diffraction analysis (Figure S14).

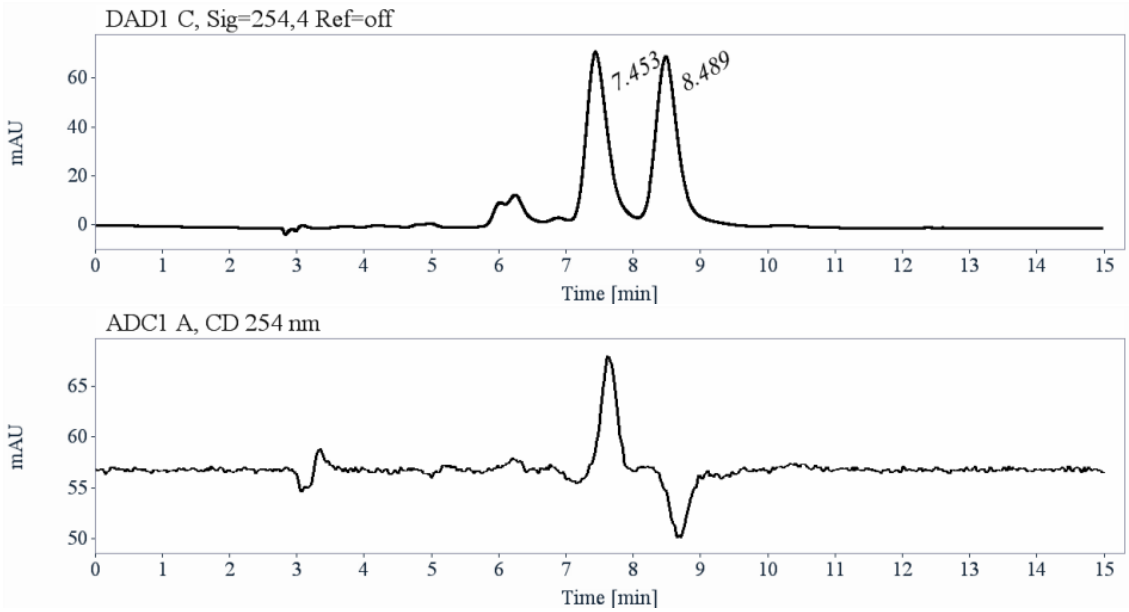


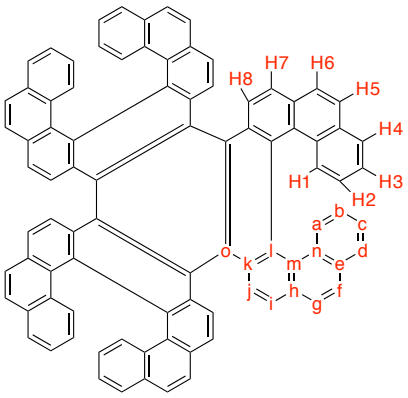
Figure S3. HPLC analysis of rac-C_2-**2**. Conditions: (*S*,*S*)-Whelk-O1 (250 x 4.6 mm), heptane/2-PrOH/dichloromethane (4:3:3) as mobile phase, flow rate = 1 mL/min, UV and circular dichroism detection at 254 nm.

2. Characterization data

2.1. NMR spectroscopy

(+)-*(P,P,P,M,M,M)*-D_3-**2**:

The nanographene (+)-*(P,P,P,M,M,M)*-D_3-**2** was found only moderately soluble in organic solvents, and the best solvents identified were chloroform, bromoform and dichloromethane with a solubility roughly estimated at ca. 1–2 mg/mL for each. Although possible, the ^{13}C NMR analyses of the product were thus complicated by a low signal/noise ratio. All resonances were attributed on the basis of COSY, HSQC, and HMBC 2D experiments (Figure S4-d–f).



^{1}H NMR (600.13 MHz, $CDCl_3$, ppm, Figure S4-a): δ = 8.96 (d, 6H, *J* = 8.5 Hz, H8), 8.03 (d, 6H, *J* = 8.6 Hz, H7), 7.77 (d, 6H, *J* = 8.4 Hz, H6), 7.62 (d, 6H, *J* = 8.3 Hz, H1), 7.58 (d, 6H, *J* = 8.3 Hz, H5), 7.43 (d, 6H, *J* = 7.5 Hz, H4), 7.08 (ddd, 6H, *J* = 7.8, 6.9, 0.9 Hz, H3), 6.73 (ddd, 6H, *J* = 8.4, 6.8, 1.2 Hz, H2).

^{1}H NMR (400 MHz, $CDBr_3$, ppm, Figure S4-b): δ = 8.89 (d, 6H, *J* = 8.5 Hz), 8.05 (d, 6H, *J* = 8.6 Hz), 7.78 (d, 6H, *J* = 8.5 Hz), 7.59 (d, 6H, *J* = 8.5 Hz), 7.52 (d, 6H, *J* = 8.4 Hz), 7.43 (d, 6H, *J* = 7.8 Hz), 7.09 (dd, 6H, *J* = 7.3, 7.3 Hz), 6.73 (dd, 6H, *J* = 7.7, 7.7 Hz).

^{13}C NMR (150.90 MHz, $CDCl_3$, ppm, Figure S4-c): δ = 132.6 (e), 131.8 (h), 131.4 (k), 129.9 (n), 129.2 (o or l), 128.8 (m), 128.0 (f), 127.7 (j), 127.6 (i), 127.2 (d), 126.1 (g), 125.6 (c), 125.4 (a), 124.8 (o or l), 123.9 (b).

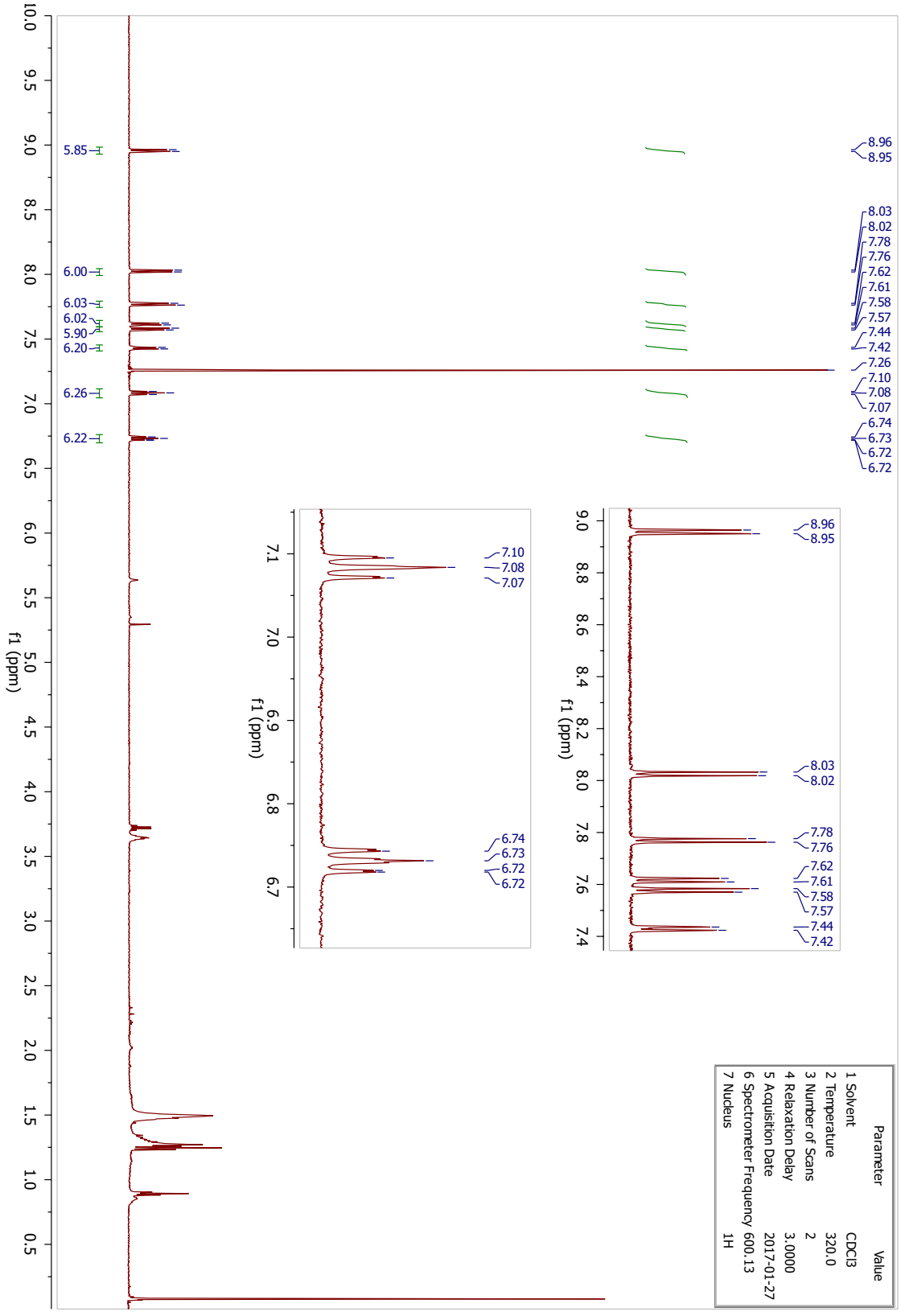


Figure S4-a. ^{1}H NMR (600 MHz, $CDCl_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**. The resonance at 7.26 ppm was attributed to residual $CHCl_3$ in the deuterated solvent, the resonance at 5.30 ppm was attributed to residual CH_2Cl_2 in the deuterated solvent, the resonances at 3.72, 1.32 & 1.25 ppm were attributed to traces of ethanol present in the sample, the broad resonance at 1.56 ppm was attributed to water present in the sample and/or the deuterated solvent, the resonances at 0.86 & 1.26 ppm were attributed to traces of grease present in the sample and/or the deuterated solvent, and the resonance at 0.07 ppm was attributed to traces of silicon grease in the sample.

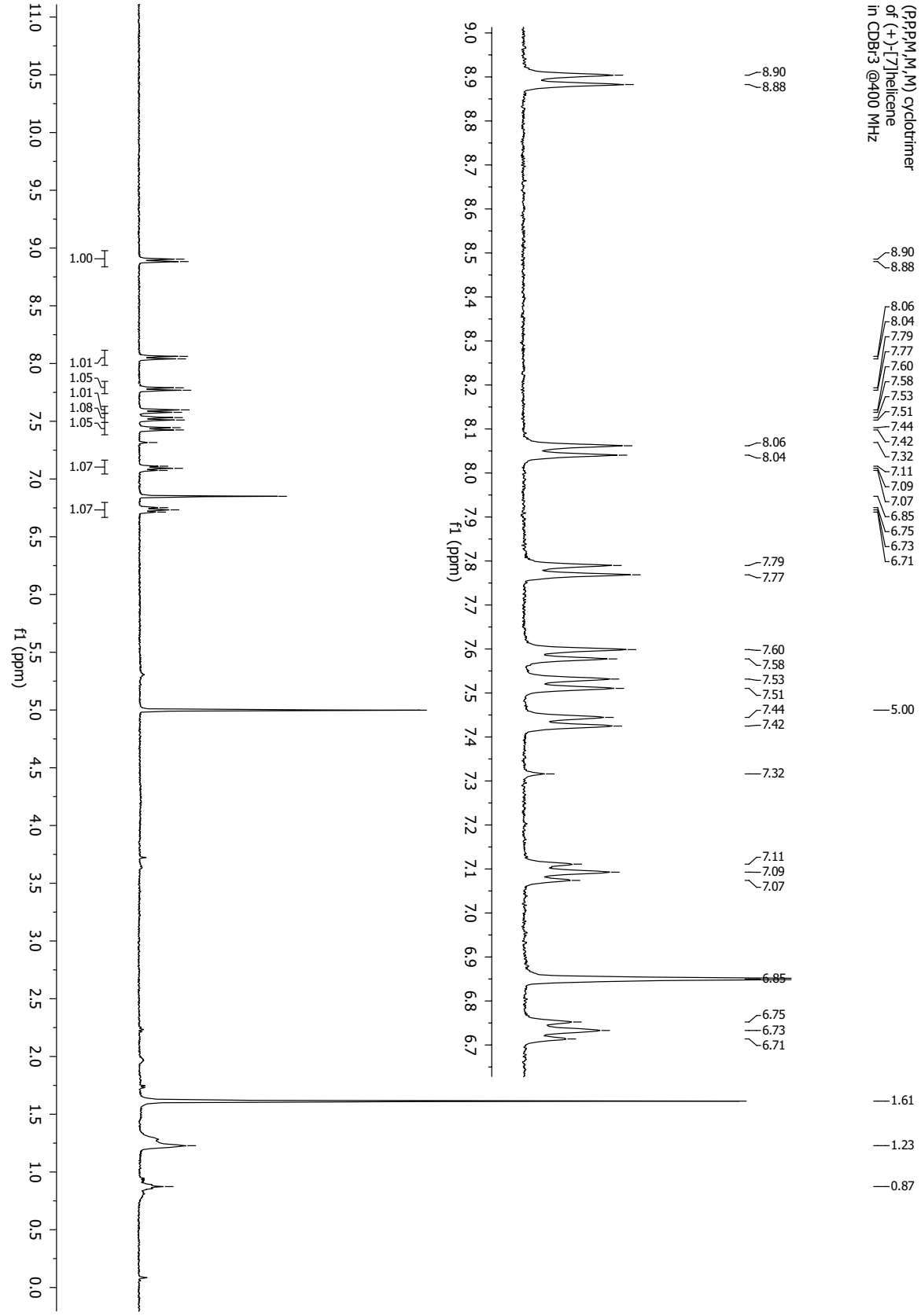


Figure S4-b. ^{1}H NMR (400 MHz, $CDBr_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**. The resonance at 7.32 ppm was attributed to residual $CHCl_3$ in the sample, the resonance at 6.85 ppm was attributed to residual $CHBr_3$ in the deuterated solvent, the resonance at 5.00 ppm was attributed to CH_2Br_2 present in the deuterated solvent, the resonance at 1.61 ppm was attributed to water present in the sample and/or the deuterated solvent, and the resonances at 0.87 & 1.23 ppm were attributed to traces of grease present in the sample and/or the deuterated solvent.

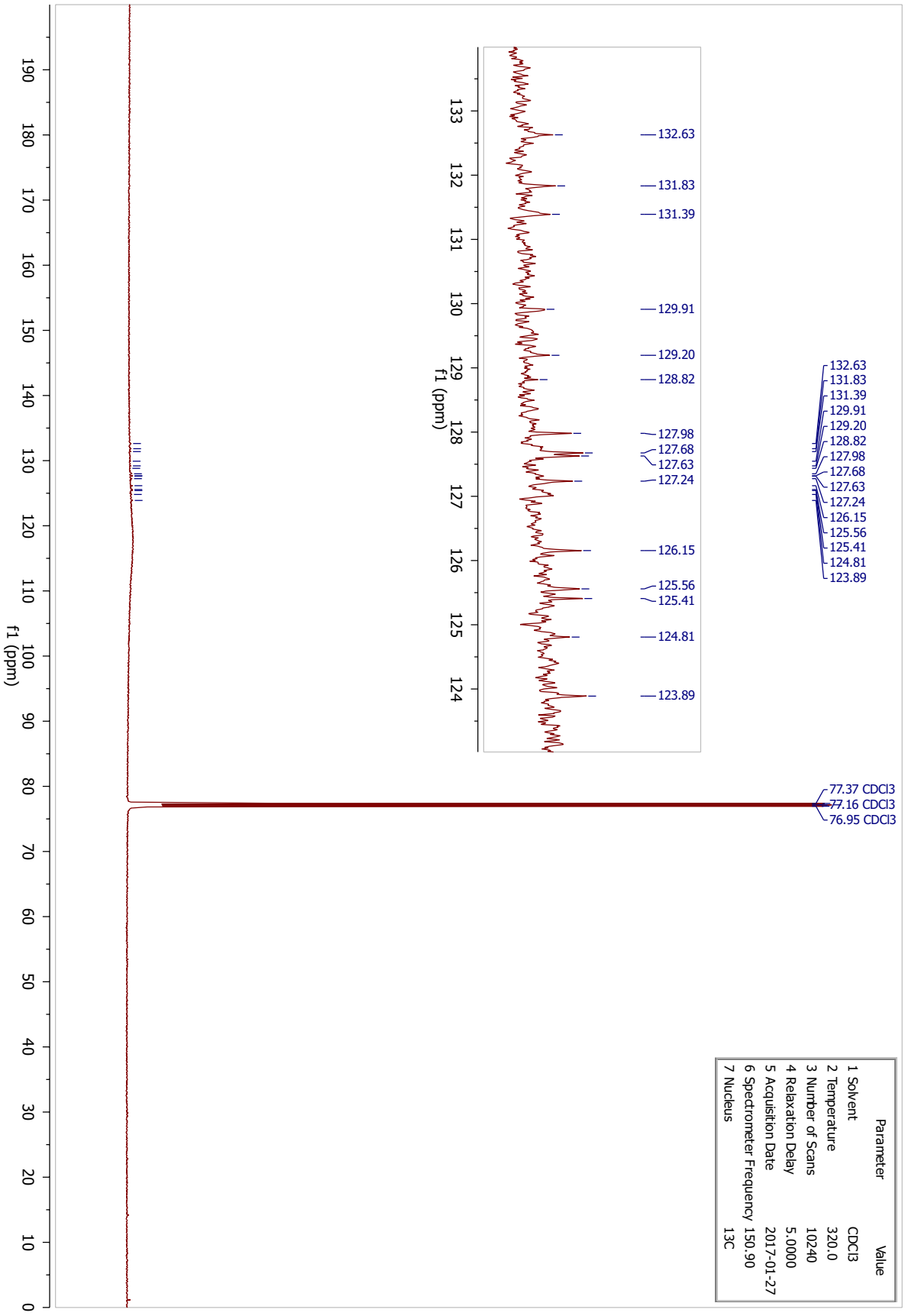


Figure S4-c. ^{13}C NMR (150 MHz, $CDCl_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**. The very low signal/noise ratio obtained after >10k scans is partly due to moderate solubility of the sample in $CDCl_3$, and the broad resonance at 110–125 ppm was attributed to the signal from the glue of the NMR probe.

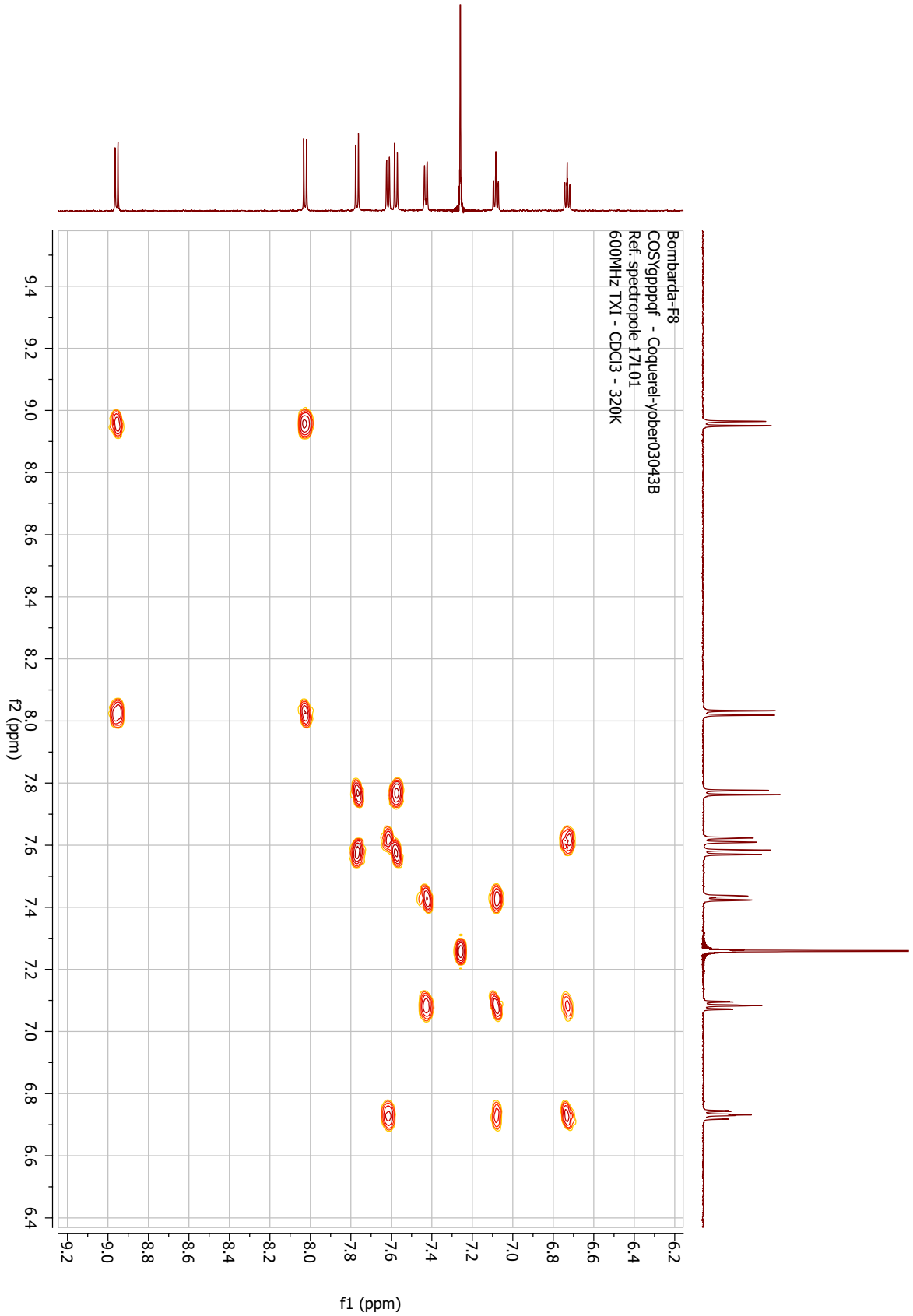


Figure S4-d. COSY experiment (600 MHz, 600 MHz, $CDCl_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**.

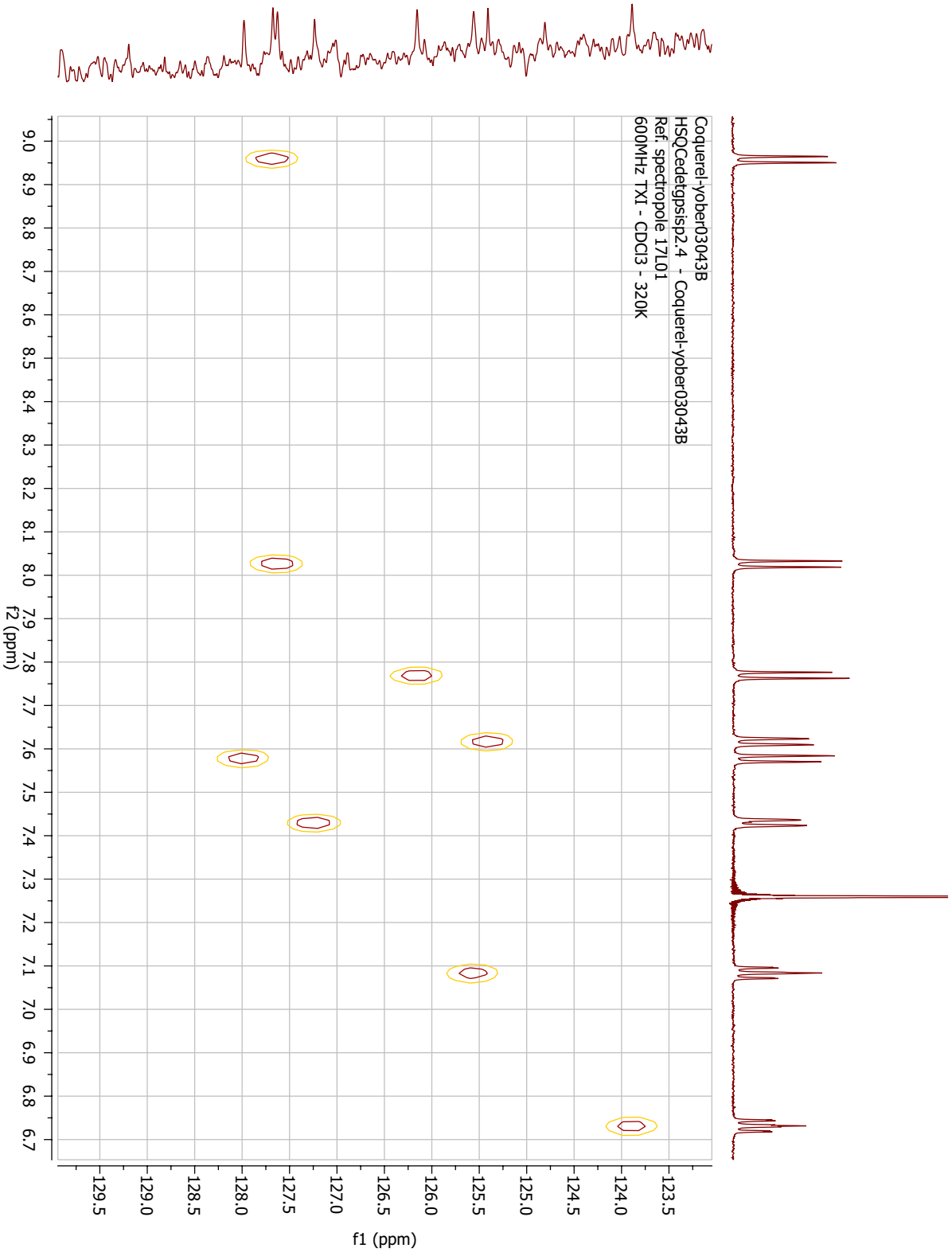


Figure S4-e. HSQC experiment (600 MHz, 150 MHz, $CDCl_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**.

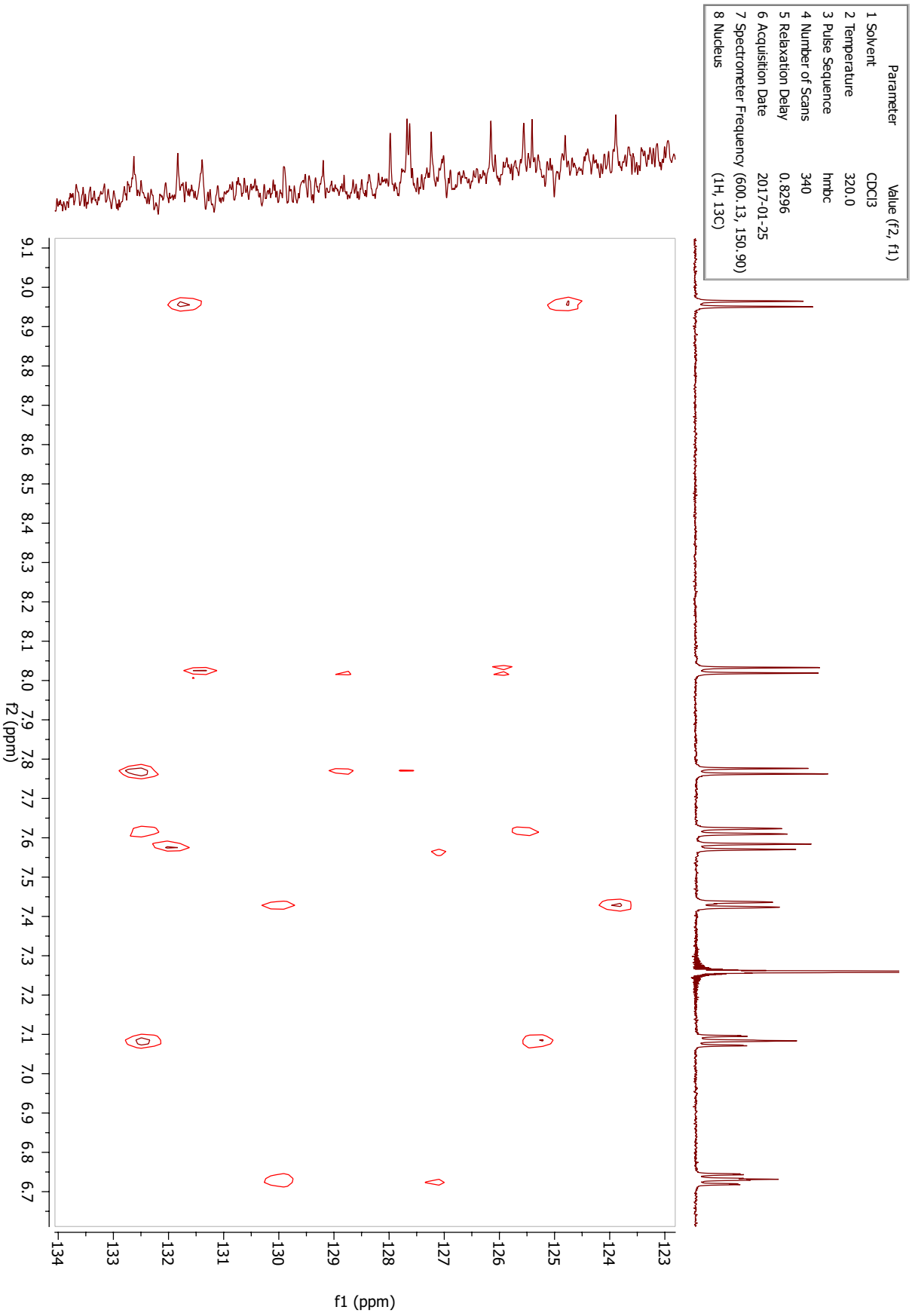
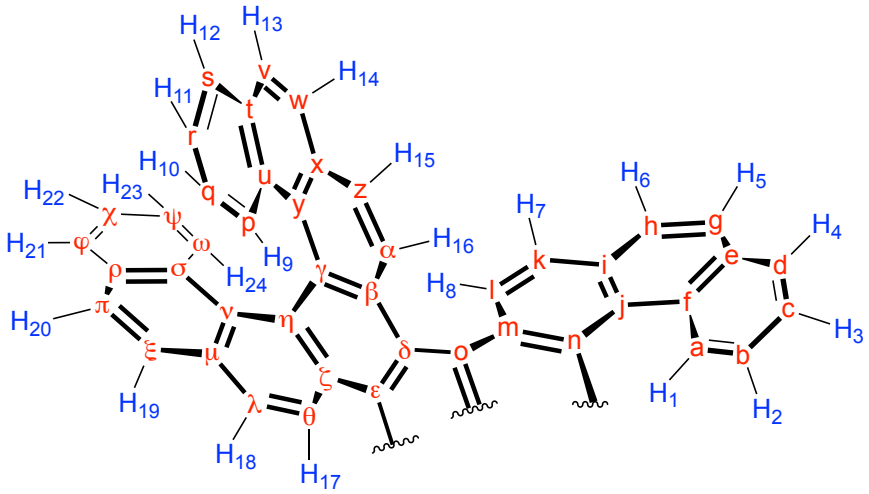


Figure S4-f. HMBC experiment (600 MHz, 150 MHz, $CDCl_3$) of (+)-*(P,P,P,M,M,M)*-D_3-**2**.

rac-*(P,M,P,P,P,M)*-C_2-**2**:

The nanographene rac-*(P,M,P,P,P,M)*-C_2-**2** was found only moderately soluble in organic solvents, and the best solvents identified was chloroform with a solubility estimated at ca. 1–2 mg/mL. The full ^{13}C NMR analysis was not possible because of too low signal/noise ratio, and only methines (CH) resonances could be identified, notably by a DEPT135 experiment (Figure S5-b). All identified resonances were attributed on the basis of COSY, NOESY, HSQC, and HMBC 2D experiments (Figure S6-a–d) and was hampered by the superimposition of proton signals.



^{1}H NMR (400.13 MHz, $CDCl_3$, 323K, ppm, Figure S5-a): δ = 9.35 (d, 2H, *J* = 8.7 Hz, H_{16} or H_8), 8.93 (d, 2H, *J* = 8.6 Hz, H_{17}), 8.59 (d, 2H, *J* = 8.5 Hz, H_8 or H_{16}), 8.12 (d, 2H, *J* = 8.7 Hz, H_{15} or H_7), 8.07 (d, 2H, *J* = 8.4 Hz, H_9), 8.00 (d, 2H, *J* = 8.7 Hz, H_{18}), 7.96 (d, 2H, *J* = 8.6 Hz, H_7 or H_{15}), 7.90 (d, 2H, *J* = 8.5 Hz, H_{14} or H_6), 7.81 (d, 2H, *J* = 8.6 Hz, H_6 or H_{14}), 7.79 (m, 2H, H_1), 7.68 (d, 2H, *J* = 8.6 Hz, H_{19}), 7.62 (d, 4H, *J* = 8.4 Hz, H_5 and H_{13}), 7.49-7.44 (m, 6H, H_4, H_{12} and H_{20}), 7.25 (m, 2H, H_{21}), 7.13 (dd, 2H, *J* = 7.3, 7.3 Hz, H_{11}), 7.10 (dd, 2H, *J* = 7.3, 7.3 Hz, H_3), 6.90 (ddd, 2H, *J* = 7.0, 7.0, 1.1 Hz, H_{10}), 6.85 (ddd, 2H, *J* = 6.9, 6.9, 0.8 Hz, H_{22}), 6.74 (ddd, 2H, *J* = 7.0, 7.0, 1.0 Hz, H_2), 6.31 (ddd, 2H, *J* = 6.9, 6.7, 0.7 Hz, H_{23}), 6.20 (d, 2H, *J* = 8.3 Hz, H_{24}).

^{13}C NMR - DEPT135 (100.63 MHz, $CDCl_3$, 323K, ppm, Figure S5-b): δ = 128.5 θ, 128.4 α or l, 128.2 v or g , 127.9 (2C) v or g and d or s or π, 127.5 d or s or π, 127.33 d or s or π, 127.28 k or z, 127.0 λ, 126.6 l or α, 126.4 h or w or φ, 126.3 φ or h or w, 126.1 p, 125.8 w or h, 125.7 c, 125.38 a or r or ξ, 125.36 a or r or ξ, 125.33 a or r or ξ, 125.2 z or k, 125.1 q, 125.0 ω, 124.8 χ, 123.9 b, 123.6 ψ ppm.

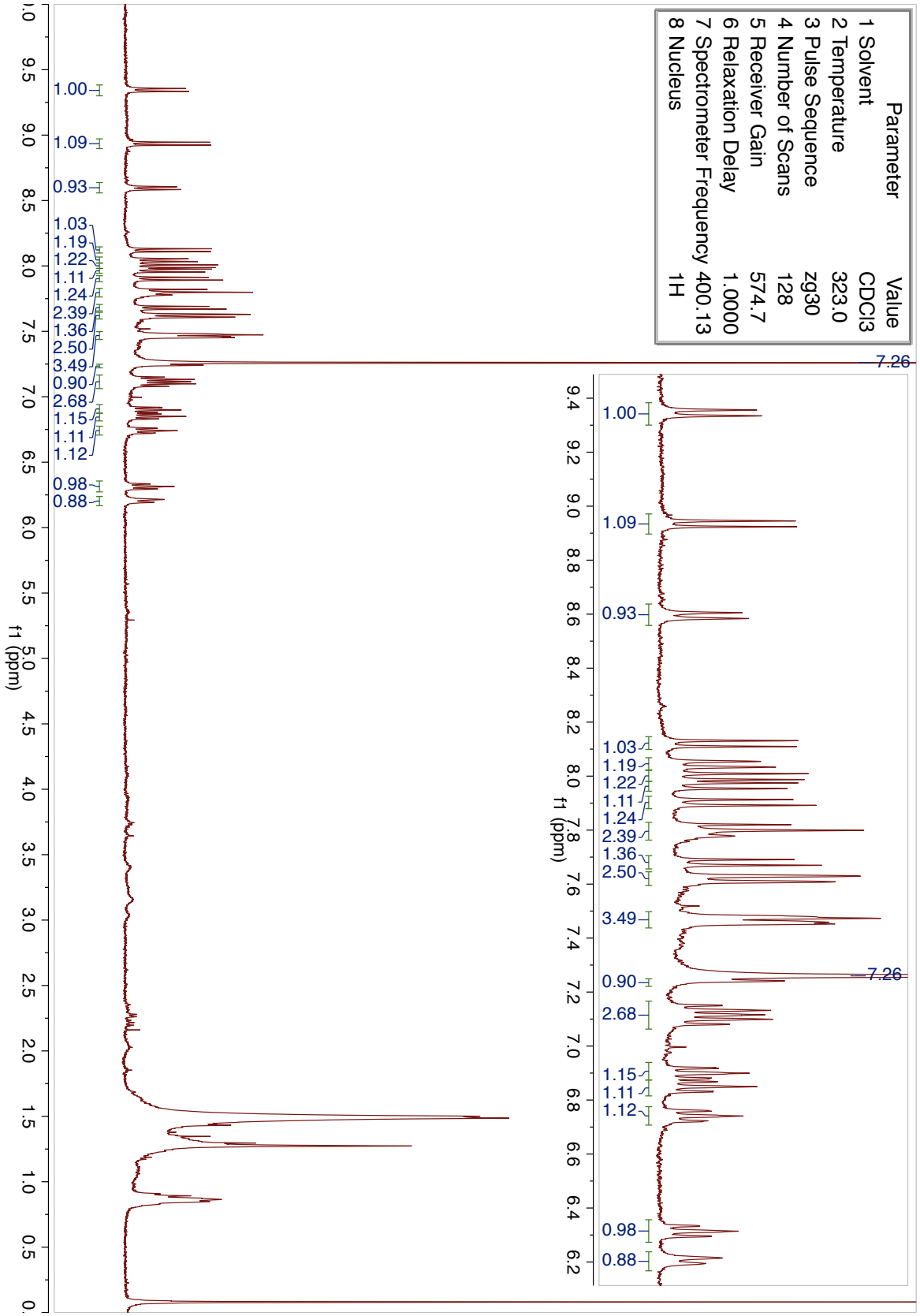


Figure S5-a. ^{1}H NMR (400 MHz, $CDCl_3$) of (+)-*(P,M,P,P,P,M)*-C_2-**2**. The resonance at 7.26 ppm was attributed to residual $CHCl_3$ in the deuterated solvent, the resonance at 5.30 ppm was attributed to residual CH_2Cl_2 in the deuterated solvent, the broad resonance at 1.56 ppm was attributed to water present in the sample and/or the deuterated solvent, the broad resonances at 0.86 & 1.26 ppm were attributed to traces of grease that accumulated over the multiple analyses performed on that sample, and similarly the resonance at 0.07 ppm was attributed to traces of silicon grease.

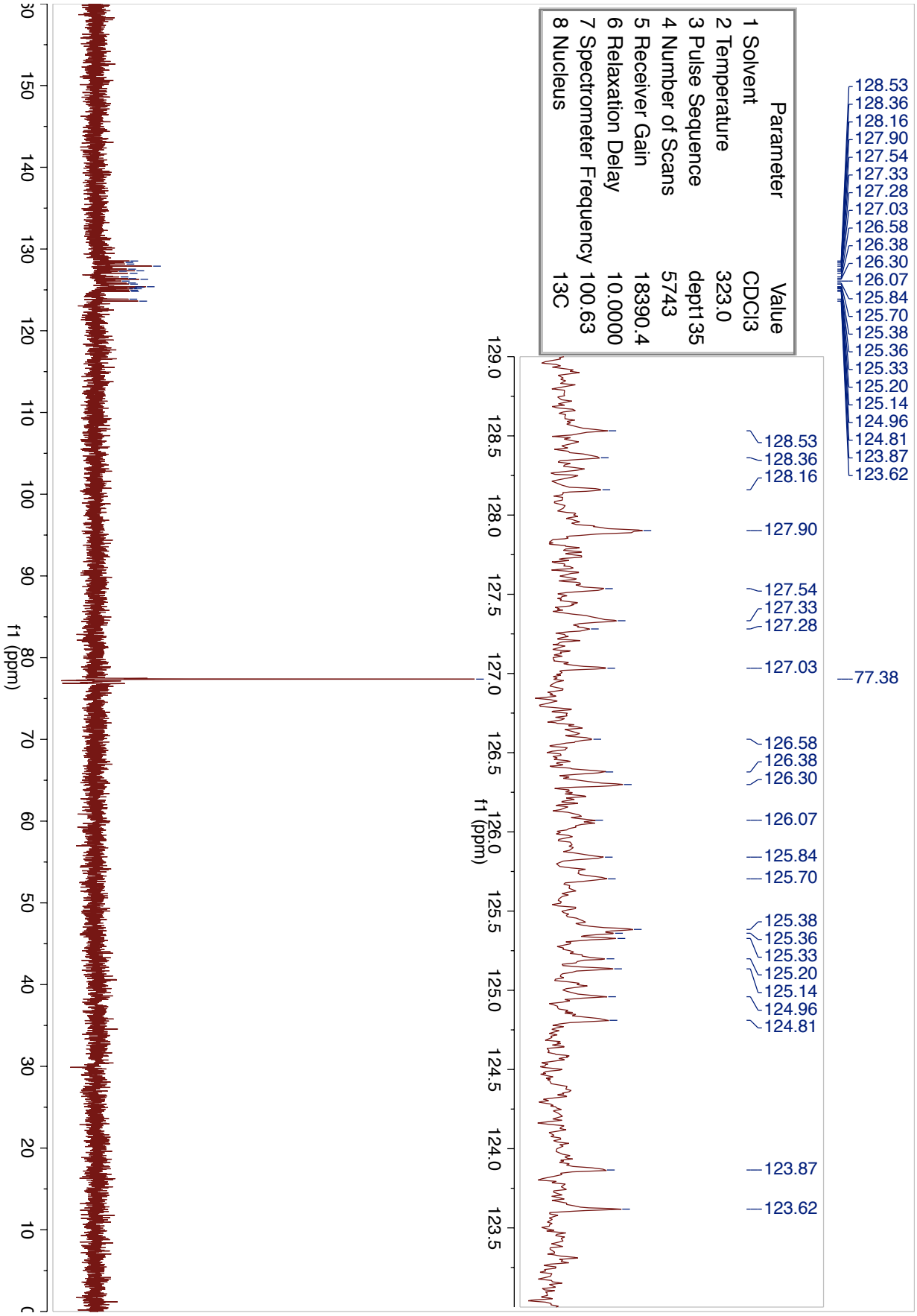


Figure S5-b. ^{13}C NMR – DEPT135 (100 MHz, $CDCl_3$) of rac-*(P,M,P,P,P,M)*-C_2-**2**. The resonance at 77.38 ppm was attributed to residual $CHCl_3$ in the deuterated solvent.

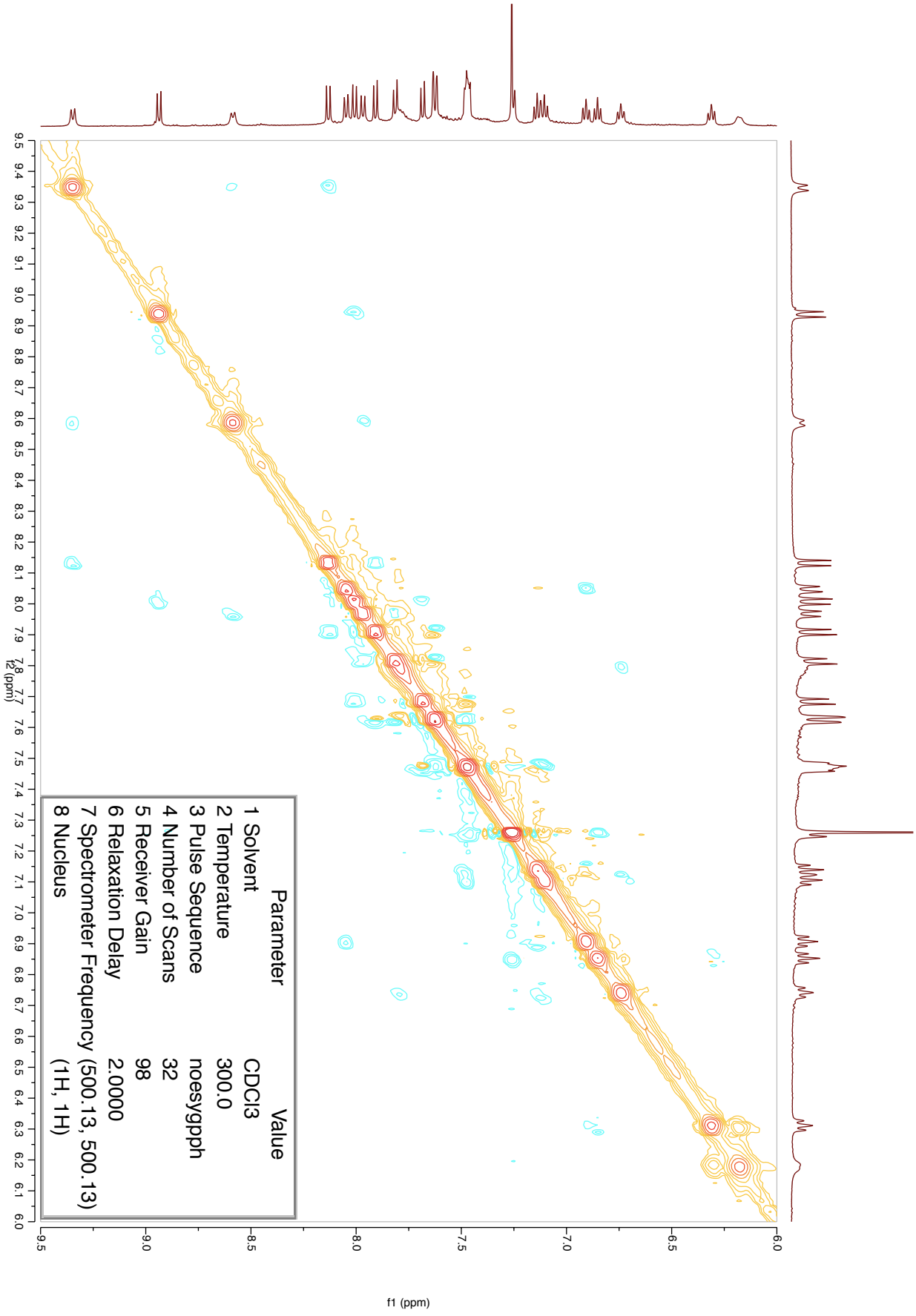


Figure S6-a. NOESY experiment (500 MHz, 500 MHz, $CDCl_3$) of rac-*(P,M,P,P,P,M)*-C_2-**2**.

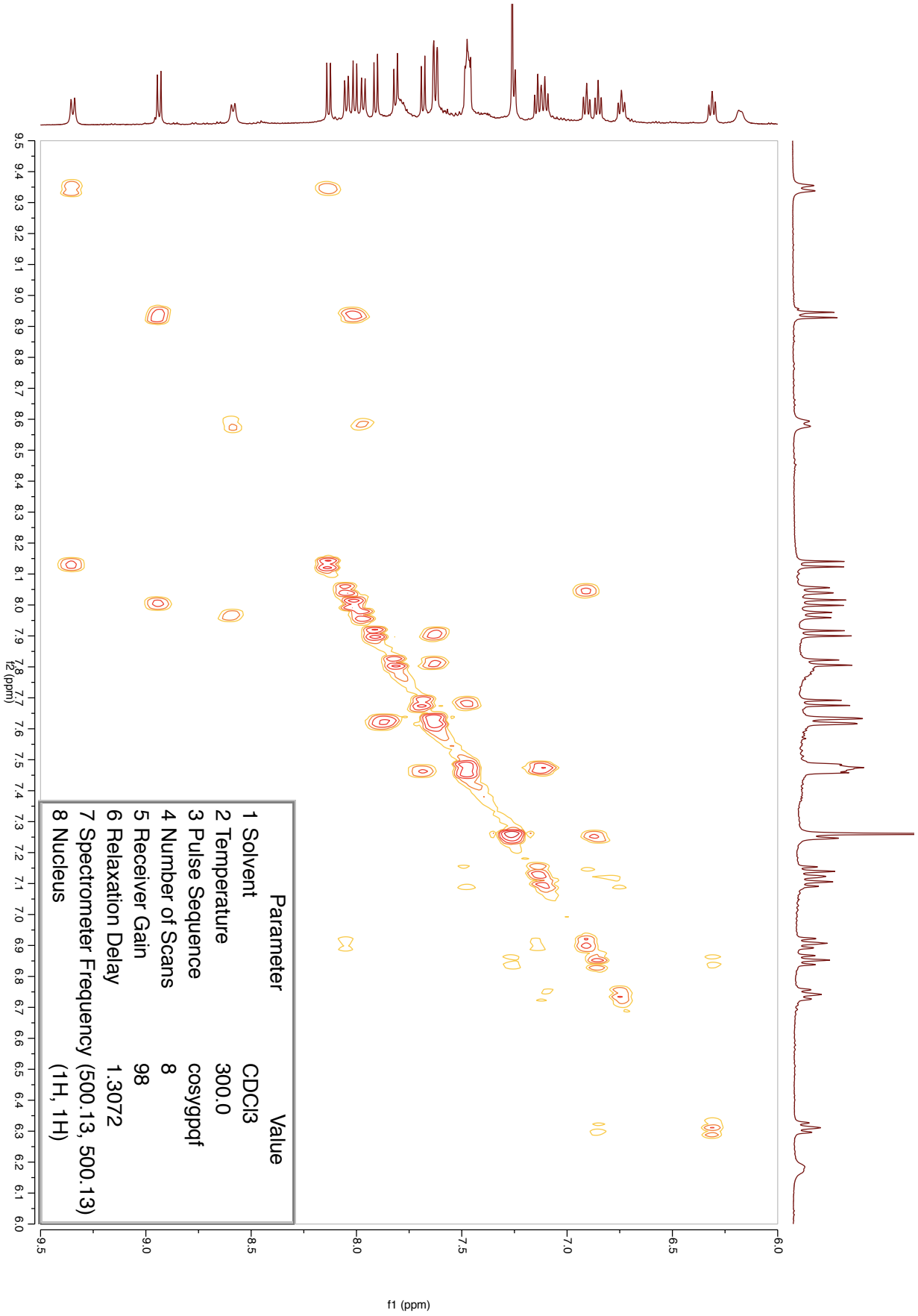


Figure S6-b. COSY experiment (500 MHz, 500 MHz, $CDCl_3$) of rac-*(P,M,P,P,P,M)*-C_2-**2**.

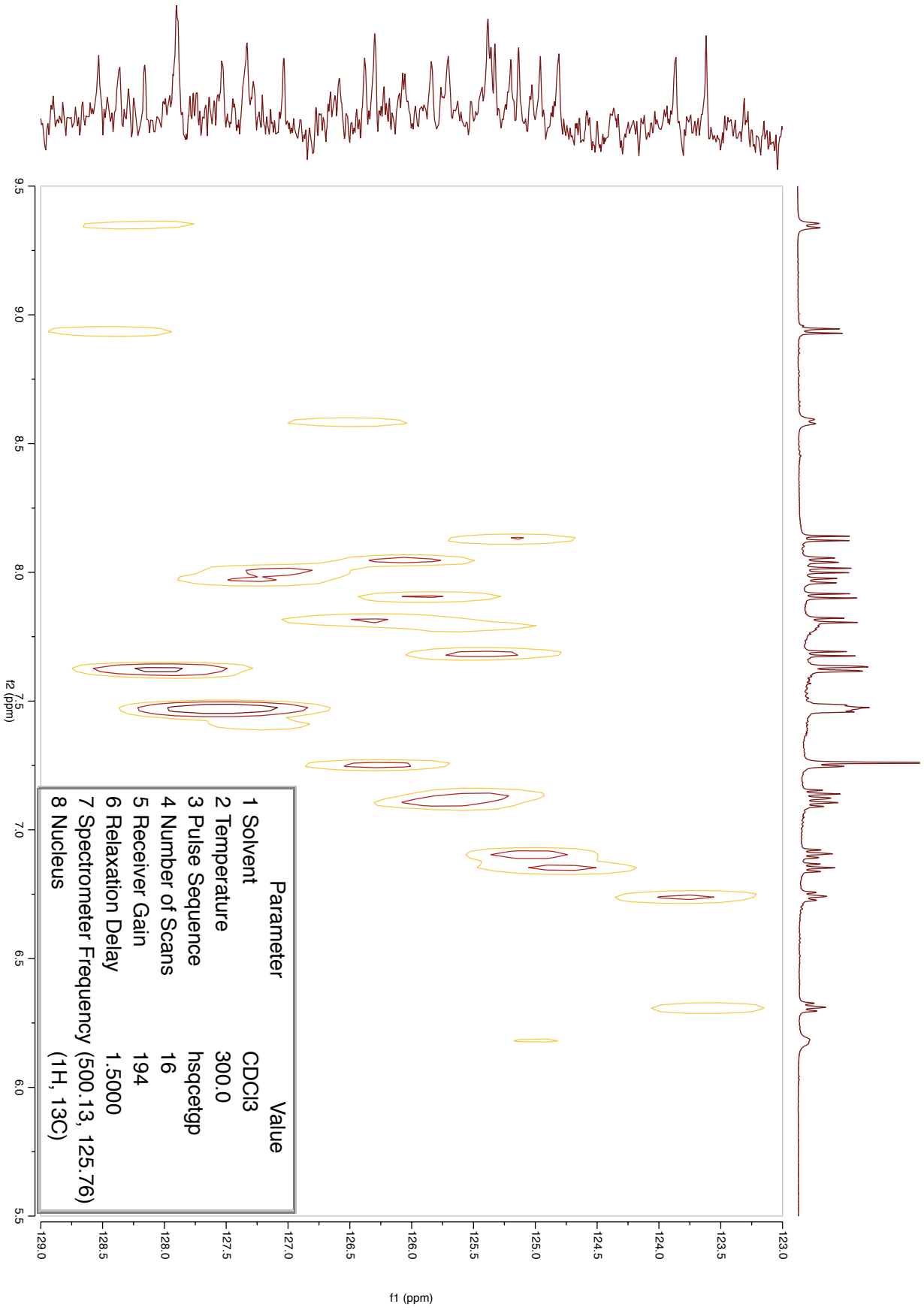


Figure S6-c. HSQC experiment (500 MHz, 125 MHz, $CDCl_3$) of rac-*(P,M,P,P,P,M)*-C_2-**2**.

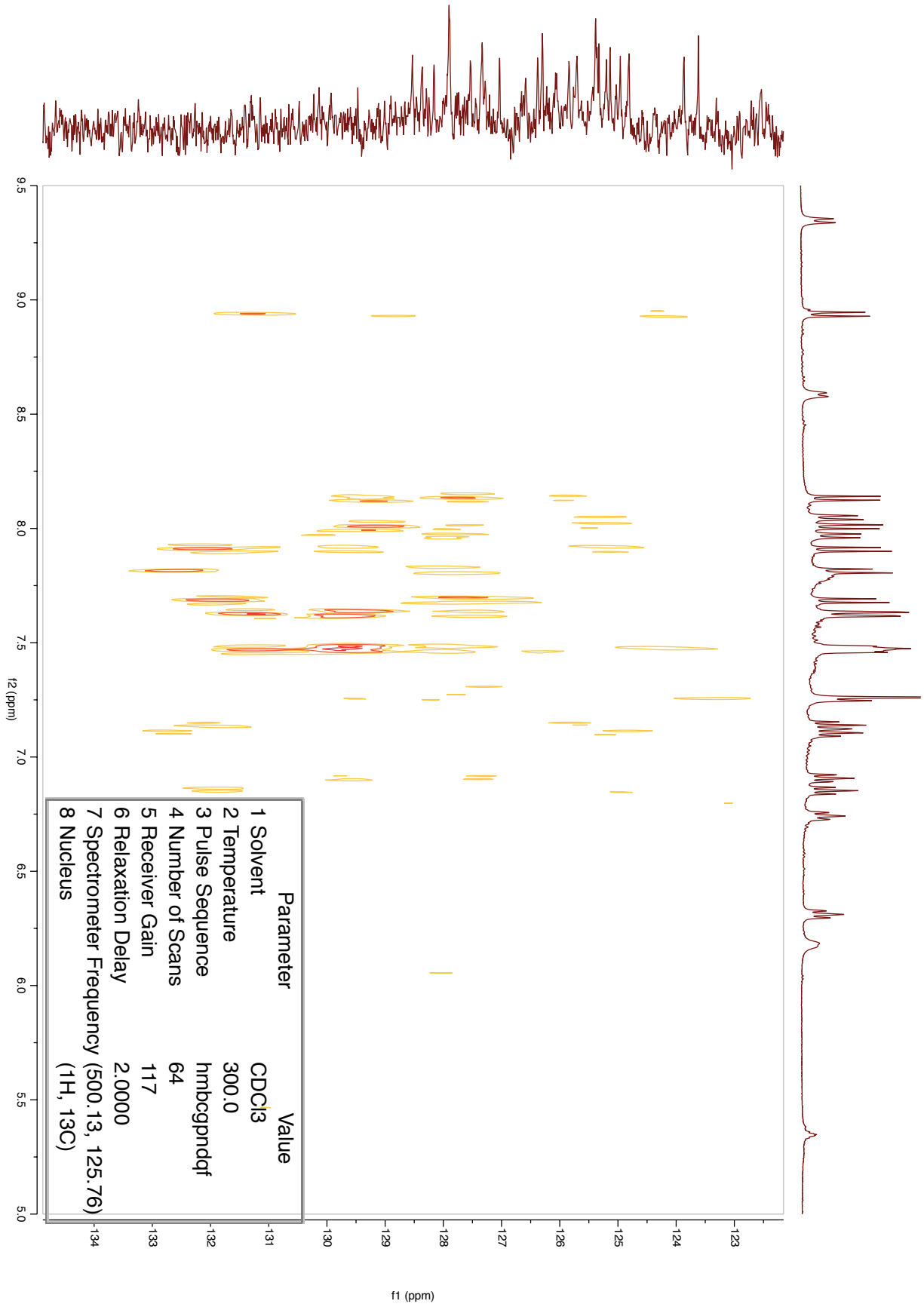


Figure S6-d. HMBC experiment (500 MHz, 125 MHz, $CDCl_3$) of rac-*(P,M,P,P,P,M)*-C_2-**2**.

2.2. X-ray diffraction analysis on monocrystal

(–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**

The crystallographic information file (CIF) for this compound is available from The Cambridge Crystallographic Data Centre (CCDC 1835903, deposited on April 9, 2018).

Monocrystals of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** were obtained by recrystallization in *d1*-chloroform at –18 ºC. A suitable crystal was mounted on a Rigaku Oxford Diffraction SuperNova diffractometer and measured at 203K at the Cu radiation (λ = 1.54184 Å). Data collection, reduction and multiscan ABSPACK correction were performed with CrysAlisPro (Rigaku Oxford Diffraction). Using Olex2[2] the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with ShelXL[4] using least-square minimization (Figure S7). The molecule was found to lie on a crystallographic two-fold axis bisecting the central cycle bearing the three [7]helicene moieties, the asymmetric unit being thus composed of one half of the molecule. Compound (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** co-crystallized with several $CDCl_3$ solvent molecules but only two of them could be localized in the asymmetric unit and refined, the remaining electronic density was modeled with a solvent mask.[2] All H and D atoms were found experimentally and refined with riding coordinates to their parent atoms and their Uiso parameters constraint to 1.2 Ueq (parent atoms). The absolute configuration of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** was assigned to (*M,M,M,P,P,P*) by the unambiguous determination of the Flack parameter estimated from a strong and clear anomalous signal (Figure S8) and confirmed by the Hooft statistics (Figure S9).[5]

The structural analysis of compound (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** reveals that the crystallographic two-fold axis bisects the central benzene ring in the middle of the C17-C17^{i} bond (symmetry code i: y, x, 1 - z) thus providing the molecule with a *C*$_2$ symmetry in the solid state. (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** adopts a propeller-shaped conformation: the absolute configurations for the three [7]helicenes on the outer crown were determined as (*M,M,M*) while the three [5]helicenes on the inner crown were determined as (*P,P,P*). The interplanar angles between the two terminal rings of each helicene subunit are equal to 36.95° and 41.12° for the [7]helicenes, and 62.01° and 65.05° for the [5]helicenes, respectively (Figure S10). These value should be compared with the 32.01º and 46.0º interplanar angle in isolated [7]helicene and [5]helicene, respectively.[6] The triphenylene core in (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** exhibits a chair conformation with a mean puckering angle (angle between the mean plane defined by four coplanar atoms and the plane defined by one atom out of the previous plane and the two atoms directly attached to it) of 14.0º, and impressive torsion angles of 32.06° and 32.93° as discussed in the main text (Figure S10). A superimposition of the structures of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** and its previously synthesized lower order analog of identical symmetry, namely *D*$_3$-hexanaphthotriphenylene (*D*$_3$-**HNTP**),[10,11] is provided in Figure S11, allowing a qualitative appreciation of the differences in geometries between the two structures. Tabulated data for selected experimental parameters (Table S1), bond lengths (Table S2) and torsion angles (Table S3) are provided herein for (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**.

The distortion of the helicene units in (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** and its propeller-shaped structure render difficult the formation of intra or inter-molecular π-π interactions. Hence the only relevant contacts observed in the crystal are weak inter-molecular CH/π(ring) interactions between benzene units of two symmetry-related molecules (C24–Cg1^{ii} = 3.492(4) Å and C24-H24..Cg1^{ii} = 138° where

[2] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339.
[3] G. M. Sheldrick, *Acta Cryst.* **2015**, *A71*, 3.
[4] G. M. Sheldrick, *Acta Cryst.* **2015**, *C71*, 3.
[5] R. W. W. Hooft, L. H. Traver, A. L.; A. L. J. Spek, *Appl. Cryst.* **2010**, *43*, 665.
[6] a) M. J. Fuchter, M. Weimar, X. Yang, D. K. Judge, A. J. P. White, *Tetrahedron Lett.* **2012**, *53*, 1108; b) R. Kuroda, *J. Chem. Soc. Perkin Trans. 2* **1982**, 789.

$Cg1^{ii}$ = centroid of ring C33/C34/C35/C36/C37/C38 with symmetry code ii: 1/2 + x, 1/2 – y, 5/4 – z), two weak halogen/π(ring) interactions between two $CDCl_3$ and two benzene units of symmetry-related molecules (Cl2-$Cg1^{iii}$ = 3.7430(16) Å and C47-Cl2..$Cg1^{iii}$ = 164.03(15)°; Cl3-$Cg2^{ii}$ = 3.2561(17) Å and C47-Cl3...$Cg2^{ii}$ = 146.98(18)° where $Cg1^{iii}$ = centroid Cg1 with symmetry code iii: 1 + y, x, 1 - z; $Cg2^{ii}$ = centroid of ring C18/C19/C20/C21/C22/C23 with symmetry code ii) and two very weak C-Cl…D bonds between the two determined molecules of chloroform. The crystal packing highlights the lack of interactions between individual molecules, which are embedded into $CDCl_3$ solvent channels organized along the a and b crystallographic axes (Figure S12). Moreover with regards to the stacking of the graphene units it is attractive to note that they form (*P*)-configured supra-helices within the crystal: the geometrical locus defined by the centroids of the central rings of all the symmetry-related molecules in the unit cell defines an helix whose axis is parallel to the crystallographic 4-fold axis and pitch the length of the unit vector c, i.e. 27.2785(2) Å (Figure S13).

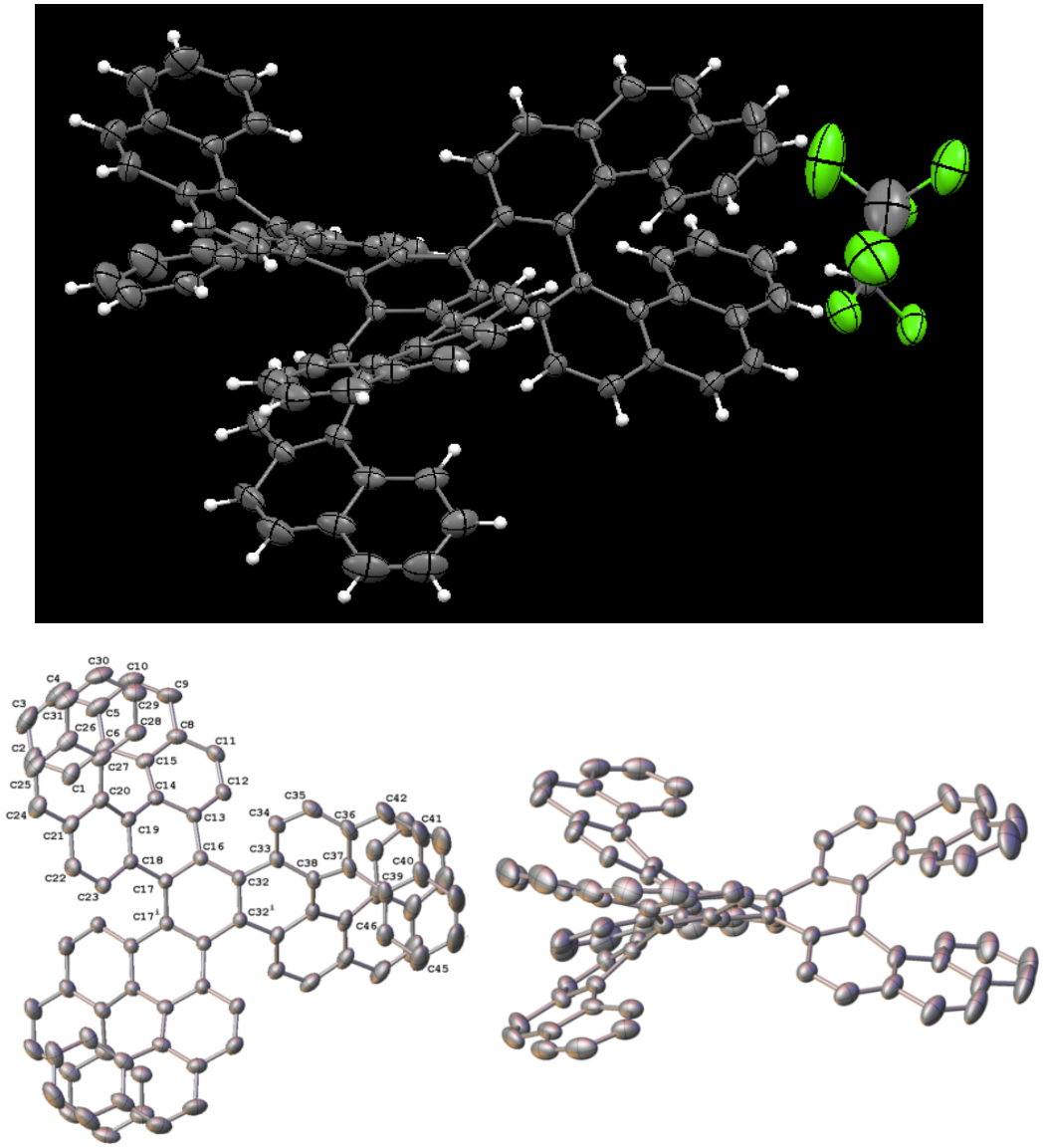


Figure S7. ORTEP view of (–)-(*M,M,M,P,P,P*)-D_3-**2**. Top: C and Cl atoms are drawn at 50% probability level, and H atoms are drawn as fixed-size spheres of radius 0.15 Å. Bottom: the $CDCl_3$ solvate and the H atoms were omitted for clarity.

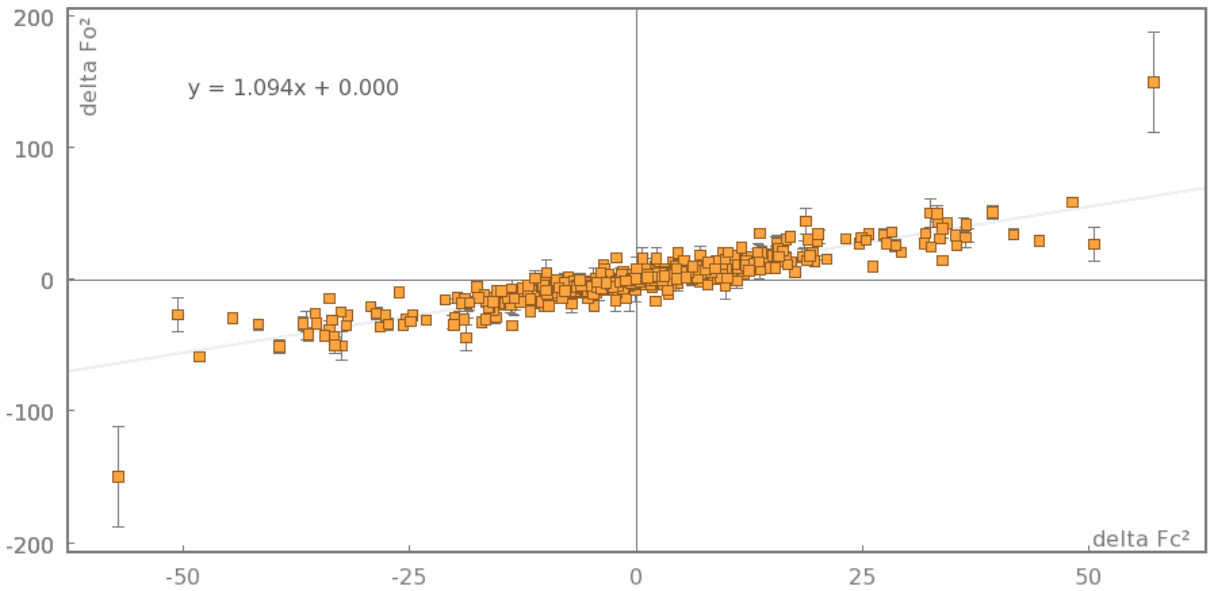


Figure S8. Bijvoet differences scatter plot for (–)-(*M,M,M,P,P,P*)-D_3-**2**

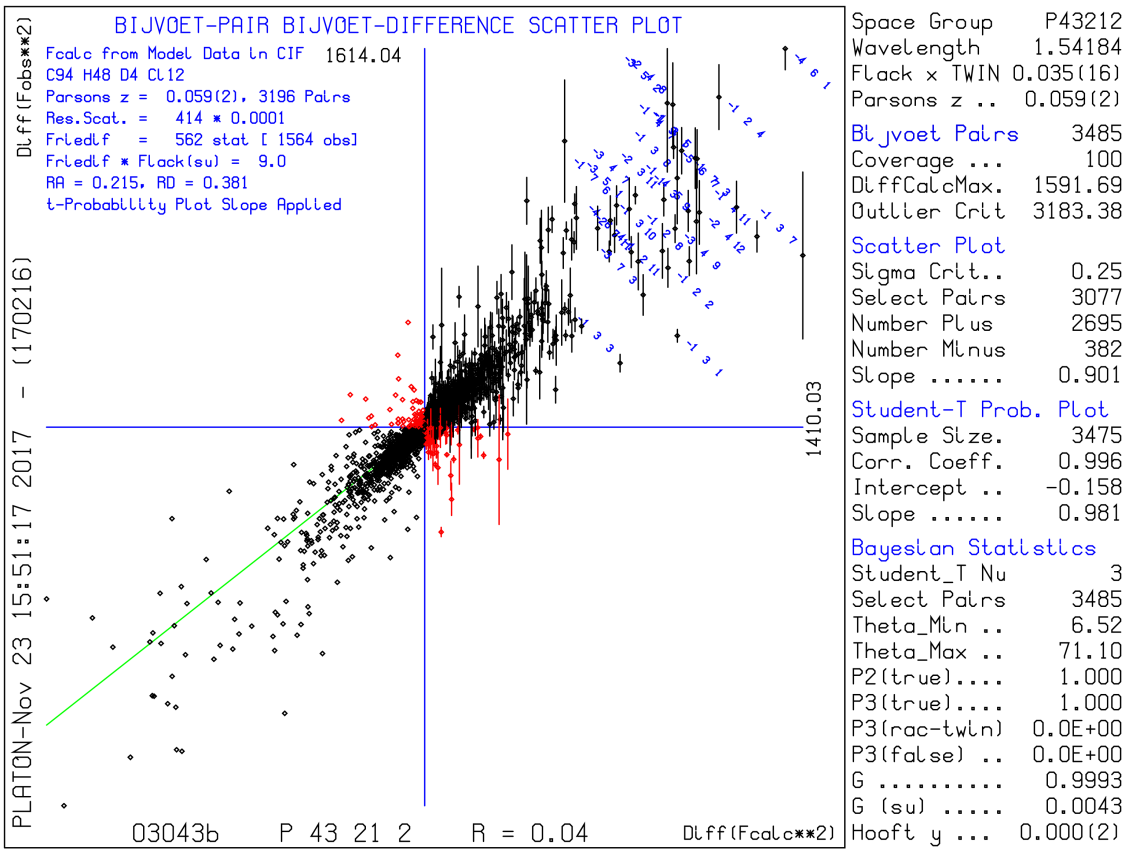


Figure S9. Hooft statistics for (–)-(*M,M,M,P,P,P*)-D_3-**2**

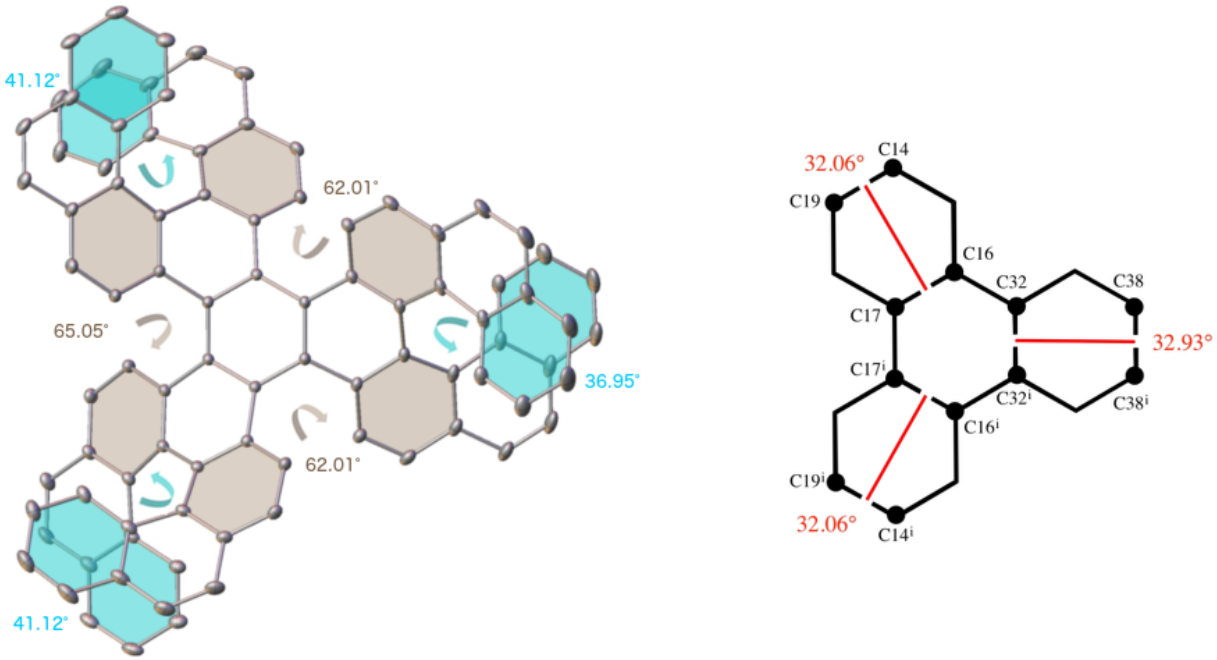


Figure S10. Distortion in (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**. Left: interplanar angles between the two terminal rings of each helicene, blue colored for [7]helicenes, grey-colored for [5]helicenes. Right: remarkable torsion angles. Symmetry code: i = y, x, 1 - z

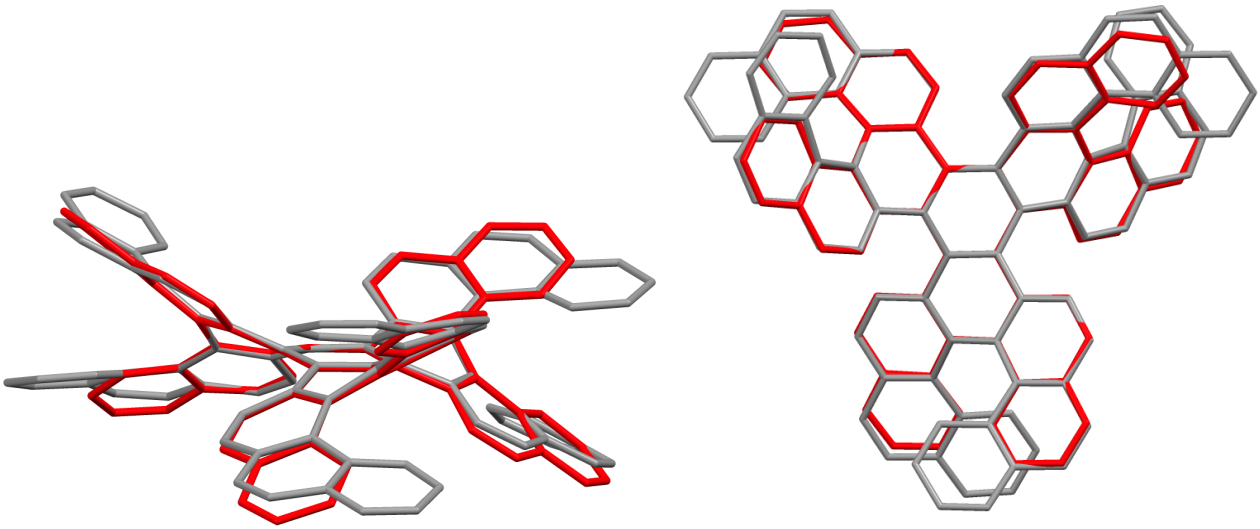


Figure S11. Superimpositions of the carbon backbones of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** (in grey) and its previously synthesized lower order analog *D*$_3$-**HNTP**[10] (in red).

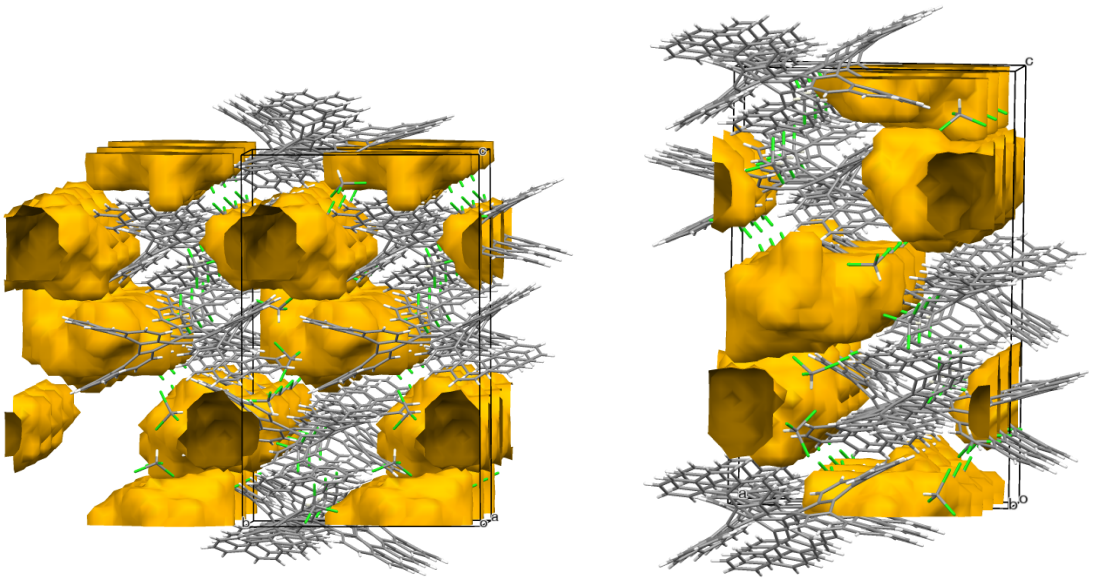


Figure S12. Crystal packing of (–)-*D*$_3$-**2** and representation of the solvent channels along the a (left) and b (right) axes. The content of the channels is a mix of explicitly determined chloroform molecules and the calculated mask of solvent (yellow voids).

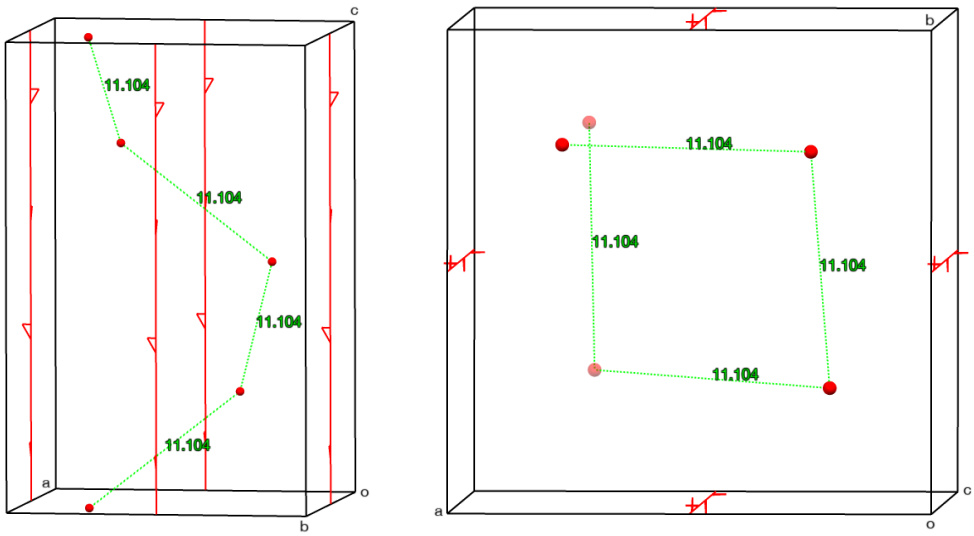


Figure S13. Representation of the *(P)*-configured supra-helix (pitch = 27.2785 Å) in the crystal packing of (–)-*D*$_3$-**2** with side view along the c axis (left) and top view (right), the four-fold 4_3 screw axis is in red, the centroids of the central rings of each molecule are represented as red dots and the distances between them (Å) are noted in green.

Table S1. Selected XRD experimental parameters for (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**

Formula	$C_{45}H_{24}$, 2($CDCl_3$)
M_w	805.39
Crystal system	tetragonal
Measurement temperature/ K	203
Space group	P 4_32_12
a/ Å	17.50350(10)
b/ Å	17.50350(10)

c/ Å	27.2785(2)
V/ Å^3	8357.38(11)
Z	8
Dc/g.cm^{-3}	1.28
Crystal colour	orange
Crystal size/mm^3	0.12*0.2*0.2
μ(Mo-Kα)/mm^{-1}	3.99
N° of refl. measured	147451
N° of unique refl.	8086
N° of observed refl.[$F^2 > 4\sigma F^2$]	7647
N° parameters refined	479
R_1 [$F^2 > 4\sigma F^2$]	0.0431
wR_1 [$F^2 > 4\sigma F^2$]	0.1282[a]
R_2 [all refl.]	0.0452
wR_2 [all refl.]	0.1311
Flack	0.035(16)
Goodness of fit [all refl.]	1.035
Residual Fourier/e. Å^{-3}	-0.503; 0.311

[a] $w=1/[\sigma^2(Fo^2)+(0.09P)^2+2.0293P]$ where $P=(Fo^2+2Fc^2)/3$

Table S2. Bond lengths for (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** obtained by XRD

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Cl1	C47	1.744(4)	C20	C27	1.453(4)
Cl2	C47	1.766(4)	C21	C22	1.414(4)
Cl3	C47	1.737(4)	C21	C24	1.429(4)
Cl4	C48	1.727(9)	C22	C23	1.359(4)
Cl5	C48	1.761(9)	C24	C25	1.353(5)
Cl6	C48	1.728(10)	C25	C26	1.417(5)
C1	C2	1.384(5)	C26	C27	1.418(4)
C1	C6	1.409(5)	C26	C31	1.411(5)
C2	C3	1.401(7)	C27	C28	1.415(5)
C3	C4	1.346(8)	C28	C29	1.377(4)
C4	C5	1.410(6)	C29	C30	1.405(6)
C5	C6	1.427(5)	C30	C31	1.366(6)
C5	C10	1.418(6)	C32	C32^1	1.413(5)
C6	C15	1.447(4)	C32	C33	1.465(3)
C8	C9	1.426(4)	C33	C34	1.421(4)
C8	C11	1.415(5)	C33	C38	1.415(4)
C8	C15	1.406(4)	C34	C35	1.361(4)
C9	C10	1.361(6)	C35	C36	1.419(5)
C11	C12	1.354(4)	C36	C37	1.405(5)
C12	C13	1.428(4)	C36	C42	1.432(4)
C13	C14	1.414(4)	C37	C38	1.441(4)
C13	C16	1.468(4)	C37	C39	1.459(4)
C14	C15	1.430(4)	C38	C38^1	1.455(6)
C14	C19	1.463(4)	C39	C40	1.421(5)
C16	C17	1.400(3)	C39	C46	1.415(5)

C16	C32	1.431(4)	C40	C41	1.423(7)
C17	C17[1]	1.432(5)	C40	C43	1.416(6)
C17	C18	1.461(3)	C41	C42	1.338(7)
C18	C19	1.406(4)	C43	C44	1.334(9)
C18	C23	1.421(4)	C44	C45	1.411(7)
C19	C20	1.445(4)	C45	C46	1.382(5)
C20	C21	1.411(4)			

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

Table S3. Bond angles for (–)-(*M,M,M,P,P,P*)-D_3-**2** obtained by XRD

Atom	Atom	Atom	Angle (˚)	Atom	Atom	Atom	Angle (˚)
Cl1	C47	Cl2	110.6(2)	C20	C21	C22	120.2(3)
Cl3	C47	Cl1	111.3(3)	C20	C21	C24	121.0(3)
Cl3	C47	Cl2	109.62(19)	C22	C21	C24	118.8(3)
Cl4	C48	Cl5	109.7(6)	C23	C22	C21	121.2(3)
Cl4	C48	Cl6	112.8(4)	C22	C23	C18	120.1(3)
Cl6	C48	Cl5	108.2(5)	C25	C24	C21	120.3(3)
C2	C1	C6	121.4(3)	C24	C25	C26	120.8(3)
C1	C2	C3	119.8(4)	C25	C26	C27	120.1(3)
C4	C3	C2	120.5(4)	C31	C26	C25	119.8(3)
C3	C4	C5	121.3(4)	C31	C26	C27	120.1(3)
C4	C5	C6	119.5(4)	C26	C27	C20	119.1(3)
C4	C5	C10	120.3(4)	C28	C27	C20	123.6(3)
C10	C5	C6	119.9(3)	C28	C27	C26	117.1(3)
C1	C6	C5	117.4(3)	C29	C28	C27	121.2(3)
C1	C6	C15	123.5(3)	C28	C29	C30	120.8(4)
C5	C6	C15	118.8(3)	C31	C30	C29	119.1(3)
C11	C8	C9	120.4(3)	C30	C31	C26	121.1(3)
C15	C8	C9	120.2(3)	C16	C32	C33	123.7(2)
C15	C8	C11	119.3(3)	C32[1]	C32	C16	119.28(15)
C10	C9	C8	120.7(3)	C32[1]	C32	C33	115.99(17)
C9	C10	C5	120.2(3)	C34	C33	C32	120.6(2)
C12	C11	C8	121.4(3)	C38	C33	C32	119.8(3)
C11	C12	C13	120.1(3)	C38	C33	C34	118.9(2)
C12	C13	C16	120.7(2)	C35	C34	C33	120.5(3)
C14	C13	C12	118.7(2)	C34	C35	C36	121.3(3)
C14	C13	C16	119.6(2)	C35	C36	C42	120.2(4)
C13	C14	C15	119.5(2)	C37	C36	C35	119.4(3)
C13	C14	C19	117.0(2)	C37	C36	C42	120.5(4)
C15	C14	C19	123.6(2)	C36	C37	C38	118.1(3)
C8	C15	C6	117.5(3)	C36	C37	C39	117.3(3)
C8	C15	C14	117.7(3)	C38	C37	C39	124.6(3)
C14	C15	C6	124.7(3)	C33	C38	C37	119.5(3)
C17	C16	C13	115.2(2)	C33	C38	C38[1]	116.16(18)
C17	C16	C32	119.4(2)	C37	C38	C38[1]	124.3(2)

C32	C16	C13	124.5(2)	C40	C39	C37	119.0(4)
C16	C17	C17[1]	119.29(15)	C46	C39	C37	123.0(3)
C16	C17	C18	117.4(2)	C46	C39	C40	117.8(3)
C17[1]	C17	C18	122.67(16)	C39	C40	C41	119.5(4)
C19	C18	C17	119.7(2)	C43	C40	C39	118.6(5)
C19	C18	C23	119.7(2)	C43	C40	C41	121.8(4)
C23	C18	C17	120.0(2)	C42	C41	C40	121.1(4)
C18	C19	C14	115.7(2)	C41	C42	C36	120.8(4)
C18	C19	C20	119.8(2)	C44	C43	C40	121.8(4)
C20	C19	C14	124.5(2)	C43	C44	C45	121.1(4)
C19	C20	C27	125.5(3)	C46	C45	C44	118.5(5)
C21	C20	C19	117.3(3)	C45	C46	C39	121.8(4)
C21	C20	C27	117.1(2)				

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

rac-*(P,M,P,P,P,M)*-C_2-**2**

The crystallographic information file (CIF) for this compound is available from The Cambridge Crystallographic Data Centre (CCDC 1902495, deposited on March 3, 2019).

Crystals for compound rac-*(P,M,P,P,P,M)*-C_2-**2** were obtained from a saturated hexane / *d1*-chloroform (ca. 3:1) solution stored at –18 ºC as orange prisms. A suitable crystal was mounted on a Rigaku Oxford Diffraction SuperNova diffractometer and measured at 173K at the Cu radiation (λ=1.54184 Å). Data collection, reduction and multiscan ABSPACK correction were performed with CrysAlisPro (Rigaku Oxford Diffraction). Using Olex2[2] the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with ShelXL[4] using least-square minimization. Compound rac-*(P,M,P,P,P,M)*-C_2-**2** co-crystallized with partial hexane and $CDCl_3$ solvent molecules (respective occupations 0.85 for hexane and 0.15 for $CDCl_3$) and a half disordered hexane in the asymmetric unit (Figure S14). All H-atoms except those for solvent molecules were found experimentally and refined with riding coordinates to their parent atoms and their Uiso parameters constraint to 1.2Ueq (parent atoms). Tabulated data for selected experimental parameters (Table S4), bond lengths (Table S5) and torsion angles (Table S6) are provided herein for rac-*(P,M,P,P,P,M)*-C_2-**2**.

As mentioned in the main text, the maximal torsion angle in the molecule was measured at 36.9º for the peripheral ring of the triphenylene core on the molecular C_2 axis in C_2-**2** (Figure 2b,d in the main text). This establishes a new record of torsion for a benzene ring. The naphthalene unit aligned with the molecular C_2 axis in C_2-**2** exhibits a severe end-to-end torsion of 66.7º (Figure 2c in the main text). This end-to-end torsion is to be compared with torsions of other naphthalene units found in distorted triphenylenes (Figure S16).

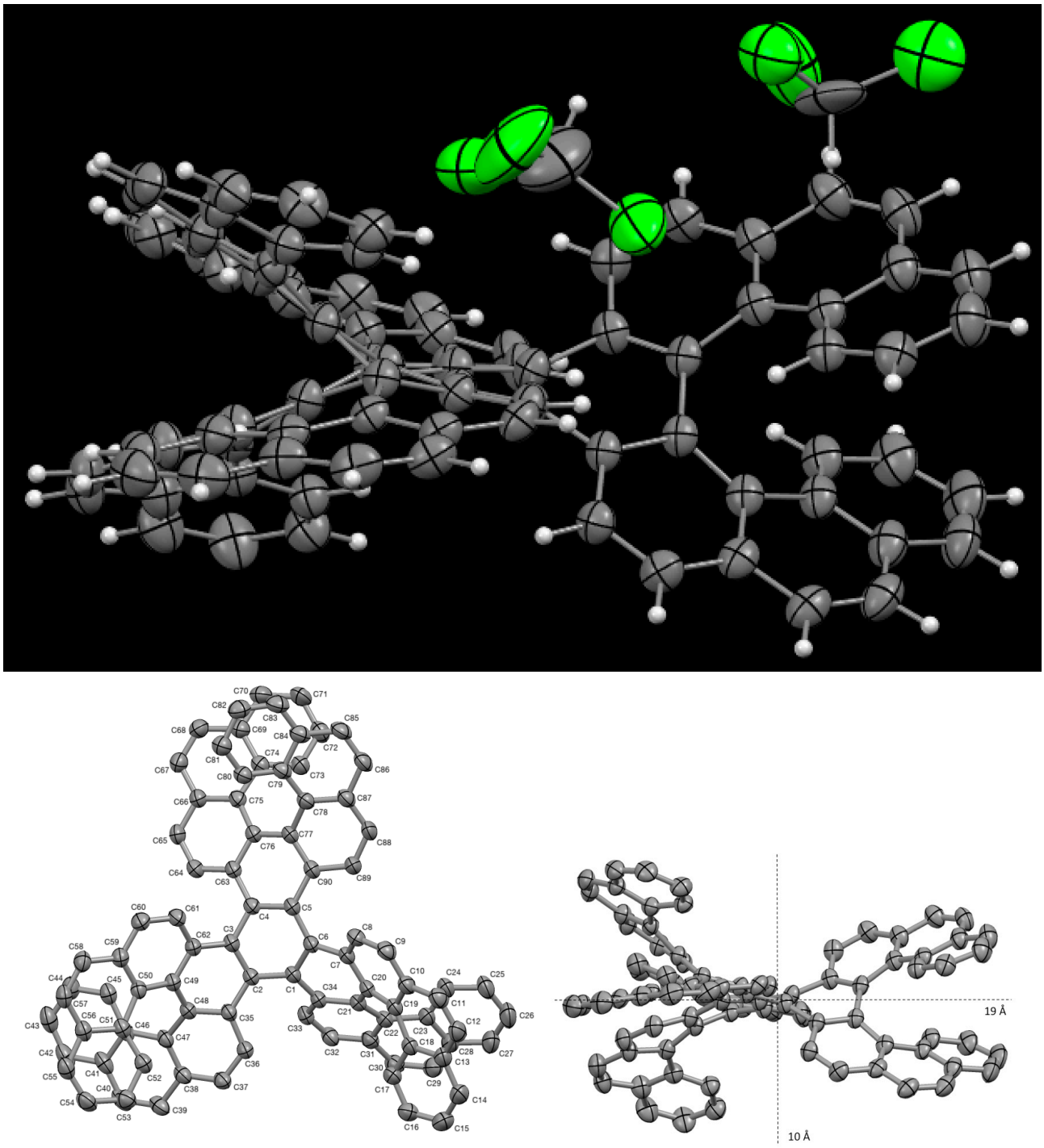


Figure S14. ORTEP view of rac-*(P,M,P,P,P,M)*-C_2-**2**. Top: C and Cl atoms are drawn at 50% probability level, H atoms are drawn as fixed-size spheres of radius 0.15 Å, and hexane molecules were omitted for clarity. Bottom: hexane and $CDCl_3$ molecules, and the H atoms were omitted for clarity. The molecule dimensions (length and thickness) were measured including the H-atoms.

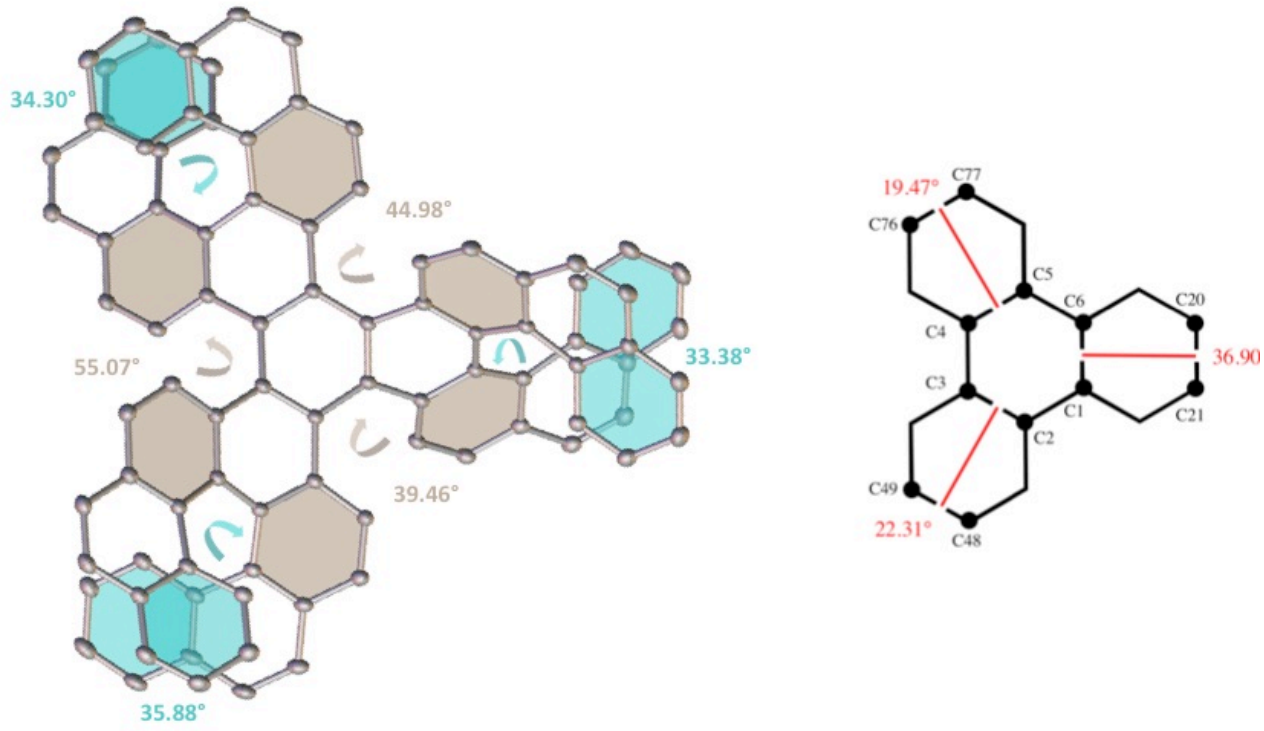


Figure S15. Distortion in rac-*(P,M,P,P,P,M)*-C_2-**2**. Left: interplanar angles between the two terminal rings of each helicene, blue colored for [7]helicenes, grey-colored for [5]helicenes. Right: remarkable torsion angles.

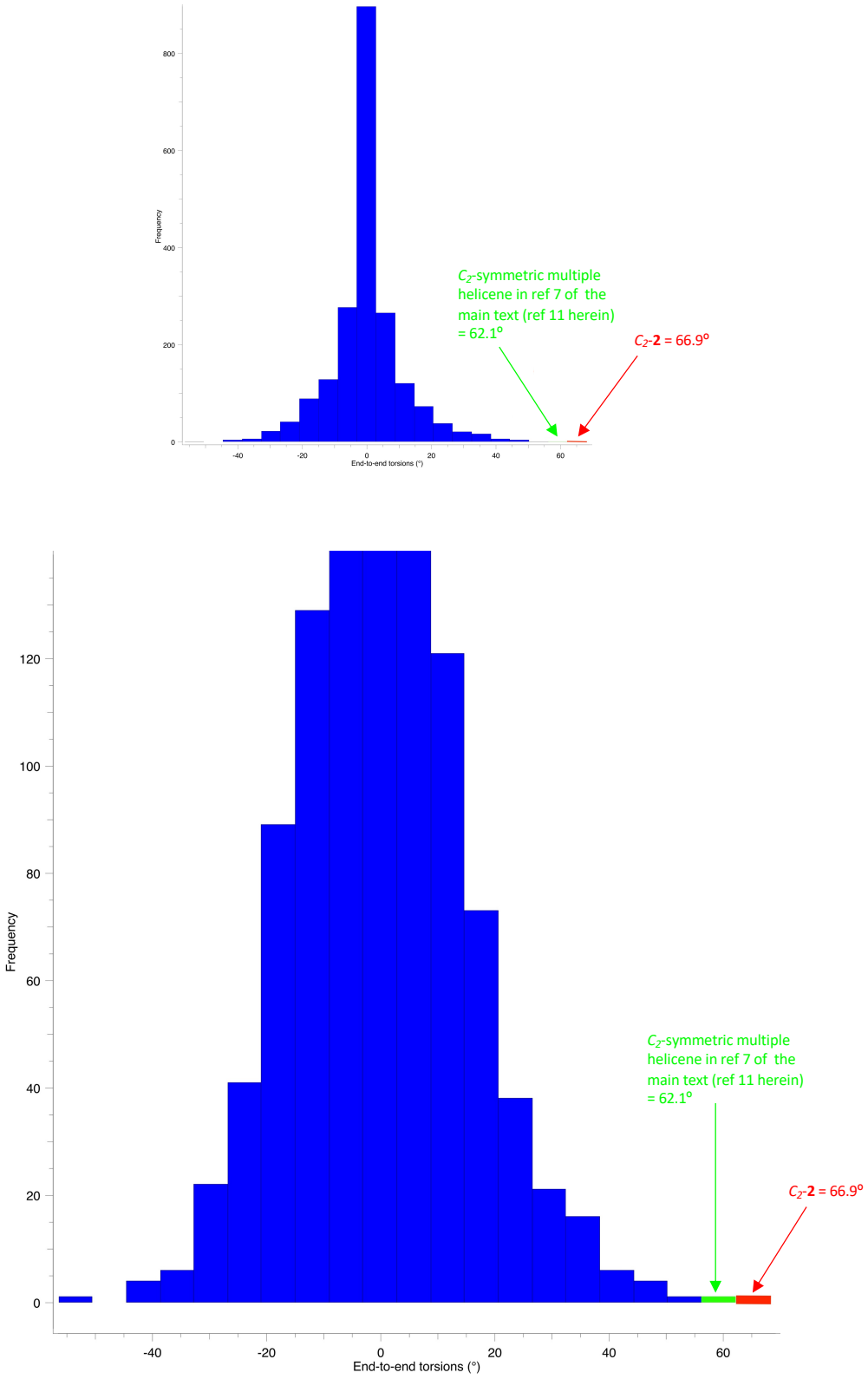


Figure S16. Abundance and end-to-end torsions of naphthalene subunits included in triphenylenes (or larger PAHs) in The Cambridge Crystallographic Data Centre (CCDC, February 2019). More than 800 hits were found (top image). Bottom image : cutoff at 130 hits for clarity.

Table S4. Selected XRD experimental parameters for rac-*(P,M,P,P,P,M)*-C_2-**2**

Formula	$C_{90}H_{48}$,0.85(C_7H_{16}),0.3($CDCl_3$),($C_{3.5}H_{7.5}$)
M_w	1299.85
Crystal system	triclinic
Measurement temperature/ K	173
Space group	P -1
a/ Å	11.3090(6)
b/ Å	14.2803(7)
c/ Å	22.3360(12)
α/ °	73.204(4)
β/ °	87.078(4)
γ/ °	88.529(4)
V/ Å^3	8357.38(11)
Z	2
Dc/g.cm^{-3}	1.252
Crystal colour	orange
Crystal size/mm^3	0.015*0.05*0.14
μ(Mo-Kα)/mm^{-1}	0.848
N° of refl. measured	24308
N° of unique refl.	12937
N° of observed refl.[$F^2 > 4\sigma F^2$]	8572
N° parameters refined	964
R_1 [$F^2 > 4\sigma F^2$]	0.0706
wR_1 [$F^2 > 4\sigma F^2$]	0.1721[a]
R_2 [all refl.]	0.1050
wR_2 [all refl.]	0.2013
Goodness of fit [all refl.]	1.049
Residual Fourier/e. Å^{-3}	-0.417; 0.530

[a] $w=1/[\sigma^2(Fo^2)+(0.0698P)^2+0.9934P]$ where $P=(Fo^2+2Fc^2)/3$

Table S5. Bond lengths for rac-*(P,M,P,P,P,M)*-C_2-**2** obtained by XRD

Atom	Atom	Length (Å)	Atom	Atom	Length (Å)
Cl1	C99	1.7503(10)	C48	C49	1.445(4)
Cl2	C99	1.7499(10)	C49	C50	1.442(4)
Cl3	C99	1.7500(11)	C49	C62	1.407(3)
Cl4	C98	1.7499(10)	C50	C51	1.463(4)
Cl5	C98	1.7499(11)	C50	C59	1.401(4)
Cl6	C98	1.7499(11)	C51	C52	1.408(4)
C1	C2	1.453(3)	C51	C56	1.425(4)
C1	C6	1.404(4)	C52	C53	1.376(4)
C1	C34	1.449(4)	C53	C54	1.395(4)
C2	C3	1.402(4)	C54	C55	1.359(5)
C2	C35	1.457(3)	C55	C56	1.414(4)
C3	C4	1.451(3)	C56	C57	1.421(4)
C3	C62	1.453(3)	C57	C58	1.351(4)

C4	C5	1.406(4)	C58	C59	1.429(4)
C4	C63	1.447(4)	C59	C60	1.427(4)
C5	C6	1.437(4)	C60	C61	1.358(4)
C5	C90	1.462(3)	C61	C62	1.411(4)
C6	C7	1.464(4)	C63	C64	1.430(4)
C7	C8	1.423(4)	C63	C76	1.410(3)
C7	C20	1.403(4)	C64	C65	1.346(4)
C8	C9	1.358(4)	C65	C66	1.421(4)
C9	C10	1.411(4)	C66	C67	1.428(4)
C10	C11	1.431(4)	C66	C75	1.405(4)
C10	C19	1.424(4)	C67	C68	1.352(4)
C11	C12	1.341(5)	C68	C69	1.425(4)
C12	C13	1.438(5)	C69	C70	1.411(4)
C13	C14	1.397(4)	C69	C74	1.427(4)
C13	C18	1.422(4)	C70	C71	1.376(5)
C14	C15	1.368(5)	C71	C72	1.389(5)
C15	C16	1.407(5)	C72	C73	1.379(4)
C16	C17	1.364(4)	C73	C74	1.409(4)
C17	C18	1.413(4)	C74	C75	1.459(4)
C18	C19	1.446(4)	C75	C76	1.449(4)
C19	C20	1.443(4)	C76	C77	1.452(4)
C20	C21	1.475(4)	C77	C78	1.443(4)
C21	C22	1.431(4)	C77	C90	1.404(4)
C21	C34	1.424(3)	C78	C79	1.443(4)
C22	C23	1.464(4)	C78	C87	1.416(4)
C22	C31	1.418(4)	C79	C80	1.403(4)
C23	C24	1.412(4)	C79	C84	1.420(4)
C23	C28	1.420(4)	C80	C81	1.365(4)
C24	C25	1.380(4)	C81	C82	1.403(4)
C25	C26	1.387(5)	C82	C83	1.364(5)
C26	C27	1.354(6)	C83	C84	1.395(5)
C27	C28	1.415(4)	C84	C85	1.437(4)
C28	C29	1.427(5)	C85	C86	1.342(5)
C29	C30	1.356(5)	C86	C87	1.441(4)
C30	C31	1.422(4)	C87	C88	1.406(4)
C31	C32	1.422(4)	C88	C89	1.366(4)
C32	C33	1.355(4)	C89	C90	1.431(4)
C33	C34	1.421(4)	C91	C92	1.424(8)
C35	C36	1.420(4)	C92	C93	1.473(8)
C35	C48	1.416(3)	C93	C94	1.399(8)
C36	C37	1.367(4)	C94	C95	1.469(10)
C37	C38	1.416(4)	C95	C96	1.454(11)
C38	C39	1.433(4)	C96	C97	1.506(14)
C38	C47	1.406(4)	C100	C101	1.529(8)
C39	C40	1.350(5)	C101	C102	1.467(8)
C40	C41	1.417(5)	C105	C106	1.507(8)

C41	C42	1.418(4)	C105	C104	1.531(9)
C41	C46	1.429(4)	C106	C103	0.720(8)
C42	C43	1.362(5)	C106	C103[1]	1.519(12)
C43	C44	1.400(5)	C102	C103[1]	1.852(14)
C44	C45	1.375(4)	C102	C103	1.437(8)
C45	C46	1.409(4)	C103	C106[1]	1.519(12)
C46	C47	1.453(4)	C103	C102[1]	1.852(14)
C47	C48	1.448(4)	C103	C103[1]	1.204(14)

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

Table S6. Bond angles for rac-*(P,M,P,P,P,M)*-C_2-**2** obtained by XRD

Atom	Atom	Atom	Angle (°)	Atom	Atom	Atom	Angle (°)
Cl2	C99	Cl1	107.1(8)	C35	C48	C49	116.7(2)
Cl3	C99	Cl1	108.4(13)	C49	C48	C47	124.5(2)
Cl3	C99	Cl2	106.3(14)	C50	C49	C48	122.6(2)
Cl5	C98	Cl4	107.4(6)	C62	C49	C48	118.2(2)
Cl6	C98	Cl4	113.2(16)	C62	C49	C50	119.2(2)
Cl6	C98	Cl5	125.2(18)	C49	C50	C51	124.0(2)
C6	C1	C2	117.1(2)	C59	C50	C49	118.3(2)
C6	C1	C34	114.9(2)	C59	C50	C51	117.7(2)
C34	C1	C2	127.9(2)	C52	C51	C50	123.9(2)
C1	C2	C35	123.7(2)	C52	C51	C56	117.7(2)
C3	C2	C1	117.3(2)	C56	C51	C50	118.1(2)
C3	C2	C35	118.7(2)	C53	C52	C51	121.1(3)
C2	C3	C4	118.5(2)	C52	C53	C54	120.3(3)
C2	C3	C62	119.1(2)	C55	C54	C53	119.9(3)
C4	C3	C62	122.1(2)	C54	C55	C56	121.4(3)
C5	C4	C3	117.7(2)	C55	C56	C51	118.6(3)
C5	C4	C63	119.9(2)	C55	C56	C57	121.5(2)
C63	C4	C3	122.2(2)	C57	C56	C51	119.7(2)
C4	C5	C6	117.7(2)	C58	C57	C56	121.0(2)
C4	C5	C90	118.0(2)	C57	C58	C59	120.5(3)
C6	C5	C90	124.1(2)	C50	C59	C58	120.5(2)
C1	C6	C5	118.0(2)	C50	C59	C60	118.9(2)
C1	C6	C7	114.3(2)	C60	C59	C58	120.5(3)
C5	C6	C7	127.6(2)	C61	C60	C59	120.9(3)
C8	C7	C6	118.9(2)	C60	C61	C62	120.8(2)
C20	C7	C6	120.2(2)	C49	C62	C3	119.0(2)
C20	C7	C8	119.8(2)	C49	C62	C61	119.1(2)
C9	C8	C7	120.1(3)	C61	C62	C3	121.8(2)
C8	C9	C10	121.4(3)	C64	C63	C4	121.9(2)
C9	C10	C11	120.1(3)	C76	C63	C4	119.8(2)
C9	C10	C19	119.8(3)	C76	C63	C64	118.3(2)
C19	C10	C11	120.1(3)	C65	C64	C63	120.9(2)
C12	C11	C10	121.3(3)	C64	C65	C66	121.2(2)

C11	C12	C13	120.3(3)
C14	C13	C12	120.1(3)
C14	C13	C18	119.8(3)
C18	C13	C12	119.9(3)
C15	C14	C13	121.6(3)
C14	C15	C16	118.9(3)
C17	C16	C15	120.5(3)
C16	C17	C18	121.8(3)
C13	C18	C19	118.8(3)
C17	C18	C13	116.9(3)
C17	C18	C19	124.1(2)
C10	C19	C18	117.6(2)
C10	C19	C20	117.4(2)
C20	C19	C18	125.0(3)
C7	C20	C19	119.7(3)
C7	C20	C21	115.5(2)
C19	C20	C21	124.8(2)
C22	C21	C20	126.3(2)
C34	C21	C20	114.7(2)
C34	C21	C22	119.0(2)
C21	C22	C23	124.6(3)
C31	C22	C21	118.6(2)
C31	C22	C23	116.8(3)
C24	C23	C22	123.3(3)
C24	C23	C28	117.6(2)
C28	C23	C22	119.0(3)
C25	C24	C23	120.8(3)
C24	C25	C26	120.9(3)
C27	C26	C25	119.7(3)
C26	C27	C28	121.5(3)
C23	C28	C29	120.1(3)
C27	C28	C23	119.1(3)
C27	C28	C29	120.7(3)
C30	C29	C28	119.8(3)
C29	C30	C31	121.5(3)
C22	C31	C30	120.5(3)
C22	C31	C32	119.4(3)
C32	C31	C30	120.1(3)
C33	C32	C31	121.0(3)
C32	C33	C34	120.8(2)
C21	C34	C1	120.0(2)
C33	C34	C1	119.9(2)
C33	C34	C21	119.3(2)
C36	C35	C2	125.2(2)
C48	C35	C2	118.1(2)
C48	C35	C36	116.7(2)
C65	C66	C67	120.5(2)
C75	C66	C65	119.0(2)
C75	C66	C67	120.5(2)
C68	C67	C66	121.0(3)
C67	C68	C69	120.5(3)
C68	C69	C74	119.6(2)
C70	C69	C68	120.3(3)
C70	C69	C74	119.8(3)
C71	C70	C69	120.7(3)
C70	C71	C72	119.6(3)
C73	C72	C71	121.0(3)
C72	C73	C74	121.2(3)
C69	C74	C75	118.8(2)
C73	C74	C69	117.4(2)
C73	C74	C75	123.6(2)
C66	C75	C74	116.9(2)
C66	C75	C76	117.8(2)
C76	C75	C74	125.2(2)
C63	C76	C75	119.1(2)
C63	C76	C77	117.5(2)
C75	C76	C77	123.3(2)
C78	C77	C76	122.7(2)
C90	C77	C76	118.0(2)
C90	C77	C78	119.2(2)
C77	C78	C79	123.6(2)
C87	C78	C77	117.6(3)
C87	C78	C79	118.8(2)
C80	C79	C78	123.6(2)
C80	C79	C84	117.3(3)
C84	C79	C78	118.9(3)
C81	C80	C79	122.0(3)
C80	C81	C82	119.9(3)
C83	C82	C81	119.6(3)
C82	C83	C84	121.3(3)
C79	C84	C85	119.2(3)
C83	C84	C79	119.6(3)
C83	C84	C85	121.0(3)
C86	C85	C84	120.8(2)
C85	C86	C87	121.3(3)
C78	C87	C86	118.8(3)
C88	C87	C78	119.0(2)
C88	C87	C86	122.0(3)
C89	C88	C87	121.5(2)
C88	C89	C90	120.6(3)
C77	C90	C5	119.2(2)
C77	C90	C89	117.0(2)

C37	C36	C35	120.7(2)	C89	C90	C5	123.8(2)
C36	C37	C38	121.1(2)	C91	C92	C93	106.5(12)
C37	C38	C39	121.4(3)	C94	C93	C92	123.1(8)
C47	C38	C37	119.1(2)	C93	C94	C95	129.6(7)
C47	C38	C39	119.4(3)	C96	C95	C94	125.9(6)
C40	C39	C38	120.7(3)	C95	C96	C97	121.5(10)
C39	C40	C41	121.8(3)	C102	C101	C100	113.2(9)
C40	C41	C42	121.8(3)	C106	C105	C104	116.5(10)
C40	C41	C46	119.6(3)	C105	C106	C103[1]	116.3(8)
C42	C41	C46	118.5(3)	C103	C106	C105	166.4(14)
C43	C42	C41	121.7(3)	C103	C106	C103[1]	51.1(11)
C42	C43	C44	120.1(3)	C101	C102	C103[1]	154.6(8)
C45	C44	C43	119.7(3)	C103	C102	C101	114.0(7)
C44	C45	C46	122.1(3)	C103	C102	C103[1]	40.5(5)
C41	C46	C47	118.0(3)	C106	C103	C106[1]	128.9(11)
C45	C46	C41	117.8(3)	C106	C103	C103[1]	101.2(13)
C45	C46	C47	124.1(2)	C102	C103	C102[1]	139.5(5)
C38	C47	C46	119.7(2)	C103[1]	C103	C106[1]	27.7(4)
C38	C47	C48	117.6(2)	C103[1]	C103	C102[1]	50.9(6)
C48	C47	C46	122.7(2)	C103[1]	C103	C102	88.6(8)
C35	C48	C47	118.5(2)				

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

3. Enantiomerization of *D*$_3$-**2**

3.1. Experimental determination of the enantiomerization barrier

A solution of enantiopure (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** (1.0 mg) in 1,2-dichlorobenzene (25 mL) was heated at 182 ºC. Aliquots (20 µL) were periodically withdrawn from the solution and analyzed by HPLC on a chiral stationary phase to determine the enantiomeric ratio. A very clean racemization was observed without detectable degradation. The decrease in the proportion of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** is monitored over time (Table S7), allowing for the experimental determination of the rate of enantiomerization $\mathbf{k_{enantiomerization}}$, the corresponding activation Gibbs free energy of enantiomerization $\mathbf{\Delta G^{\neq}_{enantiomerization}}$ and the corresponding half-life $\mathbf{t_{1/2}}$ (Figure S17).

Table S7. Proportion of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** over time at 182 ºC[a]

Time (min)[b]	% (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2**	ln ((%t-%e)/(%0-%e))
0	89.14	0.00000
344	85.17	-0.10695
1418	75.62	-0.42377
1575	74.52	-0.46766
1867	72.51	-0.55319
2922	66.7	-0.85174
5783	57.32	-1.67653

[a]HPLC conditions: (*S,S*)-Whelk-O1 column eluted with heptane / ethanol / dichloromethane (1:4:5) at 1 mL/min, detection by UV at 290 nm. [b]Time = 0 min corresponds to the first analysis, not the beginning of heating.

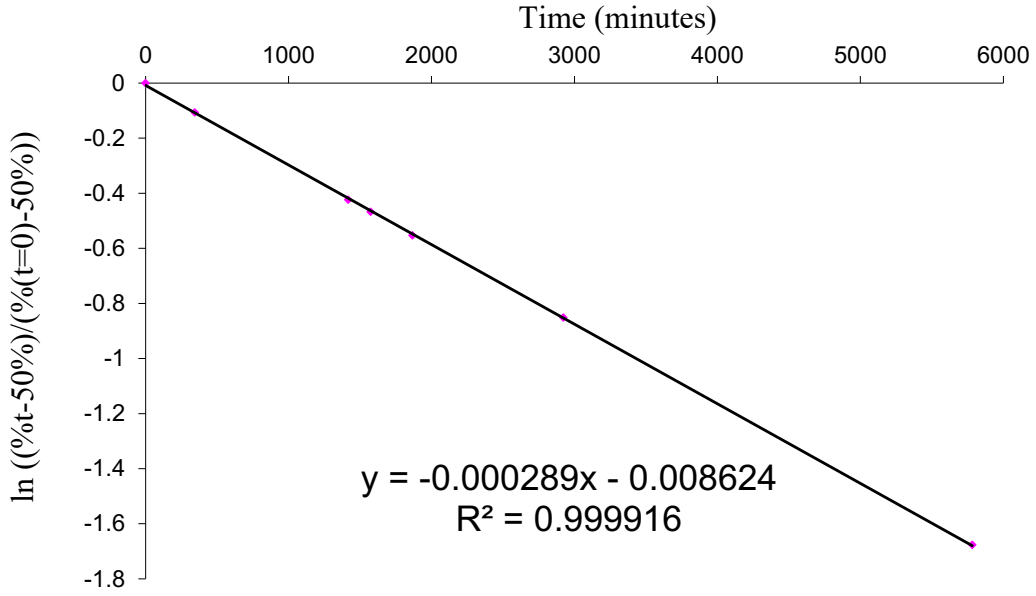


Figure S17. Kinetic line for the enantiomerization of (–)-(*M,M,M,P,P,P*)-*D*$_3$-**2** at 182 ºC

$\mathbf{k_{enantiomerisation}}$ = 4.816 × 10^{-06} s^{-1} (@ 182 °C in 1,2-dichlorobenzene)

$\mathbf{\Delta G^{\neq}_{enantiomerization}}$ = 162.0 kJ/mol (@ 182 °C in 1,2-dichlorobenzene)

$\mathbf{t_{1/2}}$ = 40.0 h (@ 182 °C in 1,2-dichlorobenzene)

3.2. Computer-assisted modeling of the enantiomerization process

The DFT calculations reported in this section were performed with the Gaussian 09 program.[7] All geometries were fully optimized using the B3LYP hybrid density functional using the 6-31G(d) basis set in the gas phase. The second derivatives were analytically calculated in order to determine if a minimum (zero negative eigenvalue) or a transition state (one negative eigenvalue) existed for the resulting geometry. The connection between the transition states and the corresponding minima was confirmed by intrinsic reaction coordinate (IRC) calculations.[8] Free Gibbs energies include thermal corrections and are expressed in kJ/mol (1 Ha = 2625.5 kJ/mol). The Cartesian coordinates, number of negative eigenvalues and free Gibbs energies expressed in Hartrees of all stationary points are reported below. The computed geometries of (*M,M,M,P,P,P*)-D_3-**2** and *(P,M,P,P,P,M)*-C_2-**2** were compared with the geometries obtained from single-crystal X-ray diffraction analyses, which showed a very good agreement.

In the nomenclature used herein to describe the chiral information in hextuple helicenes ***2****, the helicities of the three external [7]helicene units precede the helicities of the three internal [5]helicene units in going clockwise from the top external [7]helicene unit and from the top-right internal [5]helicene unit as illustrated in Figure S18 below with* (*M,M,M,P,P,P*)-D_3-**2** *(left),* (*P,M,P,P,P,M*)-C_2-**2** *(middle), and diastereomer (P,M,M,M,P,P)-*C_1-**2** *(right, diastereomer* ***C*** *in Table S5).*

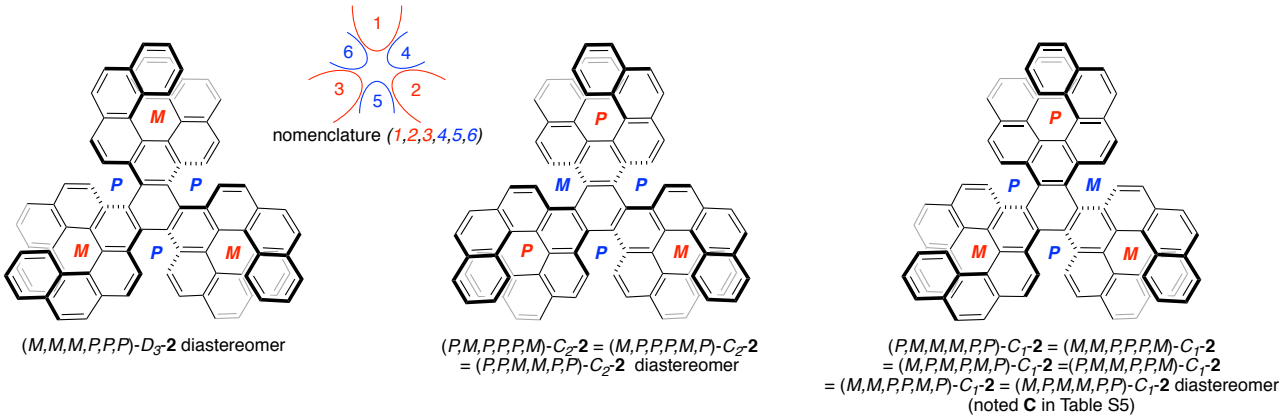


Figure S18. Proposed nomenclature for hextuple helicene **2**.

The hextuple helicene **2** can exist as 10 possible diastereomers: 2 of D_3 symmetry, 6 of C_2 symmetry, and 2 of C_1 symmetry, with relative energies ranking from 0.0 to 108.3 kJ/mol as listed below (Table S8). As expected, the (*M,M,M,P,P,P*)-D_3-**2** diastereomer was found to be the more stable (thermodynamic product), and the *(P,M,P,P,P,M)*-C_2-**2** diastereomer has a relative energy of +32.2 kJ.mol^{-1}.

[7] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

[8] S. Maeda, Y. Harabuchi, Y. Ono, T. Taketsugu, K. Morokuma, *Int. J. Quantum Chem.* **2015**, *115*, 258.

Table S8. Possible diastereomers of hextuple helicene **2**. B3LYP/6-31G(d) DFT calculations in the gas phase.

Diastereomer	ID	Relative free Gibbs energies in kJ.mol^{-1}	Symmetry
(*M,M,M,P,P,P*)	D_3-**2**	0.0	D_3
(*M,M,M,M,P,P*) (*M,M,M,P,P,M*) (*M,M,M,P,M,P*)	**B**	62.6	C_2
(*M,P,M,M,P,P*) (*P,M,M,P,P,M*) (*M,M,P,P,M,P*) (*M,P,M,P,M,P*) (*P,M,M,M,P,P*) (*M,M,P,P,P,M*)	**C**	46.8	C_1
(*P,P,M,M,P,P*) (*P,M,P,P,P,M*) (*M,P,P,P,M,P*)	C_2-**2**	32.2	C_2
(*M,P,M,P,P,P*) (*P,M,M,P,P,P*) (*M,M,P,P,P,P*)	**E**	31.3	C_2
(*M,P,P,P,P,P*) (*P,P,M,P,P,P*) (*P,M,P,P,P,P*)	**F**	62.5	C_2
(*M,M,M,M,P,M*) (*M,M,M,P,M,M*) (*M,M,M,M,M,P*)	**G**	76.5	C_2
(*P,P,M,P,P,M*) (*P,M,P,P,M,P*) (*M,P,P,M,P,P*) (*P,P,M,P,M,P*) (*P,M,P,M,P,P*) (*M,P,P,P,P,M*)	**H**	89.0	C_1
(*M,M,M,M,M,M*)	**I**	96.9	D_3
(*P,M,P,M,M,P*) (*M,P,P,M,P,M*) (*P,P,M,P,M,M*)	**J**	108.3	C_2

The most favorable enantiomerization path for (–)-*(M,M,M,P,P,P)-D*$_3$-**2** was calculated as illustrated in Figure S19. It is a symmetric process and the calculated enantiomerization barrier is $\Delta G^{\neq}$ = 160.6 kJ/mol (@ 25 ºC in the gas phase). Unexpectedly, an ephemeral high energy conformer **Int** (and **ent-Int**) could be located at step 2 (or 5) of the process with the configurational inversion of the corresponding external [7]helicene unit being calculated as a two-step process. This oddity was also found in the isomerization **H** → **G** (not shown). For the present study, no effort was pursued on this matter.[9]

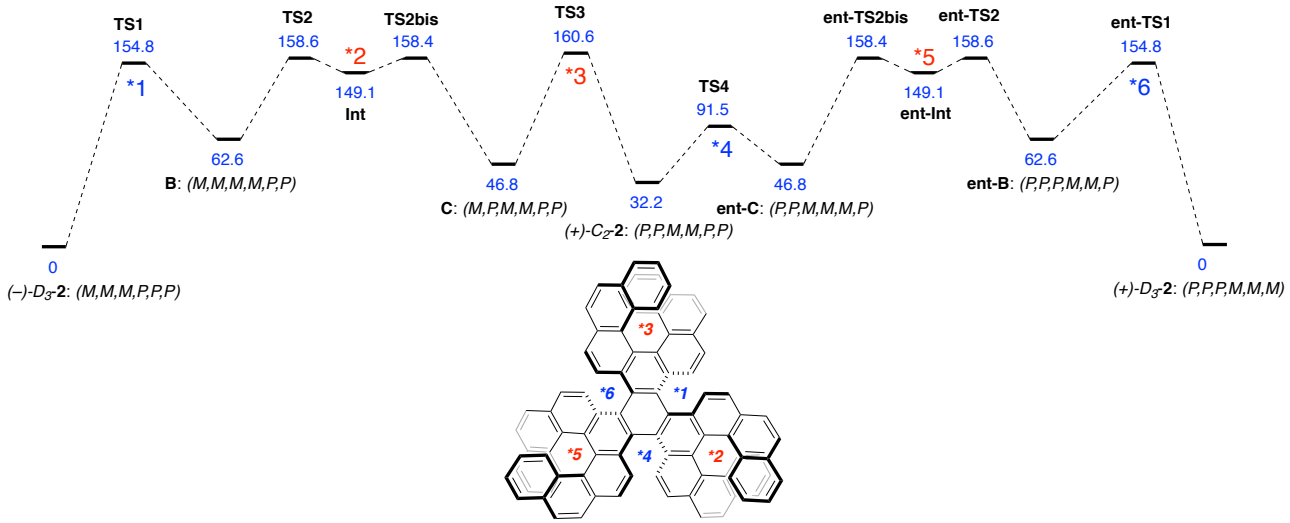


Figure S19. Enantiomerization path for (–)-*(M,M,M,P,P,P)-D*$_3$-**2**. B3LYP/6-31G(d) DFT calculations in the gas phase, relative free Gibbs energies are reported in kJ.mol^{-1}.

In our previous Communication we proposed an enantiomerization path for the lower-order analogue *D*$_3$-**HNTP** involving the alternative inversion of configuration of neighboring internal and external [5]helicene units, with an enantiomerization barrier calculated at $\Delta G^{\neq}$ = 163.8 kJ/mol (@ 25 ºC in the gas phase) for an experimentally determined barrier at $\Delta G^{\neq}$ = 147.0 kJ/mol (@ 182 ºC in 1,2-dichlorobenzene).[10] In light of the above results on the enantiomerization path of (–)-*(M,M,M,P,P,P)-D*$_3$-**2**, as well as the enantiomerization path of *D*$_3$-**HNTP** proposed by Tsuruzaki, Kamikawa and their co-workers,[11] we now confirm that the most favorable enantiomerization path for this lower-order analogue is indeed as determined by Tsuruzaki, Kamikawa and their co-workers. Our own recent calculations on the enantiomerization process of this lower-order analogue perfectly matched the previous calculations of Tsuruzaki, Kamikawa and their co-workers, and are summarized on Figure S20.

[9] Merino and co-workers recently demonstrated that [n]helicenes racemize by multi-step processes for n ≥ 8. See: J. Barroso, J. L. Cabellos, S. Pan, F. Murillo, X. Zarate, M. A. Fernandez-Herrera, G. Merino *Chem. Commun.* **2018**, *54*, 188.

[10] V. Berezhnaia, M. Roy, N. Vanthuyne, M. Villa, J.-V. Naubron, J. Rodriguez, Y. Coquerel, M. Gingras, *J. Am. Chem. Soc.* **2017**, *139*, 18508.

[11] T. Hosokawa, Y. Takahashi, T. Matsushima, S. Watanabe, S. Kikkawa, I. Azumaya, A. Tsurusaki, K. Kamikawa, *J. Am. Chem. Soc.* **2017**, *139*, 18512.

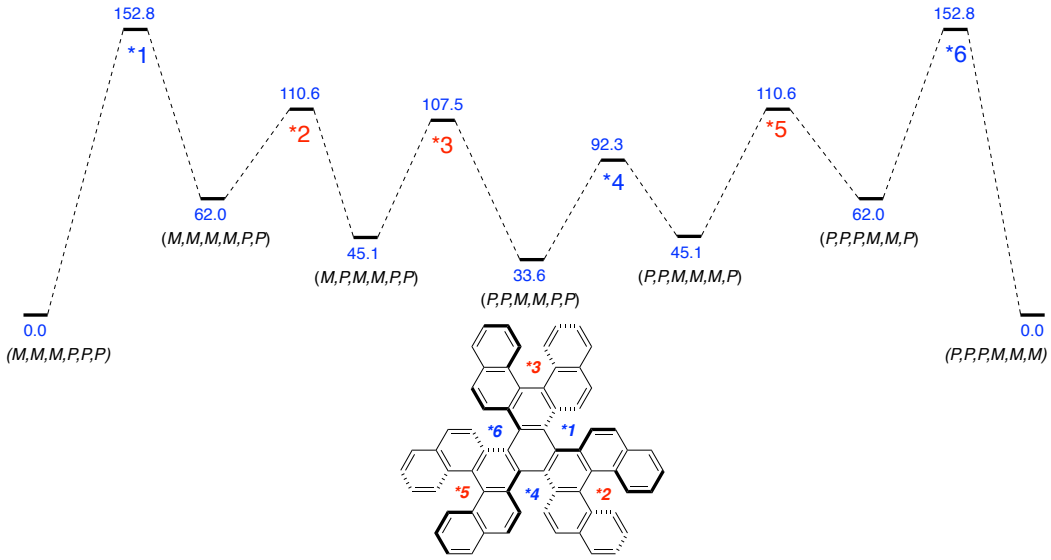
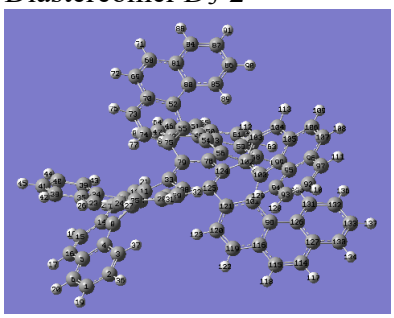


Figure S20. Enantiomerization path for the lower-order analogue *D*$_3$-**HNTP**. B3LYP/6-31G(d) DFT calculations in the gas phase, relative free Gibbs energies are reported in kJ.mol^{-1}.

Diastereomer *D*$_3$-**2**



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3	6	0	-4.680381	-3.821350	1.498867
4	6	0	-3.582618	-4.700781	1.673208
5	6	0	-3.847830	-5.945468	2.328102
6	6	0	-5.178179	-6.307384	2.648125
7	6	0	-3.660992	-3.234900	-1.325034
8	6	0	-2.204360	-4.358820	1.325089
9	6	0	-1.811253	-3.262048	0.473130
10	6	0	-2.697712	-2.577575	-0.474627
11	6	0	-0.486905	-2.759021	0.544105
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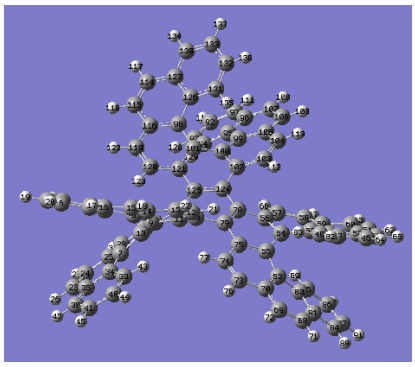
0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.628515

Diastereomer **B**



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73	6	0	1.309542	4.963635	0.332287
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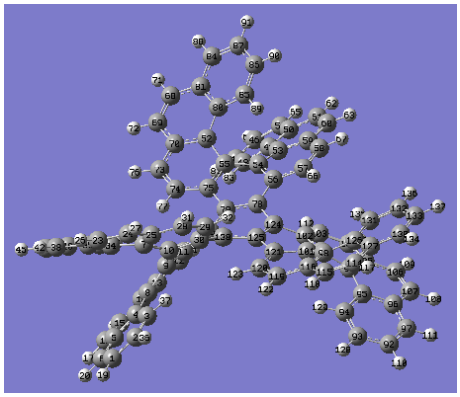
134	1	0	-2.871829	-8.992816	1.908643
135	1	0	-2.936425	-4.046545	2.151813
136	1	0	-4.530629	-5.346497	3.459571
137	1	0	-4.580241	-7.838878	3.289813
138	6	0	1.243380	-0.612690	-0.350151

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.604658

Diastereomer **C**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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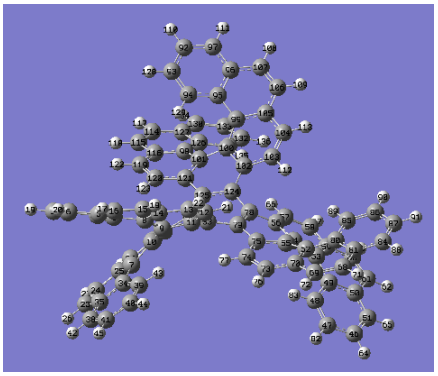
2	6	0	7.115376	2.131267	0.914695
3	6	0	5.733107	2.150729	0.896183
4	6	0	4.986172	3.025330	1.723709
5	6	0	5.724154	3.824593	2.653843
6	6	0	7.139161	3.810907	2.632185
7	6	0	3.897152	2.863810	-1.500448
8	6	0	3.525067	3.072325	1.745126
9	6	0	2.663505	2.492732	0.745755
10	6	0	3.053374	2.097191	-0.615539

11	6	0	1.301367	2.246162	1.060106
12	6	0	0.743489	2.792941	2.248775
13	6	0	1.512780	3.555440	3.084453
14	6	0	2.907749	3.700267	2.866325
15	6	0	3.685122	4.470221	3.789164
16	6	0	5.033795	4.578091	3.654975
17	1	0	5.615831	5.185550	4.343655
18	1	0	3.164426	4.977381	4.597817
19	1	0	8.919168	2.981114	1.768504
20	1	0	7.672225	4.445897	3.336059
21	1	0	-0.296235	2.595496	2.484714
22	1	0	1.075256	4.009019	3.970352
23	6	0	5.891713	4.065399	-3.166531
24	6	0	5.413174	2.828907	-3.465919
25	6	0	4.393940	2.216193	-2.668451
26	1	0	6.688506	4.513606	-3.754962
27	1	0	5.804812	2.269987	-4.312415
28	6	0	3.857984	0.965103	-3.065479
29	6	0	2.877719	0.352628	-2.333405
30	6	0	2.482138	0.879332	-1.073512
31	1	0	4.194774	0.527977	-4.002257
32	1	0	2.396399	-0.542334	-2.708720
33	6	0	0.546977	1.262803	0.295730
34	6	0	4.243246	4.274970	-1.326918
35	6	0	5.286424	4.840830	-2.127501
36	1	0	7.648041	1.439552	0.267708
37	1	0	5.215275	1.458325	0.247618
38	6	0	5.660078	6.194330	-1.950432
39	6	0	3.532235	5.163855	-0.482950
40	6	0	3.891233	6.492724	-0.353072
41	6	0	4.987310	7.011421	-1.066228
42	1	0	6.474003	6.588346	-2.554696
43	1	0	2.665616	4.809148	0.056290
44	1	0	3.312920	7.140192	0.300459
45	1	0	5.277205	8.051851	-0.947169
46	6	0	-7.756843	2.744971	2.677677
47	6	0	-6.379852	3.041954	2.651773
48	6	0	-5.514033	2.294370	1.877839
49	6	0	-5.971377	1.214258	1.080694
50	6	0	-7.357209	0.870392	1.176615
51	6	0	-8.228305	1.667105	1.959258
52	6	0	-3.974129	3.187013	-0.643543
53	6	0	-5.090907	0.390630	0.265078
54	6	0	-3.709813	0.719330	-0.035385
55	6	0	-3.173333	2.065856	-0.179584
56	6	0	-2.813254	-0.354175	-0.273458
57	6	0	-3.356200	-1.574249	-0.783441
58	6	0	-4.706389	-1.774412	-0.831101
59	6	0	-5.594817	-0.846700	-0.215347
60	6	0	-6.985353	-1.156460	-0.098901
61	6	0	-7.844124	-0.308763	0.532280
62	1	0	-8.903651	-0.542079	0.603987
63	1	0	-7.342186	-2.088357	-0.530884
64	1	0	-8.434408	3.343786	3.280217
65	1	0	-9.280565	1.395115	2.000126
66	1	0	-2.679192	-2.333230	-1.155889
67	1	0	-5.114042	-2.681511	-1.269840
68	6	0	-5.607341	5.493118	-1.059404
69	6	0	-4.349528	5.632934	-0.559756
70	6	0	-3.494855	4.497507	-0.388869
71	1	0	-6.267694	6.351035	-1.159633
72	1	0	-3.967183	6.609911	-0.274096
73	6	0	-2.134113	4.676710	-0.029109
74	6	0	-1.289205	3.607794	0.067465
75	6	0	-1.782630	2.268721	0.057067
76	1	0	-1.749729	5.688607	0.073619
77	1	0	-0.232395	3.789771	0.183945
78	6	0	-1.396098	-0.175831	-0.033586
79	6	0	-0.890071	1.121033	0.198955
80	6	0	-5.195821	3.081044	-1.435304
81	6	0	-6.037357	4.229925	-1.575195
82	1	0	-5.990376	3.859127	3.252899
83	1	0	-4.457926	2.528690	1.899862
84	6	0	-7.241820	4.136542	-2.313643
85	6	0	-5.537350	1.935993	-2.198276
86	6	0	-6.695724	1.883192	-2.949872
87	6	0	-7.580786	2.978003	-2.980145
88	1	0	-7.878412	5.016030	-2.377931

89	1	0	-4.858476	1.093922	-2.226919
90	1	0	-6.915763	0.991284	-3.530099
91	1	0	-8.500247	2.923267	-3.556648
92	6	0	2.814892	-7.823670	2.322823
93	6	0	3.218082	-6.555661	1.862288
94	6	0	2.280163	-5.595268	1.533828
95	6	0	0.888795	-5.843514	1.644407
96	6	0	0.496792	-7.087322	2.234586
97	6	0	1.473029	-8.072266	2.520240
98	6	0	1.760266	-4.621656	-1.206929
99	6	0	-0.136799	-4.855398	1.322539
100	6	0	0.054437	-3.685806	0.484456
101	6	0	1.154969	-3.540362	-0.459473
102	6	0	-0.811428	-2.570912	0.641970
103	6	0	-1.951118	-2.701727	1.492123
104	6	0	-2.281210	-3.906826	2.041858
105	6	0	-1.396562	-5.015200	1.958108
106	6	0	-1.750856	-6.259553	2.569553
107	6	0	-0.862613	-7.288683	2.631093
108	1	0	-1.144866	-8.245338	3.063825
109	1	0	-2.754425	-6.363629	2.974906
110	1	0	3.556280	-8.581950	2.559748
111	1	0	1.143393	-9.020469	2.938743
112	1	0	-2.569592	-1.837546	1.691331
113	1	0	-3.192201	-4.011147	2.626058
114	6	0	3.182740	-6.739690	-2.487097
115	6	0	3.822595	-5.576446	-2.186535
116	6	0	3.126451	-4.491078	-1.570043
117	1	0	3.719905	-7.568511	-2.941778
118	1	0	4.880616	-5.451855	-2.404178
119	6	0	3.808165	-3.279346	-1.274153
120	6	0	3.121684	-2.176674	-0.844673
121	6	0	1.723338	-2.238536	-0.560724
122	1	0	4.878743	-3.219803	-1.453123
123	1	0	3.653675	-1.248345	-0.698380
124	6	0	-0.469823	-1.293281	0.039941
125	6	0	0.877558	-1.070529	-0.338311
126	6	0	1.043439	-5.808140	-1.655072
127	6	0	1.776318	-6.874084	-2.267864
128	1	0	4.275374	-6.321259	1.774159
129	1	0	2.623974	-4.617549	1.223999
130	6	0	1.096773	-8.036732	-2.705690
131	6	0	-0.368068	-5.935758	-1.609212
132	6	0	-1.009892	-7.072060	-2.062220
133	6	0	-0.273102	-8.146811	-2.596621
134	1	0	1.680204	-8.838613	-3.152331
135	1	0	-0.964090	-5.117677	-1.227151
136	1	0	-2.093913	-7.129720	-2.012713
137	1	0	-0.782898	-9.041991	-2.942256
138	6	0	1.333773	0.302154	-0.373773

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.610678

Diastereomer C_2-**2**



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5	6	0	-0.582931	-6.975679	2.396249
6	6	0	-1.444831	-8.092941	2.288818
7	6	0	-0.173686	-4.723249	-1.628467
8	6	0	0.171064	-4.723314	1.628436
9	6	0	0.268774	-3.638805	0.683813
10	6	0	-0.270772	-3.638665	-0.683864
11	6	0	0.897894	-2.426131	1.071194
12	6	0	1.596727	-2.364821	2.307879
13	6	0	1.702474	-3.476112	3.099349
14	6	0	1.000507	-4.667910	2.786357
15	6	0	1.118579	-5.800172	3.654436
16	6	0	0.402802	-6.934217	3.432497
17	1	0	0.517183	-7.801674	4.077849
18	1	0	1.808067	-5.732076	4.492416
19	1	0	-3.155670	-8.962384	1.329383
20	1	0	-1.278013	-8.938930	2.951616
21	1	0	2.041915	-1.427903	2.620392
22	1	0	2.278367	-3.438152	4.020708
23	6	0	-0.406672	-6.934054	-3.432481
24	6	0	-1.121804	-5.799607	-3.654447
25	6	0	-1.003095	-4.667394	-2.786388
26	1	0	-0.521544	-7.801461	-4.077814
27	1	0	-1.811253	-5.731135	-4.492429
28	6	0	-1.704385	-3.475203	-3.099400
29	6	0	-1.598004	-2.363957	-2.307952
30	6	0	-0.899216	-2.425647	-1.071263
31	1	0	-2.280251	-3.436929	-4.020764
32	1	0	-2.042650	-1.426790	-2.620487
33	6	0	0.623167	-1.195963	0.330839
34	6	0	0.746416	-5.855849	-1.520706
35	6	0	0.579034	-6.976057	-2.396225
36	1	0	-3.584528	-6.934753	-0.067288
37	1	0	-2.104882	-5.009294	0.059217
38	6	0	1.440296	-8.093808	-2.288757
39	6	0	1.874843	-5.876912	-0.663741
40	6	0	2.723271	-6.966774	-0.599601
41	6	0	2.490899	-8.103338	-1.395350
42	1	0	1.273001	-8.939719	-2.951536
43	1	0	2.102065	-5.010489	-0.059210
44	1	0	3.580613	-6.936800	0.067366
45	1	0	3.150613	-8.964215	-1.329267
46	6	0	7.685534	2.854208	-2.729991
47	6	0	6.970676	1.724917	-2.286401
48	6	0	5.669835	1.847551	-1.836758
49	6	0	5.008520	3.101124	-1.801528
50	6	0	5.701873	4.217245	-2.369130
51	6	0	7.048445	4.075774	-2.783608
52	6	0	4.807465	1.474896	0.972081
53	6	0	3.631540	3.274381	-1.349928
54	6	0	2.894150	2.333109	-0.525690
55	6	0	3.526060	1.322681	0.313263
56	6	0	1.475283	2.331129	-0.589073
57	6	0	0.814035	3.395254	-1.273981
58	6	0	1.519519	4.448315	-1.780050
59	6	0	2.939705	4.417210	-1.830832
60	6	0	3.656090	5.507107	-2.419168
61	6	0	5.002128	5.441116	-2.609010
62	1	0	5.549178	6.283067	-3.026109
63	1	0	3.095742	6.394442	-2.703716
64	1	0	8.714698	2.754550	-3.064126
65	1	0	7.560532	4.948014	-3.183373
66	1	0	-0.263319	3.375699	-1.369192
67	1	0	1.000987	5.290276	-2.232168
68	6	0	7.452225	1.598312	2.039417
69	6	0	6.899766	0.393210	1.730405
70	6	0	5.566755	0.302040	1.222441
71	1	0	8.472651	1.664166	2.408984
72	1	0	7.465260	-0.526607	1.858768
73	6	0	4.998087	-0.968407	0.932678
74	6	0	3.675214	-1.084180	0.606664
75	6	0	2.857012	0.070245	0.412046
76	1	0	5.615099	-1.857409	1.035735
77	1	0	3.247446	-2.066686	0.468937
78	6	0	0.724046	1.213908	-0.050267

79	6	0	1.407970	0.016654	0.264101
80	6	0	5.338670	2.745576	1.446936
81	6	0	6.678468	2.797026	1.947825
82	1	0	7.437941	0.744215	-2.307633
83	1	0	5.134716	0.954701	-1.542630
84	6	0	7.213110	4.025320	2.407009
85	6	0	4.567237	3.931928	1.539811
86	6	0	5.104435	5.112686	2.014468
87	6	0	6.448553	5.172154	2.431071
88	1	0	8.240319	4.040167	2.764127
89	1	0	3.524469	3.911892	1.252461
90	1	0	4.478700	5.999075	2.074631
91	1	0	6.868791	6.106611	2.792901
92	6	0	-7.683816	2.858226	2.730148
93	6	0	-6.969552	1.728574	2.286518
94	6	0	-5.668670	1.850544	1.836813
95	6	0	-5.006727	3.103788	1.801566
96	6	0	-5.699482	4.220254	2.369209
97	6	0	-7.046109	4.079471	2.783739
98	6	0	-4.806663	1.477559	-0.972126
99	6	0	-3.629682	3.276339	1.349912
100	6	0	-2.892838	2.334688	0.525624
101	6	0	-3.525319	1.324632	-0.313350
102	6	0	-1.473973	2.331932	0.588984
103	6	0	-0.812134	3.395692	1.273898
104	6	0	-1.517031	4.449133	1.779992
105	6	0	-2.937232	4.418796	1.830811
106	6	0	-3.653028	5.509054	2.419188
107	6	0	-4.999094	5.443761	2.609079
108	1	0	-5.545688	6.285991	3.026209
109	1	0	-3.092206	6.396092	2.703735
110	1	0	-8.713015	2.759085	3.064328
111	1	0	-7.557733	4.951969	3.183534
112	1	0	0.265214	3.375554	1.369083
113	1	0	-0.998030	5.290810	2.232100
114	6	0	-7.451386	1.602404	-2.039391
115	6	0	-6.899555	0.396999	-1.730440
116	6	0	-5.566583	0.305112	-1.222502
117	1	0	-8.471787	1.668813	-2.408925
118	1	0	-7.465538	-0.522515	-1.858804
119	6	0	-4.998602	-0.965644	-0.932763
120	6	0	-3.675795	-1.082146	-0.606746
121	6	0	-2.856958	0.071826	-0.412139
122	1	0	-5.616102	-1.854311	-1.035807
123	1	0	-3.248566	-2.064883	-0.469010
124	6	0	-0.723353	1.214306	0.050168
125	6	0	-1.407941	0.017429	-0.264198
126	6	0	-5.337207	2.748537	-1.446929
127	6	0	-6.676995	2.800705	-1.947778
128	1	0	-7.437319	0.748111	2.307775
129	1	0	-5.134013	0.957424	1.542646
130	6	0	-7.211005	4.029294	-2.406907
131	6	0	-4.565152	3.934482	-1.539793
132	6	0	-5.101740	5.115536	-2.014406
133	6	0	-6.445842	5.175724	-2.430963
134	1	0	-8.238217	4.044697	-2.763994
135	1	0	-3.522388	3.913887	-1.252475
136	1	0	-4.475540	6.001596	-2.074563
137	1	0	-6.865596	6.110412	-2.792754
138	6	0	-0.623809	-1.195623	-0.330923

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0 negative eigenvalue
Sum of electronic and thermal Free Energies=       -3457.616248
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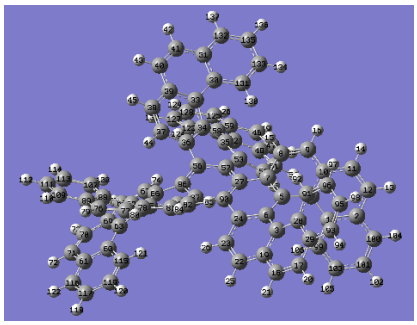
Diastereomer **E**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	7.210099	2.102601	-0.768614
3	6	0	4.885603	-1.583646	0.039766
4	6	0	4.887529	1.577672	-0.039789
5	6	0	3.713517	0.722922	0.074075
6	6	0	3.712635	-0.727484	-0.074040
7	6	0	2.474589	1.367901	0.331601
8	6	0	2.495247	2.633273	0.996117
9	6	0	3.672854	3.275461	1.252529
10	6	0	4.882874	2.808162	0.667734
11	6	0	6.080489	3.582506	0.779109
12	6	0	7.220705	3.211369	0.133763
13	1	0	8.133398	3.793315	0.235964
14	1	0	6.055853	4.479541	1.393161
15	1	0	1.561741	3.048810	1.355135
16	1	0	3.687827	4.189930	1.839750
17	6	0	7.216839	-3.220121	-0.133848
18	6	0	6.076174	-3.589877	-0.779191
19	6	0	4.879474	-2.814113	-0.667786
20	1	0	8.128835	-3.803154	-0.236076
21	1	0	6.050455	-4.486872	-1.393257
22	6	0	3.668874	-3.279970	-1.252510
23	6	0	2.492046	-2.636376	-0.996024
24	6	0	2.472918	-1.370979	-0.331513
25	1	0	3.682713	-4.194463	-1.839720
26	1	0	1.558034	-3.050805	-1.355001
27	6	0	1.208401	0.702930	0.057266
28	6	0	6.028521	-1.311546	0.899034
29	6	0	7.207562	-2.111371	0.768568
30	6	0	-2.968360	5.063746	1.798535
31	6	0	-3.993776	5.769925	2.504149
32	6	0	-1.695560	4.615348	-1.267197
33	6	0	-3.190737	3.666650	1.430416
34	6	0	-2.352383	2.902341	0.540292
35	6	0	-1.414425	3.471007	-0.433231
36	6	0	-2.392805	1.485710	0.582777
37	6	0	-3.436065	0.847383	1.309859
38	6	0	-4.396748	1.587208	1.944664
39	6	0	-4.292056	2.998622	2.036830
40	6	0	-5.284781	3.736447	2.757430
41	6	0	-5.172232	5.080168	2.931981
42	1	0	-5.942071	5.640621	3.456728
43	1	0	-6.138985	3.193184	3.154257
44	1	0	-3.464984	-0.233170	1.366442
45	1	0	-5.218122	1.091539	2.456262
46	6	0	-1.979232	7.111320	-2.636415
47	6	0	-0.760774	6.512748	-2.563208
48	6	0	-0.596795	5.248127	-1.912882
49	1	0	-2.095552	8.085642	-3.104681
50	1	0	0.120180	6.987874	-2.988015
51	6	0	0.665158	4.603270	-1.940949
52	6	0	0.848241	3.379553	-1.357535
53	6	0	-0.173497	2.793243	-0.557495
54	1	0	1.473384	5.064796	-2.502918
55	1	0	1.779043	2.851411	-1.512282
56	6	0	-1.254438	0.713724	0.078389
57	6	0	-0.038314	1.418629	-0.055992
58	6	0	-3.028924	5.146684	-1.548350
59	6	0	-3.149542	6.424488	-2.182168
60	6	0	-2.974726	-5.060043	-1.798510
61	6	0	-4.001048	-5.764924	-2.504110

62	6	0	-1.701238	-4.613337	1.267174
63	6	0	-3.195345	-3.662685	-1.430340
64	6	0	-2.356001	-2.899447	-0.540226
65	6	0	-1.418719	-3.469305	0.433249
66	6	0	-2.394651	-1.482765	-0.582684
67	6	0	-3.437111	-0.843117	-1.309747
68	6	0	-4.398740	-1.581716	-1.944543
69	6	0	-4.295836	-2.993261	-2.036716
70	6	0	-5.289510	-3.729824	-2.757300
71	6	0	-5.178659	-5.073683	-2.931874
72	1	0	-5.949220	-5.633162	-3.456601
73	1	0	-6.143042	-3.185479	-3.154090
74	1	0	-3.464656	0.237471	-1.366327
75	1	0	-5.219492	-1.085001	-2.456127
76	6	0	-1.987936	-7.109047	2.636234
77	6	0	-0.768752	-6.511953	2.563065
78	6	0	-0.603240	-5.247491	1.912815
79	1	0	-2.105438	-8.083262	3.104429
80	1	0	0.111626	-6.988178	2.987834
81	6	0	0.659496	-4.604173	1.940914
82	6	0	0.844064	-3.380653	1.357554
83	6	0	-0.176953	-2.793073	0.557527
84	1	0	1.467161	-5.066705	2.502863
85	1	0	1.775507	-2.853647	1.512321
86	6	0	-1.255319	-0.712202	-0.078299
87	6	0	-0.040070	-1.418616	0.056058
88	6	0	-3.035246	-5.143055	1.548324
89	6	0	-3.157413	-6.420753	2.182057
90	6	0	1.207535	-0.704464	-0.057178
91	6	0	5.997451	-0.369479	1.958557
92	1	0	5.084559	0.177313	2.155624
93	6	0	8.329973	-1.850122	1.591969
94	1	0	9.222973	-2.455963	1.456205
95	6	0	8.285611	-0.880093	2.570600
96	6	0	7.093380	-0.156446	2.771600
97	1	0	7.028324	0.568039	3.578763
98	1	0	9.149455	-0.697714	3.204051
99	6	0	5.997900	0.362122	-1.958558
100	6	0	8.332192	1.840000	-1.592022
101	6	0	8.286668	0.870001	-2.570626
102	1	0	9.150289	0.686573	-3.204078
103	6	0	7.093571	0.147768	-2.771598
104	1	0	9.225910	2.444785	-1.456279
105	1	0	7.027653	-0.576658	-3.578745
106	1	0	5.084362	-0.183601	-2.155599
107	6	0	-4.234091	-4.418199	1.333543
108	1	0	-4.185866	-3.404718	0.960449
109	6	0	-4.438761	-6.965098	2.437173
110	1	0	-4.499306	-7.949230	2.896191
111	6	0	-5.586239	-6.255512	2.151542
112	1	0	-6.563994	-6.680253	2.362047
113	6	0	-5.474293	-4.955848	1.624117
114	1	0	-6.367330	-4.361569	1.450504
115	6	0	-1.751139	-5.744847	-1.591821
116	6	0	-3.817173	-7.125667	-2.847058
117	6	0	-2.633529	-7.777851	-2.571942
118	1	0	-2.501535	-8.820314	-2.848650
119	6	0	-1.582871	-7.065332	-1.964894
120	1	0	-0.625824	-7.550595	-1.793501
121	1	0	-0.912961	-5.219781	-1.155251
122	1	0	-4.624085	-7.642002	-3.362000
123	6	0	-4.228648	4.423315	-1.333474
124	1	0	-4.181648	3.409803	-0.960306
125	6	0	-4.430231	6.970382	-2.437276
126	1	0	-4.489589	7.954558	-2.896354
127	6	0	-5.468202	4.962465	-1.624036
128	6	0	-5.578570	6.262225	-2.151554
129	1	0	-6.555809	6.688153	-2.362052
130	1	0	-6.361960	4.369297	-1.450342
131	6	0	-1.743942	5.747029	1.591742
132	6	0	-3.808197	7.130455	2.847025
133	6	0	-1.574023	7.067326	1.964729
134	1	0	-0.616391	7.551402	1.793248
135	6	0	-2.623767	7.781168	2.571804
136	1	0	-2.490477	8.823483	2.848449
137	1	0	-4.614444	7.647811	3.361985
138	1	0	-0.906446	5.220896	1.155148

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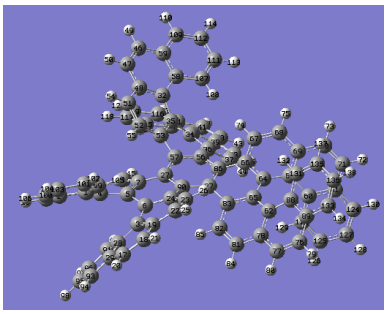
0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.616655

Diastereomer **F**



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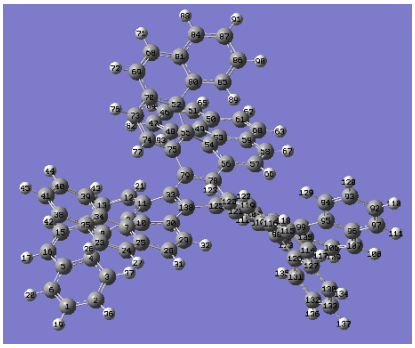
3	6	0	-3.526222	-3.741113	-0.074944
4	6	0	-5.069099	-0.982533	-0.064145
5	6	0	-3.624197	-1.157264	-0.135281
6	6	0	-2.920514	-2.420479	0.038511
7	6	0	-2.848540	0.010603	-0.360300
8	6	0	-3.463342	1.119935	-1.019936
9	6	0	-4.795398	1.109644	-1.320296
10	6	0	-5.641357	0.100445	-0.781163
11	6	0	-7.059730	0.190859	-0.943543
12	6	0	-7.895224	-0.695556	-0.335058
13	1	0	-8.971526	-0.634178	-0.476243
14	1	0	-7.454490	0.990438	-1.565767
15	1	0	-2.841150	1.944658	-1.344988
16	1	0	-5.236219	1.911126	-1.907382
17	6	0	-4.767577	-6.305244	0.081837
18	6	0	-3.623196	-6.059021	0.778062
19	6	0	-2.954905	-4.798800	0.678458
20	1	0	-5.281233	-7.259135	0.173686
21	1	0	-3.190791	-6.819271	1.424081
22	6	0	-1.703744	-4.597671	1.326433
23	6	0	-0.973083	-3.473076	1.070227
24	6	0	-1.530997	-2.377934	0.337200
25	1	0	-1.302618	-5.383569	1.960958
26	1	0	0.021795	-3.371115	1.484924
27	6	0	-1.423401	0.035439	-0.066758
28	6	0	-4.621347	-4.072165	-0.973691
29	6	0	-5.262392	-5.346055	-0.855153
30	6	0	-0.011507	5.929492	-1.679868
31	6	0	0.506135	7.065142	-2.380848
32	6	0	-0.783742	4.823935	1.386146
33	6	0	0.879153	4.807295	-1.386702
34	6	0	0.567153	3.707753	-0.506287
35	6	0	-0.494151	3.718360	0.505663
36	6	0	1.293036	2.492961	-0.607545
37	6	0	2.461339	2.458480	-1.420187
38	6	0	2.901781	3.585904	-2.058361
39	6	0	2.129695	4.774896	-2.065424
40	6	0	2.602760	5.921576	-2.779840
41	6	0	1.846985	7.047213	-2.880409
42	1	0	2.221192	7.926020	-3.399824
43	1	0	3.590237	5.871258	-3.232256
44	1	0	3.002567	1.530305	-1.544731
45	1	0	3.822885	3.559612	-2.635385
46	6	0	-1.705606	7.082898	2.880219
47	6	0	-2.484163	5.972884	2.779631
48	6	0	-2.034625	4.816930	2.064979
49	1	0	-2.061766	7.969051	3.399841
50	1	0	-3.472381	5.942574	3.232205
51	6	0	-2.830648	3.643860	2.057724
52	6	0	-2.413189	2.507724	1.419512
53	6	0	-1.244297	2.518343	0.606964
54	1	0	-3.752082	3.636149	2.634774
55	1	0	-2.973357	1.590875	1.544270

56	6	0	0.712121	1.253467	−0.075666
57	6	0	−0.688351	1.267317	0.075204
58	6	0	0.129589	5.927774	1.679244
59	6	0	−0.364791	7.073641	2.380384
60	6	0	5.925809	−1.895219	−0.761632
61	6	0	7.342073	−1.803241	−0.579871
62	6	0	3.451602	−3.809114	0.073204
63	6	0	5.048039	−1.080920	0.066141
64	6	0	3.599977	−1.227742	0.136091
65	6	0	2.871952	−2.476841	−0.039518
66	6	0	2.847012	−0.045116	0.361053
67	6	0	3.482720	1.051938	1.021398
68	6	0	4.814120	1.015812	1.322710
69	6	0	5.640691	−0.009537	0.784023
70	6	0	7.060433	0.053013	0.947749
71	6	0	7.878949	−0.849510	0.339894
72	1	0	8.956101	−0.809398	0.482215
73	1	0	7.470202	0.844472	1.570638
74	1	0	2.876438	1.888521	1.346291
75	1	0	5.269987	1.808461	1.910298
76	6	0	4.642893	−6.396850	−0.085155
77	6	0	3.504119	−6.127640	−0.782073
78	6	0	2.860438	−4.854724	−0.681714
79	1	0	5.137874	−7.360515	−0.177454
80	1	0	3.057453	−6.878694	−1.429146
81	6	0	1.613852	−4.628791	−1.330295
82	6	0	0.905012	−3.490423	−1.073455
83	6	0	1.483735	−2.406998	−0.339184
84	1	0	1.197940	−5.406227	−1.965714
85	1	0	−0.087609	−3.368775	−1.488304
86	6	0	1.422870	0.007525	0.066508
87	6	0	0.711675	−1.204316	−0.047872
88	6	0	4.539242	−4.162426	0.972513
89	6	0	5.155537	−5.448387	0.853173
90	6	0	−0.735915	−1.190188	0.046591
91	6	0	−5.017899	−3.243912	−2.054631
92	1	0	−4.485740	−2.319489	−2.237576
93	6	0	−6.335049	−5.677100	−1.718934
94	1	0	−6.821007	−6.641961	−1.593199
95	6	0	−6.735092	−4.818487	−2.720444
96	6	0	−6.046438	−3.602630	−2.903372
97	1	0	−6.316544	−2.944857	−3.724987
98	1	0	−7.552249	−5.089209	−3.383567
99	6	0	−5.511187	−2.582885	1.842621
100	6	0	−8.255354	−2.436572	1.377483
101	6	0	−6.390718	−3.303170	2.626846
102	1	0	−6.008112	−3.899939	3.450323
103	6	0	−7.776538	−3.257750	2.375979
104	1	0	−8.462282	−3.838552	2.986859
105	1	0	−4.455548	−2.610224	2.079489
106	1	0	−9.325139	−2.346077	1.203547
107	6	0	1.519877	5.894603	1.405638
108	1	0	1.957391	5.006016	0.972703
109	6	0	0.495838	8.164529	2.649442
110	1	0	0.085368	9.031536	3.161979
111	6	0	2.348671	6.959025	1.708324
112	6	0	1.831392	8.121942	2.308179
113	1	0	3.410145	6.888595	1.486694
114	1	0	2.483754	8.962497	2.528705
115	6	0	−1.402192	5.924502	−1.406386
116	6	0	−0.332220	8.173226	−2.649989
117	6	0	−2.209288	7.005396	−1.709370
118	1	0	−3.272010	6.956428	−1.487941
119	6	0	−1.668470	8.157602	−2.309104
120	1	0	−2.303646	9.011181	−2.529783
121	1	0	−1.857585	5.045054	−0.973202
122	1	0	0.095820	9.031819	−3.162321
123	6	0	5.460550	−2.688238	−1.841394
124	6	0	8.206562	−2.596323	−1.373322
125	6	0	6.326555	−3.425004	−2.625356
126	1	0	5.933131	−4.013459	−3.449721
127	6	0	7.712734	−3.407103	−2.373008
128	1	0	8.387559	−4.000788	−2.983661
129	1	0	4.404794	−2.694742	−2.079249
130	1	0	9.277745	−2.527026	−1.198236
131	6	0	4.950817	−3.343184	2.054731
132	1	0	4.436710	−2.408703	2.238355
133	6	0	6.220709	−5.801199	1.717619

134	1	0	6.687884	-6.775228	1.591345
135	6	0	5.971236	-3.722857	2.904162
136	6	0	6.636287	-4.951679	2.720563
137	1	0	6.253190	-3.071463	3.726884
138	1	0	7.447288	-5.239011	3.384256

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.604721

Diastereomer **G**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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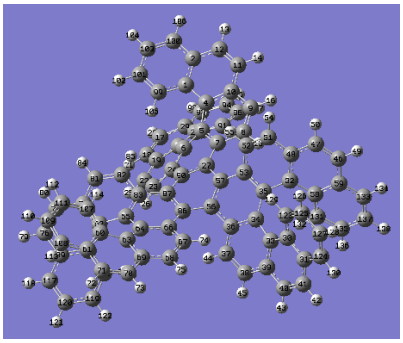
3	6	0	-2.393678	-5.465174	-1.953609
4	6	0	-3.578559	-4.688544	-1.897913
5	6	0	-4.760778	-5.266139	-2.461409
6	6	0	-4.751759	-6.615603	-2.890383
7	6	0	-1.909709	-4.677209	0.853607
8	6	0	-3.616601	-3.306917	-1.429566
9	6	0	-2.603946	-2.671351	-0.604368
10	6	0	-1.649199	-3.402723	0.214497
11	6	0	-2.469718	-1.258282	-0.648574
12	6	0	-3.467589	-0.490418	-1.322272
13	6	0	-4.584172	-1.086933	-1.831651
14	6	0	-4.690247	-2.503434	-1.895373
15	6	0	-5.848027	-3.105466	-2.482101
16	6	0	-5.913531	-4.449804	-2.684254
17	1	0	-6.807330	-4.909280	-3.099132
18	1	0	-6.679098	-2.459377	-2.754511
19	1	0	-3.597883	-8.396632	-3.201242
20	1	0	-5.672378	-7.038244	-3.286290
21	1	0	-3.346631	0.581442	-1.403449
22	1	0	-5.374492	-0.485967	-2.274809
23	6	0	-2.261936	-7.311804	1.892382
24	6	0	-1.016875	-6.873878	1.558137
25	6	0	-0.810573	-5.549363	1.063150
26	1	0	-2.416749	-8.325719	2.253231
27	1	0	-0.153111	-7.527004	1.656422
28	6	0	0.498598	-5.101942	0.733917
29	6	0	0.733671	-3.788867	0.434534
30	6	0	-0.338547	-2.850469	0.309989
31	1	0	1.325619	-5.805476	0.784500
32	1	0	1.747845	-3.464866	0.255210
33	6	0	-1.296572	-0.622115	-0.085401
34	6	0	-3.215483	-5.091761	1.347453
35	6	0	-3.383076	-6.426915	1.835992
36	1	0	-1.467562	-7.324227	-2.454602
37	1	0	-1.451152	-5.020056	-1.664475
38	6	0	-4.647262	-6.849616	2.314436
39	6	0	-4.323687	-4.214721	1.468493
40	6	0	-5.540692	-4.645430	1.959671
41	6	0	-5.717368	-5.982324	2.366641
42	1	0	-4.751173	-7.874821	2.662341
43	1	0	-4.213341	-3.175390	1.188648
44	1	0	-6.364337	-3.941177	2.040632
45	1	0	-6.680298	-6.317571	2.742266
46	6	0	-4.701987	6.846530	-2.331721
47	6	0	-4.738162	5.491667	-1.948060

48	6	0	-3.603695	4.866135	-1.468862
49	6	0	-2.370764	5.554639	-1.338296
50	6	0	-2.325667	6.907404	-1.804757
51	6	0	-3.508136	7.532804	-2.269829
52	6	0	-3.043590	3.828938	1.416035
53	6	0	-1.145795	4.930599	-0.857588
54	6	0	-1.089038	3.623792	-0.233682
55	6	0	-2.147408	3.047121	0.581349
56	6	0	0.117092	2.870937	-0.337370
57	6	0	1.324019	3.628393	-0.461061
58	6	0	1.299429	4.965128	-0.746855
59	6	0	0.077146	5.619645	-1.062540
60	6	0	0.082874	6.967166	-1.538091
61	6	0	-1.078087	7.603396	-1.855745
62	1	0	-1.071220	8.634570	-2.200431
63	1	0	1.039484	7.475245	-1.632844
64	1	0	-5.600368	7.336129	-2.697678
65	1	0	-3.449376	8.567135	-2.600925
66	1	0	2.274889	3.146485	-0.290998
67	1	0	2.227907	5.528181	-0.795477
68	6	0	-5.122567	5.313175	2.693326
69	6	0	-5.276580	3.978851	2.473785
70	6	0	-4.232566	3.204503	1.875915
71	1	0	-5.929411	5.906082	3.117100
72	1	0	-6.201105	3.472738	2.741043
73	6	0	-4.356103	1.790173	1.797498
74	6	0	-3.349515	1.026928	1.281468
75	6	0	-2.240882	1.630695	0.613327
76	1	0	-5.232441	1.319589	2.236523
77	1	0	-3.401883	-0.050949	1.355339
78	6	0	0.060531	1.415092	-0.255008
79	6	0	-1.182234	0.820169	0.046980
80	6	0	-2.781096	5.179855	1.901305
81	6	0	-3.852634	5.934114	2.477461
82	1	0	-5.662715	4.927656	-2.037396
83	1	0	-3.658012	3.817753	-1.206993
84	6	0	-3.623766	7.257854	2.925240
85	6	0	-1.485615	5.752694	1.962668
86	6	0	-1.278945	7.030772	2.445315
87	6	0	-2.361091	7.810808	2.896829
88	1	0	-4.462875	7.818686	3.330441
89	1	0	-0.628355	5.164661	1.663609
90	1	0	-0.268876	7.429102	2.486111
91	1	0	-2.194526	8.822585	3.256440
92	6	0	8.469174	1.415746	1.569809
93	6	0	7.255944	1.012082	2.162380
94	6	0	6.118106	0.856524	1.395534
95	6	0	6.125139	1.092483	-0.002834
96	6	0	7.335225	1.596515	-0.576510
97	6	0	8.497733	1.713526	0.224073
98	6	0	4.715204	-1.742416	0.831248
99	6	0	4.937854	0.973210	-0.834771
100	6	0	3.710093	0.290648	-0.440956
101	6	0	3.614412	-0.872875	0.430659
102	6	0	2.499802	0.854926	-0.933583
103	6	0	2.532469	1.614755	-2.143887
104	6	0	3.717595	1.892305	-2.762286
105	6	0	4.945521	1.654842	-2.080542
106	6	0	6.174560	2.138686	-2.629958
107	6	0	7.339812	2.057220	-1.929428
108	1	0	8.273512	2.413276	-2.357867
109	1	0	6.152646	2.582365	-3.622452
110	1	0	9.364797	1.522309	2.175835
111	1	0	9.411518	2.076227	-0.241073
112	1	0	1.591372	1.907294	-2.596218
113	1	0	3.736668	2.377771	-3.734478
114	6	0	6.906990	-3.195640	1.939191
115	6	0	5.740201	-3.087910	2.633681
116	6	0	4.606982	-2.415112	2.077051
117	1	0	7.769579	-3.695570	2.372887
118	1	0	5.642394	-3.520529	3.626501
119	6	0	3.352714	-2.454275	2.751266
120	6	0	2.230775	-1.992003	2.125422
121	6	0	2.327055	-1.237070	0.915662
122	1	0	3.288417	-2.936617	3.723039
123	1	0	1.252176	-2.130830	2.571323
124	6	0	1.220240	0.534109	-0.330242
125	6	0	1.118825	-0.717939	0.303607

126	6	0	5.871981	-2.051825	0.005764
127	6	0	6.982771	-2.742593	0.585729
128	1	0	7.209055	0.831016	3.232721
129	1	0	5.192599	0.575013	1.880795
130	6	0	8.115561	-3.044361	-0.209143
131	6	0	5.909025	-1.819840	-1.392671
132	6	0	7.010395	-2.157273	-2.154240
133	6	0	8.140879	-2.748377	-1.555415
134	1	0	8.957725	-3.547289	0.260692
135	1	0	5.042647	-1.394112	-1.881997
136	1	0	6.997773	-1.973230	-3.225026
137	1	0	9.010777	-2.997648	-2.157008
138	6	0	-0.164469	-1.404744	0.221658

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.599372

Diastereomer **H**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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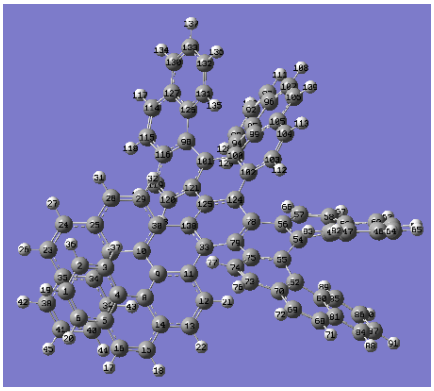
4	6	0	-0.821151	4.901390	1.124029
5	6	0	-0.788381	3.658475	0.383023
6	6	0	-1.798314	3.229438	-0.572619
7	6	0	0.359363	2.819211	0.500246
8	6	0	1.593506	3.491540	0.763571
9	6	0	1.621734	4.792343	1.185920
10	6	0	0.418826	5.485765	1.490411
11	6	0	0.462615	6.774493	2.106091
12	6	0	-0.682238	7.449757	2.400802
13	1	0	-0.644214	8.437205	2.854355
14	1	0	1.435464	7.207009	2.326987
15	1	0	2.527161	2.976919	0.599230
16	1	0	2.574420	5.289542	1.349259
17	6	0	-4.381969	5.861900	-2.770151
18	6	0	-4.623639	4.523922	-2.711201
19	6	0	-3.697082	3.634137	-2.080691
20	1	0	-5.104011	6.541129	-3.216724
21	1	0	-5.532852	4.102040	-3.132710
22	6	0	-3.895541	2.229478	-2.164492
23	6	0	-3.012279	1.360096	-1.593004
24	6	0	-1.980351	1.829881	-0.724896
25	1	0	-4.722854	1.855803	-2.762830
26	1	0	-3.105752	0.300020	-1.785827
27	6	0	0.210106	1.378087	0.309308
28	6	0	-2.156838	5.510277	-1.743695
29	6	0	-3.117052	6.381174	-2.350913
30	6	0	5.741092	-2.513535	-0.208195
31	6	0	6.774259	-3.267988	-0.848901
32	6	0	5.046501	0.538457	0.722691
33	6	0	4.561616	-2.129119	-0.969432
34	6	0	3.546140	-1.183407	-0.520215
35	6	0	3.758543	-0.044094	0.364047
36	6	0	2.214372	-1.452284	-0.941992
37	6	0	1.991205	-2.243263	-2.110804
38	6	0	3.040945	-2.793087	-2.788087
39	6	0	4.337129	-2.807557	-2.197447
40	6	0	5.394110	-3.547666	-2.815882

41	6	0	6.593886	-3.716479	-2.193942
42	1	0	7.399289	-4.265512	-2.675523
43	1	0	5.210442	-3.980121	-3.796481
44	1	0	0.977364	-2.337746	-2.485043
45	1	0	2.887175	-3.302431	-3.735847
46	6	0	7.563358	1.427814	1.729672
47	6	0	6.441559	1.553871	2.492009
48	6	0	5.158543	1.168446	1.990137
49	1	0	8.537509	1.710441	2.121123
50	1	0	6.497132	1.959536	3.499359
51	6	0	3.982636	1.447136	2.744083
52	6	0	2.754189	1.276783	2.171629
53	6	0	2.614362	0.589131	0.926658
54	1	0	4.078082	1.879830	3.736454
55	1	0	1.856323	1.607255	2.682070
56	6	0	1.078756	-0.827133	-0.300798
57	6	0	1.293191	0.400359	0.351422
58	6	0	6.198604	0.604820	-0.161929
59	6	0	7.464210	1.014321	0.365193
60	6	0	-3.102202	-5.130662	1.576355
61	6	0	-3.288805	-6.534960	1.779759
62	6	0	-4.276759	-2.817407	-0.255691
63	6	0	-1.966464	-4.673147	0.781324
64	6	0	-1.795044	-3.328363	0.256043
65	6	0	-2.915496	-2.422309	0.054554
66	6	0	-0.474821	-2.840133	0.020143
67	6	0	0.601985	-3.775982	0.089226
68	6	0	0.375740	-5.113905	0.246339
69	6	0	-0.910696	-5.600268	0.593205
70	6	0	-1.115935	-6.997788	0.824661
71	6	0	-2.295460	-7.457794	1.323041
72	1	0	-2.463763	-8.521963	1.469117
73	1	0	-0.304758	-7.681530	0.586429
74	1	0	1.620382	-3.436905	-0.006017
75	1	0	1.205840	-5.814828	0.204134
76	6	0	-7.018521	-3.548591	-0.550233
77	6	0	-6.689664	-2.369300	0.046070
78	6	0	-5.325492	-1.963505	0.175994
79	1	0	-8.057108	-3.859768	-0.632040
80	1	0	-7.461273	-1.712098	0.439850
81	6	0	-5.008870	-0.703389	0.760173
82	6	0	-3.730315	-0.224620	0.721687
83	6	0	-2.655786	-1.042422	0.252463
84	1	0	-5.812889	-0.095040	1.166364
85	1	0	-3.513564	0.777864	1.069615
86	6	0	-0.254264	-1.409044	-0.196582
87	6	0	-1.327399	-0.522023	0.007640
88	6	0	-4.632029	-3.995109	-1.033926
89	6	0	-6.009290	-4.368132	-1.143897
90	6	0	-1.062413	0.904802	-0.087025
91	6	0	-0.834688	6.004307	-1.611757
92	1	0	-0.046119	5.337527	-1.290049
93	6	0	-2.773093	7.725969	-2.630858
94	6	0	-1.495177	8.194897	-2.411214
95	1	0	-1.238920	9.225000	-2.643632
96	6	0	-0.510586	7.308406	-1.934500
97	1	0	0.517272	7.644446	-1.828970
98	1	0	-3.531892	8.374388	-3.062930
99	6	0	-3.325747	4.952911	1.503837
100	6	0	-3.139190	7.505713	2.604492
101	6	0	-4.459004	5.605278	1.949089
102	1	0	-5.421933	5.104940	1.891056
103	6	0	-4.374104	6.904487	2.486468
104	1	0	-5.270502	7.416101	2.826223
105	1	0	-3.421017	3.947126	1.116880
106	1	0	-3.047263	8.492795	3.051875
107	6	0	-3.964547	-4.257603	2.286602
108	6	0	-4.399764	-6.999041	2.524782
109	6	0	-5.264363	-6.117413	3.138430
110	1	0	-6.104689	-6.485317	3.720907
111	6	0	-5.015704	-4.734393	3.046348
112	1	0	-5.646347	-4.032785	3.585496
113	1	0	-4.534573	-8.072364	2.637388
114	1	0	-3.776273	-3.192185	2.268383
115	6	0	-3.693471	-4.749144	-1.783763
116	1	0	-2.654832	-4.445806	-1.794798
117	6	0	-6.371131	-5.515126	-1.891860
118	1	0	-7.422789	-5.787593	-1.943717

119	6	0	-4.074971	-5.849693	-2.525934
120	6	0	-5.423373	-6.256208	-2.564647
121	1	0	-5.715202	-7.129540	-3.141603
122	1	0	-3.327177	-6.398739	-3.091780
123	6	0	5.866059	-2.297510	1.187554
124	6	0	7.928960	-3.641299	-0.118702
125	6	0	6.984444	-2.706205	1.887171
126	1	0	7.038955	-2.532202	2.958291
127	6	0	8.044775	-3.356700	1.225300
128	1	0	8.929474	-3.661404	1.777771
129	1	0	5.052877	-1.828479	1.725743
130	1	0	8.712216	-4.191169	-0.635437
131	6	0	6.110925	0.404833	-1.563187
132	1	0	5.147832	0.192225	-2.009098
133	6	0	8.592497	1.081208	-0.488322
134	1	0	9.548740	1.372407	-0.059699
135	6	0	7.219039	0.509718	-2.380381
136	1	0	7.111090	0.359359	-3.451078
137	6	0	8.481516	0.822888	-1.838019
138	1	0	9.352495	0.890591	-2.484228

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.594611

Diastereomer **I**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	6	0	-5.885733	1.991332	0.824148
5	6	0	-7.304394	1.926613	0.647928
6	6	0	-8.153134	2.693508	1.483277
7	6	0	-3.385312	3.905724	0.046940
8	6	0	-5.024855	1.206055	-0.046981
9	6	0	-3.573639	1.330830	-0.108954
10	6	0	-2.826611	2.560355	0.107230
11	6	0	-2.841621	0.143696	-0.382598
12	6	0	-3.494330	-0.891491	-1.124537
13	6	0	-4.822230	-0.810219	-1.430825
14	6	0	-5.635383	0.187171	-0.822391
15	6	0	-7.056375	0.151285	-0.979224
16	6	0	-7.859452	1.028399	-0.315392
17	1	0	-8.938015	1.009065	-0.451348
18	1	0	-7.480495	-0.598769	-1.642419
19	1	0	-8.304806	4.027788	3.155086
20	1	0	-9.226265	2.646247	1.312770
21	1	0	-2.902076	-1.712209	-1.509150
22	1	0	-5.286482	-1.552004	-2.075276
23	6	0	-4.533155	6.503680	0.316509
24	6	0	-3.385210	6.194033	0.980894
25	6	0	-2.762454	4.916379	0.823193
26	1	0	-5.012266	7.470158	0.452607
27	1	0	-2.914748	6.915590	1.644450
28	6	0	-1.502271	4.653930	1.430971
29	6	0	-0.817797	3.513523	1.123253
30	6	0	-1.435623	2.457589	0.380447
31	1	0	-1.057718	5.407447	2.075763

32	1	0	0.183865	3.366172	1.506982
33	6	0	-1.422990	0.046157	-0.063948
34	6	0	-4.479408	4.308485	-0.823222
35	6	0	-5.074926	5.597750	-0.647134
36	1	0	-5.846933	3.991187	3.601328
37	1	0	-4.345027	2.715074	2.162362
38	6	0	-6.145975	5.998284	-1.483157
39	6	0	-4.914468	3.538632	-1.932172
40	6	0	-5.938845	3.965592	-2.753948
41	6	0	-6.585403	5.194396	-2.513195
42	1	0	-6.597501	6.973106	-1.313535
43	1	0	-4.414211	2.606345	-2.159726
44	1	0	-6.238680	3.351624	-3.598815
45	1	0	-7.400318	5.518495	-3.154800
46	6	0	0.835280	-8.341576	2.513627
47	6	0	0.149203	-7.134556	2.755392
48	6	0	0.338779	-6.042235	1.932082
49	6	0	1.218634	-6.091438	0.820667
50	6	0	1.983654	-7.287761	0.643653
51	6	0	1.746317	-8.405326	1.481038
52	6	0	-1.690742	-4.882088	0.049104
53	6	0	1.466511	-4.953498	-0.051052
54	6	0	0.633310	-3.758575	-0.110570
55	6	0	-0.804702	-3.725943	0.107904
56	6	0	1.295402	-2.531304	-0.384780
57	6	0	2.517155	-2.579180	-1.128691
58	6	0	3.109100	-3.770012	-1.437519
59	6	0	2.652208	-4.973193	-0.829367
60	6	0	3.392876	-6.186243	-0.987910
61	6	0	3.036641	-7.319875	-0.322245
62	1	0	3.592556	-8.244222	-0.458926
63	1	0	4.252988	-6.178925	-1.653123
64	1	0	0.671035	-9.202170	3.156416
65	1	0	2.323980	-9.310970	1.310515
66	1	0	2.932074	-1.655611	-1.512377
67	1	0	3.982640	-3.801159	-2.083360
68	6	0	-3.364784	-7.175767	0.323627
69	6	0	-3.671171	-6.025962	0.986177
70	6	0	-2.877036	-4.847463	0.826000
71	1	0	-3.961054	-8.074395	0.461784
72	1	0	-4.530629	-5.979034	1.650589
73	6	0	-3.279787	-3.624178	1.432210
74	6	0	-2.634231	-2.461629	1.122898
75	6	0	-1.411017	-2.469487	0.379951
76	1	0	-4.154152	-3.615158	2.077568
77	1	0	-3.007324	-1.520117	1.505750
78	6	0	0.671357	-1.253548	-0.065107
79	6	0	-0.729448	-1.221626	0.059566
80	6	0	-1.493481	-6.031442	-0.820856
81	6	0	-2.310801	-7.192301	-0.641621
82	1	0	-0.527094	-7.055676	3.602187
83	1	0	-0.176719	-5.118401	2.160249
84	6	0	-2.123401	-8.320761	-1.476975
85	6	0	-0.613212	-6.023029	-1.932922
86	6	0	-0.472734	-7.124053	-2.754549
87	6	0	-1.211162	-8.299211	-2.510238
88	1	0	-2.740402	-9.199689	-1.304488
89	1	0	-0.057557	-5.123280	-2.163108
90	1	0	0.205734	-7.076442	-3.601937
91	1	0	-1.085483	-9.167357	-3.151544
92	6	0	7.794853	3.104493	-2.505098
93	6	0	6.407863	3.159044	-2.748617
94	6	0	5.524266	2.484347	-1.929477
95	6	0	5.971287	1.721661	-0.820366
96	6	0	7.385287	1.591807	-0.642274
97	6	0	8.269271	2.320281	-1.475429
98	6	0	3.558239	3.747830	-0.047035
99	6	0	5.073824	0.975832	0.048458
100	6	0	3.629513	1.166412	0.108180
101	6	0	2.939273	2.428985	-0.107423
102	6	0	2.843933	0.013515	0.379745
103	6	0	3.447832	-1.050888	1.121770
104	6	0	4.777473	-1.030328	1.430285
105	6	0	5.636098	-0.070481	0.823977
106	6	0	7.053684	-0.171385	0.983096
107	6	0	7.897156	0.668500	0.321192
108	1	0	8.973488	0.599644	0.458819
109	1	0	7.441905	-0.940667	1.646253

110	1	0	8.484190	3.649364	-3.144424
111	1	0	9.338876	2.223695	-1.303646
112	1	0	2.818182	-1.844254	1.504324
113	1	0	5.206531	-1.793003	2.074797
114	6	0	4.824213	6.290178	-0.319475
115	6	0	3.662248	6.033550	-0.981986
116	6	0	2.981629	4.785913	-0.823005
117	1	0	5.347473	7.233308	-0.456884
118	1	0	3.224676	6.775611	-1.645445
119	6	0	1.710333	4.581476	-1.429724
120	6	0	0.975120	3.473227	-1.121806
121	6	0	1.544845	2.389871	-0.380166
122	1	0	1.300105	5.354568	-2.074126
123	1	0	-0.032558	3.371941	-1.504575
124	6	0	1.422304	-0.019152	0.060333
125	6	0	0.749762	1.210324	-0.062474
126	6	0	4.670399	4.100547	0.822006
127	6	0	5.324645	5.360755	0.644078
128	1	0	6.027625	3.726836	-3.593424
129	1	0	4.467099	2.517980	-2.158830
130	6	0	6.414890	5.711580	1.477523
131	6	0	5.070596	3.312585	1.931323
132	6	0	6.115299	3.692122	2.750825
133	6	0	6.818346	4.888989	2.507468
134	1	0	6.911168	6.664010	1.305826
135	1	0	4.527904	2.404727	2.160656
136	1	0	6.387569	3.065685	3.595882
137	1	0	7.648833	5.175119	3.147196
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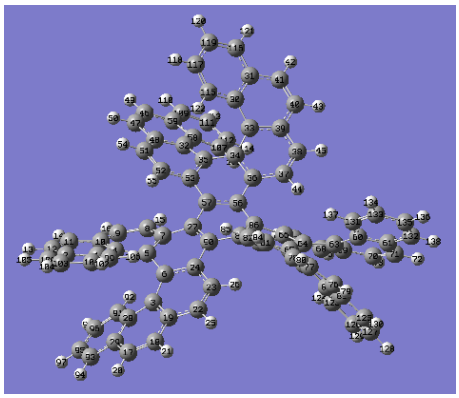
0 negative eigen value
Sum of electronic and thermal Free Energies= -3457.591615

Diastereomer **J**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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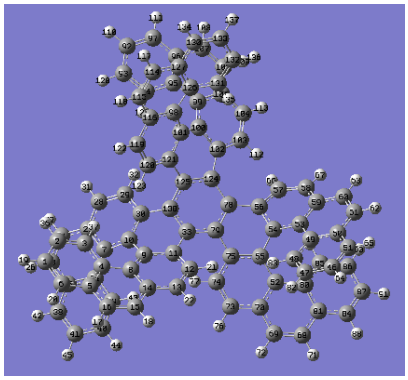
3	6	0	-1.111131	-4.993480	-0.504175
4	6	0	-3.743355	-3.449201	0.206072
5	6	0	-2.436984	-2.869913	-0.048267
6	6	0	-1.180077	-3.594758	-0.108651
7	6	0	-2.381847	-1.486440	-0.356686
8	6	0	-3.512304	-0.923472	-1.029495
9	6	0	-4.687735	-1.613033	-1.121986
10	6	0	-4.866824	-2.828559	-0.399293
11	6	0	-6.160237	-3.428797	-0.309000
12	6	0	-6.357092	-4.569927	0.408544
13	1	0	-7.341242	-5.028953	0.463312
14	1	0	-6.986596	-2.951584	-0.830370
15	1	0	-3.416142	0.051018	-1.492512
16	1	0	-5.525767	-1.200193	-1.677359
17	6	0	-0.975734	-7.835011	-0.753118
18	6	0	0.095802	-7.143266	-0.278880
19	6	0	0.069252	-5.714499	-0.196393
20	1	0	-0.970531	-8.921773	-0.785308
21	1	0	0.993770	-7.659436	0.051996
22	6	0	1.250287	-4.990286	0.105810

23	6	0	1.249879	-3.624741	0.129218
24	6	0	0.033721	-2.875291	0.115677
25	1	0	2.184155	-5.535831	0.217400
26	1	0	2.198265	-3.118530	0.183124
27	6	0	-1.189498	-0.729815	-0.033240
28	6	0	-2.116965	-5.704175	-1.288004
29	6	0	-2.075803	-7.133783	-1.340783
30	6	0	-2.117048	5.704161	1.287979
31	6	0	-2.075909	7.133770	1.340736
32	6	0	-3.743412	3.449139	-0.206048
33	6	0	-1.111205	4.993470	0.504158
34	6	0	-1.180132	3.594743	0.108651
35	6	0	-2.437027	2.869876	0.048284
36	6	0	0.033677	2.875292	-0.115674
37	6	0	1.249824	3.624758	-0.129222
38	6	0	1.250212	4.990303	-0.105828
39	6	0	0.069167	5.714503	0.196365
40	6	0	0.095695	7.143271	0.278832
41	6	0	-0.975851	7.835008	0.753059
42	1	0	-0.970665	8.921770	0.785231
43	1	0	0.993656	7.659450	-0.052052
44	1	0	2.198217	3.118560	-0.183122
45	1	0	2.184073	5.535861	-0.217424
46	6	0	-6.357171	4.569814	-0.408510
47	6	0	-6.160289	3.428696	0.309046
48	6	0	-4.866863	2.828482	0.399334
49	1	0	-7.341330	5.028820	-0.463275
50	1	0	-6.986634	2.951473	0.830429
51	6	0	-4.687747	1.612965	1.122034
52	6	0	-3.512307	0.923422	1.029534
53	6	0	-2.381865	1.486406	0.356711
54	1	0	-5.525767	1.200115	1.677419
55	1	0	-3.416124	-0.051065	1.492552
56	6	0	0.009857	1.416059	-0.252155
57	6	0	-1.189508	0.729798	0.033258
58	6	0	-3.977201	4.580810	-1.088831
59	6	0	-5.287986	5.151498	-1.157329
60	6	0	6.072844	1.579594	-0.035328
61	6	0	7.233586	2.175555	-0.622594
62	6	0	4.894041	-1.352639	0.857556
63	6	0	4.894020	1.352711	-0.857551
64	6	0	3.730069	0.574085	-0.449836
65	6	0	3.730078	-0.574029	0.449843
66	6	0	2.476204	1.027262	-0.946859
67	6	0	2.434321	1.792100	-2.152867
68	6	0	3.588004	2.165543	-2.779578
69	6	0	4.836720	2.024001	-2.108367
70	6	0	6.018668	2.600614	-2.671803
71	6	0	7.191751	2.620748	-1.980146
72	1	0	8.090329	3.047251	-2.419166
73	1	0	5.953152	3.032371	-3.667645
74	1	0	1.465989	2.018037	-2.587058
75	1	0	3.561804	2.656462	-3.748920
76	6	0	7.191793	-2.620641	1.980148
77	6	0	6.018710	-2.600526	2.671806
78	6	0	4.836752	-2.023931	2.108371
79	1	0	8.090378	-3.047130	2.419167
80	1	0	5.953201	-3.032285	3.667647
81	6	0	3.588039	-2.165495	2.779582
82	6	0	2.434349	-1.792067	2.152873
83	6	0	2.476221	-1.027226	0.946867
84	1	0	3.561847	-2.656416	3.748923
85	1	0	1.466021	-2.018021	2.587063
86	6	0	1.230045	0.617793	-0.332787
87	6	0	1.230055	-0.617775	0.332797
88	6	0	6.072868	-1.579503	0.035332
89	6	0	7.233620	-2.175445	0.622596
90	6	0	0.009879	-1.416059	0.252165
91	6	0	-3.054729	-5.056314	-2.130981
92	1	0	-3.027091	-3.978922	-2.228580
93	6	0	-3.060289	-7.841679	-2.071772
94	1	0	-3.025275	-8.928713	-2.067388
95	6	0	-4.009523	-7.175446	-2.817806
96	6	0	-3.974621	-5.768870	-2.876443
97	1	0	-4.749603	-7.729422	-3.388915
98	1	0	-4.667904	-5.235494	-3.521032
99	6	0	-2.995054	-5.099488	1.971206
100	6	0	-5.531157	-6.256082	2.010125

101	6	0	-3.263686	-6.163759	2.809215
102	1	0	-2.486593	-6.530472	3.474445
103	6	0	-4.537182	-6.767012	2.816929
104	1	0	-4.738866	-7.610460	3.471653
105	1	0	-6.531552	-6.682385	2.030868
106	1	0	-2.015482	-4.640751	2.005658
107	6	0	-2.995156	5.099422	-1.971205
108	1	0	-2.015576	4.640704	-2.005660
109	6	0	-5.531282	6.255966	-2.010118
110	1	0	-6.531685	6.682249	-2.030857
111	6	0	-4.537323	6.766905	-2.816936
112	6	0	-3.263815	6.163678	-2.809225
113	1	0	-4.739029	7.610341	-3.471669
114	1	0	-2.486735	6.530397	-3.474465
115	6	0	-3.054796	5.056298	2.130972
116	6	0	-3.060405	7.841662	2.071715
117	6	0	-3.974698	5.768851	2.876424
118	1	0	-4.667969	5.235475	3.521026
119	6	0	-4.009626	7.175425	2.817763
120	1	0	-4.749714	7.729399	3.388864
121	1	0	-3.025410	8.928696	2.067312
122	1	0	-3.027139	3.978909	2.228590
123	6	0	6.093293	-1.361212	-1.365618
124	1	0	5.196777	-1.010907	-1.860268
125	6	0	8.387364	-2.396545	-0.168571
126	6	0	7.218358	-1.620214	-2.123359
127	6	0	8.390994	-2.114318	-1.518010
128	1	0	9.278239	-2.301677	-2.116706
129	1	0	7.191985	-1.450372	-3.196222
130	1	0	9.265441	-2.827576	0.306922
131	6	0	6.093274	1.361305	1.365621
132	6	0	8.387327	2.396674	0.168572
133	6	0	7.218335	1.620324	2.123361
134	1	0	7.191966	1.450482	3.196225
135	6	0	8.390963	2.114448	1.518011
136	1	0	9.278205	2.301821	2.116707
137	1	0	5.196763	1.010986	1.860273
138	1	0	9.265396	2.827719	-0.306922

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.587274

Transition State **TS1**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.703373	-7.450406	2.446954
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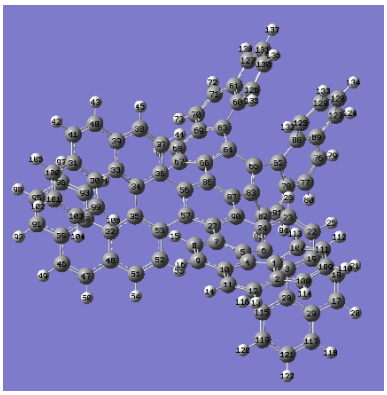
3	6	0	-2.141967	-5.346065	1.384845
4	6	0	-0.773417	-5.483820	1.727107
5	6	0	-0.423183	-6.602931	2.548397
6	6	0	-1.394177	-7.584593	2.859165
7	6	0	-1.338568	-4.582728	-1.443737
8	6	0	0.254168	-4.498488	1.390035
9	6	0	0.123353	-3.464979	0.388927
10	6	0	-0.900670	-3.450976	-0.667047
11	6	0	0.983177	-2.335870	0.429821

12	6	0	2.073272	-2.330412	1.342906
13	6	0	2.341795	-3.426424	2.116206
14	6	0	1.454088	-4.530696	2.155162
15	6	0	1.757533	-5.652251	2.991772
16	6	0	0.882288	-6.683312	3.128944
17	1	0	1.128850	-7.547806	3.740395
18	1	0	2.715120	-5.661759	3.506764
19	1	0	-3.441698	-8.205923	2.701450
20	1	0	-1.091105	-8.437072	3.462731
21	1	0	2.697343	-1.450447	1.422818
22	1	0	3.211652	-3.434804	2.768434
23	6	0	-2.541600	-6.814853	-2.767246
24	6	0	-3.174535	-5.611501	-2.756527
25	6	0	-2.584341	-4.469134	-2.127650
26	1	0	-3.005966	-7.684342	-3.225985
27	1	0	-4.150794	-5.493060	-3.220332
28	6	0	-3.246194	-3.215330	-2.200123
29	6	0	-2.680381	-2.088375	-1.667807
30	6	0	-1.488256	-2.182929	-0.900918
31	1	0	-4.180690	-3.151755	-2.751988
32	1	0	-3.128865	-1.115617	-1.835140
33	6	0	0.616254	-1.113489	-0.301956
34	6	0	-0.582296	-5.820430	-1.621112
35	6	0	-1.215770	-6.941975	-2.244606
36	1	0	-4.121171	-6.149364	1.454062
37	1	0	-2.475753	-4.460309	0.862965
38	6	0	-0.505247	-8.155012	-2.407830
39	6	0	0.791365	-5.954264	-1.300198
40	6	0	1.473271	-7.140850	-1.495737
41	6	0	0.816412	-8.264955	-2.029383
42	1	0	-1.019182	-8.996961	-2.865845
43	1	0	1.333544	-5.103376	-0.911886
44	1	0	2.527987	-7.198908	-1.240833
45	1	0	1.353237	-9.199479	-2.167804
46	6	0	6.486702	2.711967	3.745604
47	6	0	5.816872	1.594560	3.209887
48	6	0	4.979633	1.732749	2.120099
49	6	0	4.772884	2.988243	1.494693
50	6	0	5.414722	4.127116	2.078844
51	6	0	6.275909	3.955852	3.189851
52	6	0	5.219472	0.560812	-0.893271
53	6	0	3.884528	3.186348	0.360173
54	6	0	3.233584	2.104238	-0.344242
55	6	0	3.811627	0.800463	-0.631909
56	6	0	1.968228	2.357725	-0.963298
57	6	0	1.946052	3.647846	-1.586223
58	6	0	2.744086	4.682190	-1.173303
59	6	0	3.601912	4.514283	-0.053581
60	6	0	4.262411	5.623461	0.553752
61	6	0	5.154393	5.435954	1.566401
62	1	0	5.662725	6.282263	2.021967
63	1	0	4.043103	6.622262	0.184289
64	1	0	7.146511	2.595949	4.601062
65	1	0	6.759644	4.835300	3.608720
66	1	0	1.388186	3.763707	-2.502068
67	1	0	2.712138	5.636907	-1.691259
68	6	0	7.992322	-0.131474	-0.877655
69	6	0	7.049232	-1.111175	-0.905771
70	6	0	5.653770	-0.791958	-0.957474
71	1	0	9.048887	-0.373889	-0.794266
72	1	0	7.332563	-2.160432	-0.873085
73	6	0	4.698245	-1.824127	-1.140131
74	6	0	3.360518	-1.543777	-1.162191
75	6	0	2.885577	-0.251568	-0.803018
76	1	0	5.052013	-2.835346	-1.325101
77	1	0	2.652331	-2.322434	-1.412895
78	6	0	0.924622	1.303221	-0.913442
79	6	0	1.457600	-0.002120	-0.624865
80	6	0	6.227318	1.575948	-1.190264
81	6	0	7.613088	1.231675	-1.092123
82	1	0	5.949195	0.615560	3.662608
83	1	0	4.460762	0.860107	1.745254
84	6	0	8.603267	2.214725	-1.330036
85	6	0	5.920704	2.853760	-1.718329
86	6	0	6.907008	3.782767	-1.993119
87	6	0	8.261191	3.481414	-1.755704
88	1	0	9.647892	1.935234	-1.213906
89	1	0	4.895344	3.097402	-1.960508

90	1	0	6.629994	4.748203	-2.407528
91	1	0	9.030639	4.223230	-1.951613
92	6	0	-8.020728	2.664379	-1.662678
93	6	0	-7.139924	1.643554	-1.260681
94	6	0	-5.782608	1.884671	-1.156311
95	6	0	-5.224002	3.156089	-1.441826
96	6	0	-6.117224	4.156920	-1.941772
97	6	0	-7.506524	3.896055	-2.010082
98	6	0	-4.129557	2.025504	1.419517
99	6	0	-3.793642	3.456923	-1.367586
100	6	0	-2.816643	2.625562	-0.705439
101	6	0	-3.190930	1.721643	0.366330
102	6	0	-1.432968	2.663471	-1.074843
103	6	0	-1.060605	3.832849	-1.786925
104	6	0	-1.946795	4.803517	-2.175878
105	6	0	-3.338144	4.621536	-2.035624
106	6	0	-4.259624	5.591661	-2.542728
107	6	0	-5.600699	5.393646	-2.446034
108	1	0	-6.302809	6.141332	-2.806854
109	1	0	-3.858475	6.495567	-2.994731
110	1	0	-9.088581	2.474224	-1.727726
111	1	0	-8.162324	4.684741	-2.371721
112	1	0	-0.037544	4.003747	-2.013530
113	1	0	-1.576836	5.698178	-2.671083
114	6	0	-6.253225	2.370807	3.295838
115	6	0	-5.754656	1.127614	3.058403
116	6	0	-4.670238	0.930824	2.145941
117	1	0	-7.095465	2.513867	3.968433
118	1	0	-6.176913	0.254711	3.550285
119	6	0	-4.105954	-0.361894	1.984372
120	6	0	-3.027975	-0.569498	1.168013
121	6	0	-2.548479	0.472391	0.319223
122	1	0	-4.493378	-1.177496	2.590014
123	1	0	-2.535332	-1.531768	1.180506
124	6	0	-0.549985	1.486971	-0.809728
125	6	0	-1.307663	0.331447	-0.445113
126	6	0	-4.520535	3.369626	1.833450
127	6	0	-5.622248	3.525314	2.733493
128	1	0	-7.524159	0.651981	-1.036966
129	1	0	-5.134293	1.067499	-0.870764
130	6	0	-6.034653	4.820901	3.127680
131	6	0	-3.803268	4.541095	1.482886
132	6	0	-4.205511	5.793222	1.907985
133	6	0	-5.350384	5.944062	2.712974
134	1	0	-6.890083	4.910823	3.793297
135	1	0	-2.899148	4.458157	0.895259
136	1	0	-3.623010	6.665511	1.624307
137	1	0	-5.670490	6.932638	3.030830
138	6	0	-0.753046	-0.981553	-0.533765

1 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.569565

Transition State **TS2**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	2.768972	-6.600762	2.184774

3	6	0	3.725067	-3.395977	-0.653347
4	6	0	1.503370	-4.716923	1.153840
5	6	0	1.389587	-3.457769	0.438446
6	6	0	2.535058	-2.758414	-0.128954
7	6	0	0.121304	-2.820998	0.360644
8	6	0	-1.028942	-3.541393	0.801537
9	6	0	-0.941721	-4.852862	1.172701
10	6	0	0.320876	-5.475977	1.352766
11	6	0	0.392997	-6.834716	1.797017
12	6	0	1.585667	-7.402419	2.123449
13	1	0	1.643680	-8.444334	2.428674
14	1	0	-0.531752	-7.403320	1.858811
15	1	0	-1.991798	-3.052507	0.820446
16	1	0	-1.839565	-5.411497	1.425667
17	6	0	6.209607	-4.574905	-1.416019
18	6	0	6.179099	-3.296116	-0.949989
19	6	0	4.944681	-2.672090	-0.589405
20	1	0	7.152717	-5.050605	-1.673787
21	1	0	7.096688	-2.723700	-0.837768
22	6	0	4.931120	-1.327143	-0.127247
23	6	0	3.748885	-0.662935	0.049383
24	6	0	2.496200	-1.338545	-0.078217
25	1	0	5.875749	-0.809316	0.017203
26	1	0	3.761903	0.384257	0.318593
27	6	0	0.026627	-1.429735	-0.069352
28	6	0	3.739557	-4.704439	-1.292612
29	6	0	4.995746	-5.296694	-1.638441
30	6	0	-5.948845	-0.494811	1.624091
31	6	0	-7.107085	-0.095242	2.363961
32	6	0	-4.798374	-0.959890	-1.498350
33	6	0	-4.871334	0.470141	1.411535
34	6	0	-3.754703	0.282344	0.516443
35	6	0	-3.707792	-0.676383	-0.594773
36	6	0	-2.578839	1.057248	0.697405
37	6	0	-2.607637	2.171012	1.581427
38	6	0	-3.758094	2.501196	2.244179
39	6	0	-4.901201	1.662675	2.189282
40	6	0	-6.069947	2.016212	2.936569
41	6	0	-7.155418	1.198381	2.973026
42	1	0	-8.050676	1.483710	3.519989
43	1	0	-6.069635	2.964800	3.467968
44	1	0	-1.708588	2.755841	1.730338
45	1	0	-3.788342	3.381113	2.881955
46	6	0	-7.000941	-1.888802	-3.070061
47	6	0	-5.841813	-2.599090	-3.039493
48	6	0	-4.712905	-2.141509	-2.288106
49	1	0	-7.864941	-2.254568	-3.619435
50	1	0	-5.750551	-3.538660	-3.579140
51	6	0	-3.491707	-2.862197	-2.353879
52	6	0	-2.380471	-2.428221	-1.685812
53	6	0	-2.463237	-1.333375	-0.780061
54	1	0	-3.434703	-3.730590	-3.005611
55	1	0	-1.426504	-2.917884	-1.839876
56	6	0	-1.318114	0.604223	0.117185
57	6	0	-1.247446	-0.762512	-0.210283
58	6	0	-5.959832	-0.097773	-1.710112
59	6	0	-7.075101	-0.599923	-2.453840
60	6	0	1.392585	6.110795	0.590414
61	6	0	1.308133	7.488785	0.207220
62	6	0	3.502313	3.613874	-0.841104
63	6	0	0.730833	5.097210	-0.207319
64	6	0	0.958072	3.649320	-0.158237
65	6	0	2.238958	2.969833	-0.467939
66	6	0	-0.209003	2.845648	-0.324042
67	6	0	-1.353599	3.390254	-0.977769
68	6	0	-1.339283	4.668799	-1.459099
69	6	0	-0.313664	5.561771	-1.051137
70	6	0	-0.357370	6.938864	-1.446006
71	6	0	0.488706	7.858008	-0.904621
72	1	0	0.463330	8.897955	-1.220332
73	1	0	-1.094888	7.230504	-2.189903
74	1	0	-2.183706	2.733948	-1.206565
75	1	0	-2.140728	5.034181	-2.095627
76	6	0	5.665149	5.089683	-1.964733
77	6	0	5.079064	4.085171	-2.676069
78	6	0	4.057974	3.261886	-2.098959
79	1	0	6.433705	5.715895	-2.410827
80	1	0	5.390239	3.871486	-3.695903

81	6	0	3.662414	2.045529	-2.724640
82	6	0	2.851004	1.179234	-2.046036
83	6	0	2.125762	1.619339	-0.897816
84	1	0	4.091288	1.776014	-3.685999
85	1	0	2.647610	0.188085	-2.435914
86	6	0	-0.144189	1.408733	-0.088461
87	6	0	1.083201	0.773191	-0.338810
88	6	0	4.333423	4.439736	0.009196
89	6	0	5.392318	5.212912	-0.566375
90	6	0	1.210604	-0.655034	-0.139440
91	6	0	-8.219370	0.210464	-2.647322
92	1	0	-9.060849	-0.207068	-3.195417
93	6	0	-6.013459	1.262140	-1.314087
94	1	0	-5.152642	1.714990	-0.842583
95	6	0	-8.259524	1.510516	-2.189220
96	6	0	-7.129068	2.045401	-1.544031
97	1	0	-7.124775	3.085512	-1.229587
98	1	0	-9.140292	2.125527	-2.352683
99	6	0	-5.877555	-1.854537	1.230586
100	6	0	-8.171719	-1.007183	2.559599
101	6	0	-8.091758	-2.306729	2.105194
102	1	0	-8.912224	-2.999815	2.270040
103	6	0	-6.916851	-2.736478	1.461017
104	1	0	-6.817194	-3.772350	1.148240
105	1	0	-9.048693	-0.667272	3.105697
106	1	0	-4.978860	-2.227316	0.759541
107	6	0	3.833552	-4.419215	2.108990
108	6	0	3.954602	-7.126993	2.752188
109	6	0	5.046635	-6.320876	2.995322
110	1	0	5.946115	-6.732830	3.444758
111	6	0	4.964017	-4.945700	2.704489
112	1	0	5.789548	-4.286607	2.958791
113	1	0	3.785064	-3.352447	1.935620
114	1	0	3.972197	-8.178274	3.030376
115	6	0	2.566380	-5.396107	-1.687857
116	1	0	1.598953	-4.941385	-1.520507
117	6	0	5.028185	-6.572354	-2.252735
118	1	0	5.996571	-7.007717	-2.488547
119	6	0	2.624428	-6.630207	-2.305764
120	1	0	1.702615	-7.126840	-2.596426
121	6	0	3.865537	-7.240733	-2.572122
122	1	0	3.904571	-8.216423	-3.048835
123	6	0	6.249822	5.956330	0.279038
124	1	0	7.023430	6.570492	-0.176174
125	6	0	4.318383	4.297650	1.417748
126	6	0	1.901094	5.825305	1.878160
127	6	0	1.904001	8.478499	1.022930
128	6	0	6.168587	5.839619	1.652393
129	6	0	5.223184	4.963569	2.220784
130	6	0	2.403792	6.819435	2.695526
131	6	0	2.450621	8.153046	2.248407
132	1	0	3.618660	3.595534	1.858303
133	1	0	5.207912	4.806876	3.296101
134	1	0	6.861165	6.382573	2.289856
135	1	0	1.830845	4.808697	2.246339
136	1	0	2.764093	6.568738	3.689250
137	1	0	2.871264	8.927347	2.884237
138	1	0	1.863273	9.514841	0.695590

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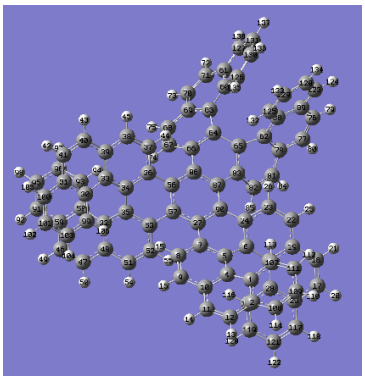
1 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.568124

Conformer **Int**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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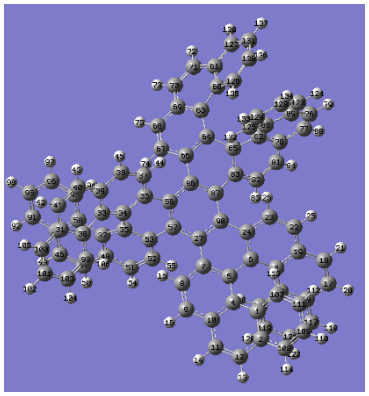
3	6	0	3.745713	-3.293850	-0.723665
4	6	0	1.498560	-4.737901	0.946797
5	6	0	1.381720	-3.441110	0.301241
6	6	0	2.529546	-2.701471	-0.204543
7	6	0	0.108153	-2.810681	0.246431
8	6	0	-1.037561	-3.562941	0.644186
9	6	0	-0.943909	-4.893817	0.935951
10	6	0	0.321752	-5.518271	1.085821
11	6	0	0.402523	-6.901302	1.445688
12	6	0	1.596910	-7.475896	1.753400
13	1	0	1.662572	-8.534162	1.993994
14	1	0	-0.516827	-7.481735	1.459303
15	1	0	-2.003490	-3.083024	0.690424
16	1	0	-1.839363	-5.471859	1.150961
17	6	0	6.268188	-4.394891	-1.475038
18	6	0	6.205802	-3.147685	-0.932144
19	6	0	4.952448	-2.561422	-0.574430
20	1	0	7.225301	-4.842428	-1.731676
21	1	0	7.111667	-2.572947	-0.755026
22	6	0	4.904816	-1.249682	-0.025509
23	6	0	3.708442	-0.608798	0.140378
24	6	0	2.470180	-1.286592	-0.085575
25	1	0	5.836120	-0.734305	0.194214
26	1	0	3.696249	0.417435	0.481619
27	6	0	0.002121	-1.402281	-0.122869
28	6	0	3.797855	-4.562109	-1.436451
29	6	0	5.072214	-5.116725	-1.778147
30	6	0	-5.922321	-0.556846	1.760332
31	6	0	-7.056791	-0.190611	2.552413
32	6	0	-4.864059	-0.906364	-1.418472
33	6	0	-4.858947	0.422293	1.543124
34	6	0	-3.769535	0.268703	0.609086
35	6	0	-3.749070	-0.649387	-0.536762
36	6	0	-2.594168	1.046161	0.778788
37	6	0	-2.605980	2.141787	1.685222
38	6	0	-3.738195	2.444272	2.391216
39	6	0	-4.872985	1.592910	2.354273
40	6	0	-6.018467	1.913369	3.150701
41	6	0	-7.094246	1.083496	3.201820
42	1	0	-7.972103	1.343954	3.787993
43	1	0	-6.008745	2.846662	3.708438
44	1	0	-1.708607	2.734689	1.813580
45	1	0	-3.758611	3.309973	3.048544
46	6	0	-7.106714	-1.795393	-2.956511
47	6	0	-5.939643	-2.492235	-2.993190
48	6	0	-4.791749	-2.052649	-2.260002
49	1	0	-7.984559	-2.148623	-3.491932
50	1	0	-5.856018	-3.407772	-3.573799
51	6	0	-3.565532	-2.754790	-2.396040
52	6	0	-2.438966	-2.338582	-1.742770
53	6	0	-2.505256	-1.287398	-0.785203
54	1	0	-3.519875	-3.592208	-3.087945
55	1	0	-1.485182	-2.810258	-1.946477
56	6	0	-1.347143	0.616818	0.156415
57	6	0	-1.277822	-0.736766	-0.220404
58	6	0	-6.039483	-0.048381	-1.559764
59	6	0	-7.173344	-0.533101	-2.286913

60	6	0	1.459079	6.268323	-0.099357
61	6	0	1.454092	7.491492	-0.845989
62	6	0	3.516568	3.583906	-0.381185
63	6	0	0.664093	5.135411	-0.546307
64	6	0	0.862548	3.714230	-0.221662
65	6	0	2.167632	3.022039	-0.338116
66	6	0	-0.285929	2.870251	-0.330812
67	6	0	-1.461675	3.335811	-0.983671
68	6	0	-1.477733	4.549463	-1.607708
69	6	0	-0.412961	5.462359	-1.417458
70	6	0	-0.423958	6.707303	-2.130008
71	6	0	0.537199	7.647910	-1.931685
72	1	0	0.551506	8.569173	-2.508565
73	1	0	-1.214945	6.862977	-2.859530
74	1	0	-2.294173	2.657097	-1.113535
75	1	0	-2.310081	4.833011	-2.246535
76	6	0	6.055740	4.803698	-0.762740
77	6	0	5.547402	3.971473	-1.716763
78	6	0	4.322899	3.259827	-1.503340
79	1	0	6.986507	5.339994	-0.929680
80	1	0	6.082537	3.803435	-2.648342
81	6	0	3.962249	2.147231	-2.318344
82	6	0	2.986948	1.296212	-1.873110
83	6	0	2.104588	1.686348	-0.819098
84	1	0	4.551070	1.913738	-3.201081
85	1	0	2.811218	0.345840	-2.365302
86	6	0	-0.186914	1.437766	-0.060210
87	6	0	1.042234	0.818641	-0.339349
88	6	0	4.185960	4.215137	0.734623
89	6	0	5.445389	4.860069	0.529420
90	6	0	1.179889	-0.615348	-0.163710
91	6	0	-8.330818	0.271918	-2.412479
92	1	0	-9.185600	-0.133357	-2.949084
93	6	0	-6.092794	1.295344	-1.111463
94	1	0	-5.221778	1.739853	-0.650847
95	6	0	-8.368173	1.553325	-1.904385
96	6	0	-7.222172	2.075295	-1.276348
97	1	0	-7.216879	3.103059	-0.923636
98	1	0	-9.259347	2.164878	-2.016209
99	6	0	-5.856827	-1.901556	1.317309
100	6	0	-8.107474	-1.117090	2.755094
101	6	0	-8.035082	-2.400028	2.254552
102	1	0	-8.844501	-3.104645	2.425015
103	6	0	-6.881645	-2.798567	1.553959
104	1	0	-6.787179	-3.822147	1.201618
105	1	0	-8.966980	-0.802442	3.342541
106	1	0	-4.973847	-2.250497	0.800443
107	6	0	3.804815	-4.470870	1.966248
108	6	0	3.950606	-7.212031	2.442370
109	6	0	5.026538	-6.408969	2.756913
110	1	0	5.922718	-6.836762	3.198064
111	6	0	4.930503	-5.019352	2.550795
112	1	0	5.741478	-4.367041	2.862826
113	1	0	3.744504	-3.395849	1.859756
114	1	0	3.976995	-8.278156	2.655834
115	6	0	2.646514	-5.244701	-1.905282
116	1	0	1.668107	-4.813504	-1.738808
117	6	0	5.140934	-6.353009	-2.465646
118	1	0	6.121979	-6.761391	-2.697466
119	6	0	2.740605	-6.438812	-2.593149
120	1	0	1.835043	-6.929624	-2.939492
121	6	0	3.997955	-7.015695	-2.859121
122	1	0	4.065127	-7.960246	-3.392092
123	6	0	6.118155	5.434268	1.635014
124	1	0	7.058044	5.952491	1.458775
125	6	0	3.750025	4.025501	2.072063
126	6	0	2.075841	6.298100	1.168613
127	6	0	2.240316	8.582131	-0.408270
128	6	0	5.633710	5.287516	2.919420
129	6	0	4.456296	4.541827	3.140129
130	6	0	2.786507	7.397630	1.613873
131	6	0	2.914416	8.534898	0.796381
132	1	0	2.856532	3.433237	2.248934
133	1	0	4.110726	4.361622	4.154688
134	1	0	6.179370	5.705146	3.761285
135	1	0	1.936318	5.452941	1.825217
136	1	0	3.242008	7.377779	2.599015
137	1	0	3.493615	9.389908	1.134710

138	1	0	2.254014	9.486291	-1.012516

0 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.571720

Transition State **TS2bis**



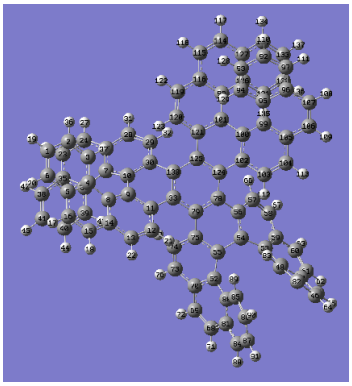
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.112850	-5.096198	1.343205
2	6	0	3.285992	-6.498077	1.573203
3	6	0	4.061917	-2.870632	-0.718392
4	6	0	1.880646	-4.625791	0.717734
5	6	0	1.670826	-3.299878	0.158802
6	6	0	2.766373	-2.429469	-0.239854
7	6	0	0.347416	-2.779764	0.098069
8	6	0	-0.736341	-3.656123	0.406225
9	6	0	-0.534365	-4.992659	0.601005
10	6	0	0.776497	-5.515643	0.749700
11	6	0	0.971161	-6.910017	1.008608
12	6	0	2.201474	-7.397561	1.325139
13	1	0	2.356236	-8.461286	1.488424
14	1	0	0.109426	-7.569463	0.938992
15	1	0	-1.741655	-3.267668	0.458176
16	1	0	-1.381471	-5.659623	0.741695
17	6	0	6.714441	-3.673407	-1.392624
18	6	0	6.503631	-2.485391	-0.760910
19	6	0	5.182645	-2.045642	-0.439578
20	1	0	7.722611	-4.009008	-1.623360
21	1	0	7.339714	-1.847028	-0.485598
22	6	0	4.978616	-0.789541	0.198996
23	6	0	3.719804	-0.270123	0.318551
24	6	0	2.568304	-1.035991	-0.045223
25	1	0	5.841760	-0.213622	0.522096
26	1	0	3.586113	0.721482	0.730511
27	6	0	0.125574	-1.365803	-0.192919
28	6	0	4.273424	-4.069302	-1.515167
29	6	0	5.611469	-4.475273	-1.821022
30	6	0	-5.801500	-1.128049	1.818349
31	6	0	-6.940488	-0.903607	2.655520
32	6	0	-4.791805	-1.198563	-1.403955
33	6	0	-4.825231	-0.054999	1.640502
34	6	0	-3.751671	-0.063067	0.676108
35	6	0	-3.682950	-0.903794	-0.526188
36	6	0	-2.641213	0.799673	0.868181
37	6	0	-2.718819	1.838540	1.835774
38	6	0	-3.852273	2.002813	2.583777
39	6	0	-4.912670	1.061196	2.521302
40	6	0	-6.058446	1.238091	3.360893
41	6	0	-7.062241	0.321341	3.384170
42	1	0	-7.942195	0.473436	4.004381
43	1	0	-6.109445	2.134116	3.974695
44	1	0	-1.870759	2.498886	1.973252
45	1	0	-3.928129	2.825174	3.290805
46	6	0	-6.983526	-2.178474	-2.961288
47	6	0	-5.761207	-2.764869	-3.065577
48	6	0	-4.639510	-2.275194	-2.323629
49	1	0	-7.839213	-2.571382	-3.504864
50	1	0	-5.611152	-3.628266	-3.709243

51	6	0	-3.360630	-2.855873	-2.529715
52	6	0	-2.259642	-2.388641	-1.867621
53	6	0	-2.395098	-1.414831	-0.838336
54	1	0	-3.258889	-3.636734	-3.279355
55	1	0	-1.273127	-2.760750	-2.117334
56	6	0	-1.380104	0.517556	0.195163
57	6	0	-1.205801	-0.802925	-0.256151
58	6	0	-6.040946	-0.440730	-1.466264
59	6	0	-7.144639	-0.974962	-2.205259
60	6	0	1.053437	6.382915	-0.686133
61	6	0	0.927353	7.420886	-1.669619
62	6	0	3.173104	3.840799	0.052254
63	6	0	0.222063	5.180898	-0.773846
64	6	0	0.512842	3.825742	-0.262556
65	6	0	1.872355	3.243929	-0.221982
66	6	0	-0.551442	2.866157	-0.290435
67	6	0	-1.813078	3.201427	-0.850135
68	6	0	-1.988648	4.374178	-1.520647
69	6	0	-0.963041	5.344053	-1.552354
70	6	0	-1.119675	6.444997	-2.458870
71	6	0	-0.156819	7.390255	-2.599304
72	1	0	-0.244026	8.182506	-3.338489
73	1	0	-2.014166	6.462069	-3.076365
74	1	0	-2.596541	2.457828	-0.877125
75	1	0	-2.903022	4.556837	-2.079119
76	6	0	5.753027	4.979315	0.415399
77	6	0	5.483964	4.239403	-0.698717
78	6	0	4.231651	3.564984	-0.853528
79	1	0	6.712694	5.476241	0.534004
80	1	0	6.237251	4.108695	-1.471918
81	6	0	4.067302	2.520759	-1.810040
82	6	0	3.045337	1.628399	-1.624502
83	6	0	1.978912	1.914642	-0.716881
84	1	0	4.831576	2.350932	-2.563168
85	1	0	3.002389	0.705486	-2.192681
86	6	0	-0.304117	1.449141	-0.017697
87	6	0	0.973789	0.946681	-0.316940
88	6	0	3.528729	4.423598	1.329724
89	6	0	4.819274	5.014315	1.498107
90	6	0	1.230228	-0.478367	-0.170340
91	6	0	-8.370951	-0.269892	-2.255524
92	1	0	-9.199011	-0.713510	-2.803574
93	6	0	-6.201768	0.860520	-0.927434
94	1	0	-5.362961	1.349878	-0.452839
95	6	0	-8.508840	0.966847	-1.661403
96	6	0	-7.398576	1.546305	-1.019777
97	1	0	-7.474984	2.545128	-0.598763
98	1	0	-9.452567	1.502633	-1.716090
99	6	0	-5.642170	-2.432918	1.288649
100	6	0	-7.909678	-1.921932	2.819943
101	6	0	-7.749994	-3.161143	2.236414
102	1	0	-8.497218	-3.937294	2.377605
103	6	0	-6.587075	-3.421958	1.488290
104	1	0	-6.421734	-4.410752	1.069094
105	1	0	-8.776117	-1.714059	3.443553
106	1	0	-4.748003	-2.677293	0.732626
107	6	0	4.101146	-4.230123	1.874761
108	6	0	4.488205	-6.975620	2.148833
109	6	0	5.466165	-6.104421	2.580207
110	1	0	6.378124	-6.481671	3.034928
111	6	0	5.246008	-4.717481	2.475977
112	1	0	5.974417	-4.020426	2.881028
113	1	0	3.941253	-3.160353	1.848252
114	1	0	4.607099	-8.048428	2.282342
115	6	0	3.218532	-4.817688	-2.097195
116	1	0	2.195844	-4.492991	-1.956768
117	6	0	5.834510	-5.641133	-2.593669
118	1	0	6.861006	-5.937008	-2.797903
119	6	0	3.462921	-5.940051	-2.864106
120	1	0	2.628073	-6.484930	-3.296601
121	6	0	4.782465	-6.373785	-3.100232
122	1	0	4.967583	-7.262706	-3.697152
123	6	0	5.171710	5.563827	2.755067
124	1	0	6.150599	6.025925	2.862338
125	6	0	2.691025	4.317244	2.471352
126	6	0	1.878896	6.673867	0.417370
127	6	0	1.782124	8.545483	-1.625003
128	6	0	4.314528	5.489548	3.834417

129	6	0	3.070523	4.839140	3.692518
130	6	0	2.669874	7.809217	0.478175
131	6	0	2.664974	8.732584	-0.579245
132	1	0	1.735403	3.810457	2.374715
133	1	0	2.411897	4.736929	4.550784
134	1	0	4.606238	5.902888	4.795926
135	1	0	1.837087	6.025040	1.273529
136	1	0	3.281877	7.984246	1.358084
137	1	0	3.302889	9.611780	-0.547232
138	1	0	1.688973	9.294295	-2.408211

1 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.568200

Transition State **TS3**



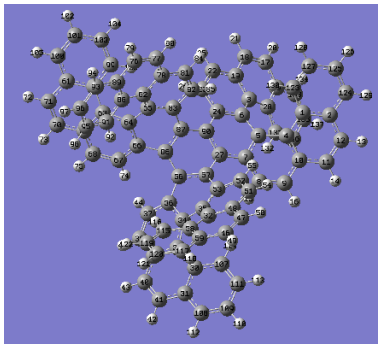
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.995099	2.104310	2.400217
2	6	0	-6.884307	2.540431	1.654699
3	6	0	-5.835422	1.680832	1.386269
4	6	0	-5.833525	0.338538	1.840724
5	6	0	-6.925110	-0.065414	2.673607
6	6	0	-8.001314	0.822841	2.909903
7	6	0	-4.879591	0.688120	-1.386154
8	6	0	-4.741748	-0.600731	1.591307
9	6	0	-3.688601	-0.406612	0.626107
10	6	0	-3.734155	0.503049	-0.525774
11	6	0	-2.481326	-1.141300	0.755376
12	6	0	-2.429354	-2.246701	1.648028
13	6	0	-3.527980	-2.589538	2.388760
14	6	0	-4.688719	-1.773434	2.398434
15	6	0	-5.793989	-2.132412	3.234184
16	6	0	-6.894069	-1.338638	3.325419
17	1	0	-7.740714	-1.628341	3.942980
18	1	0	-5.733567	-3.065251	3.789537
19	1	0	-8.823715	2.779360	2.596218
20	1	0	-8.826983	0.480250	3.529388
21	1	0	-1.509609	-2.810608	1.744652
22	1	0	-3.499013	-3.460742	3.038450
23	6	0	-7.199526	1.455039	-2.876140
24	6	0	-6.057794	2.186683	-2.974090
25	6	0	-4.872586	1.806865	-2.266636
26	1	0	-8.106566	1.763733	-3.389965
27	1	0	-6.022902	3.085973	-3.584314
28	6	0	-3.672035	2.533148	-2.473346
29	6	0	-2.516142	2.183837	-1.831477
30	6	0	-2.523508	1.188381	-0.814170
31	1	0	-3.668038	3.333569	-3.209150
32	1	0	-1.584220	2.666022	-2.096894
33	6	0	-1.266604	-0.644720	0.120420
34	6	0	-6.025315	-0.217211	-1.473046
35	6	0	-7.199413	0.209407	-2.172335
36	1	0	-6.842259	3.563769	1.291611
37	1	0	-4.986079	2.057668	0.833914
38	6	0	-8.330290	-0.639033	-2.241167
39	6	0	-6.012564	-1.553759	-1.001033
40	6	0	-7.116835	-2.378106	-1.112785

41	6	0	-8.303007	-1.910468	-1.707767
42	1	0	-9.216932	-0.276369	-2.756168
43	1	0	-5.109578	-1.958825	-0.566599
44	1	0	-7.059913	-3.398608	-0.743907
45	1	0	-9.174314	-2.556075	-1.776596
46	6	0	6.330000	-5.815583	1.390007
47	6	0	5.372421	-4.989338	2.009136
48	6	0	4.460352	-4.285991	1.246730
49	6	0	4.481280	-4.337360	-0.167339
50	6	0	5.554690	-5.055003	-0.786349
51	6	0	6.417676	-5.842059	0.012196
52	6	0	0.908071	-5.059840	-0.400099
53	6	0	3.642986	-3.465651	-0.965530
54	6	0	2.358661	-2.879040	-0.570942
55	6	0	1.097898	-3.608999	-0.290126
56	6	0	2.212233	-1.507863	-0.922640
57	6	0	2.975084	-0.955372	-1.994452
58	6	0	3.826131	-1.747733	-2.712946
59	6	0	4.216410	-3.009196	-2.182024
60	6	0	5.253264	-3.775982	-2.807784
61	6	0	5.839358	-4.827901	-2.169480
62	1	0	6.618452	-5.412211	-2.652528
63	1	0	5.574391	-3.480835	-3.803890
64	1	0	7.027270	-6.389755	1.994112
65	1	0	7.201951	-6.414043	-0.478326
66	1	0	2.766627	0.063280	-2.302911
67	1	0	4.285541	-1.391887	-3.631288
68	6	0	0.737120	-7.792102	-1.218637
69	6	0	-0.136694	-6.873125	-1.714682
70	6	0	-0.131039	-5.515451	-1.254834
71	1	0	0.740652	-8.816463	-1.582562
72	1	0	-0.869275	-7.150676	-2.468778
73	6	0	-1.193271	-4.638249	-1.599337
74	6	0	-1.239910	-3.387339	-1.052549
75	6	0	-0.095208	-2.835316	-0.402947
76	1	0	-1.995795	-4.999027	-2.237166
77	1	0	-2.096302	-2.748932	-1.230191
78	6	0	1.128851	-0.724446	-0.358884
79	6	0	-0.071567	-1.406405	-0.121933
80	6	0	1.590262	-6.091323	0.357021
81	6	0	1.542853	-7.452554	-0.087316
82	1	0	5.351953	-4.901322	3.092079
83	1	0	3.750601	-3.622448	1.728773
84	6	0	2.154566	-8.462959	0.690504
85	6	0	2.073757	-5.851968	1.663771
86	6	0	2.588078	-6.869932	2.443810
87	6	0	2.675909	-8.180086	1.937430
88	1	0	2.143205	-9.484286	0.316919
89	1	0	1.972761	-4.854840	2.075915
90	1	0	2.925945	-6.656194	3.453980
91	1	0	3.106877	-8.971928	2.544075
92	6	0	3.612789	7.234413	3.034894
93	6	0	2.394939	6.567293	2.801261
94	6	0	2.375201	5.344076	2.158518
95	6	0	3.565886	4.718627	1.710626
96	6	0	4.802417	5.344667	2.066919
97	6	0	4.795939	6.617909	2.686305
98	6	0	1.340336	4.919875	-0.563445
99	6	0	3.593201	3.421698	1.041284
100	6	0	2.464159	2.795794	0.374996
101	6	0	1.311139	3.544837	-0.104731
102	6	0	2.432539	1.378274	0.253634
103	6	0	3.613493	0.646548	0.582674
104	6	0	4.778927	1.285621	0.897046
105	6	0	4.802462	2.685179	1.130908
106	6	0	6.021144	3.329069	1.516946
107	6	0	6.033401	4.636752	1.892752
108	1	0	6.964162	5.134568	2.153498
109	1	0	6.938521	2.745846	1.493629
110	1	0	3.620674	8.205388	3.522683
111	1	0	5.750409	7.084896	2.918232
112	1	0	3.599139	-0.432569	0.559917
113	1	0	5.688875	0.713284	1.059885
114	6	0	1.288031	7.705188	-1.178356
115	6	0	0.174716	7.097878	-0.682804
116	6	0	0.165152	5.697728	-0.395679
117	1	0	1.295518	8.773563	-1.380163
118	1	0	-0.730489	7.668720	-0.490293

119	6	0	-1.017423	5.074861	0.092762
120	6	0	-1.092757	3.714100	0.198529
121	6	0	0.052618	2.890855	-0.031851
122	1	0	-1.884497	5.691203	0.316030
123	1	0	-2.026738	3.250510	0.485726
124	6	0	1.197604	0.702964	-0.127328
125	6	0	-0.012431	1.440861	-0.143793
126	6	0	2.475396	5.533130	-1.237647
127	6	0	2.448388	6.938200	-1.508323
128	1	0	1.461050	7.008747	3.138206
129	1	0	1.427438	4.837950	2.030314
130	6	0	3.547426	7.552290	-2.156898
131	6	0	3.578935	4.796986	-1.739487
132	6	0	4.628245	5.416169	-2.390185
133	6	0	4.629393	6.811731	-2.582656
134	1	0	3.509486	8.624710	-2.334069
135	1	0	3.594132	3.720421	-1.631464
136	1	0	5.453841	4.816909	-2.764499
137	1	0	5.462994	7.294082	-3.085823
138	6	0	-1.262387	0.716824	-0.239706

1 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.567329

Transition State **TS4**



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.077632	0.683601	1.420289
2	6	0	-7.225801	1.441185	1.815124
3	6	0	-5.130793	-1.444647	-0.907378
4	6	0	-5.043290	1.325989	0.620201
5	6	0	-3.924377	0.629084	0.014053
6	6	0	-3.941957	-0.762366	-0.426221
7	6	0	-2.728124	1.363600	-0.210728
8	6	0	-2.817306	2.783505	-0.333879
9	6	0	-3.989021	3.435857	-0.074674
10	6	0	-5.097687	2.738650	0.482849
11	6	0	-6.259351	3.463195	0.895836
12	6	0	-7.307224	2.831365	1.492182
13	1	0	-8.195819	3.384026	1.787290
14	1	0	-6.285785	4.535433	0.717252
15	1	0	-1.946109	3.338080	-0.660996
16	1	0	-4.066235	4.509691	-0.224997
17	6	0	-7.500621	-2.955237	-1.418586
18	6	0	-6.334731	-3.596082	-1.132356
19	6	0	-5.123709	-2.864638	-0.916854
20	1	0	-8.424957	-3.511681	-1.552961
21	1	0	-6.298917	-4.680132	-1.056048
22	6	0	-3.894187	-3.561873	-0.764923
23	6	0	-2.716789	-2.880756	-0.646545
24	6	0	-2.706463	-1.468103	-0.445282
25	1	0	-3.897413	-4.646698	-0.837028
26	1	0	-1.777938	-3.418363	-0.674992
27	6	0	-1.469828	0.662215	-0.347020
28	6	0	-6.307556	-0.787007	-1.465627
29	6	0	-7.506009	-1.545250	-1.657103
30	6	0	2.648972	5.393583	-1.295119
31	6	0	3.580304	6.327771	-1.850118
32	6	0	2.173419	3.602857	1.408139

33	6	0	2.707998	3.993526	-1.720134
34	6	0	2.029603	2.897727	-1.070905
35	6	0	1.508181	2.982212	0.291738
36	6	0	1.789975	1.676318	-1.771973
37	6	0	2.384691	1.541984	-3.051891
38	6	0	3.252635	2.477488	-3.552551
39	6	0	3.451344	3.713117	-2.898873
40	6	0	4.351408	4.682521	-3.448851
41	6	0	4.466127	5.919559	-2.898947
42	1	0	5.173011	6.644285	-3.295408
43	1	0	4.949518	4.395761	-4.310448
44	1	0	2.117997	0.717968	-3.684290
45	1	0	3.735772	2.308980	-4.512001
46	6	0	3.223251	5.145382	3.572864
47	6	0	1.922166	4.748529	3.591430
48	6	0	1.378462	3.949915	2.536483
49	1	0	3.625418	5.773017	4.364385
50	1	0	1.263698	5.038232	4.406794
51	6	0	0.040271	3.484020	2.624077
52	6	0	-0.490501	2.665365	1.665298
53	6	0	0.234681	2.387020	0.469533
54	1	0	-0.536311	3.724095	3.514073
55	1	0	-1.458492	2.209883	1.825969
56	6	0	0.819131	0.705287	-1.224261
57	6	0	-0.185219	1.325026	-0.431531
58	6	0	3.609350	3.858054	1.491360
59	6	0	4.110812	4.673991	2.554484
60	6	0	2.869615	-5.371039	-1.059246
61	6	0	3.866357	-6.271996	-1.552255
62	6	0	2.191436	-3.535834	1.564780
63	6	0	2.863831	-3.986571	-1.536326
64	6	0	2.118076	-2.901534	-0.942828
65	6	0	1.554058	-2.968811	0.405044
66	6	0	1.834301	-1.724053	-1.700517
67	6	0	2.412284	-1.628897	-2.991159
68	6	0	3.336206	-2.535815	-3.440847
69	6	0	3.608937	-3.717343	-2.716936
70	6	0	4.575667	-4.654905	-3.206130
71	6	0	4.752698	-5.856839	-2.597952
72	1	0	5.509847	-6.554486	-2.947319
73	1	0	5.172262	-4.371665	-4.069927
74	1	0	2.077526	-0.869266	-3.672182
75	1	0	3.807390	-2.395524	-4.410707
76	6	0	3.209249	-4.973710	3.814508
77	6	0	1.890089	-4.644989	3.760162
78	6	0	1.358746	-3.899559	2.661092
79	1	0	3.603019	-5.560496	4.640808
80	1	0	1.208244	-4.950163	4.550264
81	6	0	-0.007812	-3.511692	2.669704
82	6	0	-0.527845	-2.732437	1.672952
83	6	0	0.251404	-2.422617	0.520401
84	1	0	-0.618176	-3.778529	3.528999
85	1	0	-1.530240	-2.332792	1.764004
86	6	0	0.835997	-0.758294	-1.196432
87	6	0	-0.160082	-1.376612	-0.396522
88	6	0	3.631537	-3.722044	1.718832
89	6	0	4.120638	-4.484604	2.826210
90	6	0	-1.458718	-0.738530	-0.346957
91	6	0	4.595477	-3.102647	0.884948
92	1	0	4.270037	-2.439189	0.095514
93	6	0	5.512201	-4.692412	2.980682
94	1	0	5.854977	-5.293441	3.819838
95	6	0	5.951127	-3.296045	1.073594
96	6	0	6.419518	-4.120850	2.113398
97	1	0	7.485887	-4.280062	2.248600
98	1	0	6.658200	-2.796283	0.417098
99	6	0	1.867942	-5.922303	-0.222130
100	6	0	3.912978	-7.604306	-1.077961
101	6	0	2.961178	-8.084721	-0.202749
102	1	0	3.000960	-9.113508	0.144728
103	6	0	1.909684	-7.239641	0.196269
104	1	0	1.115476	-7.623107	0.831017
105	1	0	4.699865	-8.257039	-1.448885
106	1	0	1.026344	-5.312277	0.075436
107	6	0	1.643206	5.920503	-0.447124
108	6	0	3.563413	7.678790	-1.429878
109	6	0	2.610816	8.139989	-0.545291
110	1	0	2.601762	9.182470	-0.238867

111	6	0	1.622214	7.253693	-0.080440
112	1	0	4.301801	8.358804	-1.848493
113	1	0	0.827622	7.616651	0.565794
114	1	0	0.849217	5.275856	-0.096601
115	6	0	4.564562	3.257478	0.633867
116	1	0	4.237202	2.554141	-0.119352
117	6	0	5.496277	4.951210	2.638878
118	1	0	5.846715	5.592251	3.444618
119	6	0	5.916639	3.518535	0.755186
120	6	0	6.390762	4.396575	1.747612
121	1	0	7.453197	4.609550	1.829218
122	1	0	6.616851	3.031000	0.082315
123	6	0	-5.966229	-0.635079	1.929999
124	6	0	-8.245551	0.828082	2.583174
125	6	0	-8.128680	-0.476697	3.012313
126	1	0	-8.914271	-0.932697	3.608652
127	6	0	-6.961753	-1.201961	2.701773
128	1	0	-6.835642	-2.213270	3.078816
129	1	0	-9.117238	1.420634	2.851346
130	1	0	-5.069874	-1.207969	1.732758
131	6	0	-6.301222	0.543162	-1.956650
132	1	0	-5.379556	1.109320	-1.946933
133	6	0	-8.665133	-0.915377	-2.171775
134	1	0	-9.570525	-1.508131	-2.280267
135	6	0	-8.641400	0.404292	-2.570353
136	6	0	-7.433892	1.124906	-2.492743
137	1	0	-9.533765	0.873050	-2.976200
138	1	0	-7.384989	2.143654	-2.867388

1 negative eigenvalue
Sum of electronic and thermal Free Energies= -3457.593656

4. Chiroptical studies

4.1. Diastereomer *D*$_3$-**2**

The two enantiomers of *D*$_3$-**2** were directly obtained as enantiopure materials by the stereospecific syntheses described above.

Optical rotation

Optical rotations were measured on a Jasco P-2000 polarimeter with a sodium lamp (589 nm) and a halogen lamp (578 and 546 nm) in a 10 cm cell thermostated at 25 °C with a Peltier controlled cell holder (Table S9).

Table S9. Optical rotation of *(P,P,P,M,M,M)*-*D*$_3$-**2** and (*M,M,M,P,P,P*)-*D*$_3$-**2**

λ (nm)	*(P,P,P,M,M,M)*-*D*$_3$-**2** $[\alpha]_\lambda^{25}$ ($CHCl_3$, c = 0.034)	(*M,M,M,P,P,P*)-*D*$_3$-**2** $[\alpha]_\lambda^{25}$ ($CHCl_3$, c = 0.0325)
589	+ 300	- 300
578	+ 350	- 350
546	+ 700	- 700

UV-vis and electronic circular dichroism (ECD) study

UV-vis and ECD spectra were measured on a JASCO J-815 spectrometer equipped with a JASCO Peltier cell holder PTC-423 to maintain the temperature at 25.0 ± 0.2 °C. A CD quartz cell of 1 mm optical pathlength was used. The CD spectrometer was purged with nitrogen before the recording of each spectrum, which was baseline subtracted. The baseline was always measured for the same solvent and in the same cell as the samples. The spectra are presented without smoothing and further data processing (Figures S21 and S22). Acquisition parameters: 0.1 nm as intervals, scanning speed 50 nm/min, band width 1 nm, and 3 accumulations per sample.

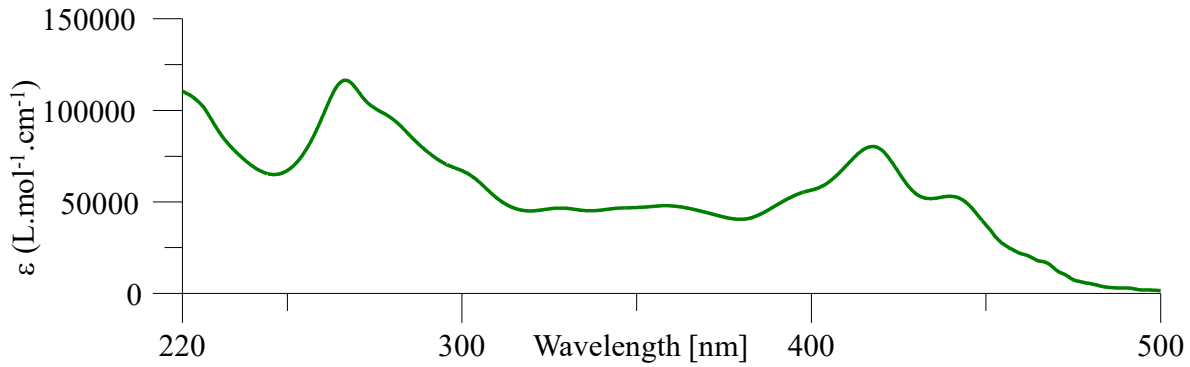


Figure S21. Experimental UV-vis spectrum of *(P,P,P,M,M,M)*-*D*$_3$-**2** (concentration = 0.0790 mmol.L^{-1} in dichloromethane).

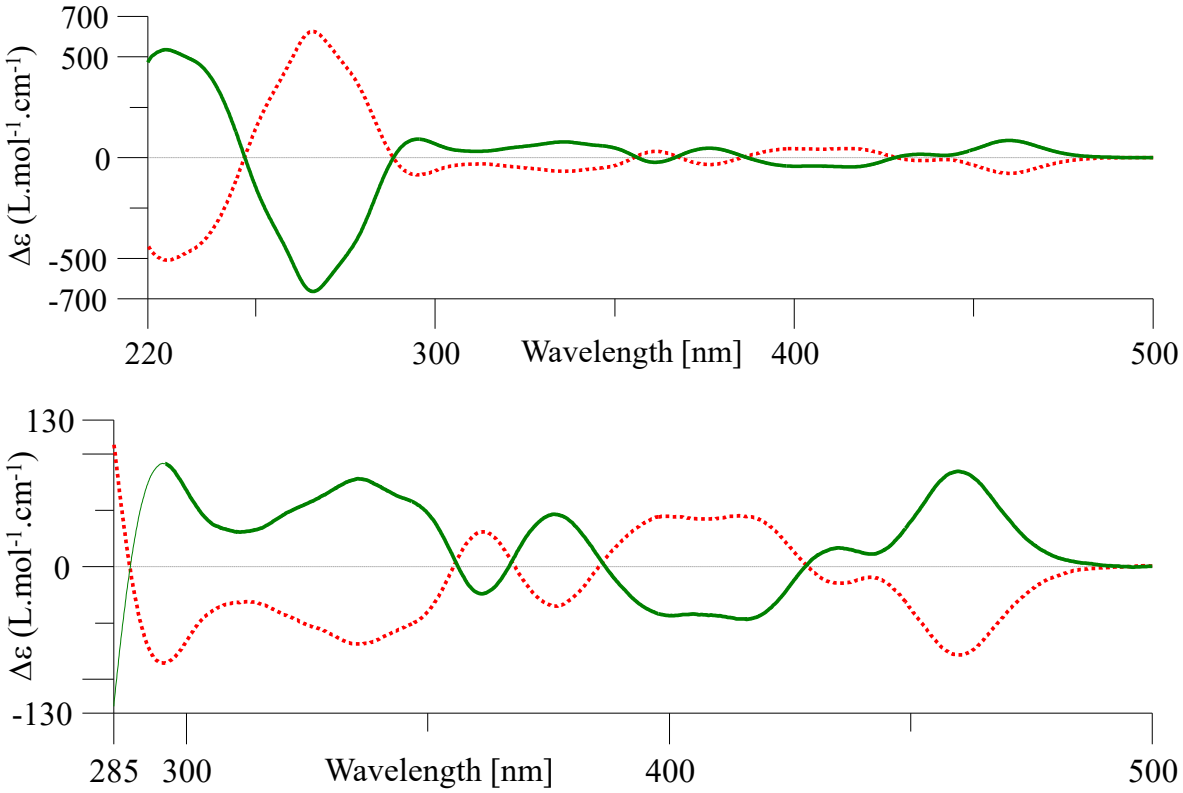


Figure S22. Experimental ECD spectra of *(P,P,P,M,M,M)*-D_3-**2** (green solid line, concentration = 0.0790 mmol.L^{-1} in dichloromethane) and (*M,M,M,P,P,P*)-D_3-**2** (red dotted line, concentration = 0.0787 mmol.L^{-1} in dichloromethane). Top = full spectra, bottom = zoom on the 285–500 nm area.

The experimental UV-vis and ECD spectra of *(P,P,P,M,M,M)*-D_3-**2** were compared with simulated spectra obtained by DFT computational methods (Figure S23). Calculations were performed with Turbomole[14] using the B3LYP functional and the def2TZVP basis set in the gas phase on optimized geometries. The symmetry point group had to be lowered to C_1 as any symmetrical ground state wave function (C_3 or C_2) was not stable. The UV/vis. and ECD spectra were computed via TD-DFT within the Tamm-Dancoff approximation on 100 excited states. The intensities reported are in arbitrary unit in the velocity representation. As can be seen from Figure S23, the UV-vis spectrum is very well reproduced by the simulation, which indicates that the computed wavelengths match the experimental ones. The simulated ECD spectrum for *(P,P,P,M,M,M)*-D_3-**2** is also in good agreement with the experimental one, which confirmed the absolute configuration of the molecule. In particular, the excitations at 461 nm, the sign change in the 375-425 nm region, the abrupt sign change around 280 nm and the large negative band at around 260 nm, are convincing evidences.

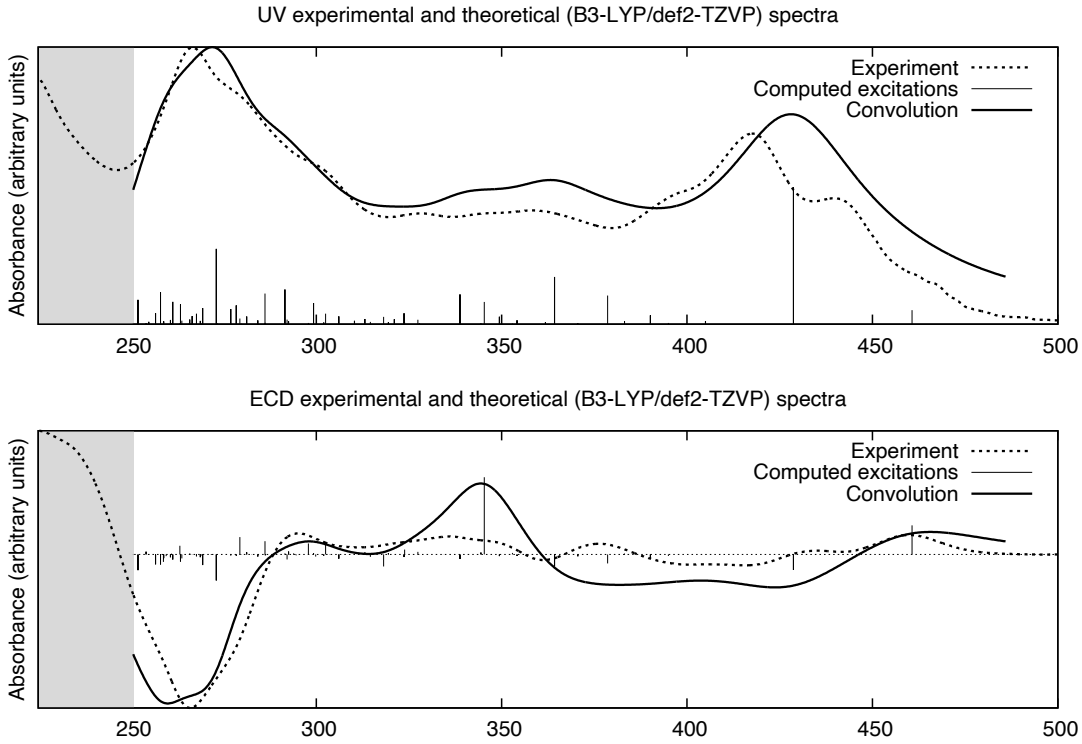


Figure S23. Comparison of the simulated and experimental UV-vis and ECD spectra of *(P,P,P,M,M,M)*-D_3-**2**. Calculations were performed at the B3LYP/def2TZVP level of theory in the gas phase. Computed wavelengths were shifted by 5%. The convolution was obtained with a fit by Lorentzian functions of half width of 0.3 eV. Theoretical intensities are given in the velocity representation. The highest computed excitation lies at 264 nm, precluding the reproduction of experimental values at higher energies (grey region).

Infrared (IR) and vibrational circular dichroism (VCD) study

Infrared (IR) and (VCD) spectra were recorded on a Bruker PMA 50 accessory coupled to a Vertex70 Fourier transform infrared spectrometer. A photoelastic modulator (Hinds PEM 90) set at l/4 retardation was used to modulate the handedness of the circular polarized light at 50 kHz. Demodulation was performed by a lock-in amplifier (SR830 DSP). An optical low-pass filter (< 1800 cm^{-1}) before the photoelastic modulator was used to enhance the signal/noise ratio. Due to its moderate solubility in standard solvents used in infrared spectroscopy, the sample of (+)-(*P,P,P,M,M,M*)-D_3-**2** was analyzed in the solid state. A pellet was prepared by mixing 1.5 mg of (+)-(*P,P,P,M,M,M*)-D_3-**2** as an orange powder with 100 mg of dry KBr. The VCD spectrum was recorded at room temperature. About 48000 scans were averaged at 4 cm^{-1} resolution (corresponding to 12 hours measurement time). The presence of vibrational linear dichroism (VLD) in the VCD spectrum was check. The VLD spectrum measurement of the pellet used for the VCD study shows that there is no significant contribution of VLD in the VCD spectrum. For IR absorption spectrum, the empty measuring compartment served as a reference. The spectra are presented without smoothing and further data processing (Figure S24).

For the simulations (Figure S24), the geometry of (–)-(*M,M,M,P,P,P*)-D_3-**2** was optimized by DFT methods using M06L/DGTZVP, and the vibrational frequencies, IR absorption and VCD intensities were calculated at the same level of theory. Computed harmonic frequencies have been calibrated using a scaling factor of 0.97 since they are generally larger than those experimentally observed. IR absorption and VCD averaged spectra were constructed from calculated dipole and rotational

strengths assuming Lorentzian band shape with a half-width at half maximum of 10 cm^{-1}. All calculations were performed using the Gaussian 16 package.[12]

Despite low-intensity spectra, a good agreement can be established between the most intense bands of the measured and calculated VCD spectra. The bands calculated for the (–)-*(M,M,M,P,P,P)*-D_3-**2** enantiomer have opposite sign to the corresponding bands of the experimental spectrum recorded for (+)-*(P,P,P,M,M,M)*-D_3-**2**, which further confirms the absolute configuration of the molecule.

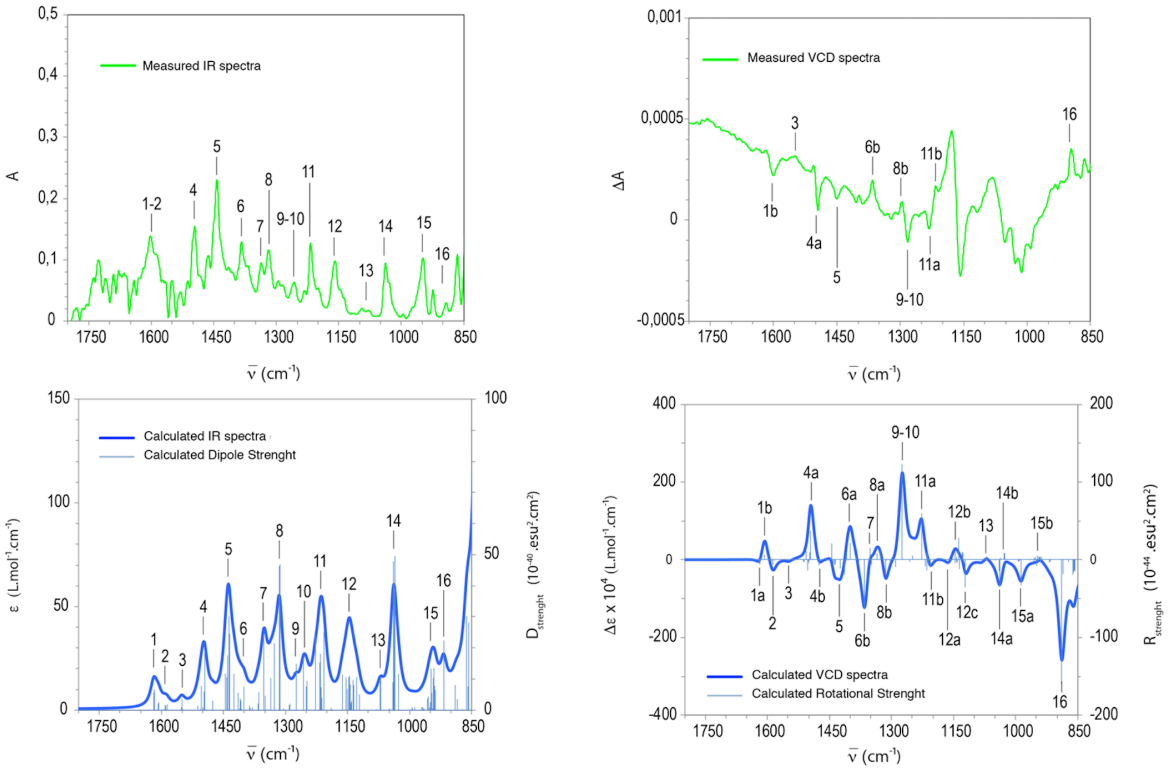


Figure S24. Top: experimental IR (left) and VCD (right) spectra of (+)-*(P,P,P,M,M,M)*D_3-**2**. Bottom: Simulated IR (left) and VCD (right) spectra of (–)-*(M,M,M,P,P,P)*-D_3-**2**.

4.2. Diastereomer C_2-2

The two enantiomers of C_2-**2** (4.6 mg) were separated by semi-preparative chiral HPLC techniques using a (*S*,*S*)-Whelk-O1 (250 x 10 mm) column eluted with (2:1:1) hexane/propan-2-ol/dichloromethane at 5 mL/min (114 stacked 70 µL injections, every 13.5 min) with UV detection at 254 nm. Using these conditions, we collected 1.8 mg of the first eluted enantiomer and 2.0 mg of

[12] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

the second eluted enantiomer, which were analysed by polarimetry and ECD, the amount of material available did not allow the recording of VCD data.

Optical rotation

Optical rotations were measured on a Jasco P-2000 polarimeter with a sodium lamp (589 nm), a halogen lamp (578 and 546 nm) in a 10 cm cell thermostated at 25 °C with a Peltier controlled cell holder (Table S10).

Table S10. Optical rotation of both enantiomers of *C*$_2$-**2**

λ (nm)	first eluted enantiopmer on (*S*,*S*)-Whelk-O1 $[\alpha]_\lambda^{25}$ (CH_2Cl_2, c = 0.0337)	second eluted enantiomer on (*S*,*S*)-Whelk-O1 $[\alpha]_\lambda^{25}$ (CH_2Cl_2, c = 0.037)
589	+ 705	- 705
578	+ 740	- 740
546	+ 885	- 885

UV-vis and electronic circular dichroism (ECD) study

UV (Figure S25) and ECD spectra (Figure S26) were measured on a JASCO J-815 spectrometer equipped with a JASCO Peltier cell holder PTC-423 to maintain the temperature at 25.0 ± 0.2 °C. A CD quartz cell of 1 mm optical pathlength was used. The CD spectrometer was purged with nitrogen before recording each spectrum, which was baseline subtracted. The baseline was always measured for the same solvent and in the same cell as the samples. The spectra are presented without smoothing and further data processing. Acquisition parameters: 0.1 nm as intervals, scanning speed 50 nm/min, band width 2 nm, and 3 accumulations per sample.

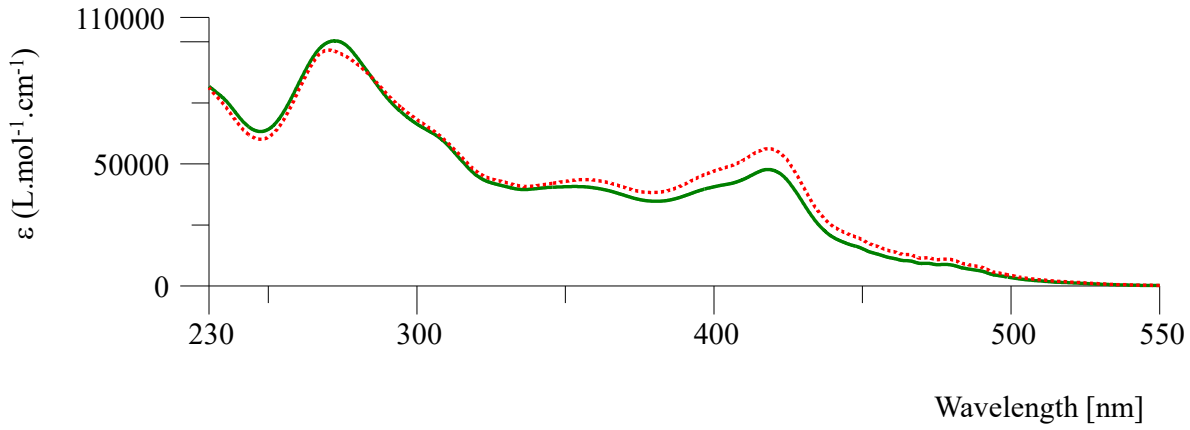


Figure S25. Experimental UV-vis spectra of both enantiomers of *C*$_2$-**2**. Data for the first eluted enantiomer (concentration = 0.129 mmol.L^{-1} in dichloromethane) are depicted with a solid green line, and data for the second eluted enantiomer (concentration = 0.124 mmol.L^{-1} in dichloromethane) are depicted with a dotted red line.

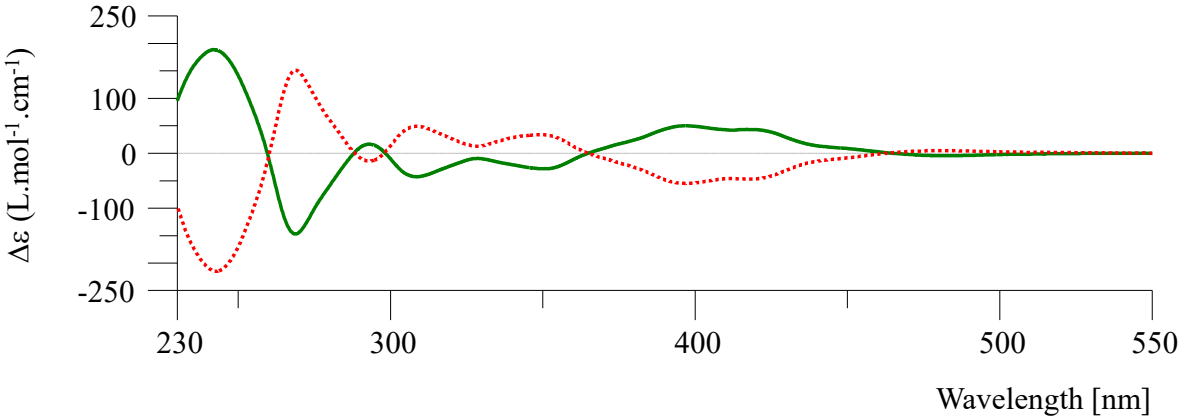


Figure S26. Experimental ECD spectra of both enantiomers of C_2-**2**. Data for the first eluted enantiomer (concentration = 0.129 mmol.L^{-1} in dichloromethane) are depicted with a solid green line, and data for the second eluted enantiomer (concentration = 0.124 mmol.L^{-1} in dichloromethane) are depicted with a dotted red line.

The experimental UV-vis and ECD spectra of C_2-**2** were compared with simulated spectra obtained by DFT computational methods for (*P,M,P,P,P,M*)-C_2-**2** (Figure S27). Calculations were performed with Turbomole[14] using the B3LYP functional augmented with an empirical dispersion term (Grimme's D3 dispersion model[13]) and the def2-SV(P) basis set on optimized geometries. The obtained wavelengths were then corrected by a factor of 0.95. As can be seen from Figure S27, the UV-vis spectrum is relatively well reproduced by the simulation, which indicates that the computed wavelengths match the experimental ones. The simulated ECD spectrum for (*P,M,P,P,P,M*)-C_2-**2** matches relatively nicely with the one of the first eluted enantiomer (the solid green line in Figure S26), which allowed attributing the absolute configuration in C_2-**2** as follow:

- The first eluted enantiomer (+)-C_2-**2** is (*P,M,P,P,P,M*)-configured. The positive sign of its $[\alpha]_D^{25}$ is in full agreement with this attribution with two (*P*)-configured [5]helicenes and two (*P*)-configured [7]helicenes in the structure, all accounting for a positive contribution to $[\alpha]_D^{25}$.
- The second eluted enantiomer (–)-C_2-**2** is (*M,P,M,M,M,P*)-configured. The negative sign of its $[\alpha]_D^{25}$ is in full agreement with this attribution with two (*M*)-configured [5]helicenes and two (*M*)-configured [7]helicenes in the structure, all accounting for a negative contribution to $[\alpha]_D^{25}$.

[13] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104.

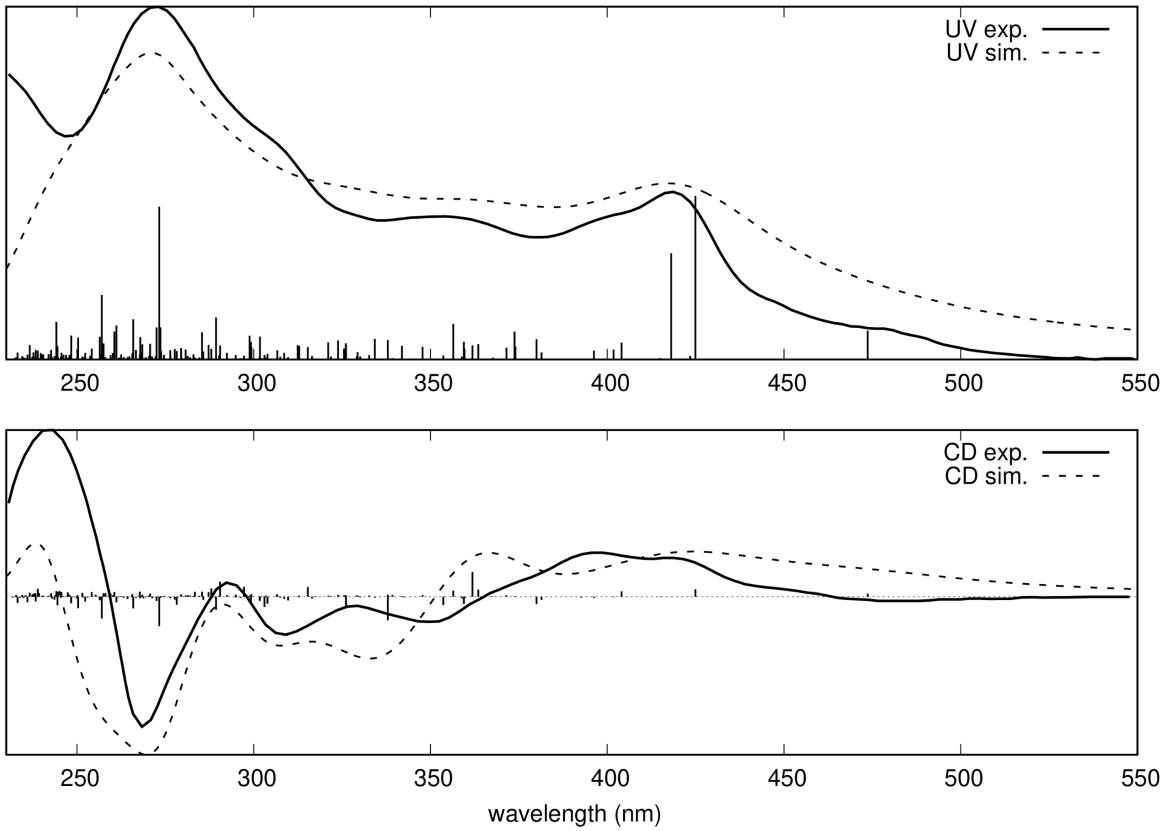


Figure S27. Comparison of the simulated and experimental UV-vis and ECD spectra of (*P,M,P,P,P,M*)-C_2-**2**. Calculations were performed at the B3LYP-D/def2-SV(P) level of theory in the gas phase. The impulses indicate the actual excitation wavelength, 200 states were computed with TD-DFT at the B3LYP-D/def2-SV(P) level, and the convolution was done on Lorentzian functions with a width at half maximum of 0.4 eV.

5. Photophysical studies

The photophysical properties of (+)-*D*$_3$-**2** (1.42 μmol.L^{-1} in dichloromethane) were evaluated (Figure S28). The absorption spectrum shows a mean absorption coefficient of 90000 M^{-1}cm^{-1} at 417 nm. The absorption and emission spectra (λ_{exc} = 400 nm) were recorded: the excitation spectrum was recorded from a solution that has absorbance lower that 0.1 in all the spectral range. There is a good overlap between absorption and emission spectra (λ_{em} = 560 nm). The quantum yield was calculated with Ru(bpy)$_3$ in water. Errors of 30–50% in the absorption coefficient and the quantum yield are certainly possible due to the small amount of material analyzed.

Absorption max: 417 nm (ε = 90000 M^{-1}cm^{-1})
Emission: max 538 nm, quantum yield 5.7%.

These values are very comparable with to the ones previously reported for lower-order analogues of *D*$_3$-**2**.[10,11]

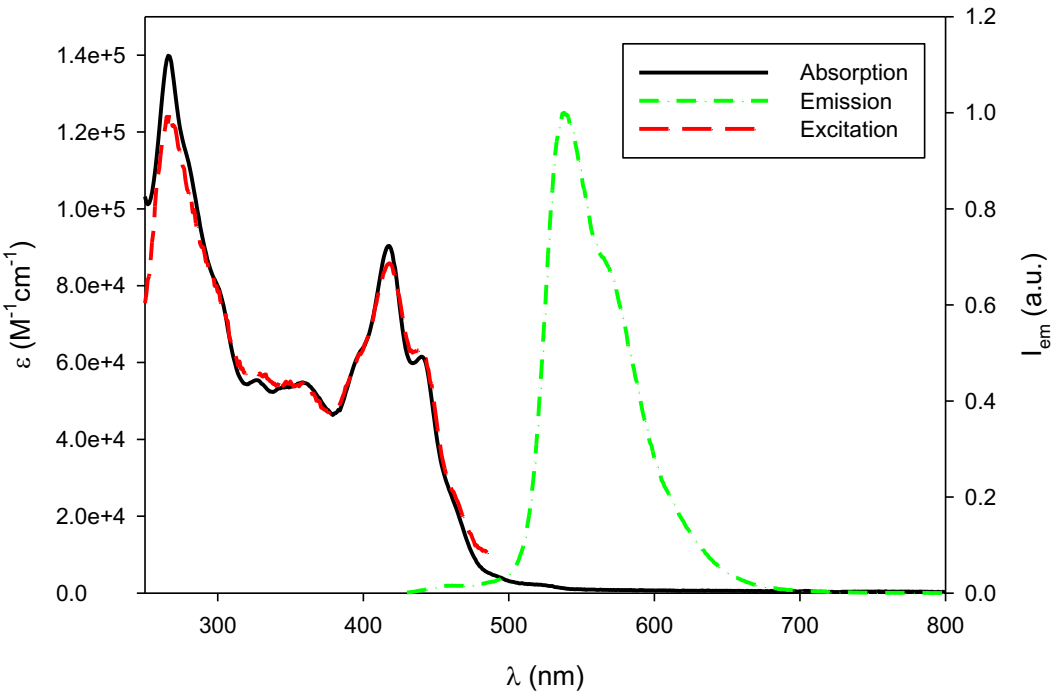


Figure S28. UV-vis absorption spectrum (solid black line) and photoluminescence (green dashed lines) of (+)-*D*$_3$-**2** in dichloromethane.

6. Evaluation of aromaticity

6.1. Calculation details

DFT calculations for geometries optimization were performed with the Turbomole v7.2 package[14] using the B3LYP functional augmented with an empirical dispersion term (Grimme's D3 dispersion model[13]) and the def2-SV(P) basis set in the gas phase with no symmetry restrictions. All calculated structures are local minima on the potential energy surfaces and were characterized by harmonic frequency calculations (i.e. no imaginary frequencies were found). The non covalent interaction (NCI) plots were obtained by using the NCIplot program[15] at the B3LYP/def2-TZVP level of calculation performed with the Gaussian 09 suite[7] on top of B3LYP-D3/def2-SV(P) optimized geometries.

For the structure-based Harmonic Oscillator Model of Aromaticity (HOMA),[16] the following parametrization was employed :

$$\mathrm{HOMA} = 1 - \frac{\alpha}{n}\sum_{i}^{n}\left(R_{\mathrm{opt}} - R_i\right)^2$$

where $\alpha = 257.7$ is an empirical normalization constant, $R_{opt} = 1.388$ Å as a reference bond length for benzene, and R_i are the computed bond lengths of the considered ring. For benzenoid rings, $n = 6$. Thus, for benzene itself HOMA = 1. For the NICS calculations, and because of the severe distortion of the systems studied, a mean plane was defined for each individual ring, and the Gauge Independent Atomic Orbitals method (GIAO)[17] was employed for chemical shifts calculations at the same level as the geometry optimization. NICS were calculated along a line perpendicular to the mean plane at 9 different positions distant of 0.5 Å: one at the center of each ring for NICS(0), and four below and four above the ring for NICS(–2) to NICS(+2). For ACID calculations, the continuous set of gauge transformation (CSGT) method was used to calculate current densities,[18] as implemented in the Gaussian 9 package.[7] The calculated current density was subsequently transformed in a rectangular grid and visualized as a cube-file with POVRAY.[19] The applied magnetic field is orthogonal to the mean plane defined by the 6 atoms of the central ring, pointing upward in all illustrations, with clockwise currents being diatropic. A standard value of 0.05 was chosen for the ACID isosurface. The density of points to compute the surface was chosen to be 160000. Finally, Shannon indexes of individual six-membered rings were computed using the Multiwfn 3.4.1 program.[20]

[14] TURBOMOLE V7.2 2017, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989-2007, TURBOMOLE GmbH, since 2007; available from http://www.turbomole.com.

[15] J. Contreras-García, E. R. Johnson, S. Keinan, R. Chaudret, J.-P. Piquemal, D. N. Beratan, W. Yang, *J. Chem. Theory Comput.* **2011**, *7*, 625.

[16] a) T. M. Krygowski, *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 7; b) T. M. Krygowski, H. Szatylowicz, O. A. Stasyuk, J. Dominikowska, M. Palusiak, *Chem. Rev.* **2014**, *114*, 6383.

[17] a) F. London, *J. Phys. Radium* **1937**, *8*, 397; b) J. R. Cheeseman, G. W. Trucks, T. A. Keith, M. J. Frisch, *J. Chem. Phys.* **1996**, *104*, 5497; c) G. Schreckenbach, T. Ziegler, *J. Phys. Chem.* **1995**, *99*, 606; d) G. Schreckenbach, T. Ziegler, *Theor. Chem. Acc.* **1998**, *99*, 71.

[18] a) T. A. Keith, R. F. W. Bader, *Chem. Phys. Lett.* **1992**, *194*, 1; b) T. A. Keith, R. F. W. Bader, *J. Chem. Phys.* **1993**, *99*, 3669.

[19] Persistence of Vision Pty. Ltd. (2004) Persistence of Vision Raytracer (Version 3.6) [Computer software]. Retrieved from http://www.povray.org/download/

[20] T. Lu, F. Chen, *J. Comp. Chem.* **2012**, *33*, 580.

6.2. HOMA

As a preamble to this part of the study, it should be noted that HOMA analyses of local aromaticity in the hextuple helicenes *D*$_3$-**HNTP** and *C*$_2$-**HNTP** were previously reported and found somewhat contradictory with the NICS analyses for the same compounds, and these discrepancies were attributed to their "highly twisted geometry".[11] Herein, we provide the HOMA analyses for the larger hextuple helicenes *D*$_3$-**2** and *C*$_2$-**2** (Figure S29). According to the HOMA values, the most aromatic rings in *D*$_3$-**2** would be the six symmetric external E rings and the least aromatic ones would be the three symmetric internal B rings, which is somehow consistent with the NICS analysis (see Figure 6a in the main text). However, the evolution of aromaticity when going from the central A ring to the external E rings is markedly different in both analyses: HOMA indicates an alternation of decrease/increase in local aromaticity (as analyzed from a Clar's perspective, see main text and below) while NICS and ACID analyses show a gradual increase in local aromaticity from non-aromatic to fully aromatic (see Figure 4 in the main text). Similarly, the HOMA analysis of *C*$_2$-**2** indicates that the external E, H and E' rings would be the most aromatic ones, and that the internal B and B' rings would be the least aromatic ones, which is not consistent with the NICS analysis, the central A ring being less aromatic than the B ring according to NICS. As for *D*$_3$-**2**, the alternation in decreased/increased local aromaticity when going from the A ring to the peripheral E, H and E' rings found in the HOMA (or Clar) analysis is not reproduced in the NICS and ACID analyses, which show a gradual increase in aromaticity from ring A to ring E, H and E'.

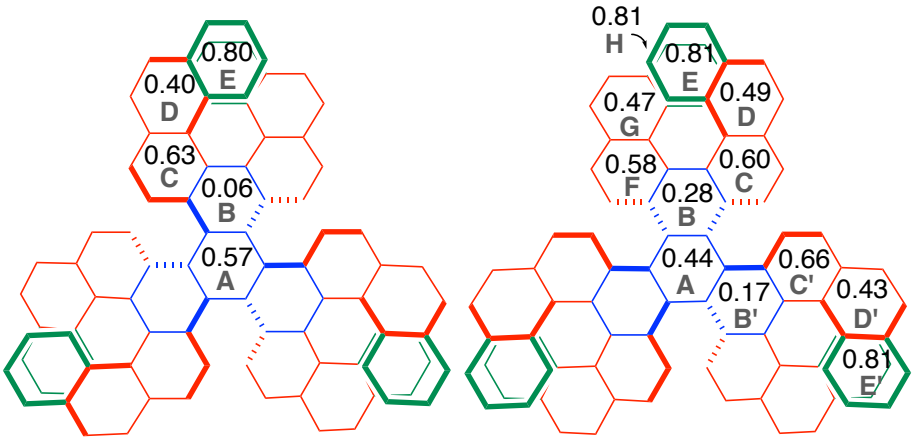


Figure S29. HOMA values for nonequivalent rings in *D*$_3$-**2** (left) and *C*$_2$-**2** (right). The color code refers to aromaticity according to NICS(0) values, indicating a clear mismatch: green = full aromaticity, red = somewhat deficient aromaticity, blue = poorly or not aromatic.

In conclusion of this part of the study, the HOMA does not appear as a suitable model for the analysis of local aromaticity in *D*$_3$-**2** and *C*$_2$-**2**. This is actually not surprising considering the definition of HOMA indices, and it was recently suggested to modify the HOMA with planarity descriptors for the analysis of simple nonplanar PAHs.[21]

[21] M. Antić, B. Furtula, S. Radenković, *J. Phys. Chem. A* **2017**, *121*, 3616.

6.3. Clar analysis

The aromaticity of PAHs can qualitatively be evaluated by their Clar's structures. These structures are built according to the so-called "Clar's rule", which states that the Kekulé resonance structure in a PAH containing the largest number of disjoint aromatic π-sextets, i.e. benzene-like moieties, displays an extra stability and is thus the most representative of its electronic distribution.[22] This simple rule is extremely useful when applied to planar PAHs. However, this method is qualitative and does not allow comparison of the relative local aromaticity of each π-sextet.

The Clar's structures containing the largest number of disjoint aromatic π-sextets of triphenylene, D_3-hexabenzotriphenylene (D_3-**HBTP**), D_3-**HNTP**, and D_3-**2** are provided in Figure S30. Note that the Clar's structures of the C_2-symmetric diastereomers are identical to those of the D_3-symmetric diastereomers although they have different spatial arrangements and torsions.

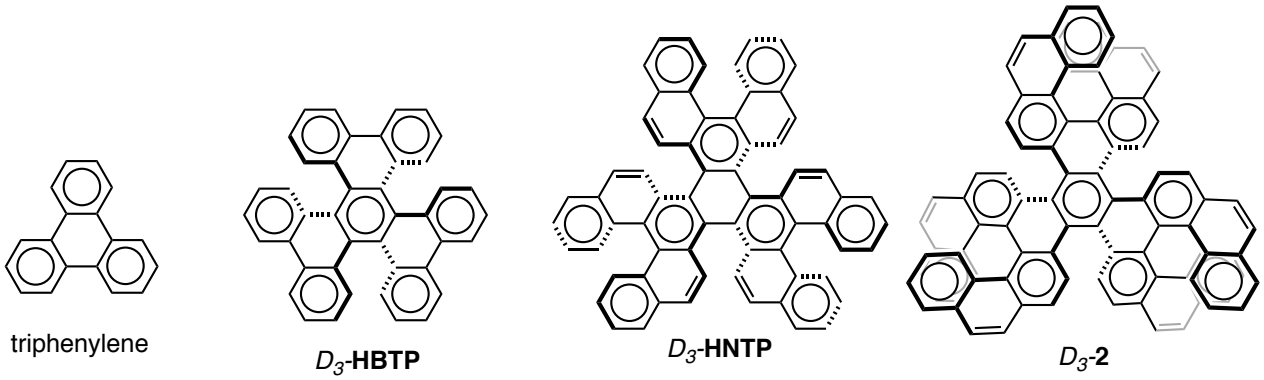


Figure S30. Clar's structures containing the largest number of disjoint aromatic π-sextets of triphenylene, D_3-**HBTP**, D_3-**HNTP**, and D_3-**2**.

[22] M. Solá, *Front. Chem.* **2013**, *1*, 22.

6.4. NICS

In order to quantitatively appreciate the evolution of local aromaticity when going from triphenylene to the described triphenylene-based propeller-shaped large hextuple helicenes, we undertook a systematic NICS analysis of triphenylene, *D*$_3$-**HBTP**, *D*$_3$-**HNTP**, and *D*$_3$-**2** at the same level of theory.

The magnetic NICS index is defined as the negative of the chemical shift computed at ghost atoms, generally located at ring centers or above (or below) the plane of the ring.[23] Any ghost atom can be viewed as a magnetic sensor at which one computes the local magnetic shielding caused by the circulation of the electrons in the ring. Thus, a significant negative NICS value in interior positions of the rings indicate the presence of so-called induced *diatropic* ring currents and is synonym of aromaticity. On the contrary, a positive NICS value denotes induced *paratropic* ring currents and is synonym of antiaromaticity. In order to reduce the influence of valence σ-electrons' contribution to the NICS index, a NICS(1) value, i.e. calculated at 1 Å above the plane where the π orbitals have their maximum density, was recommended.[23] For nonplanar systems however, the points above and below the ring center are no longer equivalent by symmetry and the NICS(1) index may introduce a bias in the measure of aromaticity. It was recently suggested to split the NICS(1) index into NICS(1) and NICS(-1) (calculated at 1 Å below the ring center) indices and use the average value $NICS(1)_{av}$ = 1/2 [NICS(1)+NICS(-1)] to characterize the aromaticity of distorted benzenoid rings.[24] For the present work we calculated NICS(–2) to NICS(2) with 0.5 Å increments as well as $NICS(1)_{av}$ for triphenylene, *D*$_3$-**HBTP**, *D*$_3$-**HNTP**, *D*$_3$-**2** and *C*$_2$-**2** (Figures S33, S34, S35, S31 and S36, respectively). From this set of data, it appeared that the presence of C–H bonds in the vicinity of the considered ghost atoms influenced significantly the magnitude of the calculated NICS. For instance, there are some important difference in the NICS(h) and NICS (-h) calculated for *D*$_3$-**HBTP**, *D*$_3$-**HNTP** and *D*$_3$-**2** as illustrated in Figure S35, S34 and S31, respectively, especially for ring C. Such behavior has already been reported for isolated [8]- and [9]-helicenes.[25] This can be explained by the deshielding of the magnetic field below these planes caused by the paratropic field generated by the C–H bond lying in a nearly parallel position to the mean plane of rings C and D. The effect on ring C is larger because a C–H bond from ring E of the other end of the [7]helicene unit is really close and nicely parallel to ring C. This is fully supported by the analysis of non-covalent interactions (NCIs) in (*M,M,M,P,P,P*)-*D*$_3$-**2** (Figure S32). Four distinct NCI surfaces appear: 1) large (*M*)-configured helicoidal surfaces inside each [7]helicene unit on the outer crown, 2) (*P*)-configured helicoidal surfaces inside each [5]helicene unit on the inner crown, 3) small more or less planar surfaces between carbon atoms at the periphery of the molecule in the [7]helicene units, and 4) inside each individual benzene ring. For NCI surfaces #1–3, the regions correspond to an increased electronic density in the space between the cycles and affect the calculated shielding below and above the mean plane of the considered rings. The value of the NCI surfaces indicates that the interactions are globally of small amplitude (green colored), with however an attractive part (blue colored) between ring C and the C–H bond of the distal ring E. For NCI surfaces #4, small amplitude repulsive surfaces are known to exit at the center of each ring as areas of nonbonded overlap.[26] For these reasons, we selected NICS(0) as the most representative, though not ideal, relative and absolute criterion of local aromaticity in *D*$_3$-**2** and its diastereomer *C*$_2$-**2**.

[23] Z. Chen, C. S. Wannere, C. Corminboeuf, R. Puchta, P. von R. Schleyer, *Chem. Rev.* **2005**, *105*, 3842.
[24] J. C. Dobrowolski, P. F. J. Lipiński, *RSC Adv.* **2016**, *6*, 23900.
[25] G. Portella, J. Poater, J. M. Bofill, P. Alemany, M. Solá, *J. Org. Chem.* **2005**, *70*, 2509.
[26] E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-García, A. J. Cohen, W. Yang, *J. Am. Chem. Soc.* **2010**, *132*, 6498.

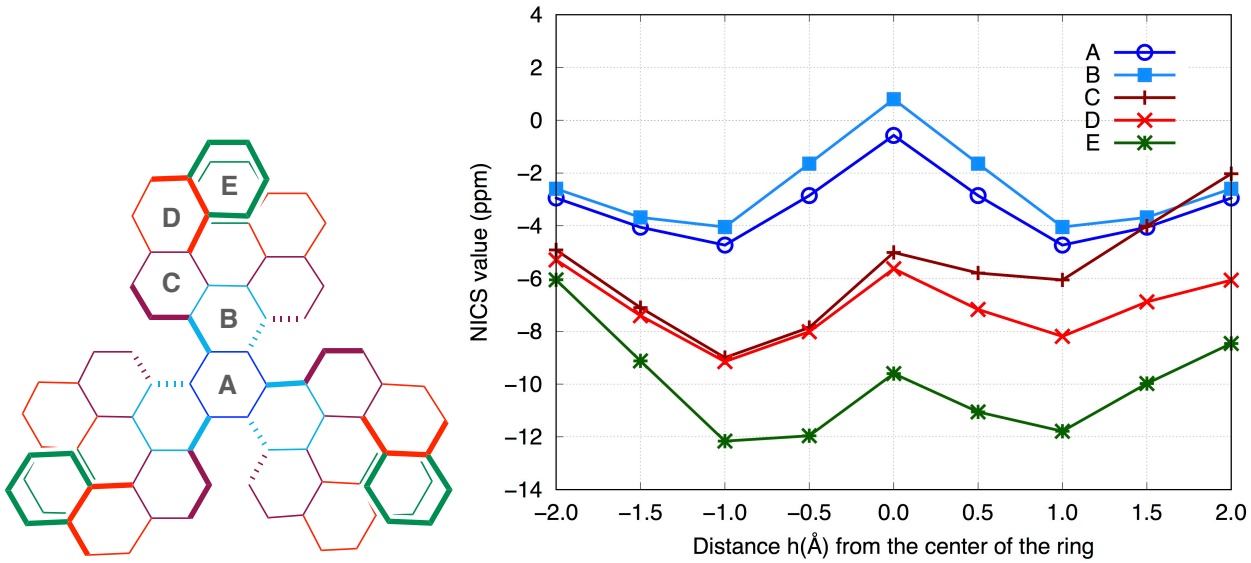


Figure S31. NICS values calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in D_3-**2**.

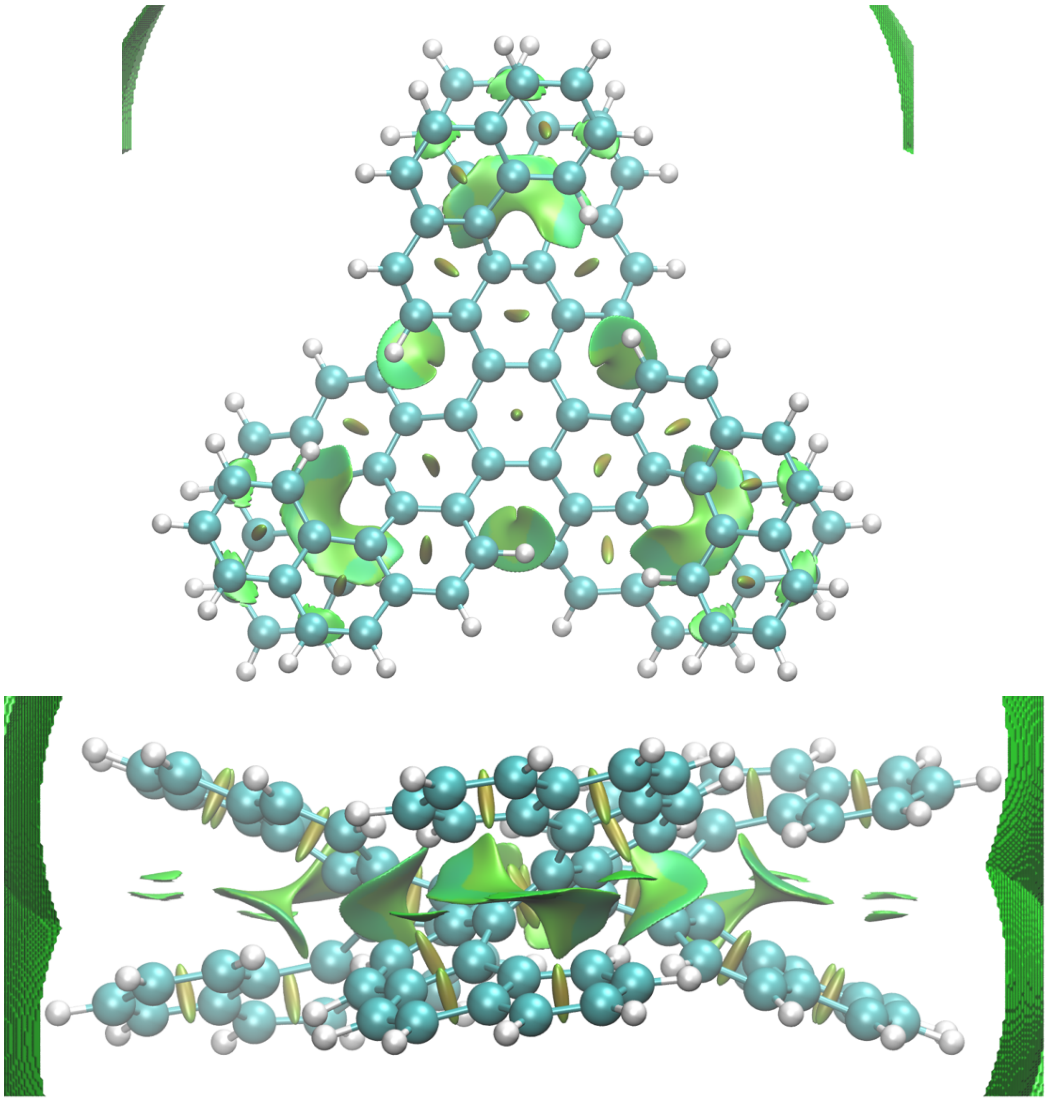


Figure S32. Top and side views of non-covalent interaction (NCI) surfaces in D_3-**2**. Blue color indicates strong attractive NCI, green color indicates weak NCI, and red color indicates strong repulsive NCI.

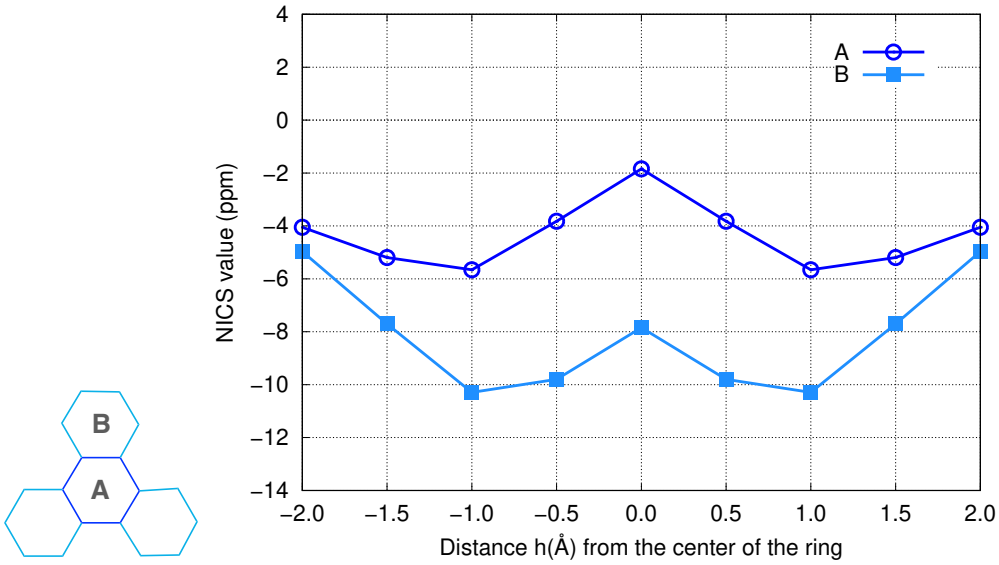


Figure S33a. NICS values for planar triphenylene calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in triphenylene.

In order to differentiate torsional effects from through-space and conjugation effects in the NICS(0) calculations of the triphenylene cores of both *D*$_3$-**2** and *C*$_2$-**2**, the NICS(0) were also computed for the virtual triphenylene molecules having the distorted geometries *D*$_3$-**2** and *C*$_2$-**2** (see Figure S33b). Comparison with the NICS(0) of triphenylene itself showed an augmentation of ca. +2 ppm for the distorted rings, showing that torsional effects have a significant contribution to the unusual NICS(0) value computed for *D*$_3$-**2** and *C*$_2$-**2**.

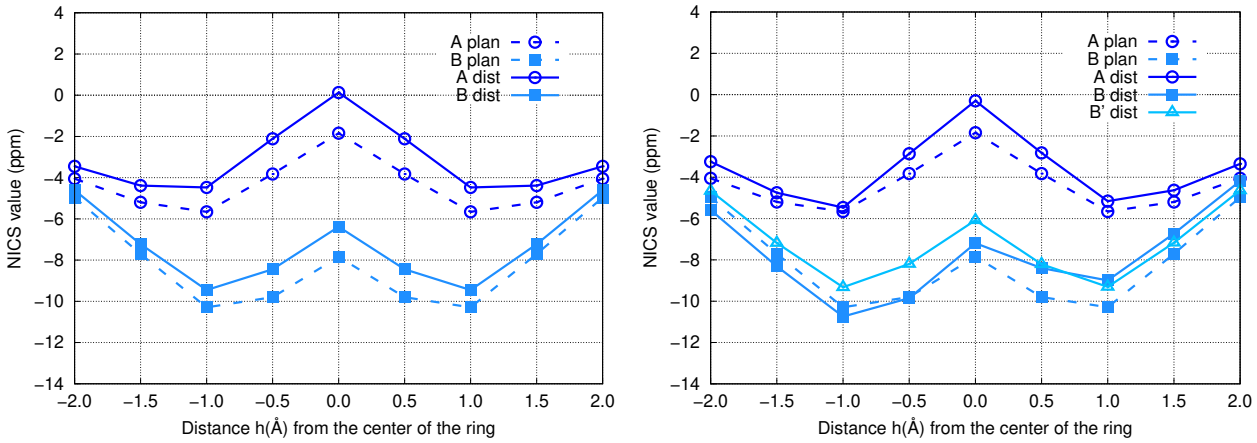


Figure S33b. NICS values for the virtual triphenylene molecules having the distorted geometries *D*$_3$-**2** (left) and *C*$_2$-**2** (right) with re-optimized geometries of the H atoms calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in triphenylene (plain lines). Dashed lines reproduce the NICS values for planar triphenylene plotted in Figure S33a.

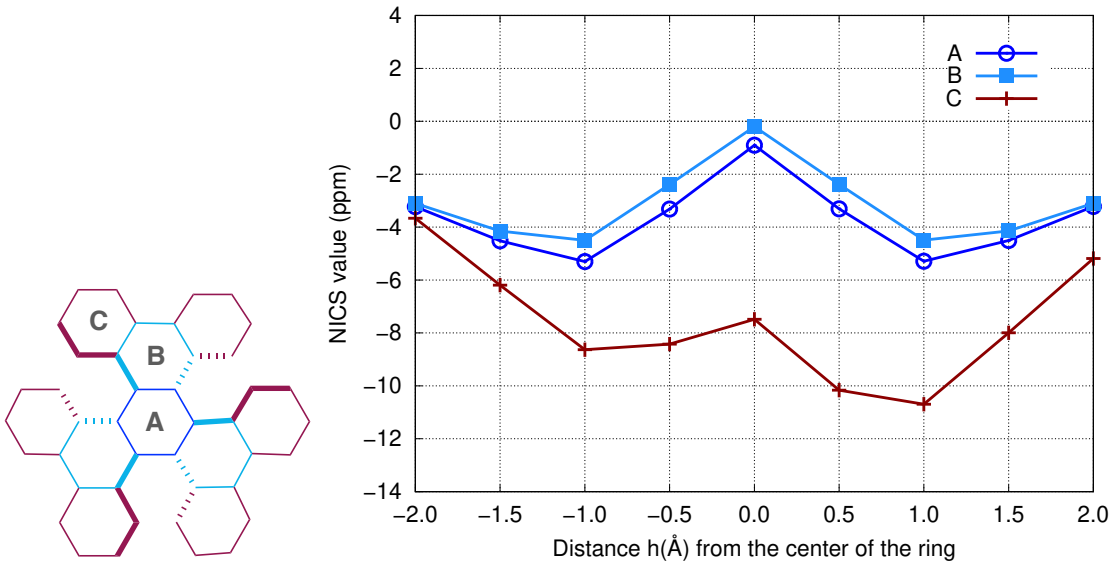


Figure S34. NICS values calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in *D*$_3$-**HBTP**.

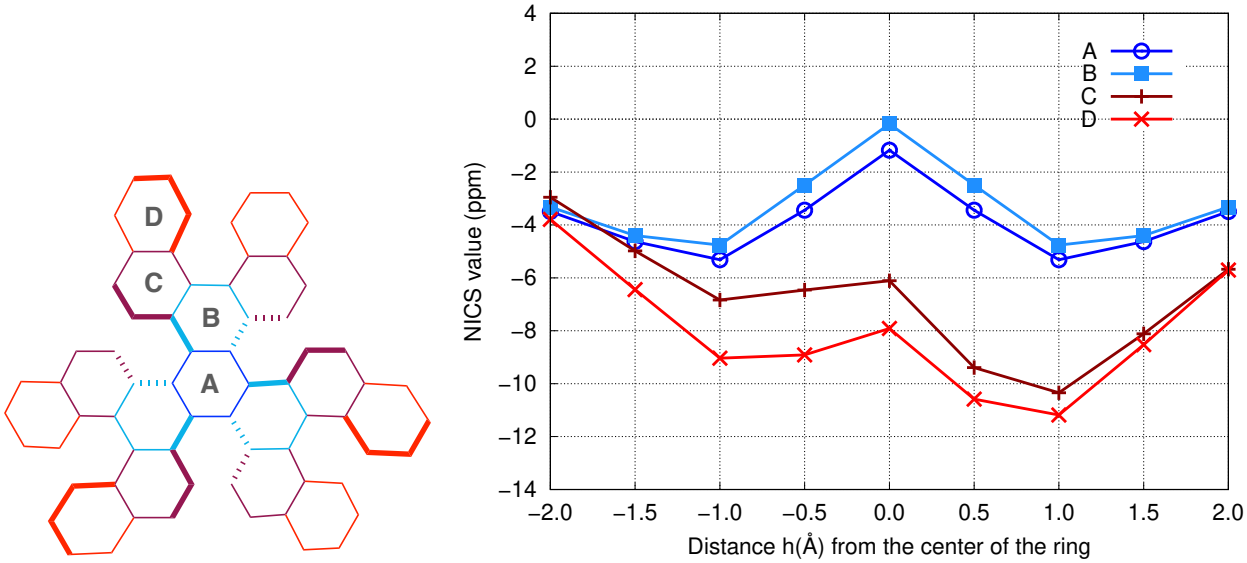


Figure S35. NICS values calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in *D*$_3$-**HNTP**.

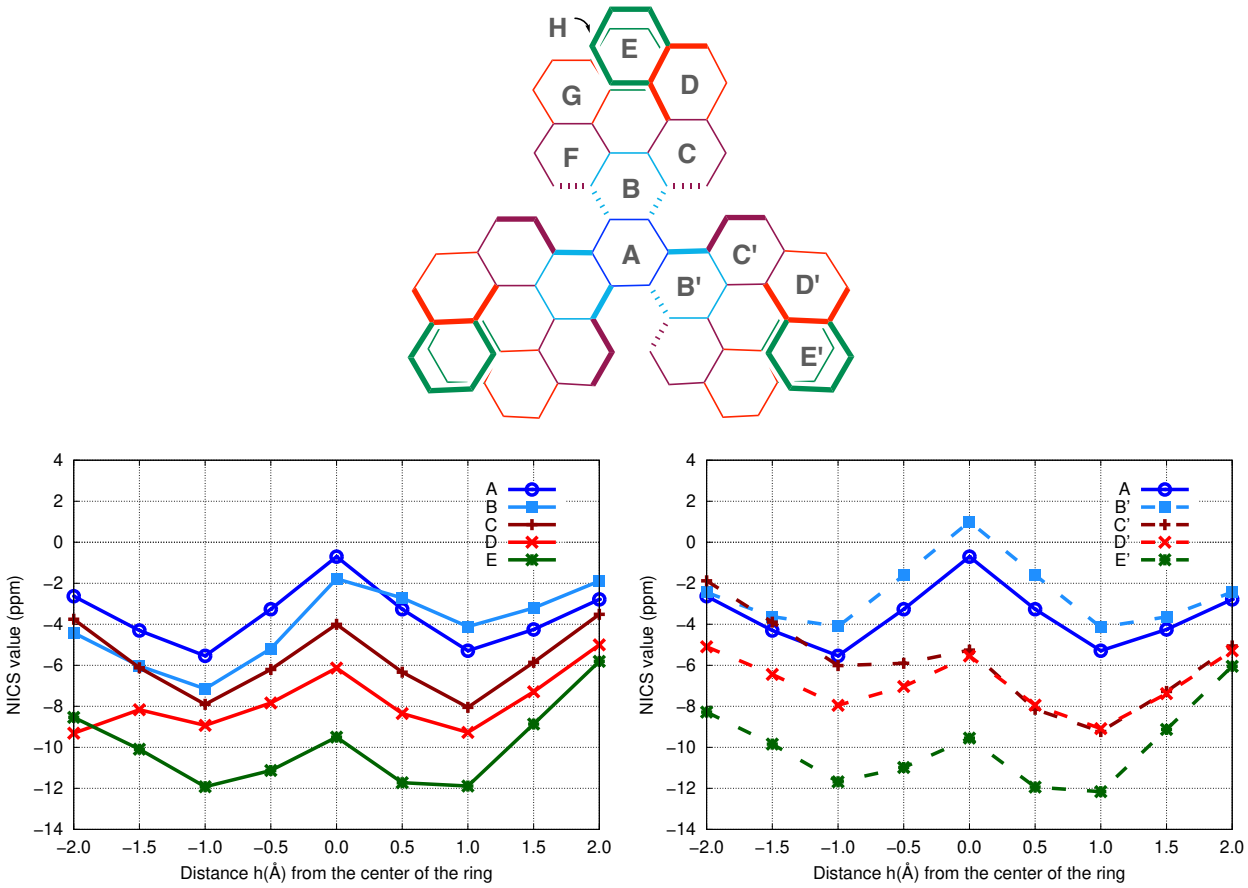


Figure S36. NICS values calculated at different distances h (in Å) below (h<0) and above (h>0) the mean plane of each ring in *C*$_2$-**2**. NICS profiles for rings F, G and H were found very similar to those of rings C, D and E and are not depicted for clarity.

6.5. ACID

ACID plots were calculated for triphenylene, D_3-**HBTP**, D_3-**HNTP**, D_3-**2** and C_2-**2** at the same level of theory for comparison (Figure S37–S41), which confirmed the respective NICS analyses. In all cases, strong macrocyclic diatropic ring currents were evidenced at the periphery of the molecule indicating global electronic delocalizations, which are certainly contributing to the thermodynamic stability of the molecules.

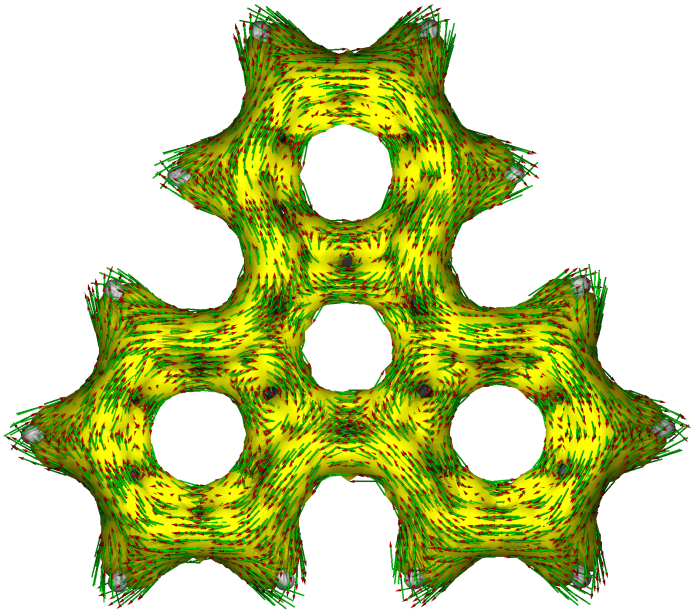


Figure S37. ACID plot of triphenylene.

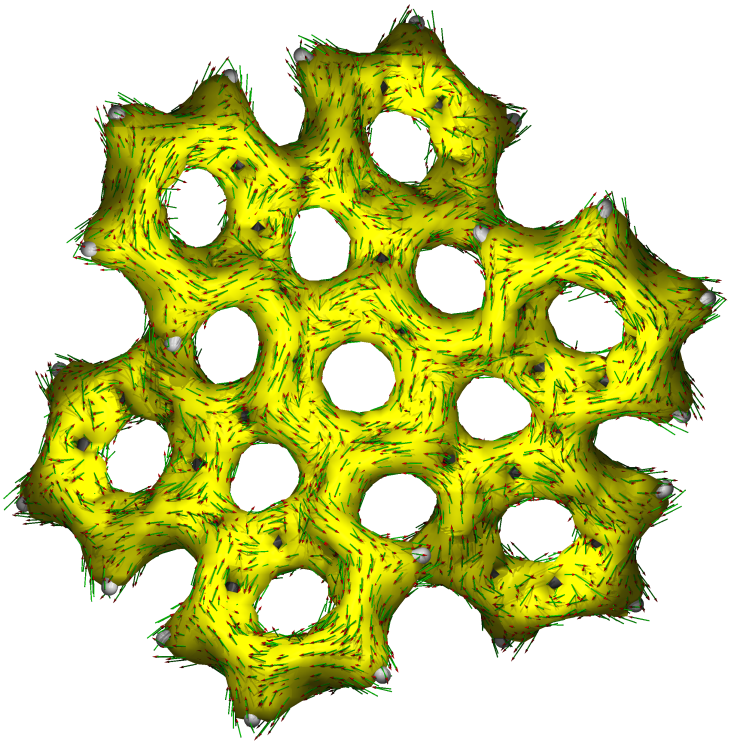


Figure S38. ACID plot of D_3-**HBTP**.

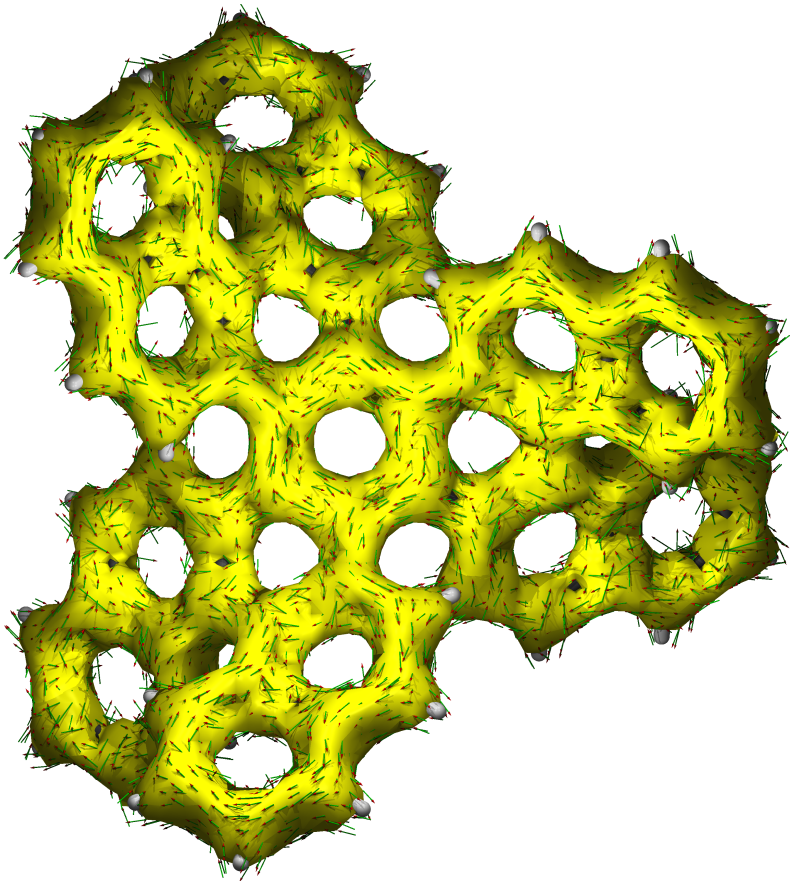


Figure S39. ACID plot of *D*$_3$-**HNTP**.

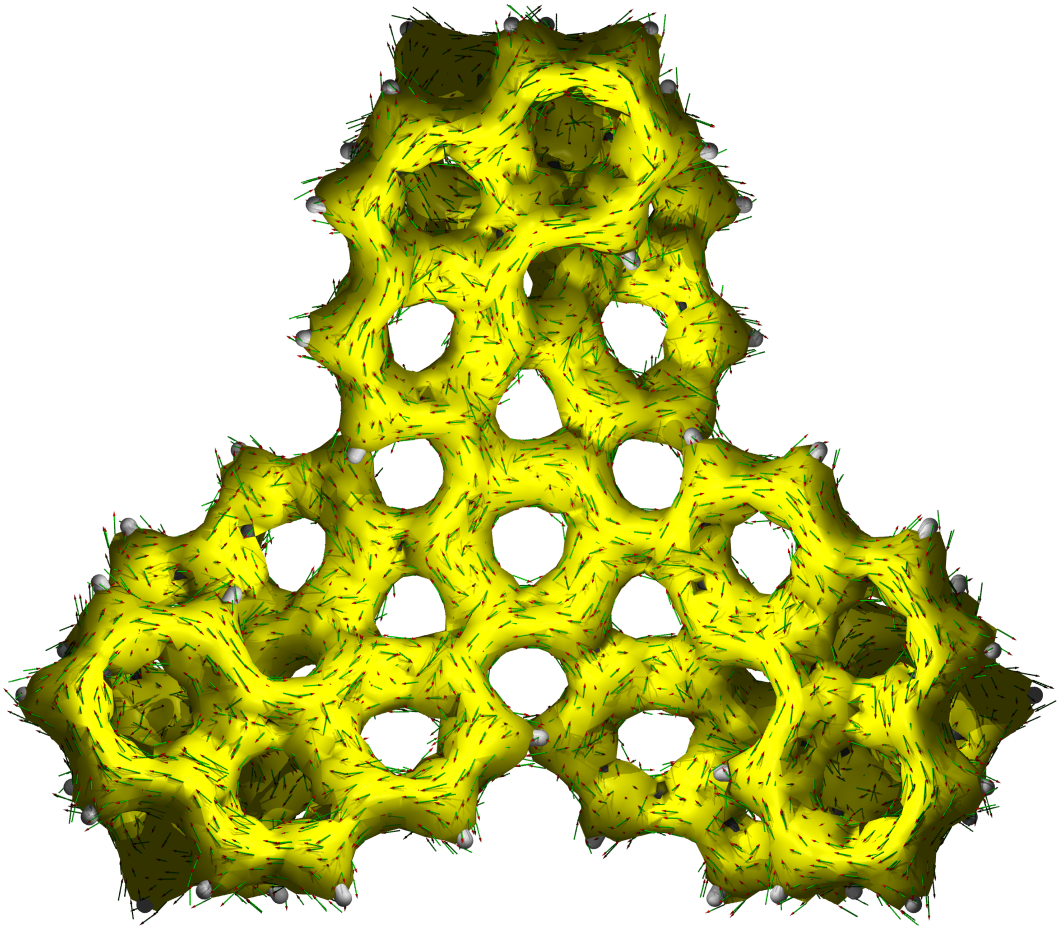


Figure S40. ACID plot of *D*$_3$-**2**.

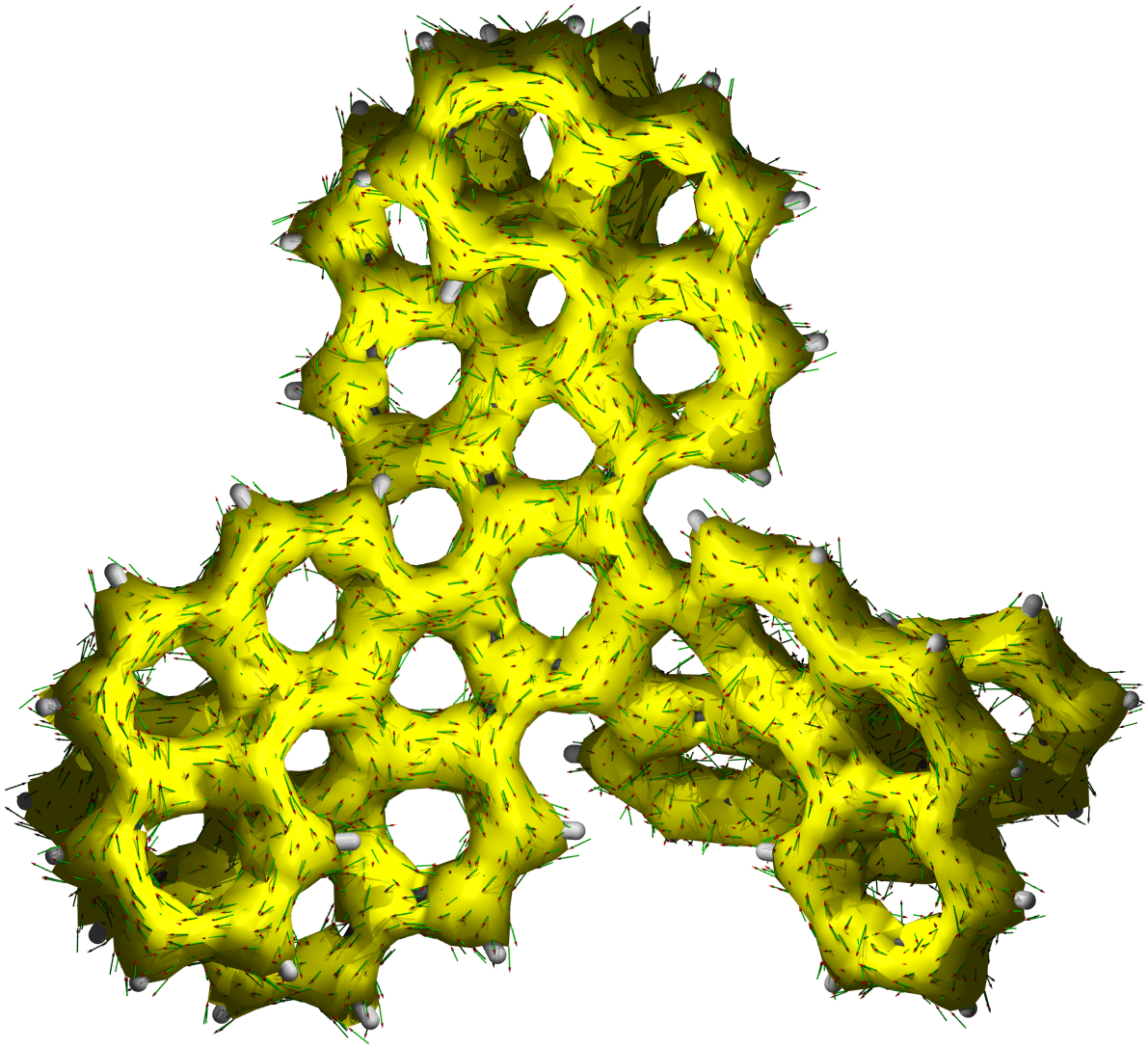


Figure S41. ACID plot of C_2-**2**.

6.6. Topological analysis: Shannon's aromacity index

In order to investigate further the electronic structure of *D*$_3$-**2**, we performed an analysis within the atoms in molecule (AIM) theoretical framework. Through this analysis, we shall be able to compute the aromaticity index of Shannon. This index comes from information theory and is based on the assumption that the entropy, as defined by Shannon, should be the same for all bonds involved in an aromatic ring. Shannon's aromaticity (SA) is computed as the difference between a hypothetical fully aromatic ring and the actual values obtained at the bonds. It takes into account the whole electronic density for the evaluation of the aromaticity. It is thus not specifically designed for planar systems. It does neither rely on the geometry (as HOMA does) nor on a specific view of what a π bond is (as NICS(1)$_{av}$ does). It was recently successfully used to study the aromaticity of various aromatic hydrocarbons.[27] To access this index, we must first find all critical points (as defined in the AIM framework) of the electronic density of the system. The critical points are defined through topological properties of the electronic density: atomic critical points (ncp$_a$) are found when the Laplacian of the density exhibits three negative eigenvalues, bond critical points (ncp$_b$) when two negative and one positive eigenvalues are found, ring critical points (ncp$_r$) when two eigenvalues are positive and one is negative and finally cage critical points (ncp$_c$) are found for three positive eigenvalues. The number of each kind of critical point must obey the necessary but not sufficient Poincaré-Hopf rule, which reads:

$$ncp_a - ncp_b + ncp_r - ncp_c = 1 \qquad (1)$$

We could find a set of critical points which obey equation (1). Using these points, we were able to compute Shannon's aromaticity indexes. Note that the index is defined such that the more aromatic cycle has an index value close to 0. As shown in Table S10, the SA values do not match either the NICS nor the HOMA trends as previously described by other authors.[27,28]

Table S10. Shannon's aromaticity indexes for *D*$_3$-**2**.

Ring	HOMA	NICS(0)	SA (x10^4)
A	0.57	-0.6	2.36
B	0.06	0.8	10.64
C	0.63	-5.0	8.54
D	0.40	-5.6	14.62
E	0.80	-9.6	5.21

The Shannon indexes suggest an alternation in aromaticity from cycle A to E, A being the most aromatic cycle followed by E, C, B and D. This description of the system is counter-intuitive and misleading. It shows how hard it is to give a proper description of the electronic structure of this system in terms of electronic delocalization and aromaticity, this later term missing a proper definition in the framework of distorted molecular systems.

[27] S. Noorizadeh, E. Shakerzadeh, *Phys. Chem. Chem. Phys.* **2010**, *12*, 4742.
[28] D. W. Szczepanik, M. Andrzejak, J. Dominikowska, B. Pawełek, T. M. Krygowski, H. Szatylowicz, M. Solà, *Phys. Chem. Chem. Phys.* **2017**, *19*, 28970.

7. Complexation studies of *D*$_3$-2

7.1. Computational study

The DFT calculations reported in this section were performed with the Gaussian 16 package.[12] All geometries were fully optimized in the gas phase using both the long-range corrected hybrid functional wB97XD that includes Grimme's D2 dispersion model with the Def2SVP basis set. The second derivatives were analytically calculated to confirm the resulting geometries as minima (zero negative eigenvalue) and thermal corrections to the free Gibbs energies were computed. Electronic energies were refined with the Def2TZVP basis set. Energies are expressed in kJ.mol^{-1} (1 Ha = 2625.5 kJ/mol).

Binding energies were determined as the difference between the energy of the complexes and the sum of the energies of an isolated Ag^+ cation and the (partially) uncomplexed ligands in their optimized geometries.

As a reference, binding energy for Ag^+ + [7]helicene → [Ag⊂[7]helicene]$^+$ = -284.7 kJ.mol^{-1}

Complex [Ag⊂[7]helicene]$^+$ was previously isolated and characterized by X-ray diffraction analysis using a $Al[OC(CF_3)_3]_4^-$ counter-anion.[29] The computed and experimental geometries were found in good agreement.

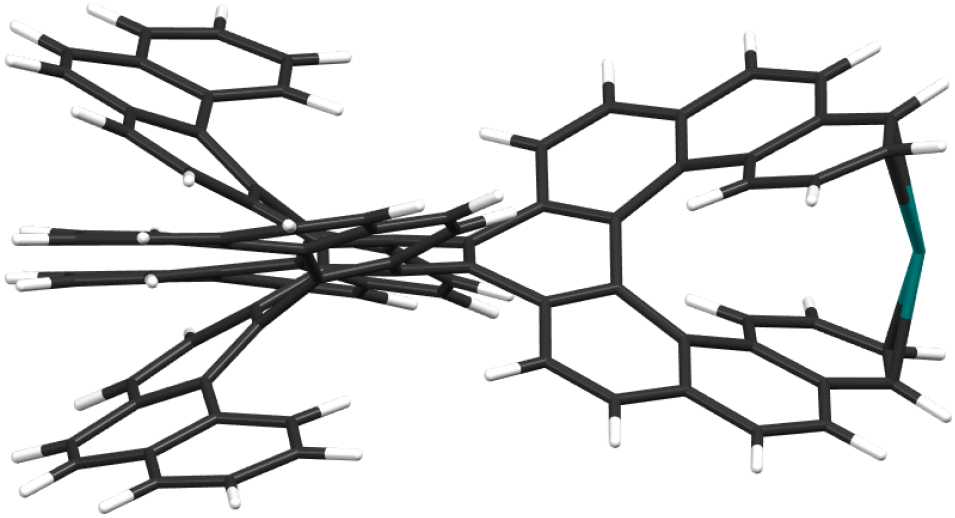
Binding energy for Ag^+ + *D*$_3$-**2** → [Ag⊂*D*$_3$-**2**]$^+$ = -297.6 kJ.mol^{-1}

Comparatively, an alternative geometry of the complex [Ag⊂*D*$_3$-**2**]$^+$ with the silver ion sandwiched by a [5]helicene unit at the inner crown gave a much lower binding energy of -257.0 kJ.mol^{-1}.

Binding energy for Ag^+ + [Ag⊂*D*$_3$-**2**]$^+$ → [2Ag⊂*D*$_3$-**2**]$^{2+}$ = -161.7 kJ.mol^{-1}

Binding energy for Ag^+ + [2Ag⊂*D*$_3$-**2**]$^{2+}$ → [3Ag⊂*D*$_3$-**2**]$^{3+}$ = -39.5 kJ.mol^{-1}

[Ag⊂*D*$_3$-**2**]$^+$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.036917	6.451505	-1.896699

[29] M. J. Fuchter, J. Schaefer, D. K. Judge, B. Wardzinski, M. Weimar, I. Krossing, *Dalton Trans.* **2012**, *41*, 8238.

2	6	0	-5.950048	5.075077	-1.617591
3	6	0	-4.721265	4.476388	-1.437919
4	6	0	-3.521347	5.223203	-1.511726
5	6	0	-3.611751	6.579237	-1.918948
6	6	0	-4.882343	7.182701	-2.068048
7	6	0	-3.870877	3.685678	1.237365
8	6	0	-2.204876	4.656228	-1.247142
9	6	0	-1.977003	3.468694	-0.469730
10	6	0	-2.959653	2.897360	0.453827
11	6	0	-0.743384	2.800828	-0.557633
12	6	0	0.322109	3.418023	-1.270459
13	6	0	0.179924	4.679776	-1.777029
14	6	0	-1.079325	5.334597	-1.762105
15	6	0	-1.211587	6.676250	-2.254293
16	6	0	-2.416056	7.301079	-2.250587
17	1	0	-2.504606	8.342228	-2.569169
18	1	0	-0.313483	7.196309	-2.595604
19	1	0	-7.012730	6.926146	-2.016699
20	1	0	-4.932493	8.237541	-2.348300
21	1	0	1.263479	2.886898	-1.407477
22	1	0	1.024388	5.177526	-2.259582
23	6	0	-6.052233	5.186591	2.256743
24	6	0	-6.113353	3.831168	2.252712
25	6	0	-5.019607	3.047943	1.752463
26	1	0	-6.908762	5.782097	2.580800
27	1	0	-7.011926	3.311172	2.592505
28	6	0	-5.086156	1.630120	1.755683
29	6	0	-4.070369	0.876171	1.238704
30	6	0	-3.002220	1.493726	0.529687
31	1	0	-5.940790	1.144382	2.231994
32	1	0	-4.090561	-0.205907	1.357333
33	6	0	-0.644106	1.416725	-0.088067
34	6	0	-3.702647	5.108014	1.509136
35	6	0	-4.829859	5.862482	1.925230
36	1	0	-6.858519	4.473489	-1.549796
37	1	0	-4.679502	3.404977	-1.249407
38	6	0	-4.716057	7.263703	2.082302
39	6	0	-2.456679	5.775173	1.434854
40	6	0	-2.359406	7.137655	1.621560
41	6	0	-3.506550	7.899643	1.910006
42	1	0	-5.603655	7.832703	2.368947
43	1	0	-1.550994	5.203912	1.238299
44	1	0	-1.384573	7.624358	1.551394
45	1	0	-3.429758	8.981418	2.035759
46	6	0	7.578872	1.490276	-2.083668
47	6	0	6.350552	2.082198	-1.723273
48	6	0	5.241744	1.293736	-1.492110
49	6	0	5.289837	-0.121993	-1.574199
50	6	0	6.482276	-0.711407	-2.088207
51	6	0	7.639465	0.108060	-2.296241
52	6	0	4.157386	0.980024	1.252921
53	6	0	4.157505	-0.980165	-1.253053
54	6	0	3.036341	-0.577993	-0.448485
55	6	0	3.036306	0.577888	0.448221
56	6	0	1.836283	-1.309090	-0.513856
57	6	0	1.824750	-2.545509	-1.220813
58	6	0	2.968603	-3.053205	-1.768109
59	6	0	4.159853	-2.283506	-1.798453
60	6	0	5.351303	-2.821183	-2.387367
61	6	0	6.495037	-2.093978	-2.464402
62	1	0	7.410389	-2.525721	-2.874357
63	1	0	5.326523	-3.849353	-2.755345
64	1	0	8.449580	2.113596	-2.299287
65	1	0	8.522244	-0.334404	-2.768613
66	1	0	0.893261	-3.100597	-1.315921
67	1	0	2.958678	-4.033654	-2.248678
68	6	0	6.494837	2.093747	2.464500
69	6	0	5.351153	2.821016	2.387306
70	6	0	4.159741	2.283383	1.798277
71	1	0	7.410168	2.525455	2.874541
72	1	0	5.326389	3.849203	2.755238
73	6	0	2.968536	3.053143	1.767756
74	6	0	1.824720	2.545484	1.220345
75	6	0	1.836272	1.309036	0.513437
76	1	0	2.958602	4.033612	2.248287
77	1	0	0.893251	3.100622	1.315336
78	6	0	0.588084	-0.702256	-0.039949
79	6	0	0.588099	0.702217	0.039441
80	6	0	5.289628	0.121799	1.574229
81	6	0	6.482037	0.711162	2.088366

82	1	0	6.274357	3.167233	-1.643769
83	1	0	4.297617	1.778373	-1.250628
84	6	0	7.639148	-0.108363	2.296573
85	6	0	5.241461	-1.293930	1.492166
86	6	0	6.350184	-2.082451	1.723519
87	6	0	7.578496	-1.490588	2.084065
88	1	0	4.297342	-1.778518	1.250552
89	1	0	6.273934	-3.167485	1.644052
90	1	0	8.449127	-2.113957	2.299865
91	6	0	-6.037235	-6.450704	1.897465
92	6	0	-5.950219	-5.074335	1.618120
93	6	0	-4.721386	-4.475859	1.438085
94	6	0	-3.521562	-5.222840	1.511746
95	6	0	-3.612083	-6.578812	1.919151
96	6	0	-4.882734	-7.182055	2.068646
97	6	0	-3.871295	-3.685551	-1.237462
98	6	0	-2.205058	-4.656067	1.246885
99	6	0	-1.977155	-3.468610	0.469360
100	6	0	-2.959864	-2.897262	-0.454128
101	6	0	-0.743473	-2.800836	0.557118
102	6	0	0.322035	-3.418105	1.269861
103	6	0	0.179797	-4.679833	1.776479
104	6	0	-1.079517	-5.334532	1.761738
105	6	0	-1.211869	-6.676134	2.254040
106	6	0	-2.416425	-7.300797	2.250614
107	1	0	-2.505061	-8.341904	2.569309
108	1	0	-0.313774	-7.196287	2.595232
109	1	0	-7.013093	-6.925176	2.017769
110	1	0	-4.932981	-8.236847	2.349060
111	1	0	1.263458	-2.887058	1.406795
112	1	0	1.024269	-5.177640	2.258960
113	6	0	-6.053078	-5.186276	-2.256219
114	6	0	-6.113978	-3.830845	-2.252399
115	6	0	-5.020025	-3.047720	-1.752448
116	1	0	-6.909759	-5.781700	-2.580024
117	1	0	-7.012527	-3.310758	-2.592113
118	6	0	-5.086393	-1.629890	-1.755826
119	6	0	-4.070457	-0.876013	-1.239043
120	6	0	-3.002309	-1.493630	-0.530081
121	1	0	-5.941029	-1.144100	-2.232081
122	1	0	-4.090531	0.206058	-1.357762
123	6	0	-0.644144	-1.416735	0.087536
124	6	0	-1.853233	-0.714488	-0.059316
125	6	0	-3.703330	-5.107954	-1.509074
126	6	0	-4.830750	-5.862307	-1.924823
127	1	0	-6.858613	-4.472618	1.550437
128	1	0	-4.679501	-3.404482	1.249409
129	6	0	-4.717224	-7.263571	-2.081701
130	6	0	-2.457459	-5.775317	-1.434979
131	6	0	-2.360464	-7.137850	-1.621479
132	6	0	-3.507796	-7.899696	-1.909541
133	1	0	-5.604980	-7.832459	-2.368078
134	1	0	-1.551589	-5.204218	-1.238849
135	1	0	-1.385692	-7.624700	-1.551473
136	1	0	-3.431213	-8.981504	-2.035132
137	6	0	-1.853213	0.714526	0.058826
138	1	0	8.521906	0.334076	2.769005
139	47	0	8.103317	-0.000456	0.000148

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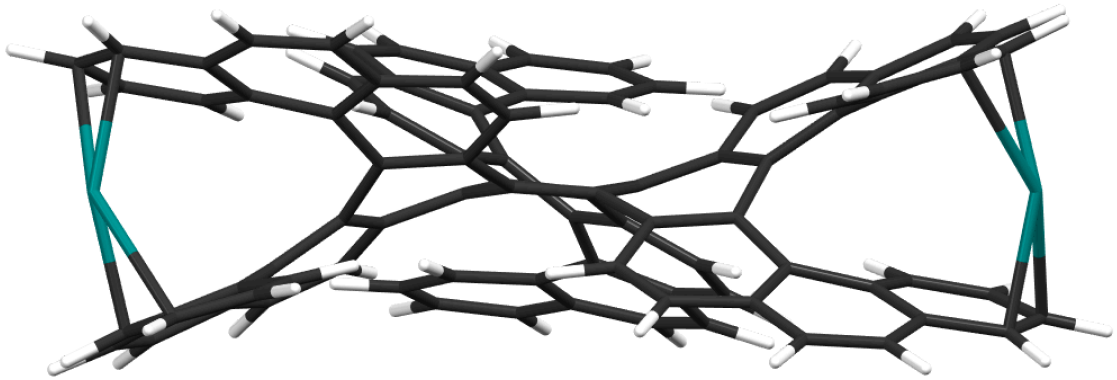
0 negative eigenvalue
Thermal correction to Gibbs Free Energy= 1.001902
E(RwB97XD) = -3605.46875730
Sum of electronic and thermal Free Energies = -3604.466855

[2Ag⊂D_3-**2**]$^{2+}$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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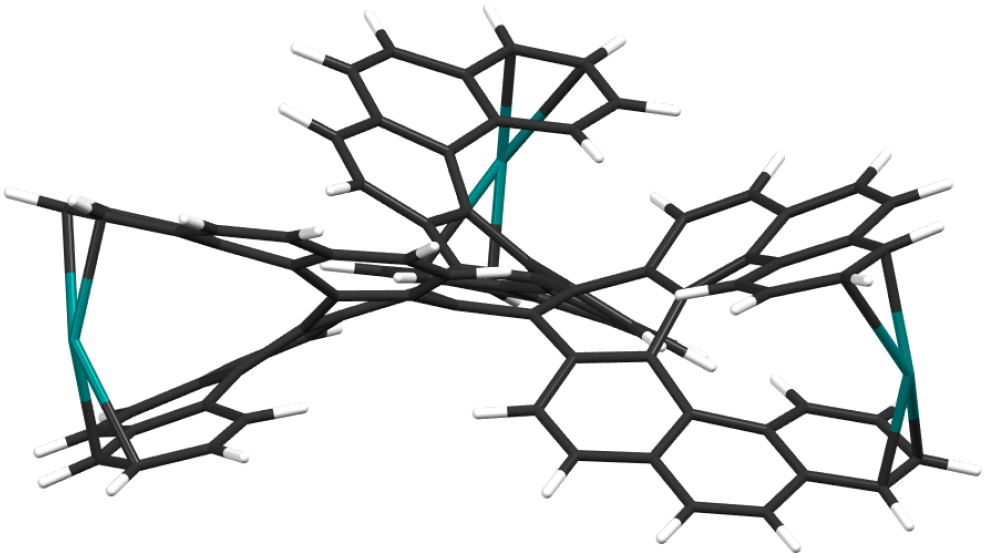
3	6	0	1.297951	6.463461	1.447266
4	6	0	-0.115006	6.509252	1.507859
5	6	0	-0.719157	7.728844	1.908720
6	6	0	0.077076	8.887276	2.066143
7	6	0	0.970081	5.361164	-1.235673
8	6	0	-0.970064	5.361165	1.235668
9	6	0	-0.569794	4.219153	0.460350
10	6	0	0.569805	4.219151	-0.460359
11	6	0	-1.308993	3.024716	0.538963
12	6	0	-2.548096	3.027103	1.238598
13	6	0	-3.055974	4.191513	1.742479
14	6	0	-2.290204	5.387056	1.736160
15	6	0	-2.851102	6.614279	2.223346
16	6	0	-2.118630	7.756680	2.226431
17	1	0	-2.565181	8.702729	2.540476
18	1	0	-3.891637	6.616899	2.555386
19	1	0	2.050087	9.731085	2.034910
20	1	0	-0.409511	9.825425	2.342585
21	1	0	-3.102231	2.098447	1.369768
22	1	0	-4.040142	4.202557	2.216398
23	6	0	2.118662	7.756678	-2.226422
24	6	0	2.851127	6.614272	-2.223345
25	6	0	2.290222	5.387051	-1.736164
26	1	0	2.565219	8.702726	-2.540462
27	1	0	3.891662	6.616888	-2.555384
28	6	0	3.055985	4.191503	-1.742488
29	6	0	2.548101	3.027095	-1.238611
30	6	0	1.308999	3.024712	-0.538975
31	1	0	4.040153	4.202544	-2.216408
32	1	0	3.102232	2.098436	-1.369783
33	6	0	-0.698979	1.778219	0.075961
34	6	0	0.115031	6.509257	-1.507859
35	6	0	0.719189	7.728849	-1.908712
36	1	0	3.148535	7.532087	1.577744
37	1	0	1.800695	5.515210	1.264325
38	6	0	-0.077037	8.887287	-2.066128
39	6	0	-1.297927	6.463475	-1.447268
40	6	0	-2.060187	7.596940	-1.634347
41	6	0	-1.444101	8.832073	-1.907961
42	1	0	0.409556	9.825434	-2.342563
43	1	0	-1.800678	5.515226	-1.264337
44	1	0	-3.148505	7.532112	-1.577741
45	1	0	-2.050043	9.731107	-2.034890
46	6	0	-7.886229	-2.164490	2.086617
47	6	0	-7.101981	-1.050875	1.712390
48	6	0	-5.750793	-1.200703	1.480357
49	6	0	-5.103155	-2.460376	1.576016
50	6	0	-5.856138	-3.551107	2.096434
51	6	0	-7.264439	-3.398494	2.307367
52	6	0	-4.649947	-0.984104	-1.271374
53	6	0	-3.694921	-2.661558	1.260323
54	6	0	-2.910251	-1.771668	0.447791
55	6	0	-3.474095	-0.777385	-0.467380
56	6	0	-1.505970	-1.820752	0.522640
57	6	0	-0.895792	-2.889544	1.238045

58	6	0	-1.648124	-3.889119	1.787044
59	6	0	-3.063652	-3.797814	1.812957
60	6	0	-3.843134	-4.845605	2.405829
61	6	0	-5.195742	-4.764081	2.478670
62	1	0	-5.786444	-5.584139	2.891887
63	1	0	-3.323337	-5.730075	2.780538
64	1	0	-8.947688	-2.039437	2.313392
65	1	0	-7.819220	-4.213069	2.783540
66	1	0	0.187271	-2.915623	1.346552
67	1	0	-1.164670	-4.736627	2.277291
68	6	0	-7.230636	-1.153160	-2.492888
69	6	0	-6.580141	0.035642	-2.432449
70	6	0	-5.280077	0.147097	-1.836303
71	1	0	-8.237721	-1.222647	-2.909159
72	1	0	-7.050890	0.941890	-2.819560
73	6	0	-4.614441	1.399654	-1.822724
74	6	0	-3.373389	1.523845	-1.267219
75	6	0	-2.788441	0.447783	-0.541834
76	1	0	-5.080636	2.252433	-2.320179
77	1	0	-2.831651	2.462215	-1.370331
78	6	0	-0.713898	-0.677759	0.054117
79	6	0	-1.406644	0.540366	-0.055320
80	6	0	-5.230480	-2.287869	-1.569075
81	6	0	-6.556909	-2.352449	-2.088854
82	1	0	-7.565342	-0.067193	1.627882
83	1	0	-5.164150	-0.318622	1.230871
84	6	0	-7.179075	-3.629570	-2.279630
85	6	0	-4.513913	-3.506689	-1.457420
86	6	0	-5.109413	-4.733965	-1.668064
87	6	0	-6.466820	-4.809368	-2.039342
88	1	0	-3.454899	-3.477774	-1.208754
89	1	0	-4.525011	-5.649061	-1.565272
90	1	0	-6.932295	-5.777367	-2.237704
91	6	0	7.886221	-2.164517	-2.086616
92	6	0	7.101977	-1.050898	-1.712393
93	6	0	5.750788	-1.200722	-1.480360
94	6	0	5.103146	-2.460393	-1.576016
95	6	0	5.856127	-3.551128	-2.096431
96	6	0	7.264428	-3.398519	-2.307363
97	6	0	4.649942	-0.984113	1.271370
98	6	0	3.694912	-2.661571	-1.260322
99	6	0	2.910244	-1.771677	-0.447793
100	6	0	3.474091	-0.777393	0.467375
101	6	0	1.505963	-1.820757	-0.522643
102	6	0	0.895783	-2.889550	-1.238045
103	6	0	1.648112	-3.889128	-1.787042
104	6	0	3.063640	-3.797827	-1.812954
105	6	0	3.843120	-4.845622	-2.405823
106	6	0	5.195728	-4.764101	-2.478663
107	1	0	5.786429	-5.584162	-2.891877
108	1	0	3.323320	-5.730091	-2.780529
109	1	0	8.947681	-2.039466	-2.313391
110	1	0	7.819208	-4.213097	-2.783534
111	1	0	-0.187280	-2.915627	-1.346553
112	1	0	1.164656	-4.736636	-2.277286
113	6	0	7.230630	-1.153172	2.492886
114	6	0	6.580138	0.035631	2.432442
115	6	0	5.280075	0.147088	1.836296
116	1	0	8.237715	-1.222661	2.909157
117	1	0	7.050890	0.941879	2.819551
118	6	0	4.614442	1.399647	1.822714
119	6	0	3.373390	1.523839	1.267208
120	6	0	2.788440	0.447777	0.541826
121	1	0	5.080639	2.252425	2.320167
122	1	0	2.831655	2.462211	1.370319
123	6	0	0.713894	-0.677761	-0.054123
124	6	0	1.406643	0.540362	0.055311
125	6	0	5.230471	-2.287878	1.569075
126	6	0	6.556899	-2.352461	2.088854
127	1	0	7.565340	-0.067217	-1.627888
128	1	0	5.164148	-0.318639	-1.230876
129	6	0	7.179062	-3.629583	2.279634
130	6	0	4.513901	-3.506697	1.457423
131	6	0	5.109398	-4.733974	1.668070
132	6	0	6.466804	-4.809380	2.039349
133	1	0	8.160313	-3.672586	2.763469
134	1	0	3.454887	-3.477780	1.208757
135	1	0	4.524993	-5.649069	1.565281
136	1	0	6.932276	-5.777379	2.237715
137	6	0	0.698981	1.778216	-0.075972

138	1	0	-8.160326	-3.672571	-2.763464
139	47	0	-7.713044	-3.664609	0.004397
140	47	0	7.713031	-3.664631	-0.004393

0 negative eigenvalue
Thermal correction to Gibbs Free Energy= 1.001322
E(RwB97XD) = -3752.28377834
Sum of electronic and thermal Free Energies = -3751.282456

[3Ag⊂*D*$_3$-**2**]$^{3+}$



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-5.808439	-1.706646	1.462816
4	6	0	-5.155504	-2.962208	1.567970
5	6	0	-5.909533	-4.052723	2.088034
6	6	0	-7.319105	-3.902903	2.295185
7	6	0	-4.676133	-1.469434	-1.268668
8	6	0	-3.743514	-3.162487	1.262820
9	6	0	-2.947991	-2.274468	0.455357
10	6	0	-3.498262	-1.274434	-0.463552
11	6	0	-1.544411	-2.339062	0.529986
12	6	0	-0.940756	-3.409062	1.248095
13	6	0	-1.702061	-4.400007	1.798705
14	6	0	-3.117169	-4.300461	1.817980
15	6	0	-3.898453	-5.347295	2.411408
16	6	0	-5.250430	-5.264286	2.478825
17	1	0	-5.842685	-6.082631	2.893327
18	1	0	-3.380555	-6.230457	2.791335
19	1	0	-9.006755	-2.550344	2.285044
20	1	0	-7.871913	-4.714449	2.779521
21	1	0	0.141752	-3.444013	1.358445
22	1	0	-1.226586	-5.249102	2.293712
23	6	0	-7.261676	-1.612052	-2.477506
24	6	0	-6.604694	-0.427305	-2.413851
25	6	0	-5.300565	-0.330369	-1.823880
26	1	0	-8.271289	-1.672220	-2.888988
27	1	0	-7.072012	0.483571	-2.793908
28	6	0	-4.624270	0.916746	-1.807750
29	6	0	-3.378968	1.027521	-1.258727
30	6	0	-2.800035	-0.055362	-0.539591
31	1	0	-5.085851	1.773092	-2.303412
32	1	0	-2.827125	1.959319	-1.370406
33	6	0	-0.738857	-1.206892	0.056721
34	6	0	-5.266875	-2.768114	-1.570691
35	6	0	-6.593179	-2.818391	-2.086882
36	1	0	-7.628576	-0.579153	1.594258
37	1	0	-5.225359	-0.822664	1.212319
38	6	0	-7.225330	-4.087621	-2.290221
39	6	0	-4.558788	-3.993570	-1.465664

40	6	0	-5.163555	-5.213387	-1.686498
41	6	0	-6.523052	-5.275170	-2.061509
42	1	0	-8.208596	-4.117992	-2.770825
43	1	0	-3.499195	-3.976784	-1.218405
44	1	0	-4.586980	-6.134588	-1.594351
45	1	0	-6.991863	-6.237847	-2.278812
46	6	0	6.290304	-5.542595	2.063240
47	6	0	4.935873	-5.422722	1.684897
48	6	0	4.384515	-4.178005	1.462937
49	6	0	5.144128	-2.984181	1.569761
50	6	0	6.465703	-3.091016	2.089517
51	6	0	7.042273	-4.386353	2.294387
52	6	0	3.611928	-3.314165	-1.267457
53	6	0	4.610011	-1.661619	1.266021
54	6	0	3.442982	-1.417402	0.458697
55	6	0	2.853042	-2.393567	-0.461292
56	6	0	2.796123	-0.170230	0.533795
57	6	0	3.419388	0.887730	1.253042
58	6	0	4.658085	0.724750	1.804159
59	6	0	5.280865	-0.549937	1.822446
60	6	0	6.578132	-0.702323	2.415994
61	6	0	7.183779	-1.914036	2.482007
62	1	0	8.188672	-2.016963	2.896560
63	1	0	7.082896	0.187912	2.797082
64	1	0	6.717224	-6.524513	2.280640
65	1	0	8.021725	-4.459053	2.778292
66	1	0	2.907304	1.842200	1.363037
67	1	0	5.154579	1.561157	2.300143
68	6	0	5.031188	-5.478163	-2.479742
69	6	0	3.676697	-5.503765	-2.415488
70	6	0	2.939179	-4.424750	-1.823825
71	1	0	5.589150	-6.321020	-2.892685
72	1	0	3.122704	-6.364293	-2.796414
73	6	0	1.521017	-4.464658	-1.807320
74	6	0	0.801130	-3.442912	-1.257423
75	6	0	1.448160	-2.399730	-0.537684
76	1	0	1.011239	-5.292802	-2.303690
77	1	0	-0.281763	-3.432024	-1.369224
78	6	0	1.413448	-0.039178	0.058975
79	6	0	0.689705	-1.235835	-0.063976
80	6	0	5.031663	-3.173925	-1.569641
81	6	0	5.740005	-4.295530	-2.087685
82	1	0	4.320590	-6.318348	1.590967
83	1	0	3.327263	-4.115207	1.213036
84	6	0	7.155084	-4.205548	-2.291303
85	6	0	5.736792	-1.947065	-1.462743
86	6	0	7.095303	-1.858058	-1.683981
87	6	0	7.830299	-3.002646	-2.061065
88	1	0	5.190543	-1.039684	-1.212803
89	1	0	7.603167	-0.897412	-1.590381
90	1	0	8.898225	-2.925218	-2.278503
91	6	0	-1.307651	8.282143	-2.064330
92	6	0	-1.933043	7.073713	-1.689066
93	6	0	-1.178085	5.941097	-1.465943
94	6	0	0.237311	5.942911	-1.568518
95	6	0	0.856447	7.116862	-2.084963
96	6	0	0.072273	8.297871	-2.290895
97	6	0	-0.870315	4.821003	1.263362
98	6	0	1.067336	4.782975	-1.264295
99	6	0	0.646841	3.665155	-0.459708
100	6	0	-0.495862	3.687887	0.457458
101	6	0	1.354489	2.451373	-0.534843
102	6	0	2.583209	2.412414	-1.251583
103	6	0	3.109961	3.546718	-1.799642
104	6	0	2.366900	4.755222	-1.817480
105	6	0	2.934701	5.933205	-2.407610
106	6	0	2.236023	7.093712	-2.473593
107	1	0	2.688336	7.998142	-2.885510
108	1	0	3.957834	5.883171	-2.786060
109	1	0	-1.907529	9.168698	-2.283156
110	1	0	0.537223	9.164385	-2.772289
111	1	0	3.115322	1.469096	-1.362423
112	1	0	4.083235	3.519065	-2.293657
113	6	0	-1.943666	7.176262	2.475005
114	6	0	-2.689183	6.045347	2.407751
115	6	0	-2.169884	4.845708	1.816610
116	1	0	-2.358750	8.098030	2.887679
117	1	0	-3.713602	6.036821	2.785924
118	6	0	-2.961429	3.668400	1.797994
119	6	0	-2.481322	2.514155	1.248753

```
    120          6           0       -1.252383    2.503854    0.531431
    121          1           0       -3.934831    3.679888    2.292396
    122          1           0       -3.050846    1.592928    1.359302
    123          6           0        0.724612    1.212514   -0.062807
    124          6           0       -0.673739    1.240923    0.057672
    125          6           0        0.006380    5.945657    1.568875
    126          6           0       -0.564181    7.143301    2.086774
    127          1           0       -3.019211    7.033760   -1.598650
    128          1           0       -1.692688    5.014750   -1.218782
    129          6           0        0.267856    8.290731    2.294575
    130          6           0        1.420496    5.885782    1.466207
    131          6           0        2.221382    6.985964    1.691195
    132          6           0        1.646030    8.218547    2.068264
    133          1           0       -0.161269    9.175106    2.776723
    134          1           0        1.896089    4.939323    1.216852
    135          1           0        3.305003    6.901608    1.600701
    136          1           0        2.281809    9.079301    2.288739
    137          6           0       -1.413023    0.018475   -0.065241
    138          1           0        7.674411   -5.040241   -2.773290
    139         47           0        7.571503   -4.575330    0.002587
    140         47           0        0.183593    8.844601    0.001716
    141         47           0       -7.750469   -4.265479    0.004322
 ---------------------------------------------------------------------
0 negative eigenvalue
Thermal correction to Gibbs Free Energy=         0.997412
E(RwB97XD) = -3899.04890949
Sum of electronic and thermal Free Energies = -3898.051497
```

7.2. Experimental study by electrospray ionization mass spectrometry

High resolution MS, MS/MS and traveling wave ion mobility spectrometry (TWIMS) experiments were performed using a Synapt G2 HDMS mass spectrometer from Waters (Manchester, UK), equipped with an electrospray ionization (ESI) source operated in the positive ion mode with the following settings (otherwise stated in text): capillary voltage, +2.8 kV; sampling cone voltage, +20 V; desolvation gas (N_2) flow, 100 L h^{-1} at 35°C; source temperature, 35°C. Importantly, these electrospray conditions did not allow the detection of the silver(I) adduct [Ag + *D*$_3$-**HNTP**]$^+$ derived from the previously synthesized hextuple helicene *D*$_3$-**HNTP**, which only proved possible under particularly harsh experimental conditions.[10]
Sample solutions were introduced at 5 μL min^{-1} in the ionization source using a syringe pump. In this Q-TOF instrument, ions were accurately mass measured using an orthogonal acceleration time-of-flight (oa-TOF) mass analyzer, and a quadrupole was used for precursor ion selection in collision-induced dissociation (CID) experiments, using argon as the collision gas. IMS-MS spectra were all recorded in the 50-1500 *m/z* range, with trap bias DC voltage of 35 V, helium cell gas flow of 180 mL min^{-1}, and the TWIMS cell operated at 3.45 mbar of N_2. Data analyses were conducted using the MassLynx 4.1 program provided by Waters. The drift timescale of the TWIMS-MS experiments was converted to a collision cross-section scale, following the calibration procedure described by De Winter.[30] The MOBCAL software[31] was used to convert Cartesian coordinates in CCS values for each DFT minimized structured. For the trajectory method in helium, a scaling factor of 0.8 was applied to the Universal Force Field for silver values.[32] As a result, the atomic distance was set at 2.5184 Å and the energy value at 1.249 meV.

[30] Q. Duez, F. Chirot, R. Liénard, T. Josse, C. Choi, O. Coulembier, P. Dugourd, J. Cornil, P. Gerbaux, J. De Winter, *J. Am. Soc. Mass Spectrom.* **2017**, *28*, 2483.

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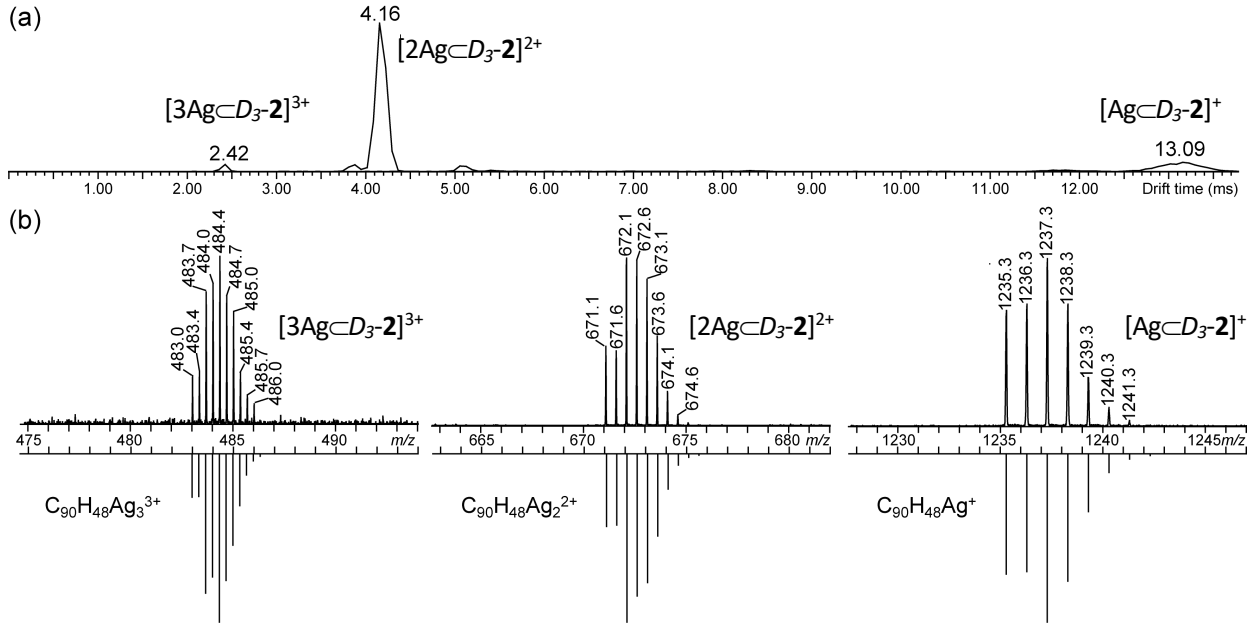

Figure S44. (a) Superimposed traces extracted at *m/z* values from the ion mobilogram recorded in positive mode ESI-IMS-MS of an equimolar solution of *D*$_3$-**2** and $AgNO_3$ in CH_3OH/CH_2Cl_2 (50/50, v/v). (b) Experimental (top) and calculated (bottom) isotopic pattern of $[3Ag\subset D_3\text{-}\mathbf{2}]^{3+}$ (left), $[2Ag\subset D_3\text{-}\mathbf{2}]^{2+}$ (middle) and $[Ag\subset D_3\text{-}\mathbf{2}]^{+}$ (right).

Table S11. Accurate mass data measured at the isotopic maximum for the silver(I) complexes of *D*$_3$-**2** (average of 3 replicates).

ion	composition	m/z_{th}	m/z_{exp}	error (ppm)
$[Ag\subset D_3\text{-}\mathbf{2}]^{+}$	$C_{90}H_{48}Ag^{+}$	1237.2823	1237.2827	+ 0.3
$[2Ag\subset D_3\text{-}\mathbf{2}]^{2+}$	$C_{90}H_{48}Ag_2^{2+}$	672.0929	672.0926	– 0.4
$[3Ag\subset D_3\text{-}\mathbf{2}]^{3+}$	$C_{90}H_{48}Ag_3^{3+}$	484.3637	484.3669	+ 6.6

Collision activation of $[Ag\subset D_3\text{-}\mathbf{2}]^{+}$ gave rise to two main competing reactions, release of *D*$_3$-**2** as a neutral to generate Ag^+ and loss of Ag(0) to produce $D_3\text{-}\mathbf{2}^{\bullet+}$, as previously reported for [6]helicene.[33] The same dissociation pattern applied to $[2Ag\subset D_3\text{-}\mathbf{2}]^{2+}$ which was observed to release 2 Ag(0) in a consecutive manner. Reliable MS/MS experiments could not be performed for $[3Ag\subset D_3\text{-}\mathbf{2}]^{3+}$ which was of too low abundance.

After appropriate calibration, drift times measured for each charge state of the complexes in IMS were converted in collision cross sections (CCS). Experimental CCS values were found at 296 Å^2 for $[Ag\subset D_3\text{-}\mathbf{2}]^{+}$, 295 Å^2 for $[2Ag\subset D_3\text{-}\mathbf{2}]^{2+}$, and 310 Å^2 for $[3Ag\subset D_3\text{-}\mathbf{2}]^{3+}$. A slightly more compact conformation was found for $[Ag\subset D_3\text{-}\mathbf{2}]^{+}$ and $[2Ag\subset D_3\text{-}\mathbf{2}]^{2+}$compared to $[3Ag\subset D_3\text{-}\mathbf{2}]^{3+}$ but this difference remained of low significance owing to the ± 10 Å^2 uncertainty associated with these measurements.

[33] E. Makrlík, J. Jaklová Dytrtová, P. Vaňura, J. Sýkora, V. Církva, J. Storch, *Chem. Phys. Lett.* **2015**, *633*, 105.