Supporting Information

π-Extended [12]Cycloparaphenylenes: from a Hexaphenylbenzene Cyclohexamer to its Unexpected $C_2$-symmetric Congener

Florian E. Golling‡, Silvio Osella§, Martin Quernheim‡, Manfred Wagner‡, David Beljonne§, Klaus Müllen‡,*

‡ Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz (Germany)
‡ Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128 Mainz (Germany)
§ Chimie des Matériaux Nouveaux & Centre d'Innovation et de Recherche en Matériaux Polymères, Université de Mons-UMONS/Materia Nova, Place du Parc 20, 7000 Mons (Belgium)

Contents

1. General Information ..........................................................................................S2
2. Synthesis ..............................................................................................................S4
3. X-Ray Crystallographic Analysis ........................................................................S13
4. 2D-NMR Spectra ................................................................................................S16
5. Computational Results .....................................................................................S22
6. NMR Spectra .....................................................................................................S82
7. MALDI-MS spectra ..........................................................................................S91
8. Optical and Electronic Properties .....................................................................S103
9. Literature ...........................................................................................................S105
1. General Information

Unless otherwise stated, the commercially available reagents and dry solvents were used without further purification. The reactions were performed using standard vacuum-line and Schlenk techniques, work-up and purification of all compounds was performed under air and with reagent-grade solvents. Column chromatography was done with silica gel (particle size 0.063-0.200 mm from Macherey-Nagel) and silica coated aluminum sheets with fluorescence indicator from Macherey-Nagel were used for thin layer chromatography. Preparative thin layer chromatography was done with PLC silica gel 60, F254, 2 mm sheets on glass from Merck. Melting points were determined on a Büchi hot stage apparatus. The $^1$H-NMR and $^{13}$C-NMR spectra were recorded on a Bruker AVANCE 250, Bruker AVANCE 300, Bruker AVANCE 500 and Bruker AVANCE 700 spectrometer in the listed deuterated solvents. Trimethylsilane (δ 0.00 ppm) or the deuterated solvent was used as an internal standard. Field desorption (FD) mass spectra were obtained on a VG Instruments ZAB 2 SE-FPD. MALDITOF mass spectra were recorded on a Bruker Reflex II-TOF spectrometer using trans-2-[3-(4-tert-butylphenyl)-2-methyl-2-propenylidene]-malononitrile (DCTB; Aldrich, >99%) as matrix. High resolution MALDI mass spectrometry measurements were performed on a Solarix ESI-/MALDI-ICR (9.4T) system (Bruker Daltonics, Germany), with a SmartBeam laser II. The system was internally calibrated in positive mode using sodium trifluoroacetate (Fluka, >99%) or sodium perfluoroheptanoate (Fluka, >99%) on quadratic calibration mode. A total of 10-400 shots were accumulated for each mass spectrum. The results were calculated using Data Analysis software (Bruker Daltonics, Germany). High-performance liquid chromatography (HPLC) was performed on a HPLC facility from Shimadzu (LC-20AD), using a GPC column from JAI Co., Ltd. Packed with highly cross-linked polystyrene/divinylbenzene.
1.1. General Information for the 2D NMR experiments

$^1$H-NMR (700 MHz) and $^{13}$C-NMR (176 MHz) measurements were executed on Bruker Avance III 700 NMR spectrometers with a 5 mm QXI probe endowed with a z-gradient. The spectra were received with $\pi/2$-pulse lengths of 13.8 $\mu$s ($^1$H) and 16 $\mu$s ($^{13}$C) and a sweep width of 10500 Hz (15 ppm) for $^1$H and 35000 Hz (200 ppm) for $^{13}$C. A relaxation delay of 2s was used for both nuclei. The temperature was held at 298.3 K and calibrated with a standard $^1$H methanol NMR sample. The control of the temperature was realized with a VTU (variable temperature unit) and an accuracy of +/- 0.1K, which was checked with the standard Bruker Topspin 3.2 software. A standard proton spectrum was recorded with 1024 transients. The 2D $^1$H,$^{13}$C-HSQC (heteronuclear single quantum correlations via double inept transfer and phase sensitive using Echo/Antiecho-TPPI gradient selection with decoupling during acquisition) experiment was run with 4096 points in f2 and 512 points in f1 dimension and an averaged $^1$J-CH coupling constant of 145Hz. Before Fourier transformation, the data were zero filled to 1024 points in f1 and multiplied by a window function (q-sine bell or sine bell) in both dimensions. The assignment of the protons was realized with a 2D-$^1$H,$^1$H NOESY (nuclear overhauser enhancement spectroscopy) and 2D-$^1$H,$^1$H COSY. The used mixing time in this experiment was kept at 250 ms. The spectroscopic widths of the homo-nuclear 2D COSY and NOESY experiments were typically 10000 Hz in both dimensions (f1 and f2) and the relaxation delay was 1.3s.
2. Synthesis

2.1 Synthesis of 3',6'-dibromo-4,4''-di-tert-butyl-4',5'-bis(4-(tert-butyl)phenyl)-1,1':2',1''-terphenyl (5)[1]

Hexabromobenzene (8.27 g, 15 mmol, 1 eq) was placed into a Schlenk flask and 4-tert-butylphenylmagnesium bromide (300 mL, 150 mmol, 10 eq.) was added and the reaction was stirred for 12 h. Then, the reaction was cooled down to 0 °C and slowly quenched with bromine. After quenching the excess amount of bromine with aq. Na₂S₂O₃, the crude product was extracted with Et₂O and the combined fractions were filtered through a fritted funnel. The filter cake was washed with water, EtOH, hexane and toluene to give the title compound 5. The solvent of the filtrate was removed under vacuo. The solid residue was washed analogously to the filter cake. The reaction afforded 5 (5.1 g, 6.68 mmol 37%) as a white solid.

1H NMR (300 MHz, THF) δ [ppm] = 7.14 (d, J=8.3, 8H), 6.94 (d, J=8.3, 8H), 1.21 (s, 36H).

13C NMR (75 MHz, THF) δ [ppm] = 149.9, 144.5, 139.2, 130.5, 125.4, 124.6, 34.8, 31.4.

MS (FD, 8 kV) (m/z): obsvd. for C₄₆H₅₂Br₂ [M⁺] = found 763.9.(calcd. 764.2)

Elemental Analysis for C₄₆H₅₂Br₂: found C, 71.46 (calcd. C, 72.25); H, 6.46 (H, 6.85).

Melting Point: > 300 °C.

X-ray crystal structure: CCDC 1033268. These data can be obtained from The Cambridge Crystallographic Data Centre via https://summary.ccdc.cam.ac.uk/structure-summary-form.
2.2 Synthesis of (1’s,4’s)-4-bromo-4’-(4-bromophenyl)-3’,5’,6’-triphenyl-1’,4’-dihydro-[1,1’:2’,1”-terphenyl]-1’,4’-diol (11)

\[
\begin{align*}
\text{1,4-dibromobenzene (9.26 g, 39.3 mmol) was dissolved in THF (200 mL) and cooled down to} \quad & -78 \degree C. \text{ After addition of } n-\text{BuLi, the reaction mixture was stirred for 30 min. Then, a} \\
\text{suspension of } & 2,3,5,6\text{-Tetrakis(phenyl)benzoquinone\textsuperscript{[2]} (2.70 g, 6.54 mmol) in THF (30 mL) was slowly added. The reaction was stirred for 2 h, warmed to r.t. and stirred overnight. The} \\
\text{crude product was purified by column chromatography (6:4 DCM/hexane} & \rightarrow \text{ DCM} \rightarrow 8:2 \\
\text{hexane/EtOAc) to give 12 (2.9 g, 3.99 mmol, 61%) as a white solid.}
\end{align*}
\]

\[
\begin{align*}
\text{\textsuperscript{1}H NMR (300 MHz, CD}_2\text{Cl}_2) & \quad \delta [ppm] = 7.41 (d, J = 8.8 Hz, 4H), \quad 7.29 (d, J = 8.5 Hz, 4H), \quad 7.01 - 6.86 (m, 12H), \quad 6.87 - 6.75 (m, 8H), \quad 2.66 (s, 2H). \\
\text{\textsuperscript{13}C NMR (75 MHz, CD}_2\text{Cl}_2) & \quad \delta [ppm] = 142.06, \quad 141.05, \quad 137.47, \quad 131.85, \quad 131.19, \quad 129.42, \quad 127.26, \quad 126.82, \quad 121.67, \quad 75.26.
\end{align*}
\]

\textbf{MS (FD, 8 kV) \textit{(m/z):} obsd. for C}_{42}\text{H}_{36}\text{Br}_2\text{O}_2 [M]^+: 725.4 (726.1)}

\textbf{Elemental Analysis:} not measured due to rapid decomposition of the sample.

\textbf{Mp:} decomposes above 40 \degree C.
2.3 Synthesis of (1's,4's)-4-bromo-4'-(4-bromophenyl)-1',4'-dimethoxy-3',5',6'-triphenyl-1',4'-
dihydro-1',1':2',1''-terphenyl (13)

12 (2.9 g, 3.99 mmol) was dissolved in 30 mL THF and cooled to 0 °C. After 30 min, NaH (0.48 mg, 12.0 mmol) (60% mineral oil) was added and the solution was stirred for another 30 min until MeI (3.4 g, 24.0 mmol) was added. The reaction was stirred at 0 °C for 2 h, then warmed to r.t. and stirred overnight. After quenching with methanol, water was added and the reaction mixture was extracted with Et₂O (3 x) and the combined organic fractions were dried over MgSO₄. The crude product was filtered through a short pad of silica (6:4 → hexane/DCM) to give 13 (2.85 g, 3.78 mmol) as a white solid (95%).

**¹H NMR** (500 MHz, C₂D₂Cl₄) δ [ppm] = 7.44 (d, J = 8.5 Hz, 4H), 7.35 (d, J = 8.7 Hz, 4H), 6.91 – 6.80 (m, 12H), 6.72 (dd, J = 8.1, 1.4 Hz, 8H), 3.89 (s, 6H).

**¹³C NMR** (126 MHz, C₂D₂Cl₄) δ [ppm] = 143.15, 142.55, 138.67, 131.64, 130.87, 130.18, 127.17, 126.71, 121.38, 81.77, 52.70.

**MS** (FD, 8 kV) (m/z): obsd. for C₄₄H₃₄Br₂O₂ [M]⁺: 755.4 (calcd. 754.1).

**Elemental Analysis** for C₄₄H₃₄Br₂O₂: found C, 70.47 (calcd. C, 70.04); H, 4.54 (H, 4.30).

**Mp:** 292 °C.
2.4 Synthesis of 2,2’-((1’s,4’s)-1’,4’-dimethoxy-2’,3’,5’,6’-tetraphenyl-1’,4’-dihydro-[1,1’:4’,1”-terphenyl]-4,4’-diyl)bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolane) (4)

[Chemical structures and reaction schemes are shown here.]

13 (1.3 g, 1.72 mmol, 1 eq.), B$_2$Pin$_2$ (3.78 g, 5.17 mmol, 3 eq.), KOAc (3.38 g, 34.4 mmol, 20 eq.), and Pd(dppf)Cl$_2$ (76 mg, 0.10 mmol, 10 mol%) were dissolved in dioxane (15 mL). The reaction was heated to 80 °C and stirred for 24 h. After completion, the crude product was extracted with Et$_2$O (3x) and the combined organic fractions were dried over MgSO$_4$. After removal of solvent until complete dryness, the crude product was recrystallized from hexane/MeOH to give 4 (1.30 g, 1.53 mmol, 89%) as a white solid.

$^1$H NMR (500 MHz, C$_2$D$_2$Cl$_4$, 373 K) $\delta$[ppm] = 7.63 (s, 1H), 6.90 – 6.77 (m, 1H), 6.72 (d, $J$ = 6.9 Hz, 1H), 3.91 (s, 1H).

$^{13}$C NMR (126 MHz, C$_2$D$_2$Cl$_4$, 373 K) $\delta$ [ppm] = 145.66, 142.59, 138.55, 133.56, 131.22, 127.20, 126.35, 125.79, 83.50, 81.70, 52.01, 24.77.

MS (FD, 8 kV) (m/z): obsd. for C$_{56}$H$_{58}$B$_2$O$_6$ [M]$^+$ = 848.0 (calcd. 848.4).

**Elemental Analysis** for C$_{56}$H$_{58}$B$_2$O$_6$: found C, 80.31 (calcd. C, 79.25); H, 6.89 (H, 7.35).*

*Solvent molecules were still encapsulated with the crystals, despite prolonged drying.

**Mp**: 300 °C.

2.5 Synthesis of dikinked diboronate 6

[Chemical structures and reaction schemes are shown here.]

$^{*}$S7
5 (110 mg, 0.14 mmol, 1 eq.), 4 (732 mg, 0.86 mmol, 6 eq.) and Cs$_2$CO$_3$ (5.63 g, 17.3 mmol, 20 eq.) were added to a 25 mL Schlenk tube. After addition of toluene (6 mL), the reaction mixture was heated to 100 °C and stirred for 2 d. The crude product was extracted with DCM (3x) and the combined fractions were dried over MgSO$_4$. The crude product was filtered through a short pad of celite and washed with DCM. Finally, the crude product was fully purified by preparative GPC (eluent THF) to give 6 (114 mg, 56.0 µmol, 40%).

$^1$H NMR (500 MHz, C$_2$D$_2$Cl$_4$) δ = 7.43 (d, $J = 8.0$ Hz, 4H), 7.33 (d, $J = 7.9$ Hz, 4H), 6.88 (d, $J = 8.2$ Hz, 14H), 6.82 (dd, $J = 9.5$, 6.8 Hz, 14H), 6.79 – 6.74 (m, 10H), 6.69 (dd, $J = 17.2$, 7.6 Hz, 16H), 6.57 (d, $J = 7.4$ Hz, 8H), 3.88 (s, 6H), 3.66 (s, 6H), 1.34 (s, 24H), 1.13 (s, 36H).

$^{13}$C NMR (126 MHz, C$_2$D$_2$Cl$_4$) δ 148.10, 146.12, 143.39, 142.20, 141.25, 140.36, 139.45, 139.36, 139.20, 138.90, 138.68, 134.07, 132.13, 131.78, 131.35, 127.51, 126.86, 126.73, 126.23, 126.16, 123.46, 84.02, 82.20, 82.15, 74.62, 74.40, 74.18, 52.52, 52.46, 34.43, 31.77, 25.37.

HR-MS (MALDI) m/z obsv for C$_{146}$H$_{144}$B$_2$O$_8$ = 2048.1080 (calcd. 2048.1098).

MP: 290 °C

2.6 Synthesis of monokinked dibromide 7

![Chemical structure of 5, 4, and 7]

5 (100 mg, 0.14 mmol, 4 eq.), 4 (28 mg, 0.033 mmol, 1 eq.) and Cs$_2$CO$_3$ (215 mg, 0.66 mmol, 20 eq.) (3 M) were added to a 25 mL Schlenk tube. After addition of toluene (8 mL), the reaction mixture was heated to 100 °C and stirred for 2 d. The crude product was extracted with DCM (3x) and the combined fractions were dried over MgSO$_4$. The crude product was filtered through a short pad of celite and washed with DCM. Finally, the crude product was fully purified by preparative GPC (eluent THF) to give 7 (42 mg, 21.4 µmol, 65%).

$^1$H NMR (500 MHz, C$_2$D$_2$Cl$_4$, 373 K) δ 7.16 (d, $J = 8.6$ Hz, 8H), 7.01 (d, $J = 8.4$ Hz, 8H), 6.90 (d, $J = 8.6$ Hz, 8H), 6.85 (t, $J = 7.4$ Hz, 4H), 6.76 (t, $J = 7.7$ Hz, 8H), 6.72 (d, $J = 7.2$ Hz, 8H), 6.59 (m, $J = 11.2$, 8.8 Hz, 8H), 6.47 (d, $J = 7.4$ Hz, 8H).
\( ^{13} \text{C NMR} \) (126 MHz, \( \text{C}_2\text{D}_2\text{Cl}_4 \), 373 K) \( \delta \) 149.53, 148.61, 142.90, 142.61, 142.40, 139.81, 139.51, 139.42, 138.89, 138.69, 137.88, 132.03, 131.52, 130.90, 130.76, 127.03, 126.60, 126.14, 125.05, 124.08, 123.50, 82.16, 52.37, 34.68, 34.47, 31.77, 31.65.

\( \text{HR-MS (MALDI)} \) (\( m/z \)) = obsv. for \( \text{C}_{136}\text{H}_{138}\text{Br}_2\text{O}_2 [\text{M}^+] \): 1963.9097 (calcd. 1963.9086).

Mp: > 300 °C.

### 2.7 Synthesis of triangular macrocycle 8

Dikinked diboronate 6 (18.2 mg, 8.9 \( \mu \)mol, 1 eq.), monokinded dibromide (17.5 mgf, 8.9 \( \mu \)mol, 1 eq.) and \( \text{Cs}_2\text{CO}_3 \) (116 mg, 0.36 mmol, 40 eq.) (3 \( \text{M} \)) were added to a 25 mL Schlenk tube. After addition of toluene (5 mL, 2 mM), the reaction mixture was heated to 95 °C and stirred for 2 d. The crude product was extracted with DCM (3x) and the combined fractions were dried over \( \text{MgSO}_4 \). The crude product was filtered through a short pad of celite and washed with DCM. The crude product was purified by recycling GPC (eluent chloroforom) to give 8 (10.2 mg, 2.85 \( \mu \)mol, 32%).

\( ^1\text{H NMR} \) (700 MHz, \( \text{C}_2\text{D}_2\text{Cl}_4 \), 333 °C) \( \delta \) 

\( ^{13} \text{C NMR} \) (176 MHz, \( \text{C}_2\text{D}_2\text{Cl}_4 \), 333 °C) \( \delta \) not all quarternary carbons observed.

2D-NMR: \( ^1\text{H}-^1\text{H-COSY}, \text{NOSY} \) (see section 4.2)
HR-MS (MALDI) \((m/z) =\) obsv. for C\textsubscript{270}H\textsubscript{258}O\textsubscript{6} [M\textsuperscript{+}]: 3598.0038 (calcd. 3598.9946)

Mp: > 300 °C

2.8 Congested Cyclic Hexaphenylbenzene Hexamer 2

![Chemical Structure](attachment:image.png)

To TiCl\textsubscript{4} (0.108 ml, 1.00 mmol, 600 eq.) was added THF (20 ml) at 0 °C under argon atmosphere and stirred for 30 min at ambient temperature. After cooling to 0 °C again, a solution of LiAlH\textsubscript{4} in THF (2.00 ml, 2.0 M, 4.00 mmol, 2400 eq) was added and stirred for 1h at 80 °C to generate low-valent titanium. A solution of 8 (6 mg, 1.66 µmol, 1 eq.) in THF (3 ml) was added and stirred for 3 d at same temperature under absence of light. After cooling to 0 °C, the reaction was quenched by water and 2M hydrochloric acid (Caution! Excess amount of unreacted LiAlH\textsubscript{4} can explosively lead to the formation of hydrogen gas upon addition of water. Therefore, at first, large glass adaptor or glass trap should be equipped at the top of the reactor. Additionally, several drops of water were slowly added to the reaction), and extracted with DCM. After filtration over celite, the organic layer was washed with water and brine, and dried over Na\textsubscript{2}SO\textsubscript{4}. After removing the solvent in vacuo, the crude product was subjected to preparative GPC (THF) to give 2 (2.6 mg, 76.2 µmol, 46%).
\[ ^1H \text{NMR} (500 MHz, C_2D_2Cl_4) \delta 6.75 (t, 4H, C-16), 6.71 (d, J = 7.2 Hz, 8H, C-9), 6.65 (t, J = 6.7 Hz, 8H, C-15), 6.56 (d, J = 7.1 Hz, 8H, C-14), 6.44 (d, J = 7.3 Hz, 8H, C-8), 6.36 (d, J = 7.3 Hz, 4H, C-3), 6.22 (d, J = 7.2 Hz, 4H, C-2), 1.11 (s, 36H, C((CH_3)_3)). \]

\[ ^13C \text{NMR} (126 MHz, C_2D_2Cl_4) \delta 147.4 (C-7/C-6), 141.2 (C-1/11), 140.2 (C-7/C-6), 139.9 (C-4/5), 138.5 (C-1/11), 138.2 (C-4/5), 137.1 (C-10), 131.9 (C-14), 131.7 (C-16), 131.4 (C-8), 130.5 (C-3), 130.1 (C-2), 126.6 (C-15), 125.1 (C-12), 123.2 (C-9), 34.24 ((CH_3)_3C), 31.5 (((CH_3)_3C)_2. \]

2D-NMR: see section 4.1

HR-MS (MALDI) \((m/z) = \text{obsv. for } C_{264}H_{240} [M^+] : 3411.8796 \text{ (calcd. 3411.8842)}. \)

\textbf{Mp:} > 300 °C

2.9. \textit{Synthesis of a }\textit{C}_2\text{-symmetric Cyclohexadiene Macrocycle 3}

\[ ^8 \text{ (4 mg, 1.1 } \mu\text{mol, 1 eq.) were dissolved in THF (2 mL) and cooled to – 78 °C. Sodium napthalide (0.06 mL, 55.0 } \mu\text{mol, 50 eq.) in THF (1 m) was slowly added. Upon addition, the reaction color turned blue. The reaction solution was stirred at – 78 °C for 1 h and MeOH} \]
(0.5 mL) was added. The colorless reaction solution was warmed to r.t.. After addition of water, the crude product was extracted with DCM (3x) and the combined fraction were dried over Na$_2$SO$_4$. The solvent was removed under vacuo and the product was purified by preparative GPC (THF). 3 (1.8 mg, 0.53 µmol, 48%) was obtained as a white solid.

**HR-MS** (MALDI) ($m/z$) = obsv. for C$_{264}$H$_{244}$ [M$^+$]: 3415.9074 (calcd. 3415.9154).

**X-ray** crystal structure: CCDC 1033267. These data can be obtained from The Cambridge Crystallographic Data Centre via [https://summary.ccdc.cam.ac.uk/structure-summary-form](https://summary.ccdc.cam.ac.uk/structure-summary-form).

**Mp**: > 300 °C

### 2.10 Oxidative Cyclodehydrogenation

**General Reaction Conditions:**

To a solution of 2 or 3 (1.00 µmol) in dichloromethane (5 ml) was added a solution of FeCl$_3$ (0.180 mmol) in nitromethane (1.5 ml). The mixture was reacted 1 d to 2 d under argon bubbling. Then, the reaction was quenched by MeOH and extracted with dichloromethane. The organic layer was washed with water and brine, and dried over MgSO$_4$. After removing solvent vacuum, the crude material was subjected to preparative TLC. The isolated material was used for MALDI TOF-MS analysis and UV-vis, fluorescence measurements.

### 2.10 Control experiments investigating the overreduction of 8 using sodium napthalenide

Experiments were performed according to literature: F. E. Golling, M. Quernheim, M. Wagner, T. Nishiuchi, K. Müllen, *Angew. Chem. Int. Ed.* 2014, 53, 1525-1528.
3. X-Ray Crystallographic Analysis

Details of the crystal data and a summary of the intensity data collection parameters for 5 and 3 are listed in Tables S1 and S2. In each case, suitable crystals were measured with STOE IPDS 2T diffractometer. Graphite-monochromated Mo Kα radiation was used. The structures were solved by direct methods with SIR-97 and refined by the full-matrix least-squares techniques against F\(^2\) (SHELXL-97). The intensities were corrected for Lorentz and polarization effects. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The crystals structures were visualized using Mercury 3.3.

3.1 X-ray crystal structure of 5

![Figure S1: X-ray crystal structure of 5.](image)

| Table S1: Crystallographic data and structure refinement details of 5. Single crystals of 5 were obtained from dichloromethane/MeOH and of 9. See CCDC 1033268. |
|---------------------------------------------------------------|
| **Compound** | **5** |
| Molecular Formula | C\(_{46}\)H\(_{52}\)Br\(_2\) |
| Formula Weight | 764.69 gmol\(^{-1}\) |
| Crystal Dimensions | 0.13 x 0.16 x 0.16 mm\(^3\) |
| Crystal color | colorless |
| Crystal System | monoclinic |
| Space Group | P 2\(_1\)/c |
| a | 12.9767(9)Å |
| b | 10.3514(6)Å |
| c | 15.6662(9)Å |
| β | 105.739(5)° |
| Cell Volume | V = 2025.5(2)Å\(^3\) |
| Z value | 2 |
| D\(_{calc\text{.}}\) | 1.254 gcm\(^{-3}\) |
| F (000) | 796 |
| Temperature | - 60 °C |
| Total number of Reflections | 13702 |
| Unique number of Reflections (R\(_{int}\)) | 4974 (0.052) |
| Observed number of Reflections | 3376 |
| Residuals: R\(_1\) (I>2.00σ(I)) | 0.0383 |
| Residuals: R\(_1\) (All Reflections) | 0.0726 |
| wR\(_2\) (All Reflections) | 0.1010 |
| Goodness of Fit | 1.021 |
| Max Shift / Error | 0.001 * e.s.d |
3.2.  X-ray structure of 3

**Figure S2:** X-ray crystal structure of 3 in wireframe model (side view). Hydrogen atoms and solvent molecules are omitted for clarity. Pentaphenylenes are labeled in red, whereas the bridging cyclohexadiene units are labeled in blue.

**Figure S3:** X-ray crystal structure of 2 in wireframe model (top view). Hydrogen atoms and solvent molecules are omitted for clarity. The pentaphenylene is labeled in red, whereas the bridging cyclohexadiene units are labeled in blue.

**Comments:** The structure of compound 3 is disordered. The solvent molecules (CH$_2$Cl$_2$, CH$_3$CN, H$_2$O) are severely disordered. The amount of solvent molecules cannot exactly be determined since the crystal contains large pores with varying amounts of solvent. This effect is amplified by loss of solvent (high vapor pressure of CH$_2$Cl$_2$ in combination with large pores) during crystal preparation. Thus, an accurate determination of solvent molecules within the voids is not possible. The voids of the crystal lattice are filled with a lot of scattered electron density; the SQUEEZE protocol was used to remove the void electron density for solvent molecules which could not be localized.

Due to the poor crystal quality and diffraction power, CheckCif gives 3 A and 15 B level alerts. Nearly all of these alerts (both A and B level) result from disordered solvent, large thermal movement of t-butyl and phenyl moieties, the high value of weighted R and the ratio of the observed/unique reflections.
Table S2: Crystallographic data and structure refinement details of 4 and 9. Single crystals of 4 were obtained from dichloromethane/MeCN. See CCDC 1033267.

| Compound | Molecular Formula | Formula Weight | Crystal Dimensions | Crystal color | Crystal System | Space Group | a (Å) | b (Å) | c (Å) | α (°) | β (°) | γ (°) | Cell Volume (Å³) | Z value | D (calc.) | F (000) | Temperature (°C) | Total number of Reflections | Unique number of Reflections (R_int) | Observed number of Reflections | Residuals: R(I>2.00σ(I)) | Residuals: R(I) (All Reflections) | wR2 (All Reflections) | Goodness of Fit | Max Shift / Error | Remark |
|----------|-------------------|----------------|-------------------|---------------|---------------|-------------|--------|-------|-------|-------|-------|-------|-----------------|---------|-----------|---------|----------------|-----------------------------|-------------------------------|-----------------------------|-----------------------------|----------------------------------|-------------------------------|----------------------|----------------|--------|
| 3        | C_{264}H_{244}+mCH_{2}\text{CL}_{2}+nCH_{3}CN+k*H_{2}O | 3416 gmol$^{-1}$ | 0.12 x 0.38 x 0.6 mm$^3$ | Colorless | P 21/n | monoklin | 16.1937(15)Å | 43.708(4)Å | 33.799(3)Å | 92.792(1)° | 92.792(1)° | 92.792(1)° | 23894(7)Å³ | 4 | 1.144 gcm$^{-3}$ | 8704 | 100 °C | 261715 | 56067 (0.1513) | 21529 | 0.1421 | 0.2912 | 0.3803 | 1.675 | 0.0001 * e.s.d. | Structure is disordered. Solvent molecules are disordered and amount of solvent could not be determined. |
4. 2D-NMR Spectra

4.1 Compound 2

4.1.1 $^1$H-$^1$H-COSY and NOESY

Figure S4: $^1$H-$^1$H-COSY (500 MHz) of 2 recorded at 298 K in C$_2$D$_2$Cl$_4$.

Figure S5: NOESY-spectrum of 2 recorded at 298 K in C$_2$D$_2$Cl$_4$. Intense through-space-coupling between the protons of the bridging phenylene with its neighboring 4-tBuPh and phenyl ring highlighted in black frames.
4.1.2 HSQC spectrum

Figure S6: HSQC spectrum (850 MHz/214 MHz) of 2 recorded at 273 K in C$_2$D$_2$Cl$_4$. 
4.1.3 HMBC spectrum

Figure S7: HMBC spectrum (850 MHz/214 MHz) of 2 recorded at 273 K in C$_2$D$_2$Cl$_4$. Neighboring C-H carbons are not detected due to the settings of the band pass filter.
4.2.  **Compound 8**

4.2.1.  $^1$H-H$^1$-COSY

The two colored rectangles belong to a split up A-B spin-system of compound 8 (see Figure S8): by integration and multiplicity (see Figure S8), these protons are attached to the phenylene ring, which bridges the cyclohexadiene and the *tetrakis*(4-tbutylphenyl)benzene moieties. However, instead of the expected two signals, the A-B spin-system is split up into a spin-system with four different signals. This splitting is due to the interlocking of the phenylene ring which renders all four protons magnetically different, as two of those point inwards, whereas the other point outwards of the macrocycle and thus experience magnetically different surroundings.

In this spectrum, only the $^4J$-couplings are highlighted by two colored rectangles, whereas the intense $^3J$ couplings are not visualized. These weak signals denote couplings between the two lightly labeled protons and the couplings between the darkly labeled protons.

*Figure S8: COSY (80°C, C$_2$D$_2$Cl$_4$, 500 MHz). The weak $^4J$ coupling is highlighted by the two rectangles.*
4.2.2. NOESY

The coupling of the backwards pointing methoxy groups with the light blue labeled protons in the aromatic region of compound 8 shows a higher coupling intensity than the more remotely lying light green labeled proton (see Figure S9). This can be explained by the distant-dependent signal intensity inherent for NOE measurement, as the nuclear Overhauser effect (NOE) scales with $1/r^6$, with $r$ being the distance between the interacting nuclei. In addition, a slight axial twisting of the phenylene ring is also necessary to give rise to through-space coupling, since the nuclei of the proton is otherwise hidden behind it. The question arises for why one does not observe the other two protons in this NOESY-spectrum. This can rationalized by two arguments: first, the kinked 1,4-dimethoxycyclohexa-2,5-diene moiety has the phenylene point away from the methoxy group (see Scheme S1). Therefore, the lightly colored protons are on the “visual axis” in between the methoxy group and the dark colored protons. Second, the distance between the protons is larger, rendering the signal intensity smaller.

![Figure S9: NOESY spectrum of compound 8 recorded at 60 °C in C$_2$D$_2$Cl$_4$ (700 MHz).](image-url)
Scheme S1: 3D-representation of macrocycle 8 based on the 2D-NMR spectra discussed above. The expected angle of around 90° between the phenylenes the cyclohexadiene unit is labeled with red semicircles.
5. Computational Results

The geometry optimization of all structures reported in Scheme S2 has been performed using Density Functional Theory (DFT) with the B3LYP hybrid functional and the 6-31G(d) Pople’s basis set. To reduce computation time, the methoxy groups of the synthesized structures have been removed and substituted by hydrogen atoms while we considered phenyl rings as R substituents.

Scheme S2: structural overview of computed structures within this chapter.
5.1 Geometrical analysis

Here, the opening of the nanoring of the macrocycle is considered with the aim to understand whether the equilibrium structure of 10c is rather close to compound 3 or 9. By going from 3 to 10c, there is a nanoring opening of about 4 Å (see Figure S10). In contrast, the nanoring opening of the neutral structure 9 is 13 Å. Hence, we can conclude that the equilibrium structure of the tetraanionic intermediate 10c is shifted toward 3 in comparison to 9, due to its oval shape. To support this result, a dianionic structure 11 was analyzed and it was found that the doubly negatively charged macrocycle has a similar shape to 3, but with a smaller opening of the nanoring due to constrains of the two remaining hydrogen atoms bounded to the sp<sup>3</sup>-carbons.

![Figure S10: Nanoring opening for the different structures studied with different charge.](image)

The bond length analysis of the structures 3 and 10c shows two peculiar situations (see Figure S11): when the negatively charged structures 10c is considered, the bond length is close to the aromatic bond length, in between 1.4-1.45 Å (see Figure S11, top view left, black double arrows); on the other hand, for the neutral structure 3, the bond length differs significantly. In fact, the bonds between the sp<sup>3</sup>-carbon and the neighboring atoms is 1.53 Å, while the distance between the two sp<sup>2</sup>-carbon atoms of the ring is 1.35 Å (see Figure S11, top view right, green double arrows). These results are in agreement with the bond angle analysis of the cyclohexadiene moieties. In fact, for the charged structures, the angles are close to the aromatic ring values, in
between 116-120 degrees, while for neutral structures the angles decrease to 110-113 degrees, close to a sp$^3$ hybridization of the carbon atoms (see Figure S11, top view, red dotted curves). The torsional angles analysis enforces this conclusion; in fact, the value of the out-of-plane bending of the phenyl substituents, bonded with the cyclohexadiene moiety, of ~38 degrees increases to ~65 degrees when passing to the neutral structure (see Figure S11, side view, black curves). Hence, we can conclude that the tetraionic structure 10c is a resonant form in between 3 and 9, with a strong aromatic character of the anionic carbons that are sp$^2$ hybridized.

Figure S11: geometrical analysis of structures 3 (sp$^2$) and 10c (sp$^3$, tetraanion). Black double arrows refer to the double bond length, while green double arrows refer to the single bonds length. Red dotted curves refer to the bond angles of the cyclohexadiene moieties, while black lines refer to the out-of-plane torsion angles.
5.2 Frontier Orbital Analysis

The frontier orbitals of the neutral structures 8a and 3 are depicted in Figure S12.

Figure S12: frontier orbital of 8a (above) and 3 (below)
The HOMO of the neutral structures 8a and 3 is localized over the ring bridging the sp³-carbon atom, while the LUMO is localized over the sp² part of the macro ring. Due to the high symmetry of the structures, the last three occupied orbitals (namely HOMO-2, HOMO-1 and HOMO) are quasi-degenerate, as well as the first three virtual orbitals (LUMO, LUMO+1 and LUMO+2). Interestingly, for the neutral structure 9 (see Figure S13) both the HOMO and the LUMO are localized over the aromatized ring (previously sp³ in 8a; see upper image Figure S12).

When the tetraanionic species 10c is considered, the HOMO is localized over two aromatic rings, bridging the charge, while the LUMO is delocalized over the remaining part of the macro ring (see Figure S13). As for structures 3 and 8a, the strong symmetry of the system leads to a quasi-degeneracy of the orbitals.

Figure S13: frontier orbitals of neutral structure 9.
When an intermediate case is considered, in which two negative charges are removed (structure 11), the HOMO is localized over the charged part of the molecule, while the LUMO is mainly localized over the cyclohexadiene moiety (see Figure S14).

Figure S15: frontier orbital of dianionic macrocycle 3b.
5.3 Electrostatic Potential (ESP) Analysis

To gain insight into the formation of structure 3 from structure 8 when a mild reductive aromatization was performed, we need to analyze the distribution of charges of our molecules. The electrostatic potential (ESP) analysis is therefore performed to assess the charge migration proposed in the mechanism. To analyze the charge distribution, we consider the charge on different subunits of the structure; in particular, the charge over tetraphenyl-1,4-phenylene moieties as one group and the phenylene ring linking them as a second group (see Figure S16, top).

![Image of electrostatic potential analysis]

Interestingly, we did observe a strong localization of the charge (~2e) over the cyclohexadiene moieties (see Figure S16, red circles) while the remaining charge (~2e) is delocalized over the substituted aromatic phenyl rings (see Figure S16, blue circles).

5.4 Energy analysis

The total energy of compound 8a and of the two isomers 9 and 3 are reported in the following table. Since 8a has two hydrogen atoms more than 9 and 3, we added the energy of H2 to the total energy of 9 and 3 to be comparable to 8a. The energy difference (in kcal/mol) is also reported.

|      | 8a              | 9            | 3            |
|------|-----------------|--------------|--------------|
| Total energy (Hartree) | -8321.3240 | -8321.2853   | -8321.3201   |
| ΔE (kcal/mol)      | 0             | 24.28        | 2.47         |
5.5 Cartesian Coordinates

**Structure 2:** Atom number: 360

Total energy (Hartree): -8317.694435

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | -7.460167 | 5.195055  | -0.731658 |
| C    | -6.611917 | 6.297382  | -0.914827 |
| C    | -5.255268 | 6.228549  | -0.579986 |
| C    | -4.778978 | 5.021084  | -0.043945 |
| C    | -5.613192 | 3.928152  | 0.124887  |
| C    | -6.976128 | 3.984572  | -0.216317 |
| H    | -8.505394 | 5.282771  | -1.011664 |
| H    | -7.019833 | 7.213700  | -1.331977 |
| H    | -3.729736 | 4.940497  | 0.227898  |
| H    | -5.201949 | 3.001654  | 0.512762  |
| C    | -4.188818 | 7.297944  | -0.745248 |
| C    | -3.771882 | 8.028969  | 0.377273  |
| C    | -3.409555 | 7.305846  | -1.921575 |
| C    | -2.466948 | 8.572366  | 0.420654  |
| C    | -2.111607 | 7.859782  | -1.884959 |
| C    | -1.589541 | 8.355166  | -0.665283 |
| C    | -0.998570 | 8.331172  | -0.471754 |
| C    | 0.756725  | 9.380562  | -0.110332 |
| C    | 0.463599  | 7.046967  | -0.582311 |
| C    | 2.117159  | 9.151486  | 0.148367  |
| H    | 0.362918  | 10.387464 | -0.009484 |
| C    | 1.805399  | 6.821263  | -0.325443 |
| H    | -0.175245 | 6.211248  | -0.850886 |
| C    | 2.662001  | 7.865932  | 0.058315  |
| H    | 2.750414  | 9.987327  | 0.431952  |
| H    | 2.205597  | 5.814471  | -0.414108 |
| C    | 4.073267  | 7.422390  | 0.331673  |
| C    | 4.356634  | 6.772732  | 1.553893  |
| C    | 5.039642  | 7.413715  | -0.697811 |
| C    | 5.475128  | 5.919440  | 1.651329  |
| C    | 6.151278  | 6.542184  | -0.606159 |
| C    | 6.290029  | 5.699521  | 0.516972  |
| C    | 6.976860  | 4.364061  | 0.392185  |
| C    | 8.341149  | 4.055795  | 0.440870  |
| C    | 6.080125  | 3.304271  | 0.175271  |
| C    | 8.791405  | 2.736266  | 0.284265  |
| H    | 9.068900  | 4.844596  | 0.604937  |
| C    | 6.524299  | 2.003171  | 0.012923  |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| H       | 5.015327  | 3.514477  | 0.128503  |
| C       | 7.891729  | 1.686211  | 0.063963  |
| H       | 9.856420  | 2.530936  | 0.342525  |
| H       | 5.802025  | 1.208275  | -0.148001 |
| C       | 8.187030  | 0.218776  | -0.079546 |
| C       | 7.816551  | -0.418104 | -1.287365 |
| C       | 8.562932  | -0.566602 | 1.031823  |
| C       | 7.577780  | -1.809970 | -1.306384 |
| C       | 8.332220  | -1.961829 | 1.008249  |
| C       | 7.733182  | -2.561644 | -0.122285 |
| C       | -7.710232 | 2.681402  | -0.062207 |
| C       | -7.664258 | 2.033331  | 1.196970  |
| C       | -8.213831 | 1.976618  | -1.179147 |
| C       | -7.839710 | 0.633766  | 1.276999  |
| C       | -8.399410 | 0.577277  | -1.094458 |
| C       | -8.096194 | -0.107359 | 0.104290  |
| C       | -7.792062 | -1.581725 | 0.061163  |
| C       | -8.624113 | -2.638519 | 0.449531  |
| C       | -6.503631 | -1.903063 | -0.393137 |
| C       | -8.182945 | -3.968297 | 0.395386  |
| H       | -9.627972 | -2.430029 | 0.808901  |
| C       | -6.061478 | -3.216854 | -0.431664 |
| H       | -5.835390 | -1.103083 | -0.700942 |
| C       | -6.887947 | -4.284174 | -0.037988 |
| H       | -8.853860 | -4.760479 | 0.712875  |
| H       | -5.043686 | -3.427089 | -0.745594 |
| C       | 7.016991  | -3.877943 | 0.025377  |
| C       | 5.743496  | -3.788295 | 0.609541  |
| C       | 7.448024  | -5.140971 | -0.395310 |
| C       | 4.923959  | -4.899939 | 0.724224  |
| H       | 5.383847  | -2.821555 | 0.951963  |
| C       | 6.626861  | -6.269946 | -0.261927 |
| H       | 8.429018  | -5.253128 | -0.848715 |
| C       | 5.338595  | -6.169694 | 0.282838  |
| H       | 3.928852  | -4.783016 | 1.140948  |
| H       | 6.992789  | -7.230019 | -0.611828 |
| C       | 4.275308  | -7.231271 | 0.345452  |
| C       | 3.756601  | -7.820113 | -0.831704 |
| C       | 3.603708  | -7.452445 | 1.574424  |
| C       | 2.438478  | -8.329427 | -0.829404 |
| C       | 2.296454  | -7.988982 | 1.579220  |
| C       | 1.664305  | -8.290367 | 0.352766  |
C  0.163406  -8.301452  0.250129
C  -0.390076  -7.139692  -0.312738
C  -0.725272  -9.278639  0.712410
C  -1.761366  -6.953535  -0.379414
H  0.273187  -6.359777  -0.676445
C  -2.113263  -9.095759  0.632036
H  -0.339349  -10.191238  1.157808
C  -2.664565  -7.921926  0.098351
H  -2.149585  -6.024720  -0.785476
H  -2.763309  -9.879012  1.005134
C  -6.215605  -5.627226  -0.044029
C  -5.939124  -6.320909  1.153608
C  -5.655715  -6.110362  -1.254669
C  -4.870669  -7.250500  1.197538
C  -4.614913  -7.056808  -1.216570
C  -4.107329  -7.498279  0.035543
C  -2.026705  9.371387  1.611912
C  -1.093336  8.894738  2.542320
C  -2.561147  10.655909  1.797088
C  -0.709063  9.679645  3.630177
H  -0.655136  7.909910  2.412299
C  -2.177498  11.441537  2.883691
H  -3.286194  11.036584  1.082988
C  -1.249330  10.954376  3.805042
H  0.023259  9.292547  4.332412
H  -2.604024  12.433591  3.008452
H  -0.947165  11.565003  4.652055
C  -4.705799  8.179529  1.538485
C  -5.893658  8.909758  1.384111
C  -4.434960  7.602051  2.786838
C  -6.781342  9.067857  2.448423
H  -6.114380  9.364762  0.422037
C  -5.324270  7.752559  3.849779
H  -3.522858  7.029298  2.923393
C  -6.499303  8.488038  3.685771
H  -7.692922  9.643542  2.309438
H  -5.099227  7.291162  4.807500
H  -7.189815  8.608166  4.516494
C  -1.271247  7.940472  -3.124857
C  -0.832339  6.807795  -3.826813
C  -0.919808  9.205750  -3.620624
C  -0.076071  6.935917  -4.991134

S31
| Atoms | X   | Y   | Z   |
|-------|-----|-----|-----|
| H     | -1.086980 | 5.818610 | -3.460356 |
| C     | -0.170398  | 9.337514  | -4.789609  |
| H     | -0.249353  | 10.092762 | -3.086548  |
| C     | 0.252182   | 8.201557  | -5.481928  |
| H     | 0.252369   | 6.044539  | -5.519395  |
| H     | 0.080965   | 10.328198 | -5.159389  |
| H     | 0.828574   | 6.300495  | -6.398281  |
| C     | -3.935130  | 6.731172  | -3.205603  |
| C     | -3.910750  | 5.354308  | -3.468948  |
| C     | -4.419527  | 7.593657  | -4.199295  |
| C     | -4.331545  | 4.857014  | -4.702995  |
| C     | -3.547914  | 4.671300  | -2.706667  |
| C     | -4.442306  | 8.663020  | -4.007984  |
| C     | -4.798131  | 5.727784  | -5.690264  |
| C     | -4.287165  | 3.788000  | -4.896200  |
| C     | -5.215193  | 7.784384  | -6.189758  |
| C     | -5.115169  | 5.341203  | -6.655520  |
| C     | 3.486644   | 6.992584  | 2.759963   |
| C     | 2.314520   | 6.258366  | 2.989035   |
| C     | 3.881850   | 7.933815  | 3.721258   |
| C     | 1.569127   | 6.446336  | 4.153675   |
| H     | 1.989101   | 5.528195  | 2.254652   |
| C     | 3.137603   | 8.126302  | 4.885653   |
| H     | 4.788432   | 8.509901  | 3.557252   |
| C     | 1.981334   | 7.377355  | 5.109660   |
| H     | 0.670900   | 5.856681  | 4.319015   |
| H     | 0.466754   | 8.855883  | 5.621042   |
| H     | 1.408099   | 7.513825  | 6.023101   |
| C     | 5.793321   | 5.218360  | 2.937825   |
| C     | 4.975211   | 4.210884  | 3.469161   |
| C     | 6.939134   | 5.92646   | 3.655288   |
| C     | 5.283014   | 3.608222  | 4.688324   |
| H     | 4.090505   | 3.89323   | 2.923517   |
| C     | 7.245706   | 4.997913  | 4.879586   |
| H     | 7.584935   | 6.368532  | 3.252877   |
| C     | 6.414729   | 4.006235  | 5.403514   |
| H     | 4.633478   | 2.831727  | 5.084143   |
| H     | 8.131751   | 5.312847  | 5.424792   |
| H     | 6.644740   | 3.548336  | 6.362222   |
| C     | 7.134372   | 6.435937  | -1.730989  |
| C     | 8.455482   | 6.870672  | -1.547845  |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | 7.675171   | 0.406408   | -2.532855  |
| C    | 8.808387   | 1.040939   | -3.064257  |
| C    | 6.450845   | 0.569079   | -3.197439  |
| C    | 8.725289   | 1.802610   | -4.229609  |
| H    | 9.763695   | 0.928424   | -2.558683  |
| C    | 6.363997   | 1.333396   | -4.360111  |
| H    | 5.559697   | 0.092516   | -2.801810  |
| C    | 7.501785   | 1.949490   | -4.883846  |
| H    | 6.168500   | 2.283431   | -4.623389  |
| H    | 5.755067   | 5.557748   | -3.132552  |
| H    | 7.434754   | 2.539384   | -5.794357  |
| C    | 7.124814   | -2.455292  | -2.584103  |
| C    | 5.776858   | -2.762779  | -2.818392  |
| C    | 8.052933   | -2.696063  | -3.606794  |
| C    | 5.363847   | -3.263287  | -4.053526  |
| H    | 5.046816   | -2.592690  | -2.032636  |
| C    | 7.644174   | -3.206170  | -4.839313  |
| H    | 9.100290   | -2.460471  | -3.439137  |
| C    | 6.295542   | -3.480297  | -5.071443  |
| H    | 4.311257   | -3.475262  | -4.224296  |
| H    | 8.378563   | -3.376496  | -5.622274  |
| H    | 5.971539   | -3.856638  | -6.038455  |
| C    | 4.301324   | -7.107544  | 2.855655   |
| C    | 3.772681   | -6.197988  | 3.784181   |
| C    | 5.534365   | -7.711652  | 3.147762   |
| C    | 4.453044   | -5.903700  | 4.964743   |
| H    | 2.821650   | -5.716674  | 3.579741   |
| C    | 6.214471   | -7.422393  | 4.330250   |
| H    | 5.959093   | -8.416659  | 2.438490   |
| C    | 5.675732   | -6.516378  | 5.244245   |
| H    | 4.025646   | -5.193146  | 5.667693   |
| H    | 7.167352   | -7.903481  | 4.534775   |
| H    | 6.204282   | -6.288535  | 6.166143   |
| C    | 1.586401   | -8.235253  | 2.877434   |
| C    | 2.005800   | -9.294011  | 3.696520   |
| C    | 0.515656   | -7.439763  | 3.307656   |
| C    | 1.377557   | -9.547473  | 4.915716   |
| H    | 2.836875   | -9.916040  | 3.375674   |
| C    | -0.108429  | -7.688059  | 4.529785   |
| H    | 0.168038   | -6.624734  | 2.679703   |
| C    | 0.318885   | -8.742368  | 5.337919   |
| H    | 1.718337   | -10.372701 | 5.535840   |
H   -0.937867   -7.062204    4.844238
H   -0.171591   -8.936723    6.288179
C    1.832788    -8.891840   -2.078674
C    1.664833    -8.118536   -3.236638
C    1.415878   -10.231357   -2.106879
C    1.103590   -10.668652   -4.387988
H    1.976250   -10.785242   -3.233307
C    0.859459   -10.785395   -3.259333
H    0.548249   -10.434386   -5.303835
C    0.701655   -10.005124   -4.405073
H    0.980333   -8.050955   -5.273843
H    0.548249   -11.826900   -3.260529
H    0.266842   -10.434386   -5.303835
C    4.603336   -7.954519   -2.063789
C    4.938745   -6.876775   -2.893289
C    5.095209   -9.228351   -2.390252
C    5.739520   -7.069059   -4.019895
H    4.585207   -5.879181   -2.651548
C    5.895253   -9.422185   -3.515870
C    4.841585   -10.072401   -1.754760
C    6.219629   -8.340616   -4.335919
H    5.996220   -6.216737   -4.641364
H    6.264055   -10.417599   -3.750055
H    6.844590   -8.486637   -5.213248
C   -4.536361   -7.917637    2.496391
C   -4.042716   -7.194888    3.591265
C   -4.775491   -9.290717    2.658028
C   -3.800422   -7.825274    4.811521
H   -3.859936   -6.129606    3.486331
C   -4.529468   -9.924744    3.876446
H   -5.175268   -9.860076    1.822541
H   -4.041520   -9.192360    4.958915
H   -3.430417   -7.244726    5.652832
H   -4.726164   -10.988691    3.980708
H   -3.854742   -9.681501    5.911168
C   -6.794702   -6.111132    2.369030
C   -7.709768   -7.117576    2.716863
C   -6.737529   -4.958199    3.162058
C   -8.538592   -6.981246    3.829838
H   -7.766547   -8.015108    2.107092
C   -7.565939   -4.820632    4.276685
H   -6.052083   -4.157890    2.899820
| At. | X       | Y       | Z       |
|-----|---------|---------|---------|
| C   | -8.467148 | -5.830313 | 4.615710 |
| H   | -9.239218 | -7.773653 | 4.080714 |
| H   | -7.514222 | -3.913306 | 4.869890 |
| H   | -9.112133 | -5.718559 | 5.483472 |
| C   | -4.065352 | -7.663373 | -2.473242 |
| C   | -3.364275 | -6.931977 | -3.442193 |
| C   | -4.271146 | -9.035541 | -2.698892 |
| C   | -2.893709 | -7.545939 | -4.602191 |
| H   | -3.175003 | -5.875687 | -3.282600 |
| C   | -3.806402 | -9.649616 | -3.860502 |
| H   | -4.810141 | -9.615440 | -1.956175 |
| C   | -3.116715 | -8.906317 | -4.81512 |
| H   | -2.349000 | -6.959124 | -5.337239 |
| H   | -3.983161 | -10.710957 | -4.015051 |
| H   | -2.752250 | -9.383437 | -5.724340 |
| C   | -6.273928 | -5.693247 | -2.561381 |
| C   | -7.439069 | -6.353083 | -2.979622 |
| C   | -5.751063 | -4.686843 | -3.384342 |
| C   | -8.056648 | -6.026799 | -4.187272 |
| H   | -7.858719 | -7.133810 | -2.350954 |
| C   | -6.368337 | -4.355000 | -4.590291 |
| C   | -6.487639 | -4.151547 | -3.077485 |
| C   | -7.521758 | -5.025896 | -4.998116 |
| H   | -8.956441 | -6.555012 | -4.492129 |
| H   | -5.946877 | -3.568323 | -5.210587 |
| H   | -8.000806 | -4.768245 | -5.938976 |
| C   | -7.719381 | -0.045254 | 2.610556 |
| C   | -6.548337 | -0.715198 | 2.992904 |
| C   | -8.770306 | 0.045019  | 3.534196 |
| C   | -6.418544 | -1.248044 | 4.275820 |
| H   | -5.728338 | -0.802835 | 2.286167 |
| C   | -8.647243 | -0.497004 | 4.813704 |
| H   | -9.681760 | 0.564688  | 3.251825 |
| C   | -7.465459 | -1.134710 | 5.193400 |
| H   | -5.494372 | -1.744243 | 4.561850 |
| H   | -9.470358 | -0.408369 | 5.517917 |
| H   | -7.359169 | -1.537680 | 6.197431 |
| C   | -7.451807 | 2.858443  | 2.431980 |
| C   | -8.398213 | 3.843498  | 2.755529 |
| C   | -6.355097 | 2.686643  | 3.289425 |
| C   | -8.261282 | 4.623006  | 3.903603 |
| H   | -9.251925 | 3.991721  | 2.099919 |

S36
Structure 8a: Atom number: 366
Total energy (Hartree): -8321.324018

C  -6.213923  3.467137  4.435851
H  -5.606912  1.935636  3.058112
C  -7.168618  4.435652  4.750436
H  -9.008408  5.377868  5.647213
H  -5.355025  3.316622  5.084942
H  -7.060705  5.040029  5.647213
C  -8.862828  -0.203665  -2.285991
C  -10.090361  0.081231  -2.244828
C  -8.096191  -0.284250  -3.457410
C  -10.543222  -1.611376  -3.343580
H  -10.696539  -0.825741  -1.344617
C  -8.544008  -1.018522  -4.554061
H  -7.142140  0.231798  -3.506698
C  -9.770465  -1.682736  -4.502954
H  -11.499349  -2.125833  -3.291997
H  -7.933410  -1.070660  -5.452274
H  -10.119900  -2.259345  -5.358860
C  -8.577478  2.701371  -2.441811
C  -9.935985  2.855434  -2.759673
C  -7.622531  3.244011  -3.311667
C  -10.329812  3.527875  -3.916236
H  -10.686724  2.439122  -2.093681
C  -8.014987  3.916539  -4.469590
H  -6.566472  3.152241  -3.076367
C  -9.368632  4.060515  -4.776441
H  -11.387460  3.634960  -4.143336
H  -7.257646  4.340293  -5.122031
H  -9.672140  4.587069  -5.677608
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| C    | -4.231606  | -3.557958  | -0.589459  |
| C    | -6.494022  | -0.647079  | 0.387780   |
| C    | -7.733568  | -0.620738  | -0.264535  |
| C    | -8.463415  | 0.562064   | -0.370998  |
| C    | -7.967322  | 1.767960   | 0.141113   |
| C    | -6.739950  | 1.734882   | 0.814266   |
| C    | -6.019330  | 0.547895   | 0.942292   |
| C    | -8.754253  | 3.075815   | -0.058200  |
| C    | -8.612342  | 4.022725   | 1.124139   |
| C    | -7.973627  | 5.204777   | 1.027275   |
| C    | -7.381427  | 5.708774   | -0.290724  |
| C    | -7.859864  | 4.933286   | -1.509973  |
| C    | -8.465009  | 3.735183   | -1.410548  |
| C    | -9.250108  | 3.544930   | 2.391660   |
| C    | -10.625476 | 3.261260   | 2.426147   |
| C    | -11.236676 | 2.803406   | 3.593024   |
| C    | -10.480272 | 2.606764   | 4.749454   |
| C    | -9.111267  | 2.876510   | 4.727930   |
| C    | -8.503616  | 3.341667   | 3.562072   |
| C    | -9.033229  | 3.023239   | -2.601886  |
| C    | -8.334964  | 2.007378   | -3.271473  |
| C    | -8.909707  | 1.343996   | -4.356782  |
| C    | -10.193421 | 1.680041   | -4.789048  |
| C    | -10.900481 | 2.686491   | -4.128789  |
| C    | -10.325107 | 3.348686   | -3.043874  |
| C    | -7.926093  | 6.189437   | 2.156261   |
| C    | -6.747664  | 6.443342   | 2.875295   |
| C    | -6.728870  | 7.396728   | 3.894858   |
| C    | -7.880957  | 8.118731   | 4.209160   |
| C    | -9.057732  | 7.878103   | 3.498137   |
| C    | -9.077927  | 6.923295   | 2.481506   |
| C    | -7.642313  | 5.621023   | -2.821543  |
| C    | -6.830784  | 5.064757   | -3.821070  |
| C    | -6.648471  | 5.716473   | -5.040995  |
| C    | -7.266696  | 6.944116   | -5.283095  |
| C    | -8.068199  | 7.515475   | -4.293601  |
| C    | -8.249697  | 6.861704   | -3.075239  |
| C    | -5.849158  | 5.828088   | -0.266274  |
| C    | -5.231287  | 7.074228   | -0.110587  |
| C    | -3.841577  | 7.193020   | -0.076796  |
| C    | -3.021250  | 6.064057   | -0.191362  |
| C    | -3.641052  | 4.816860   | -0.356850  |
| Atom | X    | Y    | Z    |
|------|------|------|------|
| C    | -5.028179 | 4.701827 | -0.403670 |
| C    | -1.524451 | 6.160823 | -0.157321 |
| C    | -0.814740 | 5.643084 | 0.948587  |
| C    | 0.596713  | 5.683888 | 0.964592  |
| C    | 1.297761  | 6.219313 | -0.137478 |
| C    | 0.589593  | 6.746920 | -1.238707 |
| C    | -0.823241 | 6.734664 | -1.241082 |
| C    | -1.560667 | 5.049278 | 2.107126  |
| C    | -1.497613 | 3.673798 | 2.372869  |
| C    | -2.192114 | 3.119210 | 3.448088  |
| C    | -2.957347 | 3.933460 | 4.284164  |
| C    | -3.023207 | 5.305607 | 4.034480  |
| C    | -2.334970 | 5.856673 | 2.952914  |
| C    | -1.574698 | 7.348970 | -2.384591 |
| C    | -2.352087 | 6.569551 | -3.252587 |
| C    | -3.055618 | 7.156870 | -4.303651 |
| C    | -2.995015 | 8.536442 | -4.505081 |
| C    | -2.223567 | 9.323642 | -3.649203 |
| C    | -1.519372 | 8.734087 | -2.599669 |
| C    | 1.351222  | 5.168183 | 2.155402  |
| C    | 2.118761  | 3.996838 | 2.078722  |
| C    | 2.819170  | 3.524024 | 3.189217  |
| C    | 2.764605  | 4.219494 | 4.399496  |
| C    | 2.005637  | 5.387920 | 4.488862  |
| C    | 1.304977  | 5.855578 | 3.376882  |
| C    | 1.340932  | 7.288050 | -2.418973 |
| C    | 2.116917  | 8.451411 | -2.316676 |
| C    | 2.821079  | 8.940043 | -3.416854 |
| C    | 2.764826  | 8.270805 | -4.640142 |
| C    | 1.996225  | 7.111735 | -4.755278 |
| C    | 1.289975  | 6.626843 | -3.654834 |
| C    | 2.797773  | 6.205313 | -0.142520 |
| C    | 3.540727  | 7.111601 | 0.624522  |
| C    | 4.934160  | 7.077703 | 0.623621  |
| C    | 5.636213  | 6.115037 | -0.114437 |
| C    | 4.891736  | 5.221925 | -0.894301 |
| C    | 3.498691  | 5.271300 | -0.914694 |
| C    | 7.173550  | 6.060026 | -0.049885 |
| C    | 7.791904  | 5.562773 | -1.349175 |
| C    | 8.429101  | 4.377346 | -1.432190 |
| C    | 8.619048  | 3.469238 | -0.214161 |
| C    | 8.385207  | 4.180524 | 1.110361 |
| Atom | X           | Y           | Z           |
|------|-------------|-------------|-------------|
| C    | 7.696749    | 5.333030    | 1.193660    |
| C    | 7.641917    | 6.490273    | -2.514631   |
| C    | 8.088207    | 7.819706    | -2.427704   |
| C    | 7.947285    | 8.698661    | -3.501232   |
| C    | 7.343500    | 8.270093    | -4.684207   |
| C    | 6.888312    | 6.954583    | -4.783539   |
| C    | 7.037715    | 6.075656    | -3.711769   |
| C    | 7.514307    | 6.062210    | 2.490779    |
| C    | 6.374378    | 5.880755    | 3.287854    |
| C    | 6.215069    | 6.593465    | 4.477276    |
| C    | 7.191089    | 7.501818    | 4.889783    |
| C    | 8.328702    | 7.694157    | 4.103783    |
| C    | 8.485577    | 6.982738    | 2.913596    |
| C    | 9.149864    | 3.928780    | -2.666809   |
| C    | 8.735656    | 2.813106    | -3.411692   |
| C    | 9.462872    | 2.390506    | -4.526020   |
| C    | 10.618547   | 3.069657    | -4.913731   |
| C    | 11.042191   | 4.179521    | -4.180404   |
| C    | 10.315667   | 4.601882    | -3.067704   |
| C    | 9.022961    | 3.528669    | 2.297453    |
| C    | 10.423691   | 3.450370    | 2.372254    |
| C    | 11.054001   | 2.862682    | 3.468280    |
| C    | 10.292659   | 2.333669    | 4.512072    |
| C    | 8.900401    | 2.394813    | 4.444704    |
| C    | 8.270757    | 2.981506    | 3.345892    |
| C    | 7.824644    | 2.153136    | -0.278579   |
| C    | 6.449027    | 2.110954    | -0.016703   |
| C    | 5.744370    | 0.909947    | -0.067968   |
| C    | 6.387581    | -0.296694   | -0.379439   |
| C    | 7.764285    | -0.254437   | -0.638189   |
| C    | 8.468985    | 0.947961    | -0.582442   |
| C    | -6.367412   | -2.139116   | 2.891659    |
| C    | -7.768132   | -2.106612   | 2.945680    |
| C    | -8.428912   | -1.616623   | 4.071919    |
| C    | -7.699141   | -1.147152   | 5.164868    |
| C    | -6.304497   | -1.175145   | 5.124160    |
| C    | -5.645608   | -1.668185   | 3.998098    |
| C    | -4.870575   | -4.646123   | 3.014067    |
| C    | -3.684230   | -4.747868   | 3.755098    |
| C    | -3.646372   | -5.467085   | 4.950034    |
| C    | -4.795357   | -6.105713   | 5.420839    |
| C    | -5.980095   | -6.019189   | 4.687748    |
|   |        |        |        |
|---|--------|--------|--------|
| 1 | -6.016924 | -5.293288 | 3.497434 |
| 2 | -3.434114 | -4.010313 | -1.778177 |
| 3 | -3.838641 | -5.103835 | -2.556338 |
| 4 | -3.086068 | -5.513373 | -3.658251 |
| 5 | -1.908716 | -4.842315 | -3.994530 |
| 6 | -1.495195 | -3.752901 | -3.226426 |
| 7 | -2.254586 | -3.393332 | -2.131714 |
| 8 | -3.449185 | -5.603846 | 0.645470 |
| 9 | -4.118989 | -6.833612 | 0.617089 |
| 10 | -3.410740 | -8.035448 | 0.590458 |
| 11 | -2.010693 | -8.051254 | 0.600755 |
| 12 | -1.341818 | -6.822021 | 0.673544 |
| 13 | -2.047866 | -5.621106 | 0.683967 |
| 14 | -1.244847 | -9.381386 | 0.521530 |
| 15 | -0.201084 | -9.536883 | 1.623196 |
| 16 | 1.119939 | -9.508716 | 1.361412 |
| 17 | 1.665640 | -9.332654 | -0.058828 |
| 18 | 0.639466 | -9.635242 | -1.139272 |
| 19 | -0.682524 | -9.653924 | -0.878818 |
| 20 | 5.637193 | -1.595898 | -0.405222 |
| 21 | 5.471488 | -2.299798 | -1.619267 |
| 22 | 4.802941 | -3.545479 | -1.631212 |
| 23 | 4.299288 | -4.087363 | -0.428488 |
| 24 | 4.433916 | -3.367548 | 0.779523 |
| 25 | 5.103907 | -2.124031 | 0.791920 |
| 26 | 6.000511 | -1.722891 | -2.899400 |
| 27 | 5.446301 | -0.552649 | -3.439515 |
| 28 | 5.918291 | -0.026364 | -4.642219 |
| 29 | 6.960740 | -0.658386 | -5.323801 |
| 30 | 7.528021 | -1.817412 | -4.790978 |
| 31 | 7.049378 | -2.345070 | -3.591949 |
| 32 | 5.251296 | -1.374579 | 2.083416 |
| 33 | 4.131127 | -0.827169 | 2.726061 |
| 34 | 4.262249 | -0.150373 | 3.938941 |
| 35 | 5.519007 | -0.010066 | 4.531648 |
| 36 | 6.641543 | -0.548426 | 3.900343 |
| 37 | 6.507724 | -1.221546 | 2.686267 |
| 38 | 4.612880 | -4.288836 | -2.920406 |
| 39 | 3.776562 | -3.775645 | -3.922697 |
| 40 | 3.585296 | -4.467975 | -5.118256 |
| 41 | 4.230783 | -5.686492 | -5.334192 |
| 42 | 5.067990 | -6.206235 | -4.345923 |
| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| H    | -5.475459 | 3.725458 | -0.559831 |
| H    | -3.390078  | 8.174997  | 0.033433  |
| H    | -3.026623  | 3.926121  | -0.456849 |
| H    | 3.023341   | 7.853399  | 1.227094  |
| H    | 5.482746   | 7.802726  | 1.217828  |
| H    | 5.404113   | -6.851431 | 0.607546  |
| H    | -1.502773  | -4.681446 | 0.716216  |
| H    | -3.956389  | -8.974914 | 0.553390  |
| H    | -0.258696  | -6.800748 | 0.725550  |
| H    | 5.922860   | 3.022377  | 0.247512  |
| H    | 9.537653   | 0.948271  | -0.781906 |
| H    | 4.680199   | 0.906453  | 0.150924  |
| H    | 8.291891   | -1.172821 | -0.879970 |
| H    | 1.876319   | -4.837049 | -1.504344 |
| H    | 5.248153   | -6.387373 | 0.655323  |
| H    | 0.775343   | -7.022920 | -1.352009 |
| H    | 4.162094   | -8.584649 | 0.776769  |
| H    | -5.844669  | 5.887753  | 2.642820  |
| H    | -9.997407  | 6.734001  | 1.934052  |
| H    | -5.808100  | 7.575564  | 4.444834  |
| H    | -9.962647  | 8.431496  | 3.736032  |
| H    | -7.862850  | 8.861257  | 5.002706  |
| H    | -11.228948 | 3.418309  | 1.535318  |
| H    | -7.437910  | 3.545797  | 3.554982  |
| H    | -12.304965 | 2.602007  | 3.598177  |
| H    | -8.510453  | 2.721350  | 5.620247  |
| H    | -10.954040 | 2.246300  | 5.658858  |
| H    | -6.341464  | 4.113983  | -3.637593 |
| H    | -8.888766  | 7.311260  | -2.318948 |
| H    | -6.024330  | 5.260331  | -5.805605 |
| H    | -8.557807  | 8.469613  | -4.471208 |
| H    | -7.126444  | 7.450742  | -6.234374 |
| H    | -7.338333  | 1.730741  | -2.941632 |
| H    | -10.875831 | 4.137272  | -2.537009 |
| H    | -8.348239  | 0.560500  | -4.858708 |
| H    | -11.899291 | 2.959811  | -4.459636 |
| H    | -10.639622 | 1.162674  | -5.634494 |
| H    | -0.896733  | 3.035557  | 1.731231  |
| H    | -2.396370  | 6.924039  | 2.760436  |
| H    | -2.131752  | 2.049972  | 3.634434  |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| H    | -3.609174 | 5.949667  | 4.685509  |
| H    | -3.495358 | 3.503668  | 5.124913  |
| H    | 2.168971  | 3.453886  | 1.139417  |
| H    | 0.712817  | 6.763026  | 3.454403  |
| H    | 3.404299  | 2.611251  | 3.109987  |
| H    | 1.953460  | 5.935071  | 5.426771  |
| H    | 3.306427  | 3.850689  | 5.266662  |
| H    | 2.171641  | 8.974322  | -1.366347 |
| H    | 6.411992  | 6.609445  | -5.697473 |
| H    | 3.419605  | 9.841478  | -3.315644 |
| H    | 1.944907  | 6.582387  | -5.703372 |
| H    | 3.318316  | 8.648577  | -5.495605 |
| H    | -2.412910 | 5.496512  | -3.096345 |
| H    | -0.918404 | 9.351490  | -1.938052 |
| H    | -3.663982 | 6.537487  | -4.956317 |
| H    | -2.169702 | 10.399337 | -3.796237 |
| H    | -3.549124 | 8.994484  | -5.320088 |
| H    | 5.602784  | 5.185140  | 2.972371  |
| H    | 9.376910  | 7.129625  | 2.308465  |
| H    | 5.321476  | 6.437243  | 5.075925  |
| H    | 9.097294  | 8.395875  | 4.417918  |
| H    | 7.067109  | 8.055999  | 5.816617  |
| H    | 11.026298 | 3.873774  | 1.572004  |
| H    | 7.187530  | 3.011121  | 3.296770  |
| H    | 12.139605 | 2.823908  | 3.509365  |
| H    | 8.297514  | 1.986006  | 5.251417  |
| H    | 10.780864 | 1.878379  | 5.369839  |
| H    | 8.570540  | 8.167736  | -1.517632 |
| H    | 6.681687  | 5.054521  | -3.800380 |
| H    | 8.311568  | 9.719067  | -3.412391 |
| H    | 0.690425  | 5.726153  | -3.751962 |
| H    | 7.229210  | 8.954963  | -5.520414 |
| H    | 7.838493  | 2.274024  | -3.125332 |
| H    | 10.646709 | 5.468030  | -2.501436 |
| H    | 9.120611  | 1.523760  | -5.085029 |
| H    | 11.939667 | 4.718248  | -4.473944 |
| H    | 11.184410 | 2.737789  | -5.780475 |
| H    | 3.148985  | -0.944190 | 2.277135  |
| H    | 7.386852  | -1.631702 | 2.197781  |
| H    | 3.380041  | 0.259358  | 4.424328  |
| H    | 7.625623  | -0.438562 | 4.346643  |
| H    | 5.620723  | 0.510893  | 5.480332  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| H    | 5.753528| -4.245670| 3.006122|
| H    | 1.810249| -3.711987| 1.395301|
| H    | 4.783063| -5.108355| 5.108475|
| H    | 0.829671| -4.560219| 3.501566|
| H    | 2.312056| -5.256489| 5.377038|
| H    | 3.276695| -2.824400| -3.763212|
| H    | 5.899760| -5.930222| -2.380885|
| H    | 2.932101| -4.053284| -5.881896|
| H    | 5.572737| -7.155808| -4.502774|
| H    | 4.082246| -6.227606| -6.264898|
| H    | 4.637034| -0.054876| -2.912812|
| H    | 7.487912| -3.253770| -3.189793|
| H    | 5.467762| 0.875088 | -5.049721|
| H    | 8.340763| -2.316597| -5.312107|
| H    | 7.321947| -0.254711| -6.266219|
| H    | 1.648805| -7.878626| 3.484244 |
| H    | 2.922879| -11.53283| 1.616619 |
| H    | 3.380763| -8.163653| 5.223320 |
| H    | 4.652526| -11.82381| 3.354293 |
| H    | 4.893361| -10.14065| 5.172827 |
| H    | 0.090529| -11.84441| 2.985955 |
| H    | -1.763829| -7.978958| 3.291210 |
| H    | -0.889368| -12.487948| 5.162102 |
| H    | -2.747080| -8.617152| 5.450587 |
| H    | -2.317703| -10.876284| 6.413331 |
| H    | 0.143135| -8.362919| -3.515354|
| H    | 2.417582| -11.583349| -1.804959|
| H    | 1.115950| -8.853186| -5.730074|
| H    | 3.387294| -12.077996| -4.015539|
| H    | 2.745817| -10.715522| -5.998445|
| H    | -1.107565| -12.158196| -1.765259|
| H    | -2.536141| -8.135903| -2.251528|
| H    | -2.818175| -12.963047| -3.363372|
| H    | -4.244424| -8.935075| -3.846527|
| H    | -4.399275| -11.351384| -4.413186|
| H    | -2.787197| -4.253275| 3.393400|
| H    | -6.944910| -5.221017| 2.937527|
| H    | -2.719763| -5.523984| 5.515645|
| H    | -6.879704| -6.513681| 5.044691|
| H    | -4.769178| -6.661761| 6.354425|
| H    | -8.343149| -2.463185| 2.096103|
| H    | -4.559720| -1.690159| 3.974439|
H    -9.515225    -1.595419     4.091854
H    -5.726143    -0.812718     5.970253
H    -8.214042    -0.761125     6.040540
H    -4.748605    -5.636515    -2.294463
H    -1.931384    -2.486108    -1.541669
H    -3.419665    -6.358135    -4.255510
H    -0.581521    -3.221877    -3.480978
H    -1.320990    -5.163549    -4.850270
H    -6.204563    -3.037057    -2.993935
H    -3.842225     0.056876    -1.184678
H    -6.252702    -1.766507    -5.115044
H    -3.875615     1.329382    -3.304677
H    -5.084720     0.425683    -5.285074
H    9.675507     3.167043    -0.232299
H    7.489185     7.106222     0.075443
H    2.468514   -10.075435    -0.168530
H    -1.997212   -10.162641     0.698990
H    -7.748516     6.739059    -0.404951
H    -9.810475     2.770970    -0.099396

Structure 9: Atom num: 364
Total energy (Hartree): -8320.10984775
C     0.405604     0.072351    -0.636821
C     0.265107    -0.132485     0.736874
C     1.390452    -0.150309     1.561566
C     2.673962     0.036270     1.030652
C     2.800937     0.264873    -0.347167
C     1.677932     0.278526    -1.175060
C     3.882742    -0.095094     1.911114
C     4.611914     1.036353     2.333733
C     5.707798     0.878631     3.210651
C     6.149984    -0.415678     3.565047
C     5.480529    -1.549413     3.058144
C     4.311141    -1.387556     2.283991
C     4.366233     2.367418     1.681460
C     3.333068     3.259337     1.990477
C     3.134688     4.427479     1.243012
C     3.954145     4.730865     0.146258
C     5.018677     3.850613    -0.126240
C     5.225874     2.705733     0.626369
C     3.742036     5.786285    -0.899798
C     4.844133     6.574975    -1.319748
| X  | Y  | Z       |
|----|----|---------|
| 4.894318 | 7.065178 | -2.643557 |
| 3.849226 | 6.735013 | -3.538119 |
| 2.618686 | 6.276740 | -3.005093 |
| 2.557480 | 5.812422 | -1.674277 |
| 5.941848 | 6.857313 | -0.340498 |
| 5.620470 | 7.435884 |  0.898165 |
| 6.609973 | 7.719502 |  1.838666 |
| 7.945039 | 7.423832 |  1.561429 |
| 8.279502 | 6.843073 |  0.336937 |
| 7.289122 | 6.564665 | -0.603678 |
| 1.243848 | 5.385675 | -1.085772 |
| 0.871831 | 4.045178 | -0.921429 |
| -0.362919 | 3.713759 | -0.362270 |
| -1.245392 | 4.715948 |  0.043672 |
| -0.885115 | 6.055038 | -0.112459 |
| 0.349942 | 6.385037 | -0.671149 |
| 6.014810 | 7.963604 | -3.080069 |
| 7.040985 | 7.558041 | -3.943582 |
| 8.047721 | 8.448849 | -4.319210 |
| 8.045560 | 9.759295 | -3.839753 |
| 7.026872 | 10.176419 | -2.981961 |
| 6.020721 | 9.285970 | -2.608436 |
| 1.401814 | 6.295406 | -3.878872 |
| 0.650871 | 5.145180 | -4.164079 |
| -0.485196 | 5.213624 | -4.968813 |
| -0.897023 | 6.435374 | -5.503634 |
| -0.156498 | 7.586836 | -5.235081 |
| 0.982800 | 7.514897 | -4.434311 |
| 4.106974 | 6.545637 | -5.005793 |
| 4.568290 | 7.476445 | -5.946321 |
| 4.920891 | 7.077539 | -7.243756 |
| 4.813386 | 5.740777 | -7.645188 |
| 4.317995 | 4.817821 | -6.711728 |
| 3.980702 | 5.208646 | -5.426921 |
| 5.214601 | 5.153058 | -8.969074 |
| 6.566206 | 4.857766 | -9.241759 |
| 6.894711 | 3.974692 | -10.294760 |
| 5.869842 | 3.357150 | -11.046806 |
| 4.529837 | 3.760535 | -10.862216 |
| 4.205960 | 4.674370 | -9.835191 |
| 7.670172 | 5.434357 | -8.403764 |
| 7.978103 | 4.903079 | -7.142982 |
| C   | 9.071138 | 5.377426  | -6.417206 |
| C   | 9.866768 | 6.402389  | -6.934813 |
| C   | 9.551830 | 6.958643  | -8.175468 |
| C   | 8.463859 | 6.475947  | -8.903435 |
| C   | 2.790757 | 5.126774  | -9.632017 |
| C   | 1.785824 | 4.251511  | -9.196596 |
| C   | 0.477496 | 4.698770  | -9.019434 |
| C   | 0.148207 | 6.029909  | -9.279497 |
| C   | 1.138968 | 6.912070  | -9.711283 |
| C   | 2.449121 | 6.464219  | -9.880807 |
| C   | 8.330469 | 3.684842  | -10.622414|
| C   | 9.161811 | 2.962556  | -9.754170 |
| C   | 10.495954| 2.720006  | -10.078395|
| C   | 11.028084| 3.201303  | -11.275909|
| C   | 10.210856| 3.920608  | -12.150366|
| C   | 8.873475 | 4.153685  | -11.827534|
| C   | 3.430883 | 3.194569  | -11.712653|
| C   | 2.798549 | 3.991917  | -12.676887|
| C   | 1.736915 | 3.493634  | -13.432324|
| C   | 1.284759 | 2.188811  | -13.230107|
| C   | 1.912444 | 1.381619  | -12.278479|
| C   | 2.980666 | 1.879035  | -11.531319|
| C   | 6.205785 | 2.184296  | -11.919937|
| C   | 6.069279 | 2.167322  | -13.312944|
| C   | 6.371598 | 1.017551  | -14.047893|
| C   | 6.805528 | -0.155729 | -13.418421|
| C   | 6.957411 | -0.132296 | -12.026581|
| C   | 6.664038 | 1.012862  | -11.293767|
| C   | 7.096562 | -1.435307 | -14.219671|
| C   | 5.978540 | -2.473662 | -14.083617|
| C   | 6.155201 | -3.650655 | -13.448561|
| C   | 7.502390 | -4.086824 | -12.891258|
| C   | 8.663392 | -3.180513 | -13.298151|
| C   | 8.481154 | -1.998870 | -13.918213|
| C   | 4.733098 | -2.161729 | -14.857902|
| C   | 4.472389 | -2.883258 | -16.035386|
| C   | 3.361101 | -2.594361 | -16.826041|
| C   | 2.487039 | -1.570540 | -16.456984|
| C   | 2.733894 | -0.844659 | -15.291531|
| C   | 3.846382 | -1.134966 | -14.499390|
| C   | 9.619601 | -1.204164 | -14.488662|
| C   | 10.033546| 0.021546  | -13.942868|
|   | C   |     |     |     |
|---|-----|-----|-----|-----|
|   | 11.067123 | 0.749195 | -14.535225 |
|   | 11.699149 | 0.273814 | -15.684682 |
|   | 11.292894 | -0.941173 | -16.238753 |
|   | 10.263075 | -1.670256 | -15.645059 |
|   | 5.051765 | -4.651694 | -13.303292 |
|   | 3.845938 | -4.309026 | -12.671692 |
|   | 2.816605 | -5.239251 | -12.533350 |
|   | 2.971663 | -6.537860 | -13.021770 |
|   | 4.167811 | -6.897223 | -13.64607 |
|   | 5.196873 | -5.965501 | -13.778059 |
|   | 10.029220 | -3.730299 | -13.028723 |
|   | 10.456824 | -4.918263 | -13.643641 |
|   | 11.728528 | -5.437235 | -13.399650 |
|   | 12.597164 | -4.780377 | -12.526501 |
|   | 12.182631 | -3.602084 | -11.903814 |
|   | 10.911178 | -3.083772 | -12.150513 |
|   | 7.482803 | -4.395555 | -11.383447 |
|   | 6.843688 | -3.570923 | -10.449871 |
|   | 6.869777 | -3.867134 | -9.085785 |
|   | 7.516802 | -5.013949 | -8.606951 |
|   | 8.140810 | -5.848746 | -9.543576 |
|   | 8.126645 | -5.542248 | -10.902174 |
|   | 6.413164 | 2.095291 | 3.729954 |
|   | 5.762125 | 2.953511 | 4.628017 |
|   | 6.401241 | 4.090390 | 5.122725 |
|   | 7.702580 | 4.392925 | 4.720437 |
|   | 8.359272 | 3.549605 | 3.822907 |
|   | 7.721077 | 2.410015 | 3.335037 |
|   | 7.350345 | -0.578470 | 4.450115 |
|   | 8.578383 | -1.010270 | 3.928864 |
|   | 9.700643 | -1.128229 | 4.749424 |
|   | 9.609611 | -0.829244 | 6.110357 |
|   | 8.389667 | -0.409370 | 6.642582 |
|   | 7.271723 | -0.281124 | 5.817988 |
|   | 3.539435 | -2.598801 | 1.846001 |
|   | 2.786611 | -3.326889 | 2.778280 |
|   | 2.062157 | -4.454487 | 2.389279 |
|   | 2.087357 | -4.880972 | 1.060189 |
|   | 2.836277 | -4.166302 | 0.123484 |
|   | 3.551360 | -3.034154 | 0.513380 |
|   | 6.049145 | -2.926818 | 3.229608 |
|   | 6.020237 | -3.637167 | 4.434600 |
|   C | 6.544958 | -4.929589 |  4.513459 |
|----|----------|-----------|-----------|
|   C | 7.121272 |  -5.549058|  3.397627 |
|   C | 7.169155 |  -4.829949|  2.197362 |
|   C | 6.637096 |  -3.546392|  2.115302 |
|   C | 7.696398 |  -6.970670|  3.486588 |
|   C | 9.142309 |  -7.034637|  3.002972 |
|   C | 9.479379 |  -7.629363|  1.841918 |
|   C | 8.458856 |  -8.369917|  0.974762 |
|   C | 7.149689 |  -8.660699|  1.693649 |
|   C | 6.795504 |  -8.016740|  2.823000 |
|   C | 7.546343 |  -5.372192|  7.147727 |
|   C | 6.775067 |  -6.458722|  6.675949 |
|   C | 6.849603 |  -6.842584|  5.317963 |
|   C | 7.727249 |  -6.167684|  4.440587 |
|   C | 8.478446 |  -5.066721|  4.905792 |
|   C | 8.375266 |  -4.657860|  6.25365 |
|   C | 5.902476 |  -7.222714|  7.627005 |
|   C | 4.803278 |  -6.615234|  8.250596 |
|   C | 4.013222 |  -7.322198|  9.156356 |
|   C | 4.307415 |  -8.653543|  9.453472 |
|   C | 5.395018 |  -9.272432|  8.835596 |
|   C | 6.184214 |  -8.562841|  7.930959 |
|   C | 9.146181 |  -3.464618|  6.737954 |
|   C | 8.816961 |  -2.178770|  6.284263 |
|   C | 9.523256 |  -1.060498|  6.727161 |
|   C | 10.576179|  -1.209060|  7.631200 |
|   C | 10.914611|  -2.483413|  8.088935 |
|   C | 10.203917|  -3.599769|  7.648561 |
|   C | 5.974092 |  -7.947475|  4.803697 |
|   C | 4.587149 |  -7.756584|  4.719149 |
|   C | 3.754188 |  -8.764100|  4.233025 |
|   C | 4.295069 |  -9.983266|  3.822836 |
|   C | 5.673285 | -10.186781|  3.904541 |
|   C | 6.504395 |  -9.177881|  4.390487 |
|   C | 9.401128 |  -4.346797|  3.966902 |
|   C | 10.791816|  -4.416214|  4.133989 |
|   C | 11.651920|  -3.754022|  3.258284 |
|   C | 11.135789|  -3.004450|  2.200060 |
|   C | 9.753496 |  -2.925540|  2.023612 |
|   C | 8.895550 |  -3.593113|  2.897680 |
|   C | 7.906858 |  -6.663995|  3.033287 |
|   C | 6.958906 |  -6.441995|  2.028123 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| C       | 7.133838  | -6.961505 | -0.743053 |
| C       | 8.255187  | -7.734689 | -0.418116 |
| C       | 9.203218  | -7.955896 | -1.427667 |
| C       | 9.040465  | -7.419954 | -2.702596 |
| C       | 10.159895 | -6.507368 | 3.968973  |
| C       | 11.075127 | -7.399497 | 4.553947  |
| C       | 11.995801 | -6.966719 | 5.506953  |
| C       | 12.017817 | -5.628393 | 5.902651  |
| C       | 11.112509 | -4.731775 | 5.334737  |
| C       | 10.191496 | -5.164563 | 4.379235  |
| C       | 5.565540  | -8.366051 | 3.604433  |
| C       | 5.541589  | -9.542445 | 4.370200  |
| C       | 4.428181  | -9.873232 | 5.142301  |
| C       | 3.316150  | -9.029758 | 5.165577  |
| C       | 3.328551  | -7.856481 | 4.410425  |
| C       | 4.443671  | -7.523219 | 3.639580  |
| C       | 10.889558 | -7.659352 | 1.343566  |
| C       | 11.541818 | -6.476935 | 0.964959  |
| C       | 12.846579 | -6.505500 | 0.472783  |
| C       | 13.526827 | -7.717975 | 0.351333  |
| C       | 12.890321 | -8.903956 | 0.723291  |
| C       | 11.582659 | -8.873706 | 1.208113  |
| C       | 6.311243  | -9.739856 | 1.080936  |
| C       | 4.991755  | -9.507050 | 0.664226  |
| C       | 4.229740  | -10.525167| 0.092393  |
| C       | 4.769489  | -11.801426| -0.073825 |
| C       | 6.080952  | -12.049503| 0.334132  |
| C       | 6.842997  | -11.027712| 0.899883  |
| H       | 2.655891  | 3.036086  | 2.810497  |
| H       | 2.311609  | 5.084871  | 1.502806  |
| H       | 5.668472  | 4.052799  | -0.971122 |
| H       | 6.045860  | 2.038934  | 0.373367  |
| H       | 4.678370  | 8.519302  | -5.666213 |
| H       | 3.639387  | 4.461976  | -4.717089 |
| H       | 5.296526  | 7.821280  | -7.941126 |
| H       | 4.221626  | 3.773715  | -6.996528 |
| H       | 5.719766  | 3.055847  | -13.831005|
| H       | 6.789095  | 1.001545  | -10.214773|
| H       | 6.255864  | 1.032367  | -15.128672|
| H       | 7.329600  | -1.011622 | -11.511447|
| H       | 5.585470  | -3.180231 | 5.319267  |
| H       | 6.678250  | -3.010809 | 1.170620  |
|    |    |    |    |    |
|----|----|----|----|----|
| H  | 6.505740 | -5.463518 | 5.459586 |
| H  | 7.635145  | -5.268832  | 1.321648 |
| H  | 6.300576  | -2.694792  | -10.790454 |
| H  | 8.626786  | -6.208742  | -11.599643 |
| H  | 6.371870  | -3.201913  | -8.385192 |
| H  | 8.638369  | -6.753123  | -9.204272 |
| H  | 6.370573  | -6.777690  | 0.006408 |
| H  | 10.081089 | -8.559635  | -1.218023 |
| H  | 7.050148  | 6.544767   | -4.333312 |
| H  | 5.230425  | 9.612167   | -1.937837 |
| H  | 8.826516  | 8.114935   | -4.997866 |
| H  | 7.012881  | 11.195054  | -2.602653 |
| H  | 8.830465  | 10.451053  | -4.134642 |
| H  | 4.582443  | 7.668390   | 1.118911 |
| H  | 7.563538  | 6.112247   | -1.550981 |
| H  | 6.335869  | 8.170140   | 2.789043 |
| H  | 9.315635  | 6.603411   | 0.111947 |
| H  | 8.718304  | 7.642684   | 2.293145 |
| H  | 0.959053  | 4.189202   | -3.753593 |
| H  | 1.554587  | 8.414696   | -4.224561 |
| H  | -1.050717 | 4.308892   | -5.176869 |
| H  | -0.464609 | 8.543804   | -5.648369 |
| H  | -1.786613 | 6.488733   | -6.125727 |
| H  | 1.554362  | 3.254808   | -1.218463 |
| H  | 0.627323  | 7.428487   | -0.794417 |
| H  | -0.625054 | 2.667608   | -0.237309 |
| H  | -1.563618 | 6.844825   | 0.199920 |
| H  | -2.206372 | 4.455114   | 0.479680 |
| H  | 7.366231  | 4.102197   | -6.737756 |
| H  | 8.236942  | 6.895464   | -9.879642 |
| H  | 9.307663  | 4.939350   | -5.450752 |
| H  | 10.160503 | 7.760800   | -8.584511 |
| H  | 10.727545 | 6.761435   | -6.376444 |
| H  | 8.760037  | 2.588852   | -8.817384 |
| H  | 8.241731  | 4.711891   | -12.513114 |
| H  | 11.122616 | 2.157237   | -9.391194 |
| H  | 10.613244 | 4.303454   | -13.084819 |
| H  | 12.070780 | 3.021174   | -11.523349 |
| H  | 3.133270  | 5.015076   | -12.823201 |
| H  | 2.065577  | -0.041957  | -14.993230 |
|   |   |   |   |
|---|---|---|---|
| H | 1.257105 | 4.129203 | -14.171959 |
| H | 1.567198 | 0.364164 | -12.113935 |
| H | 0.445833 | 1.805046 | -13.804951 |
| H | 2.031298 | 3.213129 | -8.995647 |
| H | 3.218425 | 7.154758 | -10.216320 |
| H | -0.285474 | 4.005726 | -8.675048 |
| H | 0.894343 | 7.951530 | -9.914429 |
| H | -0.872243 | 6.377542 | -9.143024 |
| H | 9.554733 | 0.406741 | -13.048860 |
| H | 9.951365 | -2.617034 | -16.077694 |
| H | 11.374039 | 1.691592 | -14.089867 |
| H | 11.777976 | -1.323812 | -17.133248 |
| H | 12.502474 | 0.843868 | -16.144443 |
| H | 9.795254 | -5.431911 | -14.337586 |
| H | 10.592680 | -2.170586 | -11.657796 |
| H | 12.042056 | -6.351978 | -13.896372 |
| H | 12.853224 | -3.080759 | -11.225139 |
| H | 13.588464 | -5.182551 | -12.334809 |
| H | 5.150661 | -3.680551 | -16.326253 |
| H | 4.020121 | -0.560483 | -13.596014 |
| H | 3.179897 | -3.168983 | -17.730910 |
| H | 3.464846 | 1.247355 | -10.791837 |
| H | 1.621300 | -1.340849 | -17.072897 |
| H | 3.718627 | -3.301402 | -12.288887 |
| H | 6.116130 | -6.260426 | -14.277923 |
| H | 1.890255 | -4.946969 | -12.045031 |
| H | 4.300579 | -7.904373 | -14.031375 |
| H | 2.167908 | -7.262348 | -12.919405 |
| H | 8.002725 | -2.057698 | -5.575320 |
| H | 10.468168 | -4.585804 | -8.018573 |
| H | 9.251844 | 0.073038 | -6.362152 |
| H | 11.730938 | -2.613178 | -8.794446 |
| H | 11.129214 | -0.339018 | -7.976010 |
| H | 11.200425 | -4.993045 | -4.958690 |
| H | 7.820828 | -3.531120 | -2.752070 |
| H | 12.726700 | -3.822970 | -3.405170 |
| H | 9.340695 | -2.343591 | -1.203259 |
| H | 11.805095 | -2.484278 | -1.519645 |
| H | 4.160559 | -6.810371 | -5.040492 |
| H | 7.576399 | -9.342428 | -4.443297 |
| H | 2.681840 | -8.594830 | -4.175461 |
| H | 6.104394 | -11.129801 | -3.579578 |
|   |   |   |   |
|---|---|---|---|
| H  | 3.649325 | -10.768395 | -3.439141 |
| H  | 4.572779  | -5.576893  | -8.031134 |
| H  | 7.030168  | -9.050192  | -7.454904 |
| H  | 3.177557  | -6.826878  | -9.642516 |
| H  | 5.633454  | -10.309134 | -9.059570 |
| H  | 3.696204  | -9.202354  | -10.165042|
| H  | 11.013677 | -5.532109  | 1.047976  |
| H  | 11.099438 | -9.803092  | 1.501524  |
| H  | 13.328894 | -5.577483  | 0.177243  |
| H  | 13.412349 | -9.853732  | 0.638330  |
| H  | 14.543808 | -7.739937  | -0.031335 |
| H  | 11.058186 | -8.443596  | 4.256066  |
| H  | 9.498519  | -4.450656  | 3.948451  |
| H  | 12.693065 | -7.677590  | 5.943220  |
| H  | 11.111118 | -3.688457  | 5.638328  |
| H  | 12.732106 | -5.288880  | 6.648382  |
| H  | 4.561364  | -8.518910  | 0.788946  |
| H  | 7.858094  | -11.240877 | 1.226102  |
| H  | 3.211436  | -10.318037 | -0.225835 |
| H  | 6.511522  | -13.040851 | 0.216994  |
| H  | 4.173545  | -12.596065 | -0.515306 |
| H  | 6.403447  | -10.204025 | 4.350794  |
| H  | 4.435994  | -6.609036  | 3.054402  |
| H  | 4.429566  | -10.791496 | 5.724134  |
| H  | 2.466854  | -7.193718  | 4.417273  |
| H  | 2.446966  | -9.286266  | 5.765741  |
| H  | 8.654334  | -1.248236  | 2.871727  |
| H  | 6.328342  | 0.060686   | 6.234674  |
| H  | 10.647235 | -1.450101  | 4.322820  |
| H  | 8.308195  | -0.174030  | 7.700544  |
| H  | 10.483607 | -0.918370  | 6.750294  |
| H  | 4.474622  | 2.723034   | 4.942139  |
| H  | 8.240864  | 1.756916   | 2.640398  |
| H  | 5.880069  | 4.740597   | 5.820718  |
| H  | 9.371228  | 3.779070   | 3.499698  |
| H  | 8.201027  | 5.280129   | 5.101860  |
| H  | 2.767907  | -3.003146  | 3.815411  |
| H  | 4.125924  | -2.479872  | -0.222947 |
| H  | 1.474166  | -4.997234  | 3.125285  |
| H  | 2.861823  | -4.488737  | -0.914249 |
| H  | 1.525650  | -5.760321  | 0.756505  |
| H  | 1.276720  | -0.331220  | 2.626816  |
Structure 3: Atom number: 364
Total energy (Hartree): -8320.144625

C  19.303699  29.996594  6.737405
C  20.141305  31.069678  6.356123
C  21.522757  30.850937  6.155579
C  22.073851  29.566954  6.357939
C  21.259482  28.522519  6.843806
C  19.875448  28.735260  7.026435
C  19.584005  32.448879  6.160783
C  18.765856  32.764858  5.067890
H  19.336835  31.989362  4.356531
C  18.292142  34.064151  4.886945
H  17.667722  34.288271  4.027372
C  18.614496  35.066665  5.802741
C  19.416702  34.760462  6.902921
H  19.672718  35.531910  7.624660
C  19.900135  33.463741  7.076283
H  20.536261  33.232987  7.926369
C  22.413158  31.970256  5.701915
C  22.268127  32.544229  4.429954
H  21.486814  32.182737  3.767782
C  23.112430  33.571069  4.008140
H  22.983601  34.001253  3.018285
C  24.115562  34.048231  4.854155
C  24.268651  33.487720  6.123366
H  25.044101  33.852929  6.791871
C  23.426704  32.456237  6.540358
H  23.554640  32.020882  7.527401
C  21.864027  27.183040  7.152906
C  22.028799  26.768620  8.481976
H  21.708563  27.423613  9.287440
C  22.593217  25.527710  8.779057
H  22.713558  25.225912  9.816339
| Atoms | X-Coordinates | Y-Coordinates | Z-Coordinates |
|-------|--------------|--------------|--------------|
| C     | 22.998262    | 24.676224    | 7.750178     |
| C     | 22.838415    | 25.076442    | 6.422092     |
| H     | 23.146418    | 24.418698    | 5.612701     |
| C     | 22.279173    | 26.320453    | 6.128721     |
| H     | 22.166999    | 26.632871    | 5.094793     |
| C     | 19.024479    | 27.610424    | 7.539277     |
| C     | 18.502284    | 27.655362    | 8.839267     |
| H     | 18.689268    | 28.528329    | 9.458510     |
| C     | 17.761570    | 26.587902    | 9.347810     |
| H     | 17.391020    | 26.630543    | 10.368467    |
| C     | 17.508617    | 25.466342    | 8.556217     |
| C     | 18.008894    | 25.417427    | 7.253469     |
| H     | 17.813625    | 24.552798    | 6.624580     |
| C     | 18.767214    | 26.476432    | 6.755315     |
| H     | 19.169579    | 26.423051    | 5.747747     |
| C     | 17.810479    | 30.151645    | 6.731570     |
| C     | 17.064861    | 29.393669    | 5.815522     |
| H     | 17.577036    | 28.702482    | 5.153123     |
| C     | 15.682234    | 29.512676    | 5.736585     |
| H     | 15.136982    | 28.907814    | 5.018369     |
| C     | 14.978084    | 30.396026    | 6.569234     |
| C     | 15.720295    | 31.155263    | 7.484824     |
| H     | 15.209495    | 31.843674    | 8.151419     |
| C     | 17.109710    | 31.036240    | 7.563525     |
| H     | 17.653246    | 31.646517    | 8.278531     |
| C     | 13.482200    | 30.444190    | 6.453400     |
| C     | 12.661611    | 30.008437    | 7.519054     |
| C     | 11.271742    | 29.848623    | 7.320449     |
| C     | 10.695485    | 30.149903    | 6.067112     |
| C     | 11.495826    | 30.688785    | 5.038137     |
| C     | 12.887904    | 30.829159    | 5.228889     |
| C     | 13.243638    | 29.720959    | 8.871559     |
| C     | 14.058819    | 28.605367    | 9.105199     |
| H     | 14.309887    | 27.941383    | 8.283091     |
| C     | 14.552850    | 28.341558    | 10.382674    |
| H     | 15.173513    | 27.465176    | 10.542681    |
| C     | 14.254841    | 29.195684    | 11.445343    |
| H     | 14.642179    | 28.988736    | 12.439614    |
| C     | 13.456585    | 30.318249    | 11.221490    |
| H     | 13.219664    | 30.992967    | 12.040151    |
| C     | 12.952719    | 30.574387    | 9.946587     |
| H     | 12.319983    | 31.441772    | 9.779935     |
H     9.677700 27.693254  5.801536
C     5.141245 28.612595  4.879715
H     4.509748 29.280370  5.478921
C     4.795266 28.894976  3.410733
C     4.736043 27.896500  2.503679
C     4.792555 26.189293  4.385542
C     4.784856 27.188115  5.293812
C     4.531845 30.327625  3.079675
C     3.540731 31.054466  3.762510
H     2.933289 30.558166  4.516109
C     3.306355 32.398366  3.471944
H     2.525984 32.935985  4.004550
C     4.069923 33.049832  1.823259
C     5.064925 32.343831  1.072600
H     5.672345 30.842590  2.108511
H     6.073374 30.459108  1.581212
C     4.237888 28.071976  1.104169
C     2.998616 26.934383  0.867309
H     2.430874 29.079393  1.707860
C     2.487498 28.814686 -0.423524
H     1.525610 29.297648 -0.576299
C     3.202294 28.313985 -1.513410
C     4.428777 27.866199 -1.294849
H     5.000003 27.291918 -2.131511
C     4.938504 27.559028 -0.002149
H     5.895302 27.069249  0.142026
C     4.517931 24.761579  4.728294
C     5.299558 24.081574  5.675793
H     6.105949 24.609505  6.175002
C     5.060099 22.740360  5.972823
H     5.683910 22.233806  6.704588
C     4.032064 22.048802  5.330051
C     3.247155 22.709948  4.383353
H     2.441072 22.183489  3.878624
C     3.493030 24.049217  4.081091
H     2.868827 24.552752  3.346687
C     4.340397 27.019565  6.712260
C     5.103211 27.501465  7.790946
H     6.068870 27.960512  7.609326
| Atoms | X     | Y     | Z     | Energy |
|-------|-------|-------|-------|--------|
| C     | 4.643858 | 27.382158 | 9.103124 |
| H     | 5.262147 | 27.751765 | 9.917300 |
| C     | 3.407345 | 26.793554 | 9.369206 |
| C     | 2.631561 | 26.324195 | 8.307479 |
| H     | 1.661458 | 25.871990 | 8.497861 |
| C     | 3.092296 | 26.437260 | 6.996999 |
| C     | 6.520843 | 26.044259 | 2.514902 |
| C     | 6.839326 | 24.687157 | 2.351201 |
| H     | 6.068325 | 23.934062 | 2.485371 |
| C     | 8.133844 | 24.280862 | 2.025282 |
| H     | 8.351390 | 23.221072 | 1.925285 |
| C     | 9.152629 | 25.220840 | 1.824629 |
| C     | 8.825757 | 26.575393 | 1.961217 |
| H     | 9.595122 | 27.324016 | 1.796939 |
| C     | 7.539740 | 26.980811 | 2.308590 |
| H     | 7.330059 | 28.038986 | 2.416710 |
| C     | 10.570156 | 24.855699 | 1.497657 |
| C     | 11.407146 | 24.310245 | 2.493588 |
| C     | 12.789158 | 24.158807 | 2.246823 |
| C     | 13.336277 | 24.538134 | 0.998622 |
| C     | 12.476675 | 24.979583 | -0.033275 |
| C     | 11.097364 | 25.150848 | 0.221473 |
| C     | 10.829858 | 23.907106 | 3.819973 |
| C     | 10.430418 | 24.869108 | 4.758273 |
| H     | 10.535641 | 25.922329 | 4.515082 |
| C     | 9.897047 | 24.490405 | 5.990495 |
| H     | 9.600727 | 25.252110 | 6.707819 |
| C     | 9.748044 | 23.137749 | 6.302776 |
| H     | 9.333521 | 22.840368 | 7.262520 |
| C     | 10.138931 | 22.170252 | 5.376105 |
| H     | 10.027678 | 21.114524 | 5.609741 |
| C     | 13.664727 | 23.580869 | 3.319899 |
| C     | 10.677258 | 22.552439 | 4.146891 |
| H     | 10.986413 | 21.794226 | 3.432764 |
| C     | 13.932475 | 24.288028 | 4.500996 |
| H     | 13.519606 | 25.284331 | 4.630740 |
| C     | 14.714467 | 23.727932 | 5.510665 |
| H     | 14.916693 | 24.298342 | 6.413421 |
| C     | 15.229215 | 22.438256 | 5.363847 |
| H     | 15.823626 | 21.991697 | 6.156895 |
| C     | 14.966678 | 21.722823 | 4.194336 |
|         |        |        |        |        |
|---------|--------|--------|--------|--------|
| C       | 18.649957 | 22.170708 | 2.156586 |
| H       | 18.406771  | 22.942494 | 2.881131 |
| C       | 18.177016 | 20.872091 | 2.344698 |
| H       | 17.579928  | 20.645022 | 3.222735 |
| C       | 18.465262 | 19.873953 | 1.412914 |
| C       | 19.232749 | 20.183827 | 0.289305 |
| H       | 19.462174 | 19.415947 | -0.445066 |
| C       | 19.715563 | 21.479683 | 0.108374 |
| H       | 20.324404 | 21.713159 | -0.760702 |
| C       | 22.279589 | 22.951842 | 1.395745 |
| C       | 23.254843 | 22.459299 | 0.516675 |
| H       | 23.346005 | 22.894913 | -0.474321 |
| C       | 24.105049 | 21.421017 | 0.898460 |
| H       | 24.849943 | 21.050534 | 0.198835 |
| C       | 23.999159 | 20.860382 | 2.172426 |
| C       | 23.034988 | 21.344435 | 3.058851 |
| H       | 22.943238 | 20.914381 | 4.052883 |
| C       | 22.181987 | 22.377904 | 2.672229 |
| H       | 21.430827 | 22.744559 | 3.365772 |
| C       | 21.703647 | 27.748043 | -0.015262 |
| C       | 21.825130 | 28.165991 | -1.347849 |
| H       | 21.475592 | 27.514635 | -2.144047 |
| C       | 22.383292 | 29.406072 | -1.659899 |
| H       | 22.469813 | 29.710737 | -2.699714 |
| C       | 22.824863 | 30.253218 | -0.642575 |
| C       | 22.708515 | 29.849331 | 0.688940 |
| H       | 23.045671 | 30.503796 | 1.489328 |
| C       | 22.155531 | 28.606088 | 0.997095 |
| H       | 22.075781 | 28.290863 | 2.033255 |
| C       | 18.849741 | 27.338110 | -0.296022 |
| C       | 18.281517 | 27.299467 | -1.576833 |
| H       | 18.442693 | 26.427590 | -2.204792 |
| C       | 17.527661 | 28.371534 | -2.055446 |
| H       | 17.120295 | 28.333498 | -3.062180 |
| C       | 17.308486 | 29.491908 | -1.252188 |
| C       | 17.855191 | 29.534766 | 0.032012 |
| H       | 17.686424 | 30.398293 | 0.670001 |
| C       | 18.625762 | 28.470829 | 0.499888 |
| H       | 19.063918 | 28.519470 | 1.492653 |
| C       | 23.365025 | 25.626123 | 1.105735 |
| C       | 24.364379 | 25.858602 | 0.152477 |
| H       | 24.117175 | 25.831509 | -0.905185 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| C       | 25.677438    | 26.124071    | 0.542756     |
| H       | 26.432567    | 26.284202    | -0.221258    |
| C       | 26.035049    | 26.194499    | 1.898057     |
| C       | 25.035340    | 25.956849    | 2.847819     |
| H       | 25.274159    | 25.994776    | 3.904776     |
| C       | 23.730209    | 25.668989    | 2.456814     |
| H       | 22.975866    | 25.478077    | 3.214555     |
| C       | 28.117613    | 25.976662    | 1.589053     |
| H       | 27.869423    | 26.019449    | 3.692383     |
| C       | 27.865255    | 26.859882    | 4.749025     |
| C       | 27.548441    | 28.351937    | 4.574691     |
| H       | 28.214434    | 28.890565    | 5.260300     |
| C       | 27.872858    | 28.850655    | 3.169838     |
| C       | 27.812893    | 28.010471    | 2.114761     |
| C       | 28.332721    | 24.598649    | 3.761345     |
| C       | 27.576257    | 23.543965    | 3.219845     |
| H       | 26.601979    | 23.742405    | 2.786584     |
| C       | 28.053265    | 22.232869    | 3.246354     |
| H       | 27.439636    | 21.436749    | 2.832324     |
| C       | 29.301316    | 21.945015    | 3.799252     |
| H       | 29.672990    | 20.923707    | 3.816045     |
| C       | 30.070669    | 22.983699    | 4.327021     |
| H       | 31.049445    | 22.776776    | 4.752487     |
| C       | 29.592376    | 24.292560    | 4.306804     |
| H       | 30.201889    | 25.093192    | 4.713501     |
| C       | 28.166283    | 26.427314    | 6.146760     |
| C       | 27.403355    | 25.431118    | 6.776322     |
| H       | 26.591447    | 24.961204    | 6.230285     |
| C       | 27.668524    | 25.049316    | 8.091018     |
| H       | 27.059277    | 24.280755    | 8.559367     |
| C       | 28.703974    | 25.654268    | 8.805313     |
| H       | 28.910352    | 25.356317    | 9.829886     |
| C       | 29.470266    | 26.648770    | 8.194376     |
| H       | 30.281692    | 27.124787    | 8.739051     |
| C       | 29.198520    | 27.035769    | 6.882240     |
| H       | 29.807687    | 27.807024    | 6.416803     |
| C       | 28.348492    | 30.266148    | 3.079878     |
| C       | 27.628850    | 31.329085    | 3.654364     |
| H       | 26.672833    | 31.141408    | 4.130984     |
| C       | 28.119025    | 32.634683    | 3.606338     |
| H       | 27.533589    | 33.437632    | 4.047185     |
| C  | 29.344431 | 32.908550 | 2.998307  |
| H  | 29.726528 | 33.925588 | 2.964823  |
| C  | 30.077590 | 31.861443 | 2.436718  |
| H  | 30.167222 | 29.750632 | 2.044902  |
| C  | 28.056995 | 28.439561 | 0.704802  |
| C  | 27.275821 | 29.441661 | 0.107916  |
| C  | 26.096952 | 28.942750 | 4.138527  |
| C  | 25.080059 | 28.904217 | 3.072154  |
| C  | 23.796047 | 29.242564 | 4.586275  |
| H  | 23.011082 | 29.440193 | 3.862219  |
| C  | 23.490614 | 29.288632 | 5.951980  |
| C  | 24.528667 | 29.047114 | 6.860631  |
| H  | 24.328538 | 29.076362 | 7.928149  |
| C  | 25.820706 | 28.768632 | 6.413190  |
| H  | 26.606735 | 28.601232 | 7.143714  |
| H  | 3.893005  | 34.098713 | 2.278704  |
| H  | 2.805061  | 28.409222 | -2.520695 |
| H  | 3.845768  | 21.003474 | 5.561750  |
| H  | 3.049414  | 26.704408 | 10.391667 |
| H  | 18.243091 | 36.078270 | 5.660787  |
| H  | 24.768717 | 34.853662 | 4.528258  |
| H  | 16.722705 | 30.327593 | -1.626623 |
| H  | 23.254291 | 31.221874 | -0.884797 |
| H  | 24.658609 | 20.049465 | 2.470871  |
| H  | 18.094314 | 18.863017 | 1.560694  |
| H  | 23.432900 | 23.707095 | 7.980941  |
| H  | 16.932915 | 24.634382 | 8.953818  |
Structure 3a: Atom numer: 360
Total energy (Hartree): -8317.4881

C 3.231026 6.552191 0.482996
C 2.024690 7.234503 0.295143
C 0.820334 6.551896 0.033469
C 0.902840 5.145273 -0.036337
C 2.098239 4.468056 0.149661
C 3.296364 5.151807 0.422831
H 4.137245 7.122420 0.674392
H 2.019762 8.319083 0.355984
H -0.003997 4.577015 -0.217363
H 2.108389 3.382844 0.093848
C -0.529462 7.163801 -0.147876
C -1.299216 6.803386 -1.297641
C -1.173825 7.927124 0.859279
C -2.691561 6.965723 -1.326839
C -2.566044 8.139368 0.819285
C -3.389001 7.505110 -0.190442
C -4.820759 7.331631 0.014592
C -5.815831 7.348484 -1.011843
C -5.324003 6.947715 1.299941
C -7.097146 6.888541 -0.823419
H -5.559727 7.743126 -1.990260
C -6.600492 6.483678 1.500890
H -4.639839 6.930851 2.143491
C -7.547458 6.312763 0.422688
H -7.780206 6.930828 -1.664488
H -6.864216 6.124787 2.489730
C -8.718975 5.534464 0.551443
C -9.432669 4.984843 -0.626578
C -9.113759 4.889918 1.827259
C -9.562684 3.606258 -0.655601
C -9.300882 3.504429 1.789373
C -9.255459 2.809282 0.522047
C -8.783987 1.423923 0.359394
C -9.110044 0.298235 1.160668
C -7.818546 1.173326 -0.652589
C -8.440309 -0.917942 1.041628
H -9.892858 0.381961 1.905093
C -7.180497 -0.048996 -0.796676
H -7.505187 2.004114 -1.276649
C -7.436081 -1.122375 0.078702
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 5.905182  | -7.079838 | -1.894564 |
| C    | 6.562713  | -6.677946 | 0.766985  |
| H    | 4.575424  | -7.223270 | 1.224232  |
| C    | 7.174124  | -6.667838 | -1.565184 |
| H    | 5.699198  | -7.294888 | -2.938561 |
| C    | 7.558818  | -6.319839 | -0.216955 |
| H    | 6.778169  | -6.505346 | 1.815708  |
| H    | 7.898769  | -6.565893 | -2.365457 |
| C    | 9.217154  | -2.877707 | 0.561361  |
| C    | 9.599202  | -3.464930 | -0.714976 |
| C    | 9.198746  | -3.775968 | 1.693762  |
| C    | 9.478777  | -4.827759 | -0.925317 |
| C    | 9.032225  | -5.149513 | 1.488018  |
| C    | 8.712865  | -5.571404 | 0.102773  |
| C    | -3.429691 | 6.475782  | -2.538775 |
| C    | -4.154246 | 5.274027  | -2.506727 |
| C    | -3.381363 | 7.187991  | -3.745450 |
| C    | -4.801833 | 4.797606  | -3.645274 |
| H    | -4.222325 | 4.723155  | -1.573818 |
| C    | -4.029302 | 6.713908  | -4.888098 |
| H    | -2.823121 | 8.119724  | -3.785587 |
| C    | -4.741861 | 5.515558  | -4.842724 |
| H    | -5.361658 | 3.867024  | -3.593665 |
| H    | -3.975036 | 7.282947  | -5.814543 |
| H    | -5.250706 | 5.144365  | -5.729792 |
| C    | -0.566715 | 6.308919  | -2.512081 |
| C    | 0.316727  | 7.175964  | -3.176205 |
| C    | -0.726089 | 5.014799  | -3.034204 |
| C    | 0.994722  | 6.778106  | -4.328462 |
| H    | 0.461589  | 8.177189  | -2.779190 |
| C    | -0.041852 | 4.608540  | -4.179844 |
| H    | -1.400433 | 4.323167  | -2.539754 |
| C    | 0.819388  | 5.488560  | -4.837568 |
| H    | 1.657894  | 7.479265  | -4.831910 |
| H    | -0.184060 | 3.599186  | -4.559010 |
| H    | 1.348145  | 5.172917  | -5.734402 |
| C    | -3.209949 | 9.110251  | 1.758457  |
| C    | -3.092901 | 9.032650  | 3.158085  |
| C    | -3.944048 | 10.191872 | 1.232689  |
| C    | -3.660138 | 9.999921  | 3.989877  |
| H    | -2.555261 | 8.199765  | 3.599205  |
| C    | -4.508964 | 11.158828 | 2.058903  |
| Element | Atomic Number | X-coordinate | Y-coordinate | Z-coordinate |
|---------|---------------|--------------|--------------|--------------|
| H       | -4.072208     | 10.257190    | 0.156216     |
| C       | -4.367953     | 11.072138    | 3.448918     |
| H       | -3.554559     | 9.904058     | 5.068933     |
| H       | -5.067053     | 11.982686    | 1.617405     |
| H       | -4.817599     | 11.821487    | 4.097516     |
| C       | -0.336727     | 8.546388     | 1.940663     |
| C       | 0.217651      | 7.776669     | 2.974178     |
| C       | 0.217651      | 9.923946     | 1.925275     |
| C       | 1.003340      | 8.366588     | 3.965012     |
| H       | 0.039431      | 6.705636     | 2.994262     |
| C       | 0.715893      | 10.517137    | 2.915900     |
| H       | -0.494818     | 10.532288    | 1.132683     |
| C       | 1.255040      | 9.739793     | 3.942494     |
| H       | 1.422699      | 7.746018     | 4.753175     |
| H       | 0.904257      | 11.588772    | 2.884965     |
| H       | 1.868037      | 10.198627    | 4.715918     |
| C       | -10.080551    | 5.901091     | -1.598579    |
| C       | -9.961429     | 5.785795     | -3.001770    |
| C       | -10.844750    | 6.990918     | -1.121489    |
| C       | -10.590147    | 6.681183     | -3.866733    |
| H       | -9.345023     | 4.996222     | -3.413953    |
| H       | -11.473954    | 7.884169     | -1.982939    |
| C       | -10.950289    | 7.110744     | -0.047881    |
| C       | -11.356640    | 7.737494     | -3.370335    |
| H       | -10.465602    | 6.556929     | -4.941716    |
| H       | -12.064403    | 8.701046     | -1.569047    |
| H       | -11.839159    | 8.440716     | -4.047102    |
| C       | -10.346092    | 2.892813     | -1.728067    |
| C       | -9.796878     | 2.484188     | -2.952796    |
| C       | -11.695726    | 2.582843     | -1.488561    |
| C       | -10.561603    | 1.798442     | -3.901286    |
| H       | -8.752545     | 2.698116     | -3.160336    |
| C       | -12.470485    | 1.915046     | -2.437159    |
| H       | -12.130373    | 2.875761     | -0.536698    |
| C       | -11.903433    | 1.515238     | -3.650644    |
| H       | -10.100886    | 1.479562     | -4.834121    |
| H       | -13.517230    | 1.700374     | -2.226537    |
| H       | -12.500314    | 0.982094     | -4.388838    |
| C       | -9.683797     | 2.727274     | 3.013688     |
| C       | -11.021718    | 2.707446     | 3.439663     |
| C       | -8.748604     | 1.990800     | 3.757960     |
| C       | -11.410218    | 1.992818     | 4.574282     |
S68

| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | -11.756773 | 3.270258 | 2.870491 |
| C    | -9.133429  | 1.264428 | 4.885597 |
| H    | -4.992304  | 1.244166 | 3.612832 |
| C    | -10.466652 | 1.265374 | 5.302992 |
| H    | -12.453272 | 2.001803 | 4.887549 |
| H    | -8.388269  | 0.688008 | 5.428554 |
| H    | -10.767295 | 0.701127 | 6.184177 |
| C    | -9.353788  | 5.749370 | 3.011561 |
| C    | -9.128594  | 5.369636 | 4.359373 |
| C    | -9.807391  | 7.080784 | 2.823693 |
| C    | -9.389023  | 6.230787 | 5.423911 |
| H    | -8.723319  | 4.391145 | 4.579292 |
| C    | -10.068595 | 7.938577 | 3.885827 |
| H    | -9.933013  | 7.436294 | 1.807051 |
| C    | -9.873242  | 7.522795 | 5.207634 |
| H    | -9.193457  | 5.885400 | 6.438754 |
| H    | -10.423799 | 8.947543 | 3.678049 |
| H    | -10.067020 | 8.195304 | 6.041533 |
| C    | -7.549448  | -2.914657 | -2.224941 |
| C    | -7.193680  | -2.518231 | -3.523125 |
| C    | -8.911820  | -3.101392 | -1.942038 |
| C    | -8.164328  | -2.319415 | -4.504893 |
| H    | -6.146510  | -2.359594 | -3.761772 |
| C    | -9.883405  | -2.907884 | -2.922240 |
| H    | -9.206603  | -3.387123 | -0.936542 |
| C    | -9.513913  | -2.514948 | -4.210391 |
| H    | -7.862572  | -2.002687 | -5.500740 |
| H    | -10.933029 | -3.048553 | -2.674525 |
| H    | -10.272240 | -2.349895 | -4.972312 |
| C    | -5.495956  | -4.973338 | -2.557932 |
| C    | -6.532683  | -5.891373 | -2.787154 |
| C    | -4.458168  | -4.896402 | -3.498365 |
| C    | -6.537808  | -6.701661 | -3.922655 |
| H    | -7.344996  | -5.959886 | -2.068906 |
| C    | -4.462975  | -5.702629 | -4.636525 |
| H    | -3.633819  | -4.210181 | -3.332462 |
| C    | -5.502568  | -6.608550 | -4.854159 |
| H    | -7.353345  | -7.405142 | -4.078387 |
| H    | -3.640320  | -5.626384 | -5.341641 |
| H    | -5.502843  | -7.240139 | -5.740170 |
| C    | -5.703858  | -1.843613 | 2.347224 |
| C    | -6.076496  | -2.471018 | 3.544293 |
| Atoms | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| C     | -5.325608 | -0.493351 | 2.392217  |
| C     | -6.057560 | -1.776503 | 4.754339  |
| H     | -6.368083 | -3.517638 | 3.525405  |
| C     | -5.298205 | 0.201261  | 3.600981  |
| H     | -5.055200 | 0.015351  | 1.472261  |
| C     | -5.660058 | -0.439349 | 4.788984  |
| H     | -6.345714 | -2.285173 | 5.671915  |
| H     | -7.712169 | 1.978027  | 3.435682  |
| H     | -5.631703 | 0.101679  | 5.731943  |
| C     | -3.694856 | -3.899723 | 2.010857  |
| C     | -2.754502 | -2.959318 | 2.457598  |
| C     | -3.732066 | -5.150620 | 2.644431  |
| C     | -1.881262 | -3.258278 | 3.502719  |
| H     | -2.708568 | -1.985057 | 1.980935  |
| C     | -2.866866 | -5.449035 | 3.697131  |
| H     | -4.446187 | -5.894837 | 2.302444  |
| C     | -1.934939 | -4.503981 | 4.130233  |
| H     | -1.155238 | -2.515955 | 3.824464  |
| H     | -2.921652 | -6.422863 | 4.178577  |
| H     | -1.253598 | -4.737106 | 4.944899  |
| C     | 0.744080  | -5.756932 | -3.460070 |
| C     | 0.922245  | -4.393257 | -3.744902 |
| C     | -0.092452 | -6.497387 | -4.311406 |
| C     | 0.301090  | -3.797622 | -4.842816 |
| H     | 1.561909  | -3.796479 | -3.102870 |
| C     | -0.706162 | -5.909259 | -5.417352 |
| H     | -0.250671 | -7.551385 | -4.099002 |
| C     | -0.513183 | -4.552161 | -5.689262 |
| H     | 0.456110  | -2.738755 | -5.036617 |
| H     | -1.332967 | -6.514248 | -6.069941 |
| H     | -0.991753 | -4.088176 | -6.549061 |
| C     | 3.603686  | -5.930435 | -3.358533 |
| C     | 3.636227  | -6.422267 | -4.670946 |
| C     | 4.308152  | -4.750066 | -3.075008 |
| C     | 4.342788  | -5.753486 | -5.672861 |
| H     | 3.094500  | -7.334810 | -4.905960 |
| C     | 5.014601  | -4.079882 | -4.072160 |
| H     | 4.313108  | -4.370351 | -2.058076 |
| C     | 5.034373  | -4.578462 | -5.377499 |
| H     | 4.350720  | -6.152378 | -6.685713 |
| H     | 5.557026  | -3.170359 | -3.826079 |
| H     | 5.588357  | -4.056423 | -6.154803 |
C 3.155889 -9.273884 0.394103
C 2.970485 -9.440009 1.778517
C 3.906922 -10.258782 -0.277594
C 3.488218 -10.547077 2.453493
H 2.417437 -8.688811 2.332732
C 4.422006 -11.364915 0.391679
H 4.087606 -10.136651 -1.341518
C 4.212916 -11.520231 1.767092
H 3.330022 -10.639602 3.526410
H 4.994230 -12.108190 -0.160800
H 4.623179 -12.379023 2.294856
C 0.279919 -8.710392 0.533539
C -0.313945 -8.121636 1.659774
C -0.001655 -10.059254 0.266837
C -1.150383 -8.859925 2.497937
H -0.124990 -7.073713 1.873099
C -0.835755 -10.800997 1.104442
H 0.454165 -10.528464 -0.600655
C -1.414108 -10.203864 2.226035
H -1.599360 -8.377886 3.362982
H -1.033064 -11.847609 0.879649
H -2.066360 -10.779029 2.880409
C 10.200369 -5.570526 -1.992022
C 10.103875 -5.279428 -3.370217
C 11.018687 -6.666843 -1.636718
C 10.803974 -6.016929 -4.325706
H 9.446618 -4.481560 -3.693807
C 11.720205 -7.402011 -2.587495
H 11.109405 -6.918919 -0.584662
C 11.622809 -7.082010 -3.947192
H 10.694569 -5.761534 -5.378897
H 12.351720 -8.229556 -2.265845
H 12.162375 -7.661170 -4.694736
C 10.425966 -2.580659 -1.611462
C 11.720705 -2.217636 -1.202326
C 9.965729 -2.061896 -2.831243
C 12.530301 -1.395475 -1.985855
H 12.082388 -2.592141 -0.248580
C 10.765170 -1.224923 -3.615369
H 8.959892 -2.304896 -3.161494
C 12.053345 -0.891805 -3.199640
H 13.533597 -1.142352 -1.646126
| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| H    | 10.372288| -0.826416| -4.548725|
| H    | 12.676730| -0.239379| -3.808867|
| C    | 9.227771 | -6.196484| 2.519446 |
| C    | 8.919306 | -6.060072| 3.897076 |
| C    | 9.725774 | -7.467626| 2.131349 |
| C    | 9.141832 | -7.089381| 4.810217 |
| H    | 8.477836 | -5.141028| 4.258380 |
| C    | 9.949170 | -8.492913| 3.042954 |
| H    | 9.919069 | -7.638021| 1.077899 |
| C    | 9.669760 | -8.316485| 4.402938 |
| H    | 8.881278 | -6.929005| 5.856093 |
| H    | 10.341546| -9.444623| 2.685588 |
| H    | 9.833747 | -9.120832| 5.118031 |
| C    | 9.481854 | -3.214246| 3.055232 |
| C    | 10.788696| -3.237330| 3.568239 |
| C    | 8.476430 | -2.638446| 3.848194 |
| C    | 11.080011| -2.717659| 4.830986 |
| H    | 11.577458| -3.677551| 2.963967 |
| C    | 8.764233 | -2.106183| 5.105520 |
| H    | 7.462648 | -2.595330| 3.462508 |
| C    | 10.067976| -2.146975| 5.605796 |
| H    | 12.100833| -2.755857| 5.208672 |
| H    | 7.967288 | -1.648368| 5.686485 |
| H    | 10.293021| -1.734499| 6.587855 |
| C    | 7.662099 | 3.235413 | -1.293178|
| C    | 7.383748 | 3.103859 | -2.662386|
| C    | 9.007149 | 3.315623 | -0.898581|
| C    | 8.411958 | 3.055356 | -3.603690|
| H    | 6.350976 | 3.032923 | -2.989413|
| C    | 10.036290| 3.270443 | -1.837114|
| H    | 9.242674 | 3.396849 | 0.158350 |
| C    | 9.743521 | 3.139420 | -3.196329|
| H    | 8.168838 | 2.942502 | -4.657853|
| H    | 11.070376| 3.321013 | -1.504158|
| H    | 10.546540| 3.089210 | -3.928070|
| C    | 5.642532 | 5.357543 | -1.385717|
| C    | 6.701938 | 6.278598 | -1.382982|
| C    | 4.663130 | 5.477189 | -2.382896|
| C    | 6.787261 | 7.280287 | -2.349973|
| H    | 7.468825 | 6.198643 | -0.617540|
| C    | 4.747688 | 6.476258 | -3.352626|
| H    | 3.821432 | 4.792167 | -2.393341|
Structure 3b: Atom numer: 362
Total energy (Hartree): -8318.89599044

C   2.955815  5.292128   0.969356
C   1.753982  5.991900   0.850373
C   0.554406  5.336066   0.523090
C   0.622416  3.942702   0.328005
C   1.814887  3.244777   0.454642
C   3.015278  3.901231   0.778509
H   3.863928  5.838056   1.210593
H   1.748385  7.065039   1.017868
H  -0.285839  3.399170   0.087025
H   1.819635  2.169500   0.301846
C  -0.786386  5.987086   0.401737
C  -1.524300  5.825617  -0.801850
C  -1.412272  6.622977   1.501648
| Element | x   | y   | z   |
|---------|-----|-----|-----|
| C       | 8.624864 | 0.172268 | 1.613268 |
| C       | 7.531143  | -0.619370 | -0.367448 |
| C       | 9.616578  | -0.792817  | 1.446558 |
| H       | 8.679689  | 0.853780   | 2.458353 |
| C       | 8.504058  | -1.605772  | -0.515881 |
| H       | 6.724417  | -0.554132  | -1.093156 |
| C       | 9.571879  | -1.712568  | 0.385297 |
| H       | 10.437286 | -0.831922  | 2.157076 |
| C       | -3.237712 | -4.122935  | -0.471188 |
| C       | -2.193431 | -3.202246  | -0.679470 |
| C       | -2.890892 | -5.484663  | -0.446881 |
| C       | -0.878055 | -3.615414  | -0.835041 |
| H       | -2.423285 | -2.142048  | -0.718804 |
| C       | -1.567360 | -5.901243  | -0.597921 |
| H       | -3.666991 | -6.231099  | -0.303077 |
| C       | -0.525952 | -4.976621  | -0.788854 |
| H       | -0.102347 | -2.870032  | -0.983303 |
| H       | -1.339330 | -6.962489  | -0.554423 |
| C       | 0.922277  | -5.335872  | -0.896986 |
| C       | 1.598866  | -5.968194  | 0.174613 |
| C       | 1.667045  | -4.926998  | -2.036464 |
| C       | 3.006630  | -6.067167  | 0.167094 |
| C       | 3.073684  | -5.041457  | -2.049478 |
| C       | 3.754992  | -5.562025  | -0.925795 |
| C       | 5.249551  | -5.527013  | -0.853823 |
| C       | 5.881277  | -4.686096  | 0.076490 |
| C       | 6.074345  | -6.304710  | -1.682184 |
| C       | 7.268647  | -4.619660  | 0.176914 |
| H       | 5.270322  | -4.072113  | 0.732609 |
| C       | 7.462292  | -6.255177  | -1.567474 |
| H       | 5.622680  | -6.964023  | -2.418475 |
| C       | 8.091580  | -5.407818  | -0.640467 |
| H       | 7.713549  | -3.955633  | 0.909748 |
| H       | 8.068796  | -6.885983  | -2.211762 |
| C       | 10.691614 | -2.765526  | 0.217239 |
| C       | 10.833610 | -3.280365  | -1.213259 |
| C       | 10.575582 | -3.895474  | 1.244925 |
| C       | 10.280065 | -4.471848  | -1.565506 |
| C       | 10.125522 | -5.123901  | 0.893016 |
| C       | 9.631101  | -5.387829  | -0.525454 |
| C       | -3.659570 | 5.807774   | -2.104643 |
C   -4.470151   4.666862   -2.200435
C   -3.520982   6.624450   -3.235199
C   -5.102640   4.338623   -3.398918
H    -4.605598   4.036579   -1.326510
C    -4.159854   6.303182   -4.434301
H    -2.894124   7.510110   -3.175951
C    -5.715715   3.442510   -3.454164
H    -4.033971   6.947634   -5.301456
H    -5.435092   4.894439   -5.459428
C    -0.811566   5.386654   -2.047937
C    0.120613   6.248970   -2.645211
C    -1.061651   4.153073   -2.669549
C    0.761071   5.904479   -3.835517
H     0.332003   7.204477   -2.172742
C    -0.412503   3.799369   -3.852071
H    -0.624486   2.837840   -4.31246
H     0.995138   4.404667   -5.373755
C    -3.448202   7.651309   2.591862
C    -3.477769   7.136061   3.897238
C    -4.056819   8.896899   2.362778
C    -4.085571   7.841800   4.935897
H    -3.024651   6.170351   4.098322
C    -4.660691   9.606040   3.399081
C    -4.058136   9.303874   1.355557
C    -4.677650   9.081417   4.693802
H    -4.100676   7.415687   5.936386
H    -5.125648   10.567547   3.193500
H    -5.156141   9.629150   5.502193
C    -0.603608   6.983130   2.713705
C    -0.118146   6.006185   3.594974
C    -0.311633   8.328337   2.985849
C    0.625030   6.365560   4.719544
H    -0.318152   4.957928   3.393496
C    0.434551   8.689228   4.108273
H    -0.685659   9.095673   2.313779
C    0.904717   7.707933   4.982080
H    0.987240   5.591130   5.390787
H    0.645458   9.738868   4.300351
| Atom | X    | Y    | Z    |
|------|------|------|------|
| H    | 1.484855 | 7.986055 | 5.858974 |
| C    | -9.707391 | 5.660198 | -2.227708 |
| C    | -8.683840 | 5.692223 | -3.186872 |
| C    | -10.759416 | 6.579219 | -2.358140 |
| C    | -8.709223 | 6.607396 | -4.239639 |
| H    | -7.843643 | 5.012616 | -3.084806 |
| C    | -10.796626 | 7.488970 | -3.416966 |
| H    | -11.557624 | 6.569752 | -1.620534 |
| C    | -9.769314 | 7.508066 | -4.362332 |
| H    | -7.891412 | 6.619687 | -4.956373 |
| H    | -11.628650 | 8.185278 | -3.500967 |
| H    | -9.792545 | 8.220736 | -5.184029 |
| C    | -11.102548 | 3.002950 | -2.345472 |
| C    | -10.673616 | 3.088704 | -3.685356 |
| C    | -12.376204 | 2.436512 | -2.123565 |
| C    | -11.480514 | 2.658990 | -4.739088 |
| H    | -9.689040 | 3.482333 | -3.906471 |
| C    | -13.183981 | 2.007657 | -3.173368 |
| H    | -12.723036 | 2.336602 | -1.099512 |
| C    | -12.743619 | 2.119021 | -4.495239 |
| H    | -11.109310 | 2.738189 | -5.759097 |
| H    | -14.163295 | 1.584274 | -2.957797 |
| H    | -13.369247 | 1.780429 | -5.318294 |
| C    | -11.058807 | 2.624464 | 2.426877 |
| C    | -12.463265 | 2.619133 | 2.387318 |
| C    | -10.434761 | 2.039475 | 3.541004 |
| C    | -13.216910 | 2.076875 | 3.428713 |
| H    | -12.961985 | 3.059890 | 1.528212 |
| C    | -11.184617 | 1.486408 | 4.580514 |
| H    | -6.284891 | 2.456712 | 2.287952 |
| C    | -12.579314 | 1.507753 | 4.533653 |
| H    | -14.303648 | 2.098589 | 3.376567 |
| H    | -10.673667 | 1.030930 | 5.426085 |
| H    | -13.163383 | 1.079009 | 5.345215 |
| C    | -9.897314 | 5.381815 | 2.571447 |
| C    | -9.434191 | 5.066110 | 3.860457 |
| C    | -10.540402 | 6.624667 | 2.408598 |
| C    | -9.626654 | 5.934236 | 4.936672 |
| H    | -8.899349 | 4.137385 | 4.020414 |
| C    | -10.737335 | 7.493464 | 3.479636 |
| H    | -10.886777 | 6.899510 | 1.416413 |
| C    | -10.283156 | 7.151096 | 4.756369 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| H | -9.248668 | 5.658860  | 5.919151  |
| H | -11.246542| 8.441469  | 3.316841  |
| H | -10.429022| 7.828755  | 5.594850  |
| C | -7.979852 | -3.463272 | -2.138464 |
| C | -7.807896 | -3.305395 | -3.522343 |
| C | -9.227095 | -3.914875 | -1.676457 |
| C | -8.841401 | -3.596726 | -4.413429 |
| H | -6.855538 | -2.948019 | -3.901797 |
| C | -10.259286| -4.211569 | -2.564399 |
| H | -9.384216 | -4.024948 | -0.607410 |
| C | -10.071059| -4.053973 | -3.939883 |
| H | -8.684019 | -3.460012 | -5.480857 |
| H | -11.215737| -4.559046 | -2.180565 |
| H | -10.878210| -4.277337 | -4.633602 |
| C | -5.453526 | -4.931575 | -2.265409 |
| C | -6.191355 | -6.124331 | -2.215825 |
| C | -4.529931 | -4.765810 | -3.308109 |
| C | -6.019299 | -7.116815 | -3.181208 |
| H | -6.912961 | -6.265716 | -1.416155 |
| C | -4.359516 | -5.754836 | -4.276637 |
| H | -3.936264 | -3.857869 | -3.355861 |
| C | -5.103157 | -6.935049 | -4.218149 |
| H | -6.604435 | -8.031877 | -3.122856 |
| H | -3.639551 | -5.599867 | -5.075963 |
| H | -4.968448 | -7.706418 | -4.973001 |
| C | -6.280993 | -0.931181 | 1.888100  |
| C | -6.458978 | -1.296079 | 3.229635  |
| C | -6.226575 | 0.433796  | 1.569804  |
| C | -6.566732 | -0.325555 | 4.226939  |
| H | -6.502352 | -2.349491 | 3.492683  |
| C | -6.331232 | 1.406397  | 2.562712  |
| H | -6.116309 | 0.733907  | 0.532187  |
| C | -6.496861 | 1.029096  | 3.898374  |
| H | -6.699072 | -0.630399 | 5.262759  |
| H | -9.351435 | 1.975023  | 3.565834  |
| H | -6.569434 | 1.786568  | 4.675425  |
| C | -3.857630 | -2.465779 | 1.838443  |
| C | -3.152763 | -1.258828 | 1.964232  |
| C | -3.618588 | -3.473186 | 2.784551  |
| C | -2.246841 | -1.059186 | 3.005747  |
| H | -3.329989 | -0.463163 | 1.247090  |
| C | -2.725465 | -3.271057 | 3.837321  |
|   | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---|--------------|--------------|--------------|
| H | -4.151996    | -4.416126    | 2.698901     |
| C | -2.033997    | -2.062992    | 3.952337     |
| H | -1.713790    | -0.114780    | 3.081687     |
| H | -2.582997    | -4.053207    | 4.579327     |
| H | -1.342401    | -1.903433    | 4.776365     |
| C | 0.949667     | -4.402572    | -3.243656    |
| C | 1.131889     | -3.087896    | -3.700692    |
| C | 0.082504     | -5.239409    | -3.962975    |
| C | 0.474347     | -2.626873    | -4.841114    |
| H | 1.796225     | -2.422690    | -3.157291    |
| C | -0.567484    | -4.784081    | -5.109462    |
| H | 0.080492     | -6.256153    | -3.616674    |
| C | -0.375470    | -3.473700    | -5.553884    |
| H | 0.627328     | -1.602532    | -5.171665    |
| H | -1.223085    | -5.456405    | -5.657553    |
| H | -0.886056    | -3.115729    | -6.444421    |
| C | 3.855613     | -4.602841    | -3.253142    |
| C | 3.783476     | -5.327326    | -4.451698    |
| C | 4.677509     | -3.467224    | -3.210029    |
| C | 4.508164     | -4.927614    | -5.575149    |
| H | 3.146941     | -6.206273    | -4.502378    |
| C | 5.401509     | -3.064580    | -4.332225    |
| H | 4.753216     | -2.900217    | -2.286724    |
| C | 5.319124     | -3.793591    | -5.520100    |
| H | 4.436672     | -5.503757    | -6.494687    |
| H | 6.030571     | -2.179543    | -4.277157    |
| H | 5.884011     | -3.480516    | -6.394725    |
| C | 3.722135     | -6.702718    | 1.321341     |
| C | 3.692973     | -6.126309    | 2.601562     |
| C | 4.439396     | -7.896382    | 1.149640     |
| C | 4.350854     | -6.727836    | 3.674896     |
| H | 3.144331     | -5.201962    | 2.755467     |
| C | 5.094018     | -8.502455    | 2.222064     |
| H | 4.479991     | -8.352360    | 0.164494     |
| C | 5.052484     | -7.920137    | 3.491426     |
| H | 4.311767     | -6.263102    | 4.657098     |
| H | 5.633630     | -9.433837    | 2.065701     |
| H | 5.564384     | -8.389687    | 4.327703     |
| C | 0.829925     | -6.556107    | 1.321163     |
| C | 0.166823     | -5.754058    | 2.259825     |
| C | 0.771613     | -7.949948    | 1.473723     |
| C | -0.520249    | -6.330507    | 3.328198     |
H  0.178320  -4.673906  2.148777
C  0.079010   -8.527798  2.538060
H  1.280560   -8.582798  0.751848
C  -0.567136  -7.718041  3.472671
H  -1.024708  -5.688034  4.043226
H  0.047211   -9.610472  2.636462
H  -1.106430  -8.163871  4.305114
C  10.246063  -4.977359  -2.966995
C  9.723471  -4.189620  -4.009208
C  10.708126  -6.267435  -3.294933
C  9.667239  -4.665530  -5.316823
H  9.353029  -3.195237  -3.780844
C  10.659964  -6.742441  -4.605223
H  11.130045  -6.899977  -2.517741
C  10.136596  -6.742441  -4.605223
H  11.033637  -7.739349  -4.828812
H  10.090065  -6.317694  -6.645662
C  11.677655  -2.449125  -2.113764
C  12.680602  -3.042810  -2.910885
C  11.583935  -1.040765  -2.139814
C  13.529566  -2.275572  -3.702512
H  12.796337  -4.121503  -2.894610
H  12.432848  -0.274317  -2.937521
H  10.826280  -0.539393  -1.548002
C  13.411127  -0.881872  -3.726639
H  14.293753  -2.768821  -4.299606
H  12.316316  0.806970  -2.943802
H  14.071949  -0.282162  -4.348024
C  10.175293  -6.315121  1.789085
C  9.072134  -7.175907  1.956355
C  11.378867  -6.665377  2.433847
C  9.169886  -8.323519  2.743484
H  8.125547  -6.937648  1.484388
C  11.475009  -7.812834  3.216577
H  12.247615  -6.026805  2.307768
C  10.368347  -8.651775  3.379108
H  8.294514  -8.957314  2.863514
H  12.420112  -8.055628  3.697616
H  10.441068  -9.547306  3.991733
C  10.985501  -3.550344  2.637047
C  12.250584  -2.995166  2.908238
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| C       | 10.108494 | -3.741567 | 3.719191 |
| C       | 12.626768  | -2.656505  | 4.207937  |
| H       | 12.954314  | -2.842201  | 2.093590  |
| C       | 10.479972  | -3.396266  | 5.017041  |
| H       | 9.122858   | -4.155147  | 3.531020  |
| C       | 11.742140  | -2.852954  | 5.270262  |
| H       | 13.614158  | -2.237953  | 4.389932  |
| H       | 9.775745   | -3.542873  | 5.832180  |
| H       | 12.030517  | -2.581076  | 6.282684  |
| C       | 7.543833   | 2.598758   | -1.049271 |
| C       | 7.320939   | 2.462347   | -2.428099 |
| C       | 8.840944   | 2.912839   | -0.616036 |
| C       | 8.358454   | 2.639371   | -3.343302 |
| H       | 6.323917   | 2.219185   | -2.783198 |
| C       | 9.879535   | 3.095395   | -1.528955 |
| H       | 9.033150   | 3.014950   | 0.448140  |
| C       | 9.642214   | 2.959260   | -2.898638 |
| H       | 8.162032   | 2.526746   | -4.406709 |
| H       | 10.874966  | 3.344732   | -1.168892 |
| H       | 10.449804  | 3.101335   | -3.612639 |
| C       | 5.325364   | 4.473113   | -0.969337 |
| C       | 6.261760   | 5.050727   | -0.818568 |
| C       | 4.399080   | 4.560621   | -2.017952 |
| C       | 6.278885   | 6.592909   | -1.694479 |
| H       | 6.985347   | 5.453420   | -0.009949 |
| C       | 4.417956   | 5.642520   | -2.897891 |
| H       | 3.651393   | 3.782693   | -2.139251 |
| C       | 5.358248   | 6.662524   | -2.740719 |
| H       | 7.013435   | 7.383376   | -1.558459 |
| H       | 3.686400   | 5.687315   | -3.699009 |
| H       | 5.369645   | 7.507233   | -3.425536 |
| C       | 5.579516   | 0.067866   | 2.830176  |
| C       | 5.830059   | 0.387448   | 4.172733  |
| C       | 5.450568   | -1.284479  | 2.481081  |
| C       | 5.947027   | -0.613240  | 5.137885  |
| H       | 5.926535   | 1.430872   | 4.459605  |
| C       | 5.564408   | -2.287622  | 3.444221  |
| H       | 5.263716   | -1.551339  | 1.445099  |
| C       | 5.813899   | -1.954501  | 4.777112  |
| H       | 6.140855   | -0.342509  | 6.173130  |
| H       | 5.456489   | -3.330150  | 3.154646  |
| H       | 5.902771   | -2.735708  | 5.528064  |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 3.278008| 1.843856| 2.837248|
| C    | 3.050886| 2.806393| 3.832074|
| C    | 2.478685| 0.690394| 2.834153|
| C    | 2.066973| 2.613848| 4.801771|
| H    | 3.650448| 3.712316| 3.842122|
| C    | 1.485807| 0.501003| 3.795491|
| H    | 2.637321| -0.064722| 2.069936|
| C    | 1.278450| 1.460992| 4.787099|
| H    | 1.918262| 3.365381| 5.573284|
| H    | 0.874825| -0.397646| 3.765430|
| H    | 0.507674| 1.314445| 5.539516|
| H    | 9.946876| -6.409503| -0.774127|
| H    | 11.622196| -2.231474| 0.449349|
6. NMR Spectra

Figure S17: $^1$H- (300 MHz) and $^{13}$C-NMR (75 MHz) spectra of 5 recorded at 298 K in THF-$d_8$. 

C$_{48}$H$_{52}$Br$_2$
MW: 764.71 g/mol
Figure S18: $^1$H-(300 MHz) and $^{13}$C-NMR (75 MHz) spectra of 13 recorded at 298 K in CD$_2$Cl$_2$. 

$\text{C}_{42}\text{H}_{30}\text{Br}_2\text{O}_2$

m.w.: 726.49 g/mol
Figure S19: $^1$H-(500 MHz) and $^{13}$C-NMR (126 MHz) spectra of 4 recorded at 373 K in C$_2$D$_2$Cl$_2$. 

$^1$H-$^1$H C$_{44}$H$_{36}$Br$_2$O$_2$

m.w.: 754.55 g/mol
Figure S20: $^1$H-(500 MHz) and $^{13}$C-NMR (126 MHz) spectra of 4 recorded at 373 K in C$_2$D$_2$Cl$_2$. 

C$_{98}$H$_{38}$B$_2$O$_6$

m.w. 848.68 g/mol
Figure S21: $^1$H-(500 MHz) and $^{13}$C-NMR (126 MHz) spectra of 6 recorded at 373 K in C$_2$D$_2$Cl$_2$. 

m.w.: 2048.32 g/mol
Figure S22: APT-\textsuperscript{13}C-NMR (126 MHz) spectra of 6 recorded at 366 K in C\textsubscript{2}D\textsubscript{4}Cl\textsubscript{2}.
Figure S23: $^1$H-(500 MHz) and $^{13}$C-NMR (126 MHz) spectra of 7 recorded at 373 K in C$_2$D$_2$Cl$_2$. 

C$_{138}$H$_{139}$Br$_2$O$_2$

m.w.: 1964.36 g/mol
Figure S24: $^1$H-(700MHz) and APT$^{13}$C-NMR (176 MHz) spectra of 8 recorded at 333 K in C$_2$D$_2$Cl$_2$. 
Figure S25: $^1$H-NMR spectrum of compound 2 recorded at r.t. in C$_2$D$_2$Cl$_4$. Despite prolonged drying at elevated temperatures, MeCN is still present within the cavities of the crystals. Also aliphatic peaks detected at 0.8 ppm and 1.2 ppm that could not be removed.

For $^{13}$C-NMR of compound 2: see p. 17 and p.18 (HSQC and HMBC).

Figure S26: $^1$H-NMR spectrum of compound 3 recorded at 500 MHz at r.t. and 100 °C. Due to the high unsymmetry of the molecule, only a fingerprint spectrum can be resolved. For structural analysis, see crystal structure on p. S14.
7. MALDI-MS spectra

7.1 Spectrum of 2 after oxidative cyclodehydrogenation

Oxidative cyclodehydrogenation of 2 for 1 d yielded a product mixture. Thus, the crude product was separated by preparative TLC to investigate the product distribution, in detail.

Figure S26: oxidative cyclodehydrogenation of 2. Upper left (Fr. 1) first fraction; bottom: starting material 2.

In Figure S26, the mass spectrum of compound 2 after dehydrogenation is shown. The separation afforded various products ranging from 3389 m/z, as the most unpolar product, to 3408 m/z, as the most polar product. The lightest fraction was subjected to FeCl₃ again. No further decrease in mass could be observed. Room temperature and high temperature approaches for cyclodehydrogenation with other oxidizing agents, such as DDQ, Sc(OTf)₃ and/or TfOH, led to
decomposition of the starting material and gave product mixtures that did not yield masses in the expected product range.

7.2 $C_2$-symmetric Congener

The $C_2$-symmetric compound 3 was oxidatively cyclodehydrogenated with FeCl$_3$. As can be seen from the crystal structure, the two pentaphenylenes that are bridged by two cyclohexa-2,5-dienes are only slightly bent. Thus, compound 3 is expected to undergo oxidative cyclodehydrogenation. In addition, cyclohexadienes are known to form phenylenes in the presence of oxidizing agents.$^{[4]}

Scheme S3: Oxidative cyclodehydrogenation of 108 with FeCl$_3$

The $C_2$-symmetric compound 3 was subjected to FeCl$_3$. The reaction progress was monitored by mass spectrometry. Spectra were recorded after 1 d and 3 d. In Figure S27, the mass spectrum of 3 after cyclodehydrogenation for 1 d is shown. Four peaks are observed at 3370 m/z, 3355 m/z, 3317 m/z and 3299 m/z. The mass of the starting material is 3415 m/z.

Figure S27: HR-MS (MALDI) spectrum of compound 3 after cyclohydrogenation (1 d). Red isotopic pattern for a cyclodehydrogenated compound with a sum formula of $C_{264}H_{182}$ and its two hydrogen atoms heavier congener: $C_{264}H_{184}$. Reaction conditions: FeCl$_3$ rt, 24 h, filtration through a short bed of silica with DCM/THF and subsequent separation by preparative GPC column.
To understand the observed masses, first, a closer look is taken at the intermediate mass of 3355 m/z. The lower masses will be discussed in the following spectra (vide infra).

Figure S28: section of the mass spectrum of compound 3 after cyclodehydrogenation for 1 d with FeCl₃ at r.t.

In Figure S28, a small section of the mass spectrum between 3350 m/z and 3360 m/z is shown. The sum formulas for two intermediates (red, left, 13; green, right, 11) are shown. These structures can be proposed based on the structure of the starting material, as the crystal structure hinted at a slightly bent pentaphenylene that should smoothly undergo cyclodehydrogenation to give a short nanoribbon segment. The sum formula of 11 the theoretical mass (green) deviates by 0.01 g/mol; such an error range has been observed for molecules with similar molecular weight, of which the structure had been confirmed by X-ray crystallography before MS measurements. Therefore, the experimental findings may very well be in agreement with the outlined sum formula. One can conclude that the above given sum formula matches with the experimental findings.
After 3 d, the spectrum shows an increase in intensity for the signals at 3318 m/z and 3396 m/z, whereas the peaks around 3353 m/z, assigned to the cyclodehydrogenated dicyclopentadiene-bridged bisribbon 11, decreased in intensity and were additionally shifted by 2 m/z to lower masses; the peaks at 3370 m/z disappeared. In the range from 3340 m/z to 3260 m/z five different peaks can be observed. The mass difference between each of them equals 22 m/z. These findings are a first indicator that a side reaction has occurred, namely a chloro-de-t-butylation, as the mass difference between a chlorine atom and a t-butyl group equals 22.1 m/z. With this having said, the peaks around 3318 m/z were more closely investigated (see Figure S30), as this mass could have also hinted at a bottom-up synthesis of an ultrashort CNT.
In Figure S30, sections of two mass spectra of 3 after cyclodehydrogenation for 3 d at r.t. are shown. In the left spectrum, the hypothetical structure of an almost fully fused CNT is depicted. The calculated mass spectrum of this structure is shown in green. The difference between the observed and calculated mass is 1 m/z; the deviation is thus beyond the error limit. From these and the above described findings, one can conclude that during oxidative cyclodehyrogeation CNT 14 has not been formed. The mass spectrum for the simulated structure of 15 hints strongly at the formation of a bis(de-tbutylated) and concomittantly dichlorinated compound, as the mass and the corresponding isotopic pattern are in good agreement. One has to state, however, that only the sum formula can be concluded and a structural hypothesis, as shown here, is entirely based on chemical intuition.
7.3 Spectrum of triangular cycle 8

Figure S31: MALDI-TOF-MS measurement of compound 8 (with internal calibration standard).
### FT05107a Florian Golling/Müllen - FEG-424 - DCTB

**Evaluation Spectra / Validation Formula:**

| # | Formula | m/z | Meas. m/z | z | mSigma | N-Rule | err [mDa] | err [ppm] |
|---|---------|-----|-----------|---|--------|--------|-----------|-----------|
| 1 | C270H259O6 | 3565.5976 | 3567.2097 | t | 12.0 | ok | -9.9 | -2.5 |
| 1 | C270H258NaO6 | 3565.5976 | 3567.2007 | t | 12.0 | ok | -9.9 | -2.5 |
| 1 | C270H258K2O6 | 3634.9215 | 3634.9215 | t | 12.0 | ok | -9.9 | -2.5 |

**Calibration Info:**

- **Date:** 16.06.2014 11:23:42
- **Polarity:** Positive
- **Calibration Spectrum:** M+; Scan
- **Reference Mass List:** ESi: Na-PFPFA
- **Calibration Mode:** Quadratic

| Reference m/z | Resulting m/z | Intensity | Error [ppm] |
|---------------|---------------|-----------|-------------|
| 2338.7423 | 2338.7423 | 103380094 | 0.002 |
| 2724.7011 | 2724.7011 | 60366012 | 0.151 |
| 3110.5659 | 3110.5659 | 64524000 | -0.336 |
| 3496.6188 | 3496.6199 | 54264923 | 0.316 |
| 3562.5776 | 3562.5776 | 44366645 | -0.107 |

**Standard Deviation:** 0.374

**Mass List:**

| # | m/z | Res. | S/N | I % | FWHM |
|---|-----|-----|-----|-----|------|
| 1 | 1566.8201 | 114515 | 1012.7 | 82.0 | 0.0137 |
| 2 | 1567.0235 | 116772 | 303.4 | 24.7 | 0.0132 |
| 3 | 1599.0470 | 92548 | 183.5 | 17.1 | 0.0203 |
| 4 | 1597.2667 | 98387 | 94.0 | 88.2 | 0.0217 |
| 5 | 1595.8715 | 94549 | 201.0 | 33.0 | 0.0207 |
| 6 | 2333.7235 | 60704 | 215.6 | 23.5 | 0.0269 |
| 7 | 2338.7422 | 71879 | 93.4 | 100.0 | 0.0326 |
| 8 | 2338.7443 | 77534 | 403.6 | 43.3 | 0.0302 |
| 9 | 2716.6223 | 68395 | 175.2 | 21.3 | 0.0395 |
| 10 | 2724.7015 | 62927 | 654.0 | 83.3 | 0.0433 |
| 11 | 2725.7001 | 63561 | 336.4 | 40.5 | 0.0426 |
| 12 | 2735.4004 | 54390 | 106.0 | 15.4 | 0.0271 |
| 13 | 3110.5659 | 48258 | 438.1 | 62.6 | 0.0645 |
| 14 | 3111.6600 | 48601 | 241.4 | 34.6 | 0.0648 |
| 15 | 3496.6043 | 53398 | 90.3 | 15.2 | 0.0651 |
| 16 | 3496.6199 | 51767 | 316.5 | 52.5 | 0.0675 |
| 17 | 3497.6234 | 52792 | 215.6 | 36.0 | 0.0662 |
| 18 | 3564.9714 | 47911 | 128.8 | 18.8 | 0.0744 |
| 19 | 3564.9776 | 49303 | 330.1 | 51.0 | 0.0722 |
| 20 | 3564.9814 | 48417 | 526.2 | 76.0 | 0.0737 |
| 21 | 3566.8846 | 46614 | 617.9 | 74.8 | 0.0718 |
| 22 | 3566.8966 | 48827 | 359.2 | 53.4 | 0.0731 |
| 23 | 3566.9504 | 49286 | 219.0 | 31.8 | 0.0724 |
| 24 | 3576.9258 | 55448 | 105.0 | 15.4 | 0.0708 |
| 25 | 3596.9977 | 45233 | 238.6 | 41.8 | 0.0795 |
| 26 | 3598.0000 | 49636 | 420.0 | 62.7 | 0.0705 |
| 27 | 3599.0071 | 46210 | 408.4 | 59.0 | 0.0797 |
| 28 | 3599.0010 | 47500 | 311.0 | 45.0 | 0.0756 |
| 29 | 3600.0075 | 47665 | 182.4 | 26.5 | 0.0755 |
| 30 | 3615.9990 | 48540 | 271.7 | 39.4 | 0.0755 |
| 31 | 3530.9292 | 46937 | 407.9 | 69.0 | 0.0771 |
| 32 | 3621.9964 | 47516 | 398.7 | 57.6 | 0.0762 |
| 33 | 3622.0011 | 47000 | 291.3 | 42.2 | 0.0770 |
| 34 | 3624.0022 | 47185 | 171.2 | 24.9 | 0.0766 |
| 35 | 3633.6623 | 46343 | 107.6 | 15.8 | 0.0736 |
| 36 | 3636.9659 | 46571 | 157.9 | 23.0 | 0.0781 |
| 37 | 3637.9678 | 47332 | 159.9 | 23.3 | 0.0769 |
| 38 | 3638.9724 | 49079 | 134.3 | 18.0 | 0.0741 |
| 39 | 3582.5772 | 47300 | 296.7 | 43.0 | 0.0821 |
| 40 | 3595.0000 | 47923 | 210.0 | 31.7 | 0.0901 |

**Figure S32:** mass list of compound 8
Figure S33: MALDI-TOF-MS measurement of compound 2 (with internal calibration standard).
**Figure S34**: mass list of compound 2
7.5 Mass spectrum of 3

Figure S35: MALDI-TOF-MS measurement of compound 3
Figure S36: MALDI-TOF-MS measurement of compound 3 (with internal calibration standard).
Figure S37: mass list of compound 3.
8. Optical and Electronic Properties

8.1 UV-Vis spectra and Emission Spectrum

In this section, UV-Vis spectra and emission spectra are shown. For compound 2 and 3, the absorption spectra are depicted. An emission spectrum can only be shown for 2; for its $C_2$-symmetric congener 3, no emission was observed.

![Graph showing absorption spectra of compounds 2 and 3.](image)

**Figure S37**: absorption spectra of the congested cyclohexamer (2, black) and its $C_2$-symmetric congener 3 (red) are shown. The emission spectrum of 2 is depicted; no emission was observed for 3.

The absorption maxima at 258 nm and 263 nm for 2 and 3, respectively, are in the same range as the values reported for polyphenylene cylinders, consisting of a [9]CPP or a [15]CPP ring (see *Angew. Chem. Int. Ed.* 2014, 53, 1525-1528). The ring size and, correspondingly, the ring strain merely influence the absorption maxima. These results are in line with size-dependent measurements, which show very small differences for the absorption maxima.\(^5\) For “naked” CPP rings, however, the absorption maxima are bathochromically shifted (ca. 350 nm), due to higher degrees of conjugation.

The emission maximum of 2 is observed at 426 nm. This value is hypsochromically shifted in comparison to the [9]CPP based polyphenylene cylinder reported in *Angew. Chem. Int. Ed.* 2014,
53, 1525-1528; in comparison to its higher homologue - the [15]CPP based polyphenylene cylinder - its value is bathchromically shifted ([12]CPP has its emission maximum at 450 nm). This observation is in line with the general trend observed for CPPs and the explanation, that upon excitation the large ring strain and the distortion of these CPP scaffolds is released by partial planarization of neighboring phenyl rings, which results in large Stokes shifts.

8.2 HOMO-LUMO energies

CV measurements of both compounds were not successful, since the materials degraded during CV measurement. Due to the apparent molecular properties, we could not even record an irreversible oxidation/reduction potential. This holds also true for the previously reported compounds in Angew. Chem. Int. Ed. 2014, 53, 1525–1528 and Angew. Chem. Int. Ed. 2015, DOI: 10/1002/anie.201500392.

|    | 2   | 3   |
|----|-----|-----|
| HOMO | -5.58 | -5.50 eV |
| LUMO | -0.94 | -1.01 eV |

Figure S38: HOMO/LUMO energies of compound 2 and 3 obtained by DFT calculations calculated at the B3LYP/6-31G(d) level of theory.

In Figure S38, the HOMO/LUMO energies of compound 2 and 3 are depicted. The values of the HOMO energies have similar values as for [12]CPP (-5.26 eV). However, the LUMO energies differ by 0.6 eV, with a higher lying LUMO of 2 and 3. This may be attributed to the increased ring strain, arising from twisted neighboring phenylene units (due to the high sterical demand exerted by phenyl substituents).

The calculated energy gaps between the HOMO and LUMO level energies of [n]CPPs are in the range of 2.5 eV (n = 4) to 3.7 eV (n = 20). For [12]CPP, the energy gap is 3.6 eV and thus significantly smaller than for 2 and 3 (4.6 eV and 4.5 eV, respectively). This can be rationalized by the computed structure of 2 and the X-ray crystal analysis of 3. Both show that neighboring phenylene units align in an almost perpendicular manner. Hence, the degree of conjugation within these macrocycles is reduced in contrast to its parent compound [12]CPP. In addition, the high sterical demand of the neighboring groups may also explain, why the emission maximum of 2 is hypsochromically shifted in comparison to [12]CPP.
9. Literature

[1] a) K. Harada, H. Hart, C. J. Frank Du, J. Org. Chem. 1985, 50, 5524-5528; b) H. Hart, G. C. Nwokogu, Tetrahedron Lett. 1983, 24, 5721-5724; c) S. Shah, T. Concolino, A. L. Rheingold, J. D. Protasiewicz, Inorg. Chem. 2000, 39, 3860-3867.

[2] I. Ullah, R. A. Khera, M. Hussain, A. Villinger, P. Langer, Tetrahedron Lett. 2009, 50, 4651-4653.

[3] T. Ishiyama, M. Murata, N. Miyaura, J. Org. Chem. 1995, 60, 7508-7510.

[4] C. Huang, Y. Huang, N. G. Akhmedov, B. V. Popp, J. L. Petersen, K. K. Wang, Org. Lett. 2014, 16, 2672-2675.

[5] E. R. Darzi, R. Jasti, Chem. Soc. Rev. 2015.

[6] T. Iwamoto, Y. Watanabe, Y. Sakamoto, T. Suzuki, S. Yamago, J. Am. Chem. Soc. 2011, 133, 8354-8361.