Supporting Information

Dynamic chiral cyclohexanohemicucurbit[12]uril

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1. General Information

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. Solvents used for flash chromatography were reagent grade, which were dried and distilled prior to use according to standard procedures. Acetonitrile of HPLC grade was used for reverse phase flash chromatography. CycHC[8][1] was synthesized from (*R,R,N,N'*)-cyclohexa-1,2-diylurea[2,3]. Synthesized products were purified using flash chromatography. Normal phase flash chromatography was run over Kieselgel 60 extra fine silica gel (0.04-0.063 mm) stationary phase whereas reversed phase flash chromatography was run using Biotage® SNAP KP-C18-HS 60g column. Identification of products were performed by RP-HPLC-HRMS on an Agilent 6540 UHD Accurate-Mass Q-TOF LC/MS spectrometer. ^{1}H, ^{13}C and 2D NMR spectra were acquired on a Bruker Avance III 800 MHz spectrometer with a Cryoprobe (D/H/C/N/P), signals referenced to solvent residual peak (*d*-Tol ^{1}H-NMR 2.09 ppm, ^{13}C-NMR 20.40 ppm). Optical rotation was measured with Anton Paar MCP 500 polarimeter by calibrating optical rotation value via calibration graph build from four parallel measurements at four different wavelengths (589, 578, 546 and 435 nm).

2. Experimental Procedure

2.1 Synthesis of cycHC[12] and its characterization data

General comments

Anionic template is in general driving size-selective formation of cycHCs[1] and formation of larger cycHC and oligomers (up to 18 units), though without successful isolation, was previously proved in fluorinated acid[4]. Using **cycHC[8]** as starting material variety of templates and reaction conditions were screened for the synthesis of large homologues. Dissociated anions from various acids were considered as templates, such as from heptafluorobutyric acid, pentafluorobutyric acid, trichloroacetic acid, tribromoacetic acid, dichloroacetic acid, chlorodifluoroacetic acid, 3,5-bis(trifluoromethyl)benzoic acid also inorganic acids like periodic acid, (4-fluorophenyl)boronic acid and some inorganic salts, like sodium hexafluoroantimonate and tetrabutylammonium trifluoromethanesulfonate. The results were more or less similar when (*R,R,N,N'*)-cyclohexa-1,2-diylurea was used in presence of fluorinated acids. None of the conditions tested could provide large macrocycles as the major product.

*Procedure of isolation of **cycHC[12]***

To the **(*R,R*)-cycHC[8]** (1.69 g, 1.39 mmol), acetic acid (15 ml, 264 mmol) and heptafluorobutyric acid (27 ml, 208 mmol) was added and the homogenous reaction mixture was stirred at room temperature for two hours. The RP-HPLC-UV chromatogram suggested that the crude product mainly contained mixture of 6-, 8-, 10-, 11- and 12-membered cycHCs (See Figure S1). To the resulting solution 300 ml of DCM was added and the reaction mixture was cooled on the ice-bath. Under stirring conditions, the reaction mixture was quenched by the addition of solid K_2CO_3 (944 mmol) over a period of 30 minutes. The mixture was further stirred for next two hours at room temperature and then filtered. As all the macrocycles were expected to dissolve in DCM, the solid residue on the filter was further washed with DCM (3 x 300 ml). The collected filtrate was evaporated and 1.5 g (89% from starting mass of **cycHC[8]**) of solid product was obtained. MS analysis from the obtained solid confirmed presence of **cycHC[12]** in addition to other macrocycles (see Table S1) and oligomers. The product was purified on reverse phase column, eluting it with step gradient from 50/50 to 100/0 CH_3CN/H_2O. Purification of product gave mainly mixture of oligomers, however along with other macrocycles 17 mg (1%) of **cycHC[12]** was isolated (see Figure S2). Structure of **cycHC[12]** was confirmed by HRMS. The presence of some amount of oligomers were noticed by NMR analysis, though their content is hard to estimate by HPLC-UV due to their low absorption.[4] To reach analytically pure sample normal phase column chromatography (1-3% DCM/MeOH) was performed affording **cycHC[12]** of higher purity by HPLC-UV (see Figure S3) and NMR.

(R,R)-cycHC[12] characterisation data

HRMS (ESI+): $[M+Na]^+$ Calc. 1848.1242 Da; Exp. 1848.1282 Da (See also section 2.3).

NMR identification details are outlined in *3. Structure elucidation of cycHC[12] by NMR* section and characterisation of ^1H and ^{13}C-NMR signals is given on page S8.

$[\alpha]_D^{25}$= -92.57° (c 0.02, $CHCl_3$).

2.2 Chromatographic analysis

The monitoring of the reaction as well as isolated products after column chromatography were done on an Agilent Technologies HPLC 1200 Series system with multiple wavelength detector, separating compounds on Kinetex C18 column (2.1x100 mm, 2.6 µm). Eluent A (CH_3CN) and B (H_2O) were used in a gradient mode for 10-minutes from 50A/50B to 100A/0B followed by additional isocratic elution of 100A/0B for 10-minutes (Figure S1) and 10 minutes gradient from 60A/40B to 100A/0B followed by 10-minutes elution with 100A/0B (Figure S2 and S3). The column temperature was set at 30 °C, the flow rate was 0.25 ml min^{-1}, injection volume 5 µl and the UV detection at 210 nm. Chromatographic data received from RP-HPLC was processed using Microsoft excel to give chromatogram with better resolution.

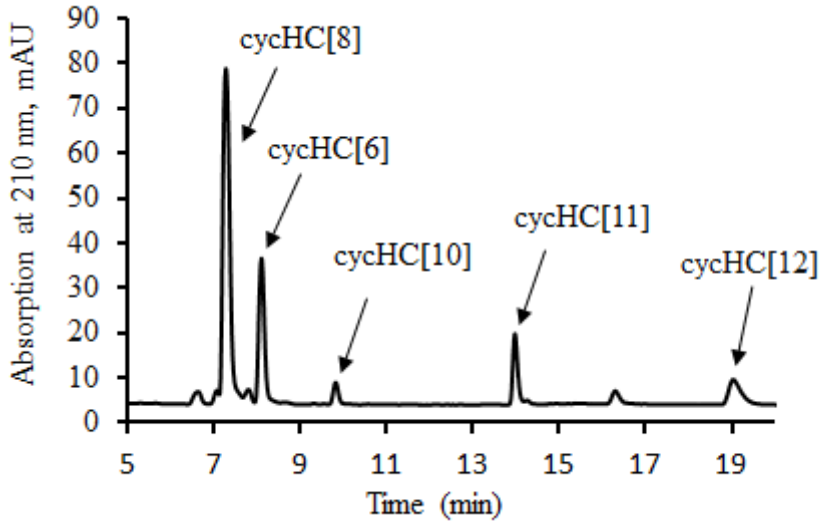


*Figure S1: HPLC-UV chromatogram of crude reaction mixture (Please note that extinction coefficient of oligomers is nearly 10 times lower than **cycHC[6]** and **cycHC[8]**,[4] thus the amount of oligomers in the reaction mixture cannot be accurately estimated).*

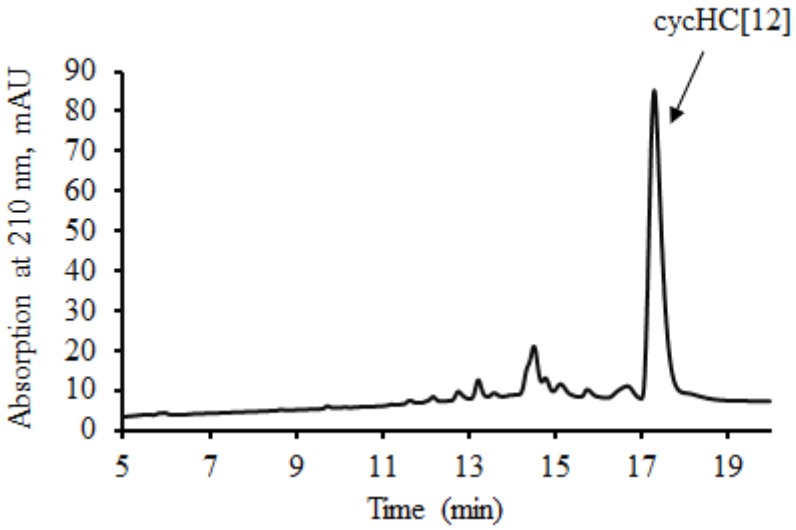


*Figure S2: HPLC- UV chromatogram of **cycHC[12]** after purification by RP column chromatography*

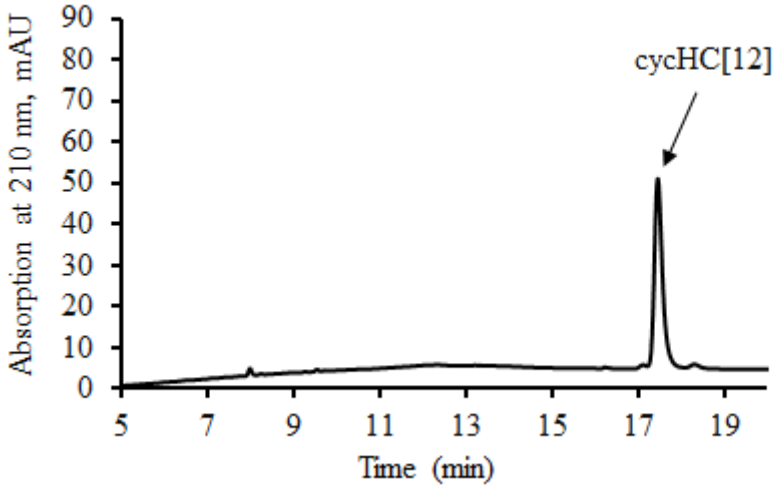


*Figure S3: HPLC-UV chromatogram of **cycHC[12]** after additional purification by normal phase column chromatography*

2.3 Mass-spectrometric analysis

Identification of reaction products and traces were performed by RP-HPLC-HRMS on an Agilent 6540 UHD Accurate-Mass Q-TOF LC/MS spectrometer with a Zorbax Eclipse Plus C18 column (2.1x150 mm, 1.8 µm) and AJ-ESI ionization. Eluent C (CH_3CN with 0.1% HCO_2H and 1.0% H_2O) and D (H_2O with 0.1% HCO_2H) in a 10-minute gradient from 50C/50D to 100C/0D was used. The column temperature was set at 30 °C, the flow rate was 0.4 ml min^{-1}, UV detection at 210 nm and the injection volume was varied depending on the concentration of analytes. The results were analysed with Agilent Mass Hunter Workstation (Version B.07.00) software. Calculated and experimental *m/z* values of different **cycHC[*n*]** observed in the crude reaction mixture are listed in Table S1. All mass-to-charge ratios are presented for $[M+Na]^+$ adducts (most abundant).

Table S1. Experimental and theoretical m/z ratios of observed macrocycles in crude reaction mixture

Compound	Calc. *m/z*	Exp. *m/z*	Compound	Calc. *m/z*	Exp. *m/z*
[**cycHC[4]**+Na]$^+$	631.3690	631.3645	[**cycHC[10]**+Na]$^+$	1543.9384	1543.9306
[**cycHC[5]**+Na]$^+$	783.4639	783.4563	[**cycHC[11]**+Na]$^+$	1696.0333	1696.0299
[**cycHC[6]**+Na]$^+$	935.5588	935.5538	[**cycHC[12]**+Na]$^+$	1848.1282	1848.1242
[**cycHC[7]**+Na]$^+$	1087.6537	1087.6471	[**cycHC[13]**+Na]$^+$	2000.2231	2000.2175
[**cycHC[8]**+Na]$^+$	1239.7486	1239.746	[**cycHC[14]**+Na]$^+$	2152.3180	2152.3119
[**cycHC[9]**+Na]$^+$	1391.8435	1391.8361	[**cycHC[15]**+Na]$^+$	2304.4129	2304.4053

3 Structure elucidation of cycHC[12] by NMR

3.1 COSY, HSQC, HMBC and NOESY spectra of cycHC[12]

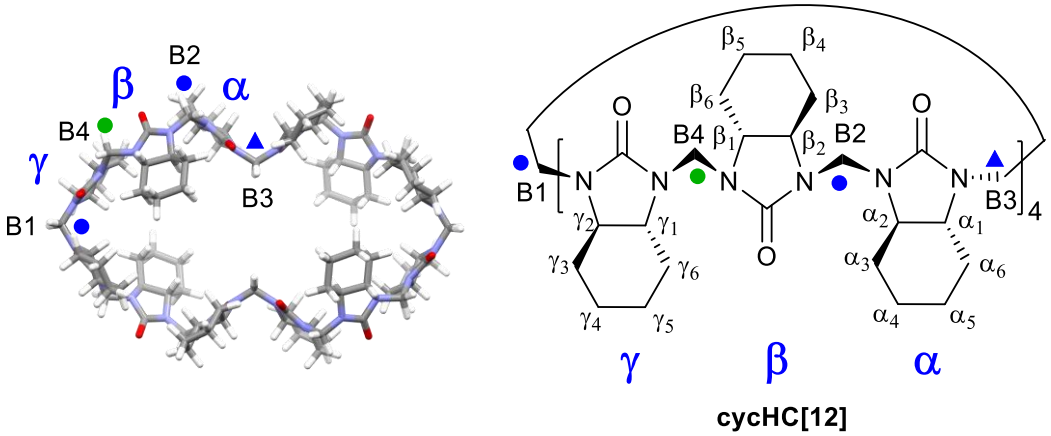


Figure S4. ***cycHC[12]*** *bridges designated with labels B1-B4, and monomers with α,β and γ, on the right structure atom numbering in each monomer is shown. Blue and green dots designate syn- and anti-configurations of bridge to cyclohexano-group, respectively. Blue triangle represent bridges directed inside the cavity in syn- configuration.*

^{1}H, ^{13}C and 2D NMR spectra were acquired on a Bruker Avance III 800 MHz spectrometer with a Cryoprobe (D/H/C/N/P). Chemical shifts were referenced to the residual solvent signal. COSY, HSQC and HMBC spectra were analysed to obtain the structure elucidation brought below. From the COSY spectrum, α_1 and α_2, β_1 and β_2, and γ_1 and γ_2 in pairs are axial protons from the same monomers in the macrocycle, respectively, connected to the chiral centres (Figures S4 and S5). From the HMBC spectrum (green cross peaks) and the HSQC spectrum (red cross peaks) in Figure S6, the monomers that contain α_2 and β_2 carbons are three bonds away from the B2 bridge proton atoms, α_1 from B3 bridge proton atoms, γ_2 from B1 proton atoms and γ_1 and β_1 from B4 proton atoms, respectively. Combining the COSY, HSQC and HMBC data, we obtain a sequence $\alpha_1\alpha_2$ B2 $\beta_2\beta_1$ B4 $\gamma_1\gamma_2$ B1 $\gamma_2\gamma_1$ B4 $\beta_1\beta_2$ B2 $\alpha_2\alpha_1$ B3 $\alpha_1\alpha_2$ B2 $\beta_2\beta_1$ B4 $\gamma_1\gamma_2$ B1 $\gamma_2\gamma_1$ B4 $\beta_1\beta_2$ B2 $\alpha_2\alpha_1$ B3 for the **cycHC[12]** macrocycle. This results in three different types of monomers for the

macrocycle that are connected with four different types of bridge moieties, with the resulting bridge integral ratios as 1:2:1:2. We suggest the macrocycle to adopt a concave octagon as shown in Figure S4. The NOESY spectrum in Figure S7 suggests that the B3 bridge hydrogens point towards the cavity of the macrocycle, which is in agreement with the proposed structure for **cycHC[12]**. The rest of the signals brought below were obtained from COSY, HSQC and HMBC spectra. Second order doublet for H_{B2} was solved via fitting with simulated spectrum, obtained by spin simulation tool in MestReNova 14.1.1-24571 software. Also for visualisation of ^{13}C-NMR signals derived from DFT modelling (main text on Figure 3) spin simulation was used with the same tool, simulating signals for 100.13 MHz, no of points 64 K and Line Width 5Hz and with frequency window 43 to 60 ppm.

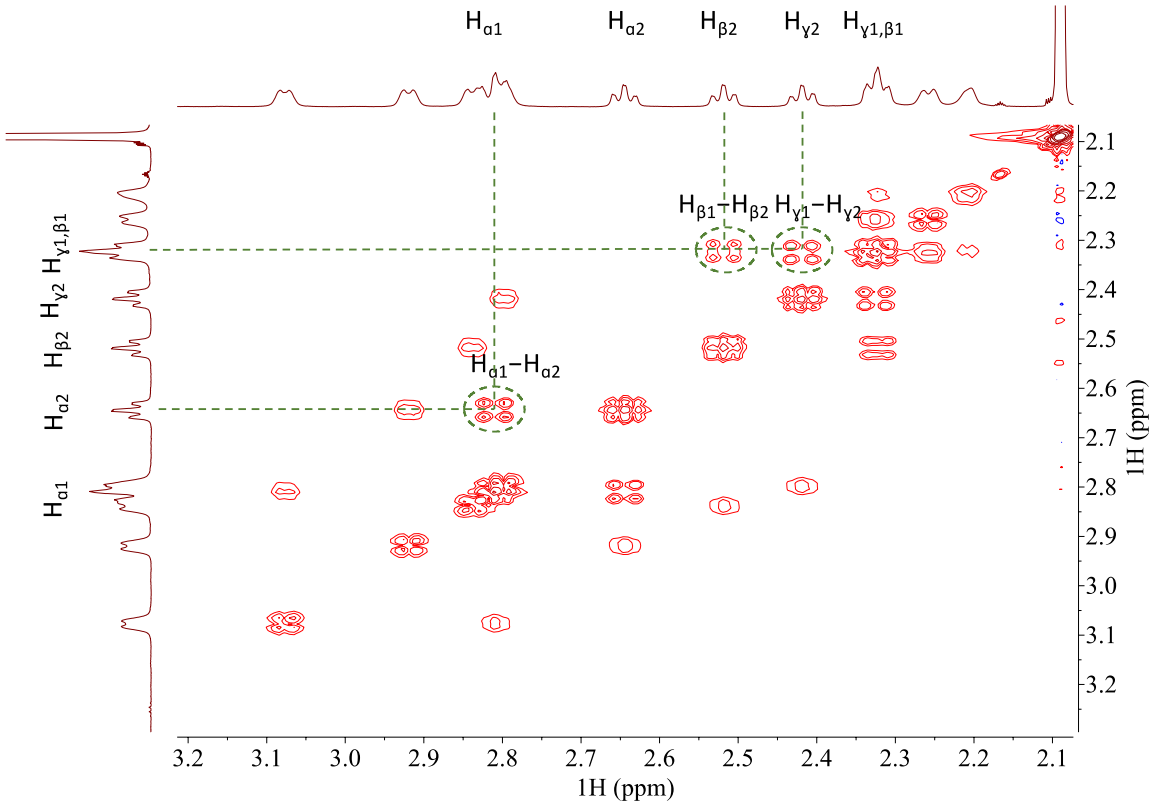


*Figure S5. COSY spectrum for **cycHC[12]** measured at 265 K in toluene-d_8 with axial protons indicated in the spectrum.*

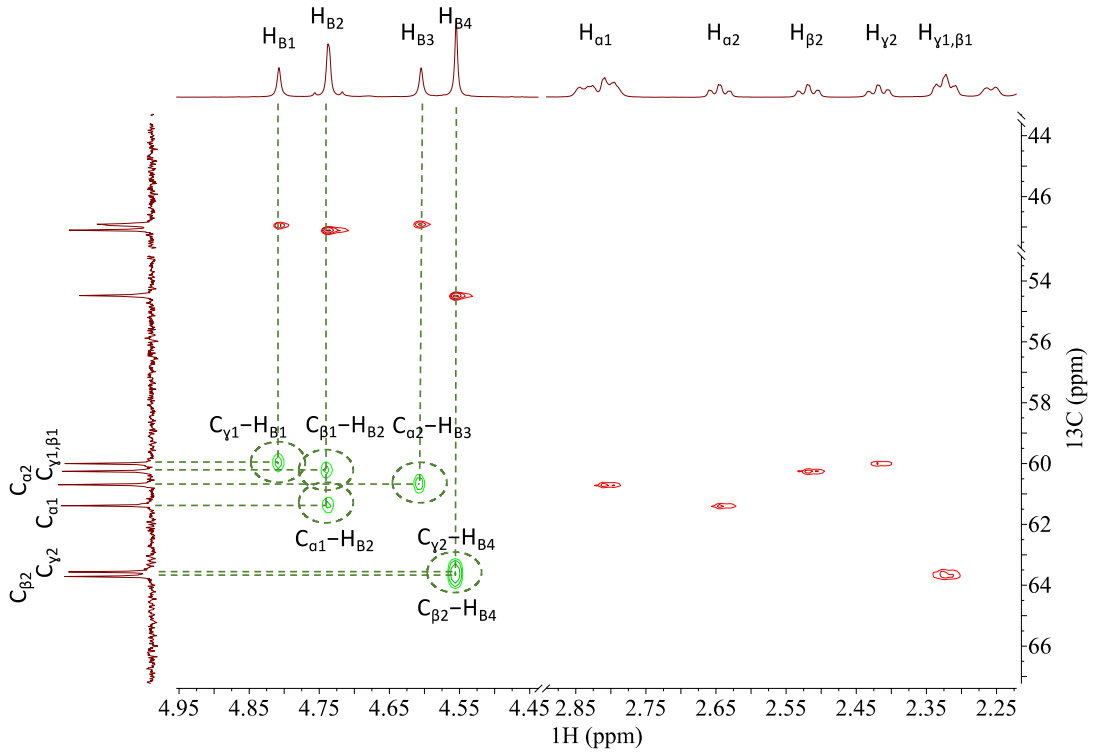


Figure S6. HSQC and HMBC spectrum for ***cycHC[12]*** *measured at 265 K in toluene-d_8 with bridge and axial protons indicated in the spectrum. Lower temperature was needed to separate the bridge proton atoms, which merge at higher temperatures, as detailed below in the VT dynamics section. In the spectra, green cross peaks are from the HMBC and red cross peaks from the HSQC spectra. The HMBC correlations are marked with correlation lines.*

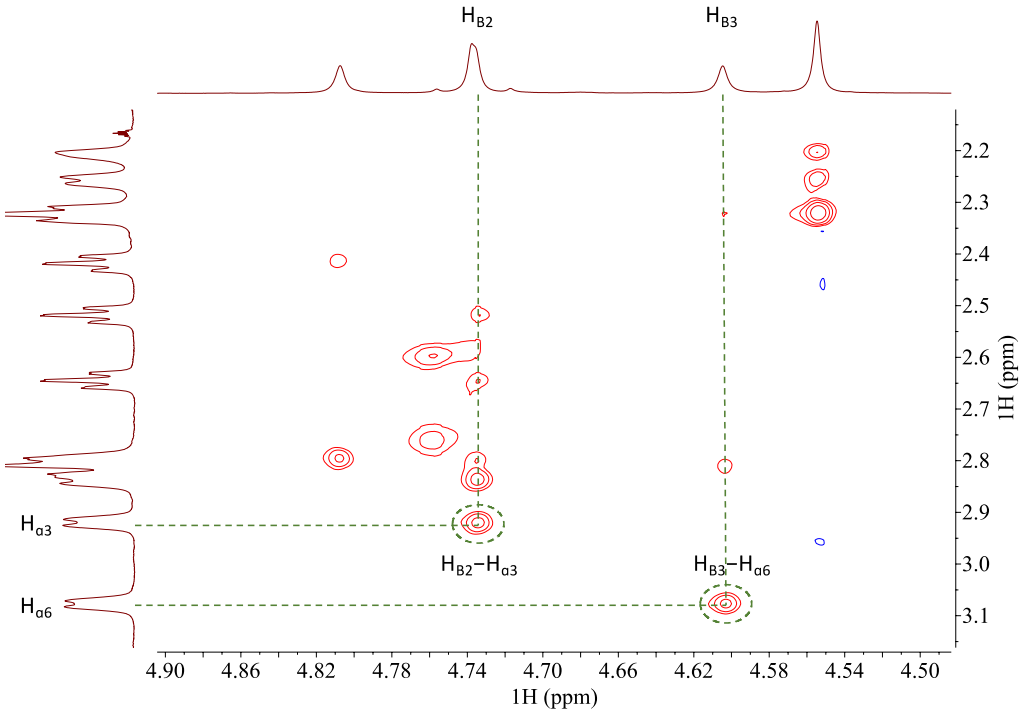


*Figure S7. NOESY spectrum with mixing time d_8 as 0.1 s for the large **cycHC[12]** macrocycle: α_6 proton gives a cross peak with B3 and α_3 proton with bridge B2, respectively. The axial α_6 proton faces towards the cavity of the macrocycle, indicating that B3 bridge proton atoms also point towards the cavity of the macrocycle, as illustrated in Figure S4. On the contrary, the axial α_3 proton atoms point away from the cavity of the macrocycle, indicating the B2 bridge atoms also point in this direction. This is in agreement with our proposed conformation for **cycHC[12]**.*

3.2 ^{1}H and ^{13}C-NMR spectra and signal characterisation for cycHC[12]

^{1}H NMR (800 MHz, Tol-d_8) δ 4.81 (s, 4H, H_{B1}),), 4.74 (d, J = 14.0 Hz, 4H, H_{B2A}), 4.73 (d, J = 14.0 Hz, 4H, H_{B2B}), 4.60 (s, 4H, H_{B3}), 4.55 (s, 8H, H_{B4}), 3.08 (d, J = 10.2 Hz, 4H, $H_{\alpha 6a}$), 2.92 (d, J = 10.5 Hz, 4H, $H_{\alpha 3}$), 2.86 – 2.79 (m, 12H, $H_{\alpha 1}$, $H_{\beta 3}$ and $H_{\gamma 3}$), 2.64 (td, J = 11.0, 2.9 Hz, 4H, $H_{\alpha 2}$), 2.52 (td, J = 11.0, 2.9 Hz, 4H, $H_{\beta 2}$), 2.42 (td, J = 11.0, 2.9 Hz, 4H, $H_{\gamma 2}$), 2.33 (dt, J = 12.2, 6.2 Hz, 8H, $H_{\gamma 1}$ and $H_{\beta 1}$), 2.26 (d, J = 11.0 Hz, 4H, $H_{\beta 6}$), 2.21 (s, 4H, $H_{\gamma 6}$), 1.68 – 1.64 (m, 4H, $H_{\alpha 5}$), 1.66 – 1.61 (m, 4H, $H_{\alpha 4}$), 1.64 – 1.61 (m, 4H, $H_{\gamma 4}$)*, 1.60 – 1.56 (m, 4H, $H_{\beta 5}$)*, 1.56 – 1.53 (m, 4H, $H_{\gamma 5}$)*, 1.37 – 1.26 (m, 4H, $H_{\alpha 5}$)*, 1.34 – 1.28 (m, 4H, $H_{\alpha 5}$)*, 1.24 – 1.19 (m, 4H, $H_{\alpha 4}$)*, 1.21 – 1.15 (m, 4H, $H_{\beta 6}$)* 1.17 – 1.12 (m, 4H, $H_{\gamma 5}$)*, 1.13 – 1.09 (m, 8H, $H_{\beta 4}$ and $H_{\beta 5}$)*, 1.11 – 1.05 (m, 8H, $H_{\alpha 6}$ and $H_{\gamma 6}$)*, 1.10 – 1.04 (m, 4H, $H_{\alpha 3}$)*, 1.08 – 1.05 (m, 4H, $H_{\beta 4}$)*, 0.98 (td, J = 11.9, 8.3 Hz, 4H, $H_{\gamma 3}$), 0.92 (td, J = 12.2, 11.6, 8.6 Hz, 4H, $H_{\beta 3}$). *Signals marked with asterisk were obtained from the HSQC spectra due to overlap in the ^{1}H NMR spectrum.

^{13}C NMR (201 MHz, Tol-d_8) δ 162.98 ($C_{\alpha CO}$), 161.45 ($C_{\beta CO}$), 161.26 ($C_{\gamma CO}$), 63.71 ($C_{\beta 1}$ or $C_{\gamma 1}$), 63.561 ($C_{\beta 1}$ or $C_{\gamma 1}$), 61.39 ($C_{\alpha 2}$), 60.70 ($C_{\alpha 1}$), 60.26 ($C_{\gamma 2}$), 60.00 ($C_{\beta 2}$), 54.48 (C_{B4}), 47.10 (C_{B2}), 46.94 (C_{B1}), 46.91 (C_{B3}), 29.73 ($C_{\beta 6}$), 29.45 ($C_{\gamma 6}$), 28.83 ($C_{\alpha 6}$), 28.00 ($C_{\alpha 3}$), 27.64 ($C_{\beta 3}$), 27.51 ($C_{\gamma 3}$), 24.87 ($C_{\alpha 5}$), 24.78 ($C_{\alpha 4}$), 24.51 ($C_{\gamma 5}$), 24.43 ($C_{\beta 4}$), 24.32 ($C_{\beta 5}$), 24.27 ($C_{\gamma 4}$).

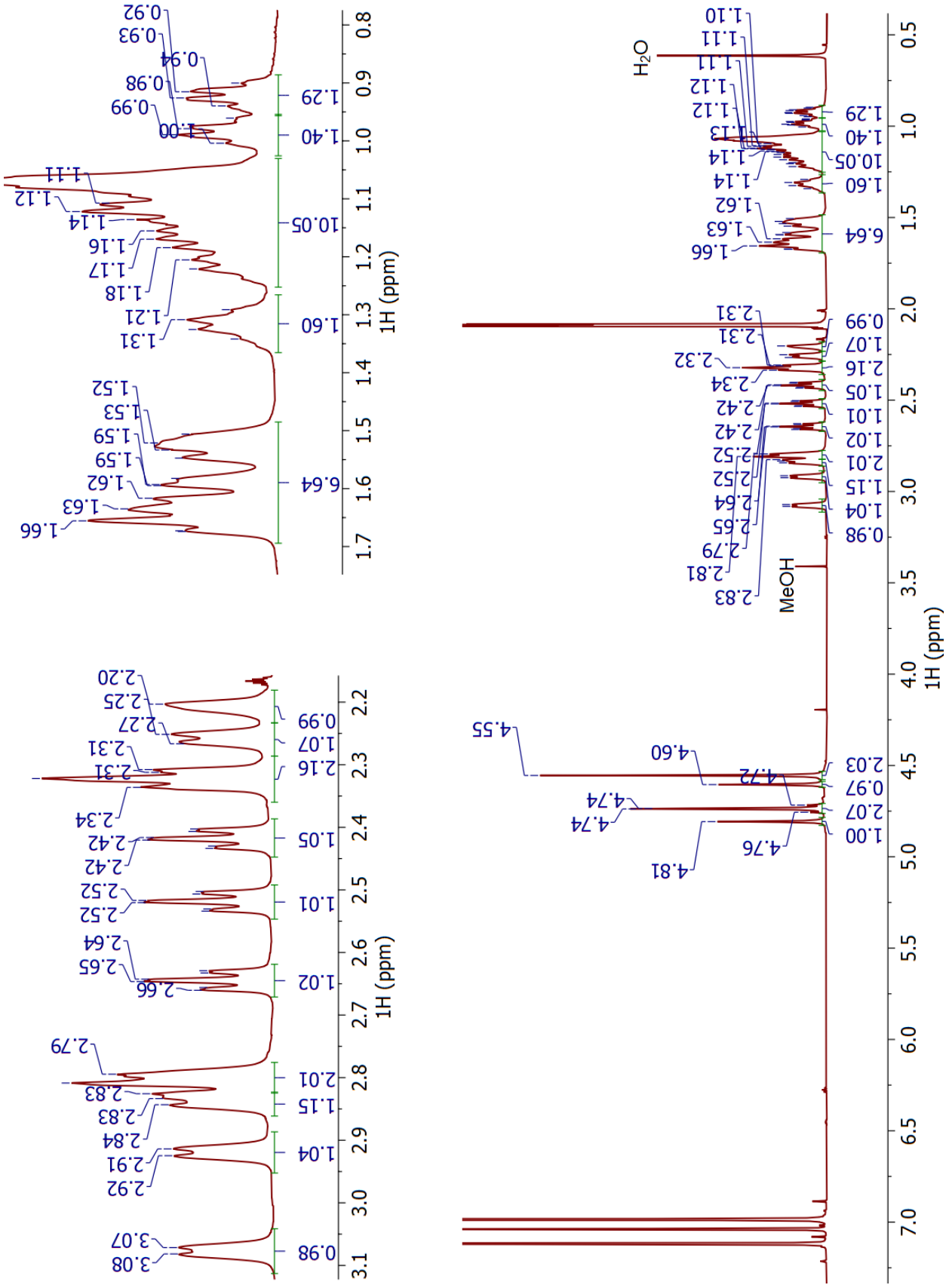


*Figure S8: ^{1}H-NMR spectrum of **cycHC[12]** in toluene-d_8 at 265 K, with insets for regions 0.8-1.7 ppm and 2.2-3.1 ppm.*

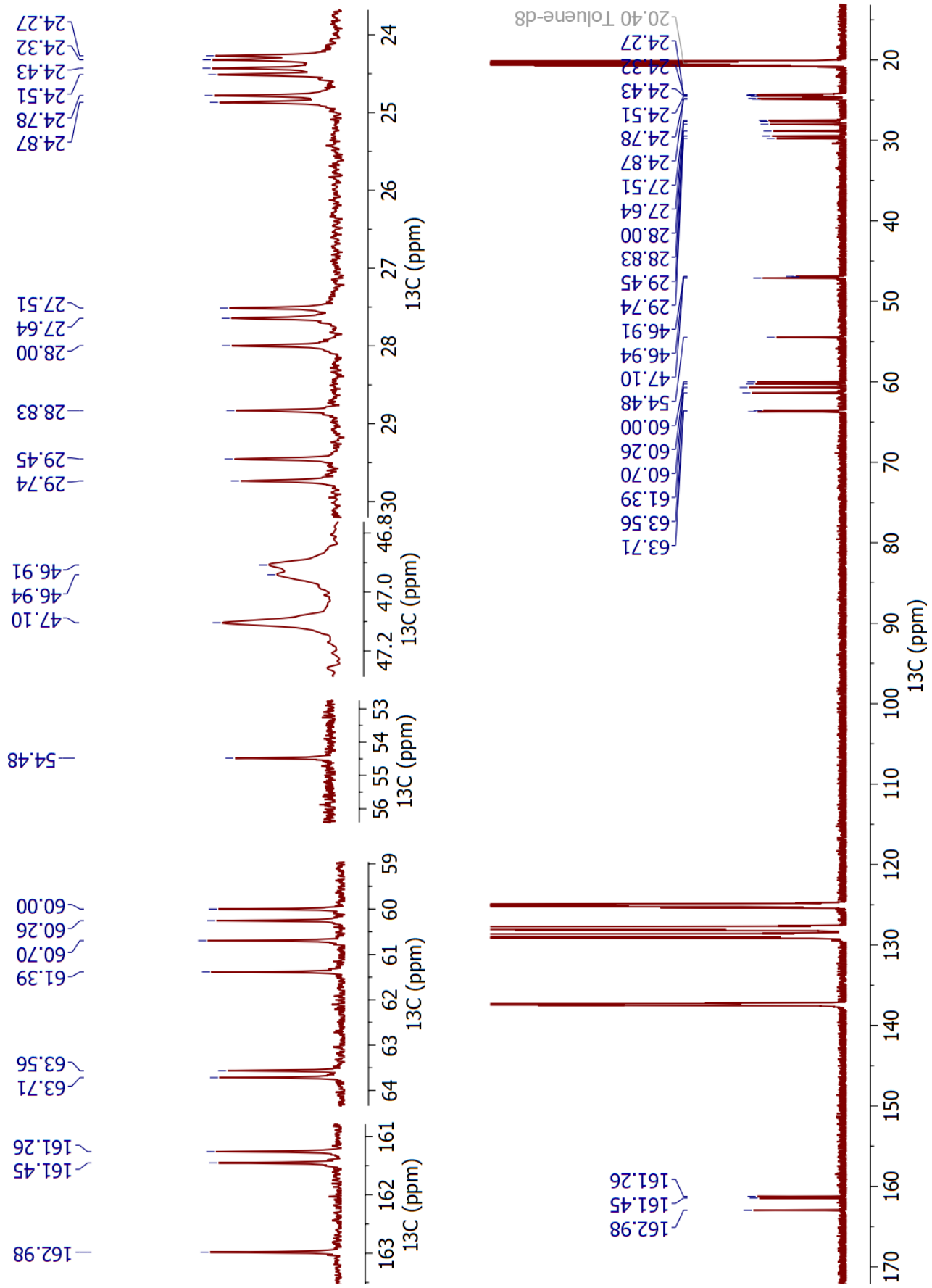


Figure S9: *^{13}C NMR spectrum of **cycHC[12]** in toluene-d_8 at 265 K, with insets for all carbon signal containing regions.*

4. cycHC[12] conformational dynamics in solution

4.1 ^{1}H NMR VT-NMR of cycHC[12] in toluene

Variable temperature ^{1}H NMR spectra were measured in the temperature region 268–348 K in 10 K intervals. Two dynamic exchange processes were observed in this region and the ^{1}H NMR proton resonances corresponding to the bridge proton atoms (H_{B1}, H_{B2}, H_{B3} and H_{B4}) in **cycHC[12]** for these regions were simulated (Figure S10 and S11) using the program WINDNMR V. 7.1.14 (Hans J. Reich. University of Wisconsin. Madison. WI. USA. **2009)** after processing the NMR spectra with NUTS. DNMR option with 2-spin was used in WINDNMR to simulate spectra with all input parameters except temperature taken from the slow-exchange or near slow-exchange limit spectra and the chemical shifts for the lower temperature bridge flip process were extrapolated using the chemical shifts for the proton atoms in the first three spectra. Adjustments of spectral amplitudes and rate constants (k_{ab}+k_{ba}) were carried out iteratively until the line shapes matched. Activation parameters for the formation of the transition states were obtained from the modified Eyring equation and are given below:

$$\ln\left(\frac{k}{T}\right) = -\Delta H^{\ddagger}\frac{1}{RT} + \left(23.76 + \Delta S^{\ddagger}\frac{1}{R}\right)$$

via a linear plot ln(*k*/T) versus 1/T.

For the first dynamic process, the bridge flip, firstly, the H_{B1} and H_{B2} atoms are in exchange with each other and secondly, the H_{B3} and H_{B4} atoms are in exchange with each other during the same conformational change of the **cycHC12** macrocycle. For atoms H_{B1} and H_{B2}, the NMR spectra at 268—298 K in 10 K increments were used for fitting. The chemical shifts for temperatures 268—288 K were taken from the NMR spectra and the chemical shifts for the signals at 298 K, where significant merging of the signals has already occurred, was extrapolated from the shifts in the temperature range 268—288 K. The rate constants at each individual temperature were thus determined, shown as left most data in Table S2. These values were used to obtain linear fits of ln(*k*/T) versus 1/T to get activation enthalpy, entropy and Gibbs free energy values for the formation of the transition state. The data point for temperature 308 K was omitted from this analysis since the extrapolated chemical shift values did not place this point on a straight line with the other points for the Eyring analysis. We hypothesize that there is an emphasized conformational change at this temperature, particularly influencing the chemical shift of the H_{B1} proton atom. The H_{B1} changes its chemical shift most as temperature increases above 268 K and we suggest that the change in its chemical shift is not dependent linearly on temperature. The same analysis was performed for the exchange between H_{B3} and H_{B4} proton atoms. As outlined in Table S2, the activation Gibbs free energy values for the exchanges between H_{B1} and H_{B2} as well as between H_{B3} and H_{B4} are quite similar at temperatures 260, 300 and 340 K, however, the activation entropy and enthalpy values differ about 10 kJ mol^{-1} for these pairs of hydrogen atoms. In DNMR analysis, the proton atoms with closer chemical shift values for the same exchange process, have a lower coalescence temperature than the proton atoms with more different chemical shift values. Since line broadening varies as the square of the chemical shift after coalescence, the obtained rates are very dependent on the chemical shift difference between the atoms at these temperatures. Therefore, the activation parameters are strongly affected by the line separation of exchanging signals (https://www2.chem.wisc.edu/areas/reich/nmr/08-tech-03-dnmr.htm). For the exchange between H_{B1} and H_{B2}, the chemical shifts do not vary linearly with temperature, particularly for H_{B1}, and the signals become closer together as temperature is raised. We therefore suggest that the analysis for the exchange between H_{B3} and H_{B4} proton atoms is more accurate. The activation parameter values derived from the exchange between H_{B3} and H_{B4} proton atoms are brought in Table S2 (right most values) and are marked in bold.

For the second dynamic process, the monomer flip, firstly, we consider the spectrum at 308 K as the slow exchange spectrum, where the monomers start to rotate. The monomer flip will take place as a concomitant process with the bridge flip, however, the bridge flip is increasingly in fast exchange at higher temperatures. We use the signals for the H_{B1} and H_{B2} proton pair as the slow exchange signal for the monomer flip at 308 K and obtain rate constants for the monomer flip for temperatures 308—348 K. Fitting all the spectra for temperatures up to 348 K, while assuming a references standard signal line width of 0.5 Hz, we obtain five

rate constants for the monomer flip process. The Eyring analysis results in the activation Gibbs free energy, entropy and enthalpy values as outlined in Table S3 (left most values). We have assumed in this analysis that at all temperatures, signal broadening arises from the monomer flip process only. This might, however, not hold true as at 308 K, for example, the bridge exchange between H_{B1} and H_{B2} proton atoms could still contribute to the broadening of the corresponding signal at lower temperatures. Hence the temperatures 308 K and 318 K are omitted from the Eyring analysis for the monomer flip process to leave three data points, 328, 338 and 348 K, and the activation parameter values are calculated again. We suggest that these values represent the activation parameters for the monomer flip more accurately since there might still be some line broadening from the bridge flip process at 308 K. The activation Gibbs free energy, entropy and enthalpy values for the analysis based on the last three temperature points is brought in Table S3 (right most values). The Eyring plots were made in Excel and the relevant activation parameters derived from the slope and the intercept of linear fits. The plots were based on the data in Tables S2 and S3 and are not brought out independently.

Based on the analysis of the spectra in WINDNMR, standard error propagation formulae were used to get estimated errors for each point in the graphs for the Eyring analysis. As was evident from this analysis, the error bar values on the Eyring plots are marginal in size, which allowed to use the LINEST function in Excel to determine the slope and the intercept as well as their respective errors for the Eyring plots. Thereafter, error propagation formulae were used to arrive at the errors in the activation enthalpy, entropy and Gibbs free energy values for both of the dynamic exchange processes. These errors at 298 K are brought in Table 1 in the main text of our manuscript.

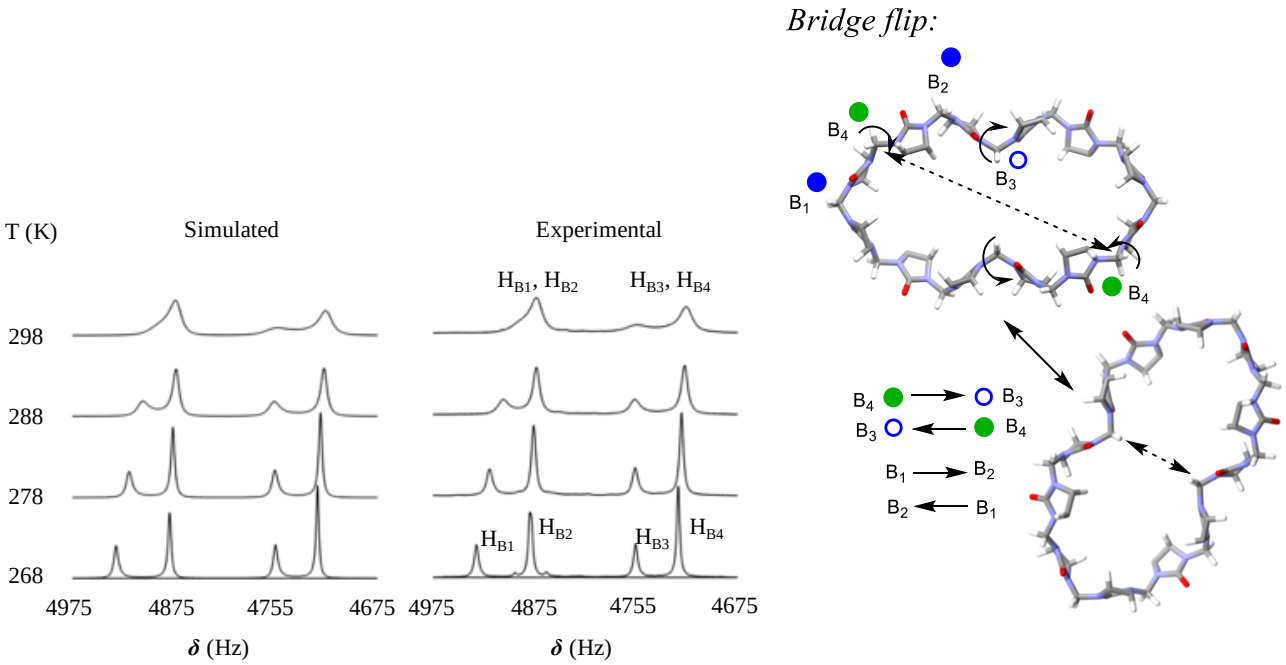


Figure S10. Example simulated and experimental spectra for ***cycHC[12]*** *for the temperature region 268–298 K for exchange between equal conformations of the* ***cycHC[12]*** *concave octagon* H_{B1} and H_{B2} and also H_{B3} and H_{B4} proton atoms *(cyclohexano groups are omitted from the structure for clarity).*

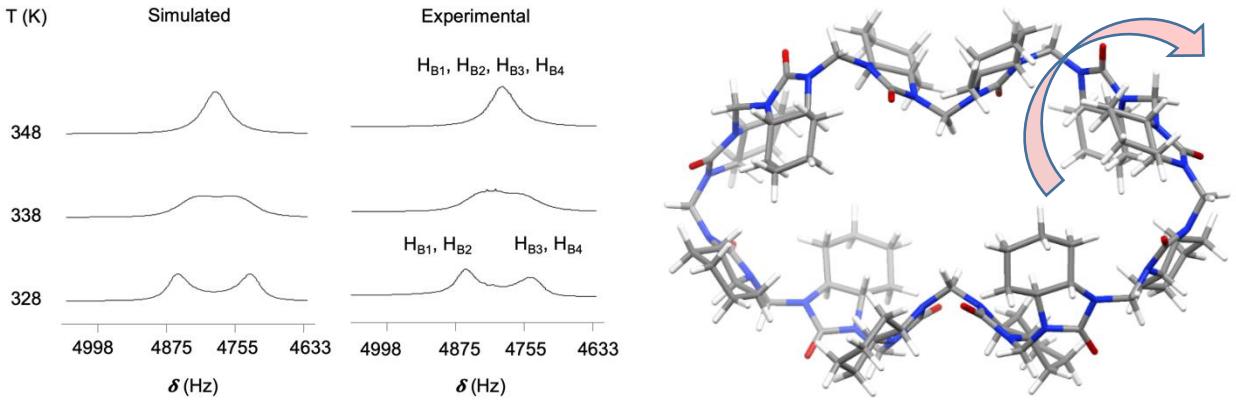


Figure S11. Simulated and experimental spectra for ***cycHC[12]*** *for the temperature region 328–348 K for fast rotation of the monomers, using 3 points, at high temperatures.*

Table S2. Activation enthalpy, entropy, and Gibbs free energy values for the ***cycHC[12]*** *bridge flip process as derived from the exchange between protons H_{B1} and H_{B2} as well as H_{B3} and H_{B4} proton atoms. The latter are values in bold are deemed to be more accurate due to the larger chemical shift difference between these proton atoms at all temperatures. Values are reported in kJ mol^{-1}.*

Bridge flip process

	$H_{B2}\rightarrow H_{B1}$			$H_{B1}\rightarrow H_{B2}$			$H_{B4}\rightarrow H_{B3}$			$H_{B3}\rightarrow H_{B4}$		
T (K)	260	300	340	260	300	340	260	300	340	260	300	340
$\Delta H^{\ddagger}$ (kJ/mol)	28.4	28.4	28.4	28.4	28.4	28.4	**38.5**	**38.5**	**38.5**	**38.5**	**38.5**	**38.5**
$T\Delta S^{\ddagger}$ (kJ/mol)	-31.3	-36.1	-40.9	-29.8	-34.4	-39.0	**-22.2**	**-25.6**	**-29.0**	**-20.7**	**-23.9**	**-27.1**
$\Delta G^{\ddagger}$ (kJ/mol)	59.7	64.5	69.4	58.2	62.8	67.4	**60.7**	**64.1**	**67.6**	**59.2**	**62.4**	**65.6**

Table S3. Activation enthalpy, entropy, and Gibbs free energy values for the ***cycHC[12]*** *monomer flip process. The more downfield signal of the two signals in Figure S11 is used for obtaining line widths for fitting since it has a smaller contribution from the bridge flip process. All temperatures between 308—348 K are used in the left most results and temperatures between 328—348 K are used for obtaining the right most results in bold. The right most results in bold are considered to be more accurate due to the smaller contribution from the bridge flip process and a larger contribution from the monomer flip process to line broadening at these temperatures. The derivation of the activation parameters is brought above in the text. Values are reported in kJ mol^{-1}.*

Monomer flip process

	$H_{B2}+H_{B2}\rightarrow H_{B3}+H_{B4}$			$H_{B2}+H_{B2}\rightarrow H_{B3}+H_{B4}$*		
T (K)	260	300	340	260	300	340
$\Delta H^{\ddagger}$ (kJ/mol)	57.9	57.9	57.9	**59.9**	**59.9**	**59.9**
$T\Delta S^{\ddagger}$ (kJ/mol)	-7.4	-8.5	-9.6	**-5.8**	**-6.7**	**-7.6**
$\Delta G^{\ddagger}$ (kJ/mol)	65.3	66.4	67.6	**65.7**	**66.6**	**67.5**

*3 point fitting results

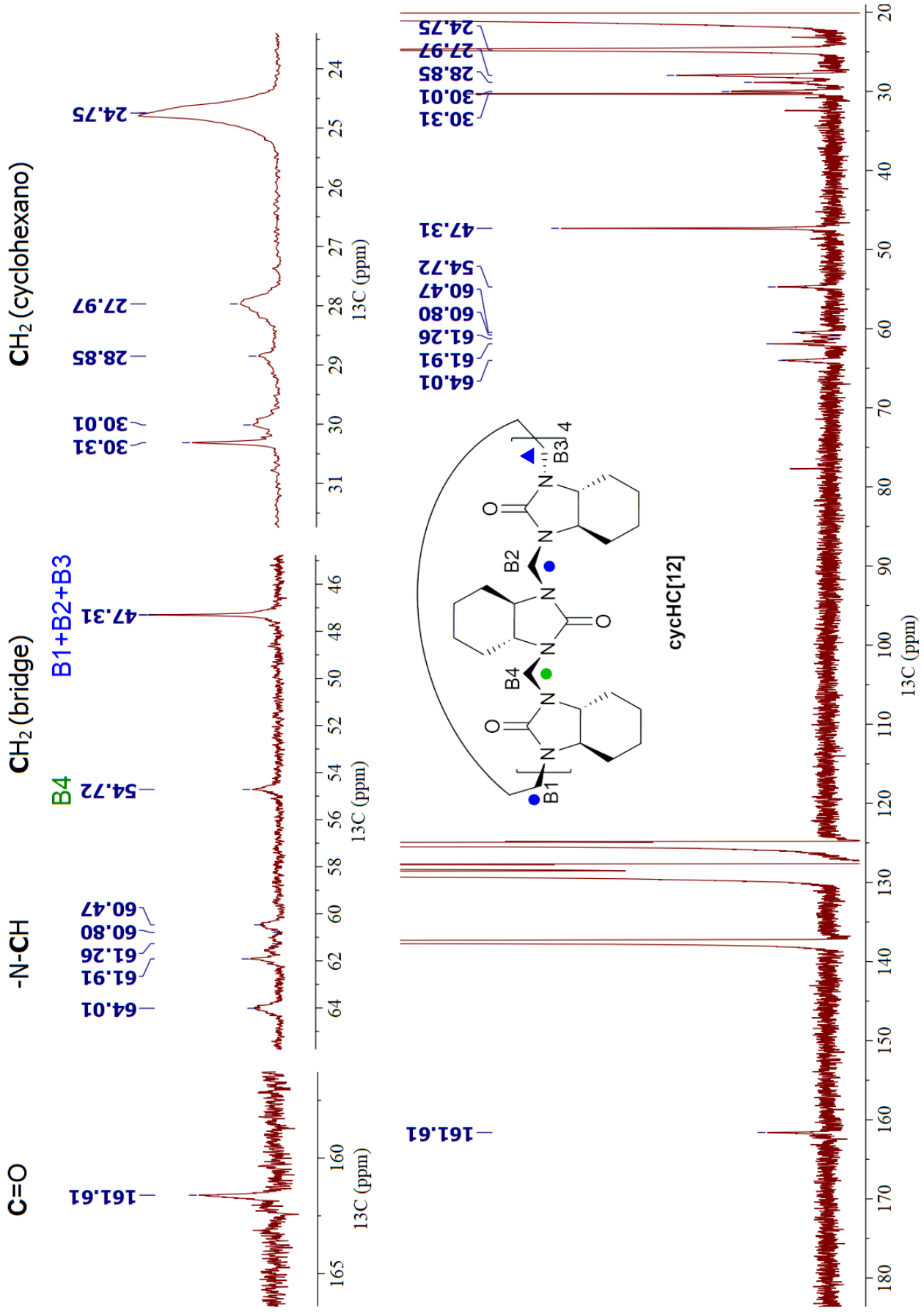


*Figure S12. ^{13}C-NMR spectrum for **cycHC[12]** in toluene-d_6 at 308K, with insets from the same spectra in upper row, the bridging carbon from B1, B2 and B3 are in exchange and their signal is at 47.31 ppm.*

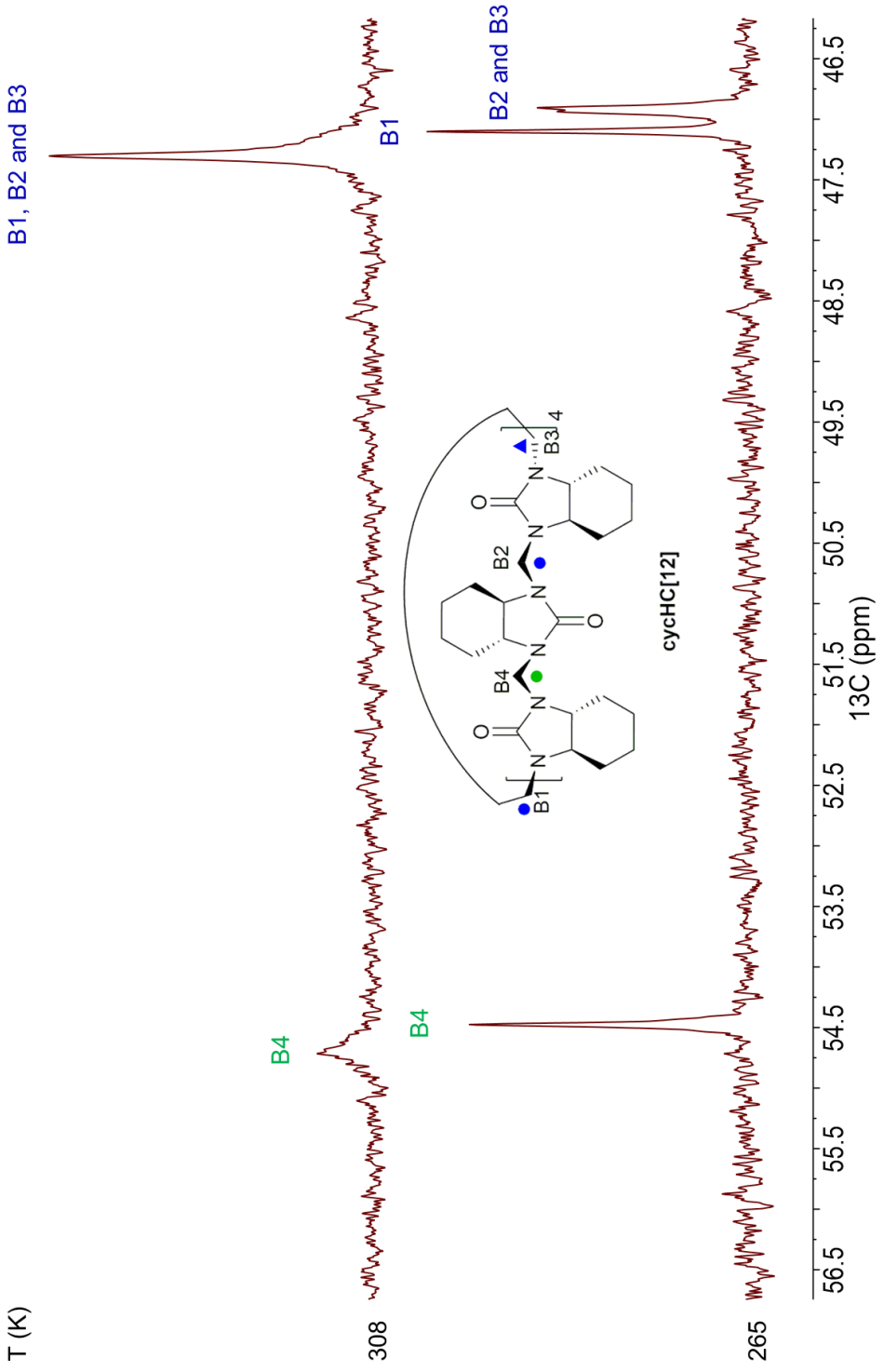


Figure S13. 13C-NMR spectra for ***cycHC[12]*** *in toluene-d6 at (a) 265K and (b) 308K*
As the temperature is increased from 265 K to 308 K, the bridging carbon from B1, B2 and B3 gets averaged at 47.31 ppm.

4.2 ^{1}H NMR VT-NMR of cycHC[12] in chloroform

Variable temperature ^{1}H NMR of **cycHC[12]** in chloroform were measured in the temperature region 264–318 K. Due to the complexity of the spectra (Figure S14) we could not use the following data to interpret the dynamics of **cycHC[12]** structure in chloroform.

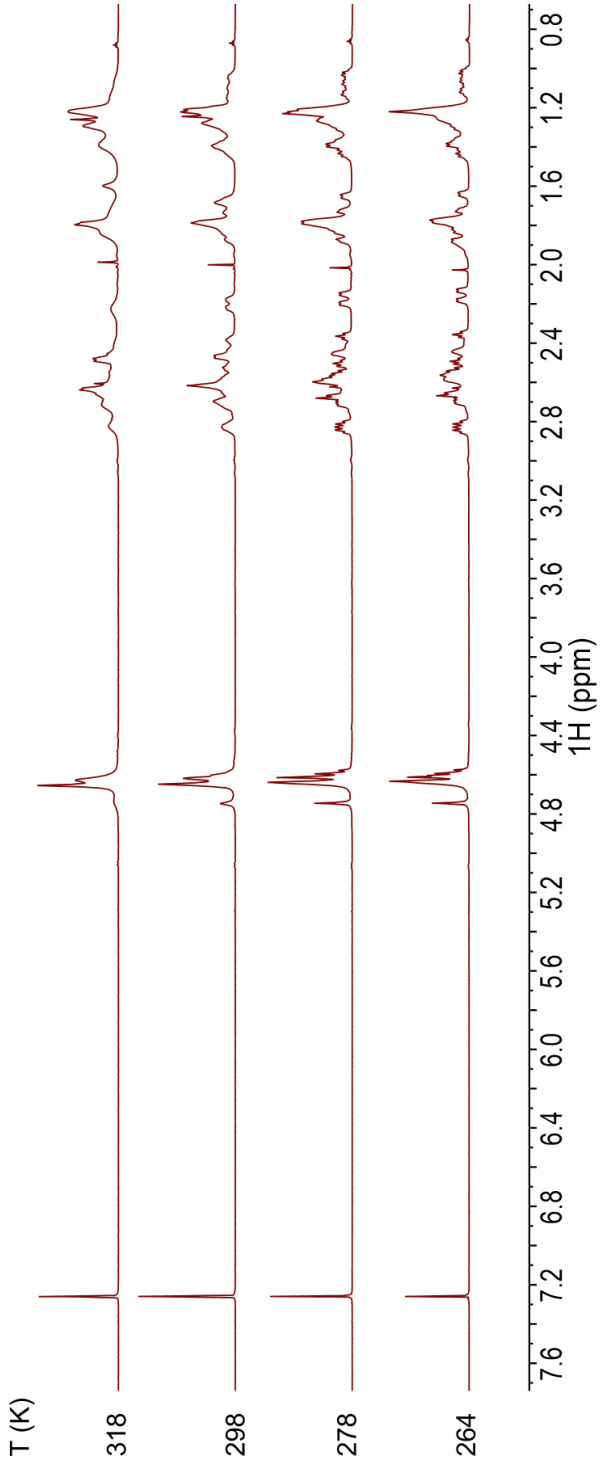


*Figure S14. Variable temperature ^{1}H NMR spectra of **cycHC[12]** in $CDCl_3$ for the temperature region 264–318 K.*

5. ^{13}C VT-NMR of cycHC[8] in toluene

Variable temperature ^{13}C NMR for **cycHC[8]** in toluene-d_8 were measured in the temperature region 273-358 K. No chemical exchange was observed for the bridging carbons present at 55.81 and 46.59 ppm respectively. However, with increase in temperature, the carbon signal at 24.55 ppm and 24.38 ppm started shifting and at 343 K got merged into a single signal (Figure S15), indicating equilibrium at portal regions of the cyclohexano monomeric unit of **cycHC[8].** No chemical exchange was observed on bridges and therefore we can conclude that neither bridge nor monomer flip occurs with **cycHC[8]** within this temperature range.

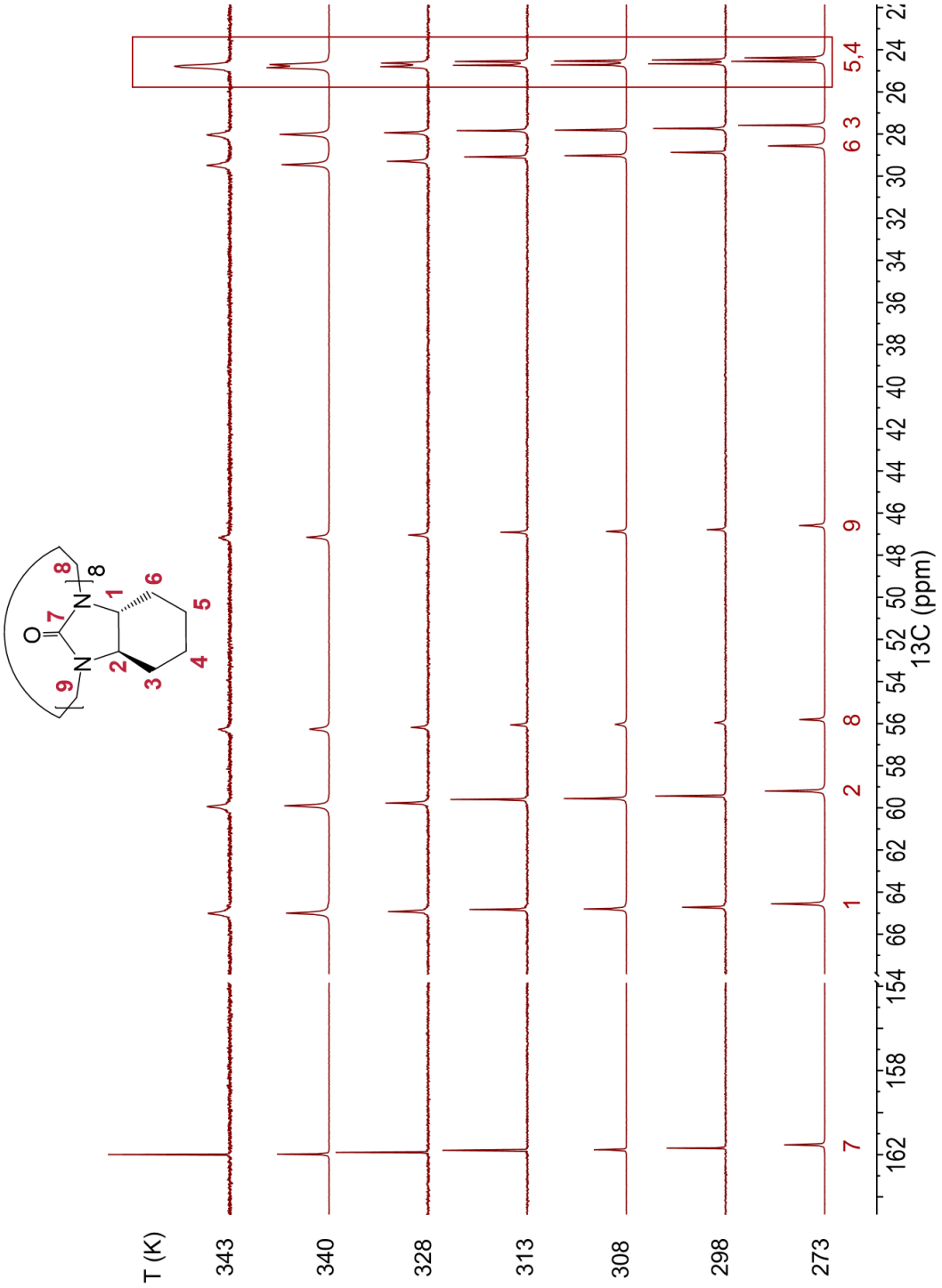


*Figure S15. Variable temperature ^{13}C NMR spectra of **cycHC[8]** in toluene-d_8 for the temperature region 273–358 K.*

6. Computation Studies

Density Functional Theory (DFT) calculations were performed to support the results obtained from the NMR study and to visualise the potential conformers of **cycHC[12]**. Taking into account the structures of the smaller homologues of cycHC and the obtained NMR results, we proposed three different conformers for **cycHC[12]**: the **regular 12-gon conformer**, which is based on the smaller homologues of cycHC and **concave octagon conformer** and **concave 12-gon conformer**, which are based on the aforementioned NMR studies. We addressed the problem by modelling the Boltzmann probabilities of the proposed conformers and then calculating the chemical shifts of the carbon atoms of the methylene bridges for relevant conformers.

6.1 Computational Details

The three conformer structures were built using the program Avogadro[5] and DFT calculations were done using the program NWChem[6]. The functional BP86[7–11] in combination with the basis set SVP[12] was used for both geometry optimisation and calculating the chemical shifts. The calculations were performed in the gas phase. The chosen methods have been previously proven to work well for the geometry optimisation of cycHCs[13]. The calculations for **cycHC[8]** were taken from the PhD thesis[14] of Mario Öeren, where the same DFT methods were used. The calculations for **cycHC[8]** were done using the program package Turbomole 6.5[15].

The geometries and NMR spectra were refined with a modern method, LC-TPSS/cc-pVTZ, recommended by Iron[16]. The goal of using a modern functional and a bigger basis was to increase the accuracy of the calculated chemical shifts and validate the trends provided by BP86/SVP. The calculations were done using Gaussian16[17]. Visualisation of ^{13}C-NMR signals of **cycHC[12]** in main text was done by spin simulation tool in MestReNova 14.1.1-24571 software from theoretical output that gave closer values to experimental.

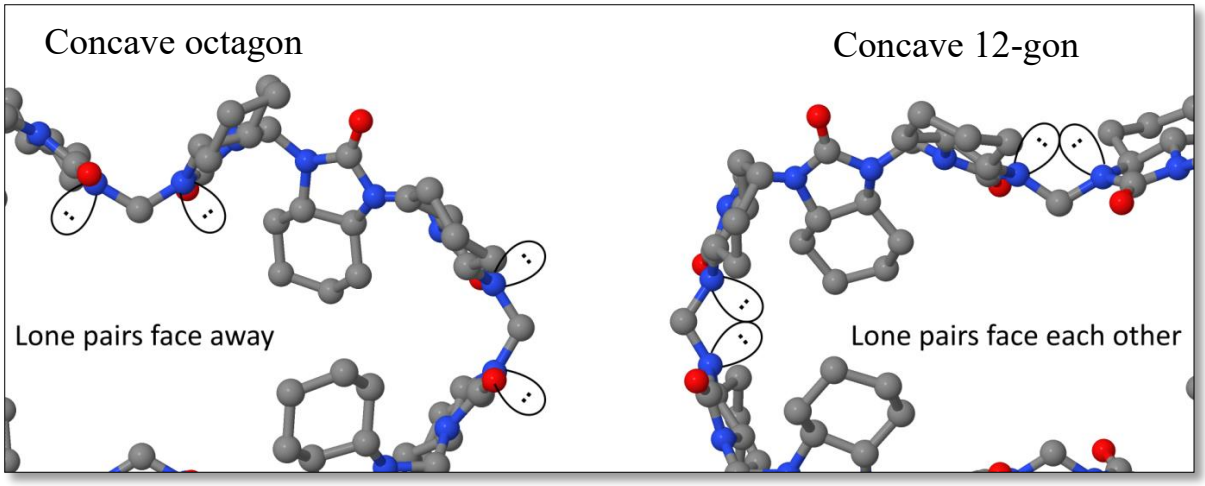
6.2 The Potential Conformers

The relative energy values, in kJ mol^{-1}, are in the following Table S5. The DFT results propose that both the regular 12-gon conformation and the concave 12-gon conformation are not favoured, and it is highly unlikely to observe them experimentally. The modern method, which takes into account the long-range interactions, in combination with a bigger basis set provided the same trends as BP86/SVP, but the energy differences between conformers were greater. This was probably due to the fact that the long-range interactions forced the cyclohexyl groups of the cycHC[12] to contract, covering the opening and reducing the overall energy of cycHC[12] in vacuum. It would be interesting to see if the same effect would be observed if the cavity of cycHC[12] would have guests or would be filled with solvent molecules. Unfortunately, such experiments fall out of the scope of the current study.

*Table S5. The relative energy values of potential conformers of **cycHC[12]***

	ΔE of Conformers (kJ mol^{-1})	
	BP86/SVP	LC-TPSS/cc-pVTZ
Concave octagon	0	0
Concave 12-gon	30	41
Regular 12-gon	52	85

The concave octagon conformer is probably favoured over concave 12-gon conformation because of the lone pairs on nitrogen atoms. In the concave octagon conformation, the lone pairs on nitrogen atoms connected to the methylene bridge are pointing away from each other, while in the concave 12-gon conformation, they point towards each other. The interaction between the two lone pairs in concave 12-gon conformation is repulsive, thus the relative energy of the conformer is higher compared to the concave octagon conformer.



Interestingly, the regular 12-gon conformer, which is the preferred conformer in smaller homologues of cycHC is over 50 kJ mol^{-1} higher than concave octagon conformer. We conclude that the void within the regular 12-gon conformations is not preferable and smaller homologues such as **cycHC[6]** and **cycHC[8]** (see Figure S15 for VT-NMR) are too rigid to go through any noticeable conformational changes, while the **cycHC[12]** is flexible enough to invert the methylene bridges and collapse on itself to **form energetically favourable concave octagon conformation**. Interestingly, there are no noticeable changes within the angles of N−CH_2−N (bridge angles) which indicates that the conformational change is probably induced to reduce the empty space within the molecule. The angles between the conformations are in the Table S6.

Table S6. Angles between the lone pairs on nitrogen atoms in different conformations of ***cycHC[12]***

Angle	Regular 12-gon conformation	Concave octagon conformation	Concave 12-gon conformation
1	117.3°	117.0°	114.4°
2	115.5°	116.9°	114.6°
3	117.5°	114.0°	115.8°
4	115.4°	117.0°	115.1°
5	117.5°	113.9°	115.8°
6	115.5°	116.9°	114.6°
7	117.3°	117.0°	114.4°
8	115.5°	116.9°	114.6°
9	117.5°	114.0°	115.8°
10	115.4°	117.0°	115.1°
11	117.5°	113.9°	115.8°
12	115.5°	116.9°	114.6°
Average:	**116.5°**	**116.0°**	**115.1°**

6.3 Comparison of calculated ^{13}C-NMR shifts of cycHC[12] in concave octagon and regular 12-gon conformers with experimental values

The bridge shifts for the concave octagon and regular 12-gon conformers were calculated. The agreement between the calculated and experimental chemical shift at 265 K values is very good. The calculated ^{13}C chemical shifts of regular 12-gon conformation deviate significantly from the experimental **cycHC[12]** spectra recorded at 308 K and are more similar to chemical shift values to the barrel-shaped **cycHC[8]**. In barrel-shape macrocycles (regular 12-gon and cycHC[8]) half of the methylene bridges are in *syn* and half in *anti* configuration to cyclohexane. Summary of these results in ppm can be found in Table S7.

Visualisation of ^{13}C-NMR signals of **cycHC[12]** derived from DFT modelling for concave octagon and regular 12-gon in Table S7 spin simulation tool in MestReNova 14.1.1-24571 software was used, simulating signals for 100.13 MHz, no of points 64 K and Line Width 5Hz and with frequency window 43 to 60 ppm (main text on Figure 2).
Surprisingly, the modern method with a bigger basis set did not provide any advantage over the BP86/SVP when calculating the NMR spectrum and the trends remained the same. It could be argued that the long-range interactions over-estimate the contraction of the cyclohexyl groups and the LC-TPSS/cc-pVTZ optimised geometry is not representative of the cycHC[12] geometry in the experiment. Thus, in this specific case, the BP86/SVP method might have an advantage, but as said before, such analysis falls out of the scope of the present study.

*Table S7. ^{13}C-NMR shifts (ppm) for experimental **cycHC[12]** and **cycHC[8]** and calculated conformers of **cycHC[12]** in concave octagon and regular 12-gon conformation.*

Bridgecarbon	cycHC[12]						cycHC[8]
	Exp.		Calc.				Exp.
			concave octagon		regular 12-gon		
	at 265 K	at 308 K	BP86/SVP	LC-TPSS/cc-pVTZ	BP86/SVP	LC-TPSS/cc-pVTZ	at 308 K
B1 (syn)	46.94	47.31	46.2	45.3	45.7	43.8	46.88
B2 (syn)	47.10	47.31	46.2	45.3	-		-
B3 (flipped)	46.91	47.31	46.0	45.4	-		-
B4 (anti)	54.48	54.72	53.7	51.8	59.4	58.7	56.04

6.4 Molecular orbitals of cycHC[12] concave octagon conformation (BP86/SVP)

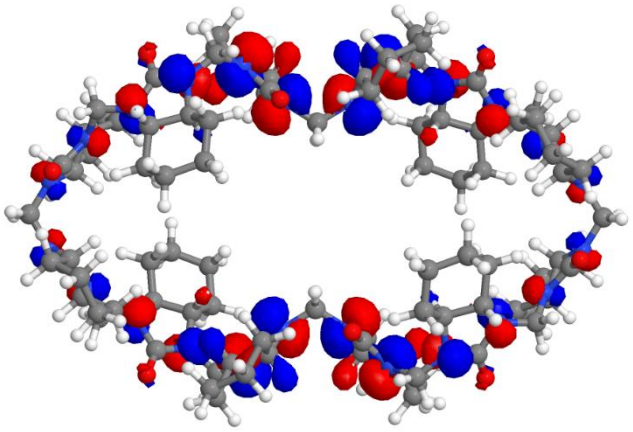


Figure S16. ***cycHC[12]*** *concave octagon HOMO orbital*

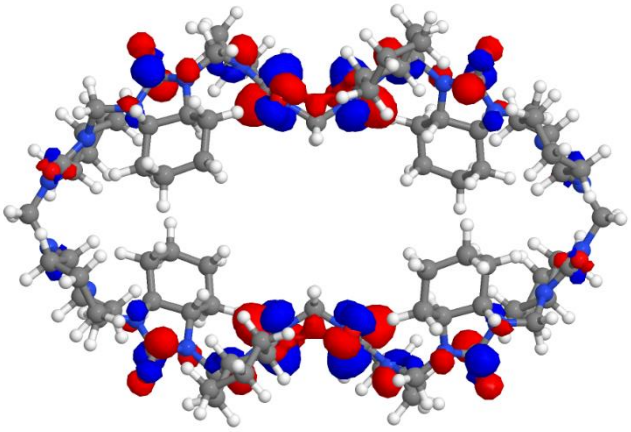


Figure S17. ***cycHC[12]*** *concave octagon LUMO orbital*

6.5 Molecular orbitals of cycHC[8]

The frontier orbitals of **cycHC[8]** were first published in Mario Öeren's PhD thesis[14] . Both orbitals are analogous to the orbitals of **cycHC[6]**[13].

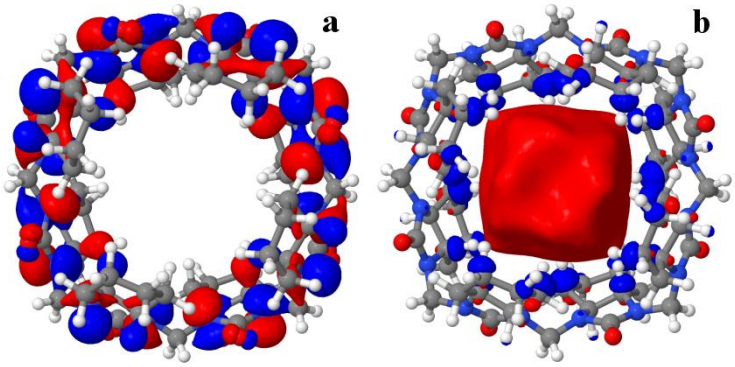


Figure S18. ***cycHC[8]*** *HOMO (a) and LUMO (b) orbitals*

6.6 Stereoview representation for BP86/SVP optimised geometries of cycHC[12]

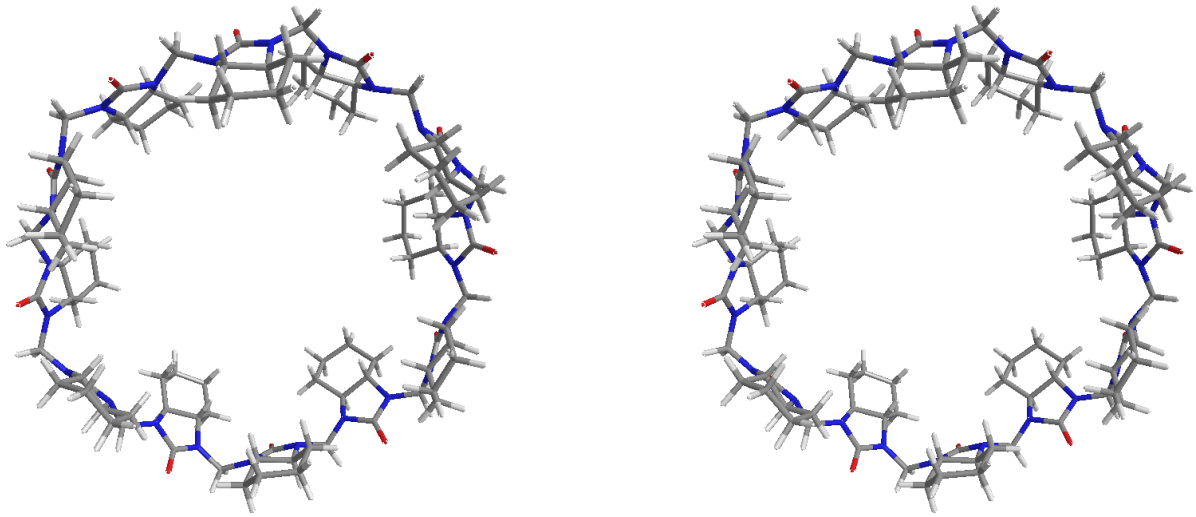


Figure S19. Regular 12-gon conformation

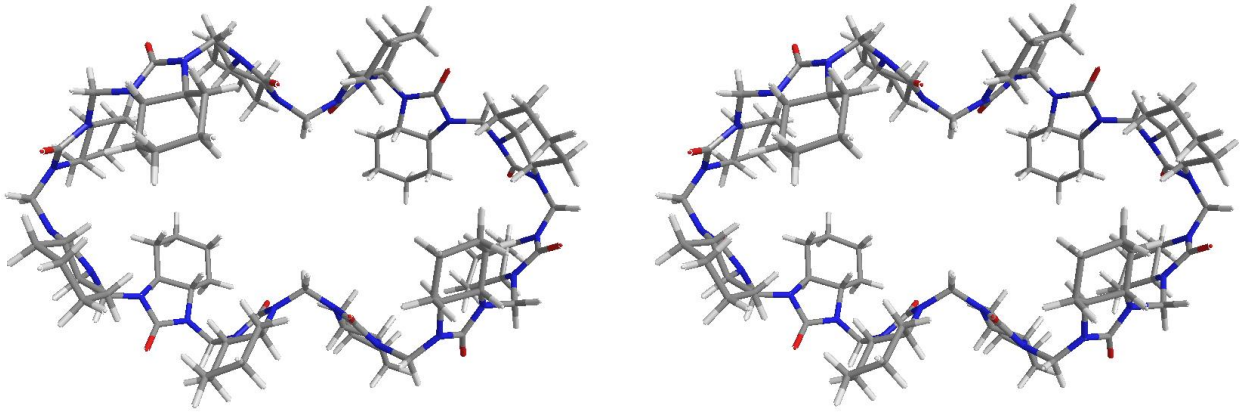


Figure S20. Concave octagon conformation

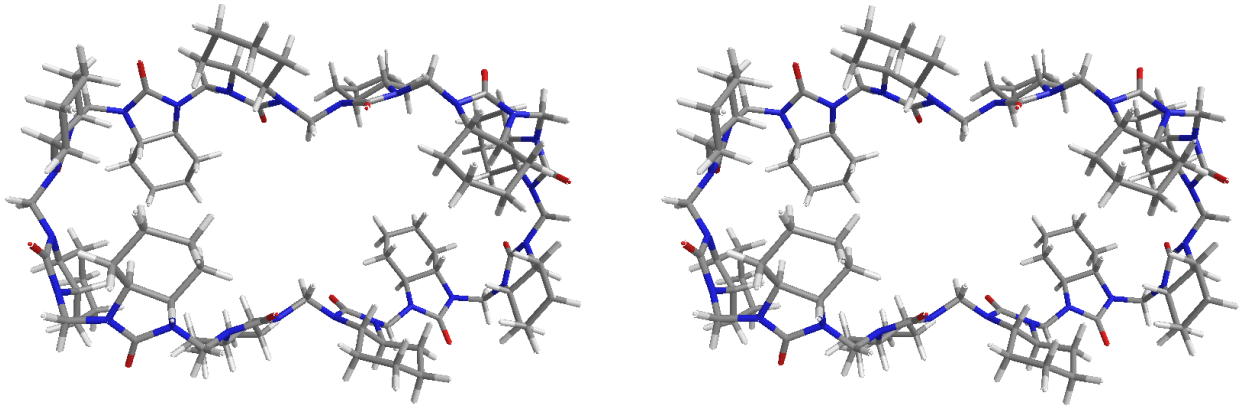


Figure S21. Concave 12-gon conformation

6.7 Stereoview representation for LC-TPSS/cc-pVTZ optimised geometries of cycHC[12]

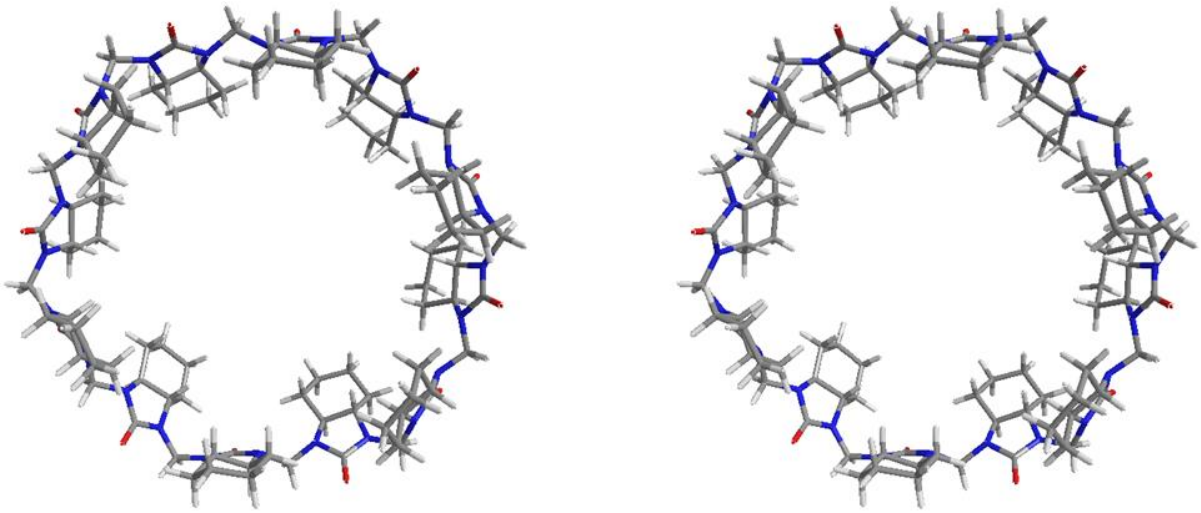


Figure S22. Regular 12-gon conformation

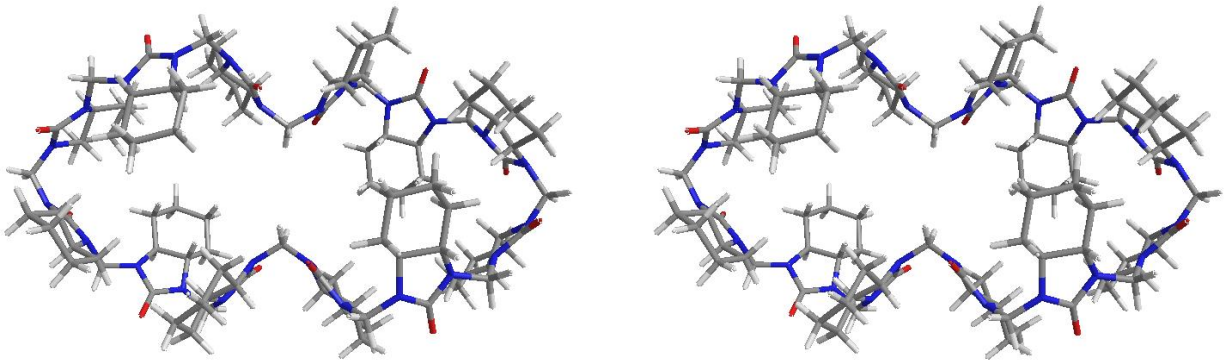


Figure S23. Concave octagon conformation

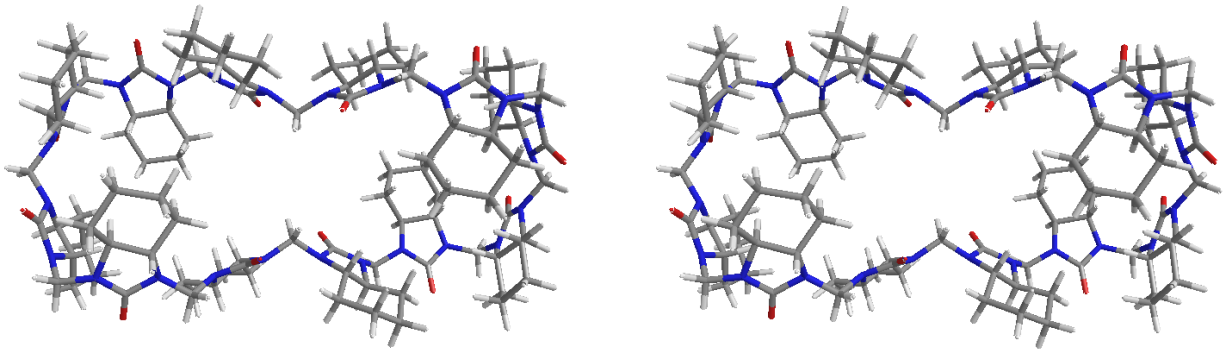


Figure S24. Concave 12-gon conformation

6.8 Optimised geometries of cycHC[12] uisng BP86/SVP

cycHC[12] in regular 12-gon conformation (Figure S19)

276

C	5.76787217	3.71708834	3.75428507
C	6.52827048	2.68852863	4.62923487
C	7.36729019	1.67617737	3.81121388
H	7.20429639	3.24539478	5.31734819
H	5.81262995	2.14275391	5.28063593
C	6.79462810	4.34427138	2.81363076
H	5.28515369	4.49188374	4.38691866
H	4.96609514	3.22382338	3.16097284
C	7.44547780	3.27110929	1.92686325
C	8.30979621	2.33881265	2.77511898
H	9.10639439	2.92454040	3.28661004
H	8.81017814	1.57293405	2.14548206
H	7.95742422	1.03545388	4.50061716
H	6.67868458	0.98868891	3.26906409
N	6.39318618	5.34852660	1.82143137
H	7.60319254	4.79008448	3.45314259
N	8.03780646	4.10648034	0.87949911
H	6.62639229	2.65236844	1.47598105
C	7.29248752	5.27782134	0.74022255
O	7.40947236	6.11881672	-0.15542198
C	7.50027035	4.14116228	-2.97797979
C	6.34143205	3.94324706	-3.98734554
C	6.43581817	2.62592721	-4.79590912
H	6.29756118	4.80767651	-4.68368961
H	5.38043056	3.95517773	-3.42424364
C	7.55679668	2.87799596	-2.11949916
H	7.33335820	5.04359893	-2.35255773
H	8.46747919	4.27775108	-3.51194429
C	7.82651972	1.64875102	-3.00147417
C	6.63456643	1.36729778	-3.91385876
H	5.73033912	1.16177674	-3.29879366
H	6.82016431	0.47090891	-4.54281240
H	5.52894003	2.50715483	-5.42662528
H	7.29300469	2.69706912	-5.50356752
N	8.58749087	2.70732479	-1.09275537
H	6.54905229	2.74847613	-1.64547542
N	8.26638811	0.66019564	-2.00978449
H	8.70137019	1.89239601	-3.66234491
C	8.88081925	1.35087918	-0.94766434
O	9.57324601	0.84144147	-0.06213115
C	9.01126722	3.69314780	-0.11495499
H	9.89030229	3.24795258	0.39465755
H	9.31468976	4.62277133	-0.63872311
C	-6.37586464	6.06964006	1.10583604
C	-5.50527752	6.17438129	-0.17168005
C	-4.26664807	7.08911480	-0.00897637
H	-6.12566957	6.53140708	-1.02120849
H	-5.16580467	5.15052562	-0.44962914
C	-5.44000944	5.66338356	2.24376736
H	-7.19098001	5.32728291	0.97231221
H	-6.85073165	7.04926045	1.33865039
C	-4.34313899	6.72297421	2.43435041
C	-3.40219721	6.75076380	1.23190645
H	-2.90701089	5.76080559	1.11835410
H	-2.60327307	7.50931290	1.37259580
H	-3.64395502	7.04434341	-0.92800898
H	-4.60689093	8.14607352	0.07830082
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H	-4.94443393	4.70338569	1.94418496
N	-3.84227510	6.39565818	3.77470147
H	-4.84703809	7.72549193	2.48591805
C	-4.90391651	5.83439418	4.51133056
O	-4.92160760	5.66423831	5.73344488
C	5.93120672	6.66257720	2.24536818
H	-9.63595647	-3.88270130	-0.78388551
H	-9.56937748	-3.98695031	1.02555427
H	-7.09483990	-1.49140417	-0.77008449
H	-6.08205371	-3.90582656	0.93389514
H	-5.47901947	-0.97767161	6.14543848
H	-9.59388189	1.40769955	1.75509264
C	-9.01162935	-3.69219070	0.11306265
H	-9.09095815	1.44392270	-2.45528654
H	-5.51069954	2.31999653	4.01176017
H	-8.46819690	-2.42932990	-2.67188380
H	-3.93963830	-6.45522087	3.00926421
O	-7.97872290	-4.80766761	-2.36483300
H	-4.07537235	-5.27420036	0.78104889
H	-9.42621591	0.13248249	3.04425430
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N	-7.84682041	-4.54589535	-0.03474741
H	-5.63418699	-0.10203678	3.78165107
H	-7.67647936	-4.18434832	2.87358605
C	-6.13544564	-0.10677780	5.93326914
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C	-8.04541353	1.08128360	-2.32903821
C	-8.75958503	-1.63057125	1.48521979
C	-6.49850334	2.42118877	4.53223965
N	-6.22790439	-5.72805360	-1.09135283
C	-8.67563005	-1.43385925	-2.22532991
O	-8.57651748	3.53263530	1.90547134
C	-4.70005606	-6.17518819	0.97122656
C	-4.91974542	-6.39204942	2.48990499
C	-7.70360862	1.09455856	-0.81753014
C	-6.22124933	2.48491938	6.03393438
C	-7.96191566	2.91205004	2.77741131
N	-7.28023968	3.46356854	3.86226962
H	-5.27090788	1.15881468	7.49628584
H	-7.05582120	-0.26305980	6.54076022
N	-8.43298513	-0.27729000	1.27394257
C	-6.53420188	-0.09794635	4.43604059
C	-7.13554856	-5.04311554	2.42268632
H	-8.26726289	-0.27049788	-4.03642173
C	-6.08061559	-5.98770423	0.34567017
C	-7.91608332	-0.31620786	-2.98350055
C	-5.44118696	1.19652853	6.39917173
C	-8.54175004	-0.00192798	-0.16358390
N	-7.84893503	1.51068751	2.86391909
H	-7.40301226	1.80929174	-2.86909465
C	-7.33871451	1.17833116	4.19960070
C	-5.79377297	-5.29974646	3.15392365
H	-5.40721248	-7.38287519	2.63568551
H	-9.77497357	-1.26621254	-2.27638152
H	-5.22158412	-4.34445845	3.18159318
H	-4.17605533	-7.04478087	0.52091632
H	-7.93047319	2.08592027	-0.37112630
H	-7.18265736	2.53326891	6.59317410
H	-7.79978034	-5.93342340	2.49628283
H	-7.13507804	-0.99702197	4.18298603
H	-6.83891171	-0.59560423	-3.03230784
H	-4.43043550	1.25514422	5.93467023
H	-9.61825659	0.21891735	-0.39561532
H	-8.20880251	1.15961491	4.90977685
H	-5.98871098	-5.56922610	4.21384985
C	-7.16367830	4.89820458	4.04817939
H	-7.25893494	5.13664145	5.12743028
H	-8.01605426	5.33971063	3.49201219
C	8.84944754	-0.60424263	-2.43539204
H	2.69770487	-7.54737026	-5.51926214
H	3.59141351	-8.09553876	-4.02996590
H	3.94843694	-5.65676086	-6.46267290
H	1.91407867	-8.92583803	-2.44071465
H	5.89404249	-4.62625066	0.54317586
H	7.64055328	-4.47592643	-5.15183029
C	2.93667264	-7.30439842	-4.45954819
H	3.69644029	-1.76867239	-6.05130052
H	9.04703942	-3.09046130	-1.19907556

H	1.53569432	-5.05208820	-6.09698355
H	-0.05856664	-7.28147663	0.51807527
O	0.34697809	-7.54477009	-5.67147257
H	0.03718375	-9.83687534	-1.24341011
H	7.53750497	-5.77846872	-3.89411013
H	5.52519537	-3.99775327	-7.20413259
O	5.49410683	-6.98280802	-3.19887808
C	3.64398372	-5.11384836	-5.52769404
C	0.50448778	-7.64043632	-4.45128988
H	6.50992004	-1.91580381	0.09561656
C	7.12293259	-4.80493050	-4.22737366
C	1.57066220	-7.85744341	-2.39363304
N	1.66979021	-7.28750591	-3.74264546
H	8.43149205	-5.40933040	-1.06619562
H	3.38385292	-7.18591017	-1.37678414
C	6.99595728	-4.77747713	0.48210922
N	3.69831344	-6.06475823	-4.41085681
C	3.92272098	-2.53168379	-6.83065192
C	5.02962113	-6.12432635	-3.95391376
C	7.99800825	-2.69725228	-1.28069555
N	-0.42051023	-8.13645033	-3.53255689
C	2.35959336	-4.35122269	-5.84509369
O	7.93708875	-2.06045358	-4.73448990
C	-0.30771241	-8.80331397	-1.01503162
C	0.41213077	-8.25246377	0.24166111
C	5.18153295	-3.32053275	-6.39011419
C	7.56344103	-2.27321377	0.12050374
C	7.77845969	-2.49000477	-3.58842526
N	7.95297924	-1.75100715	-2.40205033
H	7.33077650	-3.28757030	2.05087297
H	7.22066127	-5.64932194	1.13285233
N	5.72567601	-5.05950718	-4.52601759
C	7.36173581	-5.11161871	-0.98635751
C	2.28551665	-7.20387218	-1.21302374
H	1.79189197	-2.78129224	-7.26736605
C	0.04993529	-7.86991726	-2.17114006
C	2.67280550	-3.42034292	-7.04380596
C	7.70904644	-3.51776034	1.03190864
C	4.77928494	-4.14292596	-5.16634159
N	7.42231935	-3.79102292	-3.23305037
H	4.14121732	-1.96341652	-7.75983808
C	7.11542698	-3.84233472	-1.80137764
C	1.93279117	-8.03731516	0.04495085
H	0.23822068	-8.93221783	1.10289897
H	2.03973494	-3.76544650	-4.95476792
H	2.36400552	-7.55817800	0.94985889
H	-1.40634526	-8.84536102	-0.85829485
H	6.01997753	-2.63200543	-6.15288361
H	8.19122033	-1.43627393	0.49312994
H	1.94653893	-6.14964466	-1.10430992
H	6.75053154	-5.95735867	-1.36651811
H	-0.26434347	-6.83486891	-1.87645656
H	2.82873285	-4.05258112	-7.94741485
H	8.79384082	-3.73995615	1.15192777
H	4.39015994	-3.42841845	-4.39497766
H	6.04396504	-3.54864428	-1.65104282
H	2.43012237	-9.03016622	-0.04136510
H	-2.38229639	-5.55767184	-3.91410709
H	-1.76835055	-6.43439866	-6.20235750
H	-4.71690473	-3.20689476	-6.02354930
C	-3.02620409	-6.32800396	-4.41298665
C	-2.81563124	-6.19487360	-5.92094547
C	-4.56979342	-4.28586809	-5.80324027
H	-3.09941203	-4.59860374	-7.39454032
H	-4.16383604	-3.91538193	-3.66346222
C	-3.17101506	-4.73330259	-6.29417330
H	-3.47852661	-6.90948886	-6.45879608
C	-4.81618266	-4.55618961	-4.29755813
C	-4.48949778	-6.02772420	-4.05271256
H	-5.34823814	-4.82592839	-6.38883116
H	-2.39976838	-4.06143290	-5.85305566
H	-5.86948864	-4.33389749	-4.02446403
H	-5.13756770	-6.63183184	-4.74322193
N	-2.83815852	-7.61220131	-3.73327975
O	-3.67180325	-8.54936474	-1.74809234
C	-3.68771161	-7.68544774	-2.62930267
N	-4.59207592	-6.60850636	-2.70849323
C	-1.75199157	-8.55418954	-3.93133214
H	-1.67461830	-8.80238609	-5.00981415
H	-2.03757149	-9.46100981	-3.35957824
H	9.20263058	-0.50682450	-3.48623090
H	9.71510812	-0.79884568	-1.76333432
C	-5.89038413	-6.75553871	-2.06616530
H	-5.88604168	-7.74793866	-1.56251910
H	-6.68628421	-6.73110433	-2.84385497
H	-6.68728775	-6.89829924	0.59918708
H	1.74522594	4.36432658	7.68032717
H	-0.65105533	4.93371277	7.91930092
H	1.28996721	6.78119076	7.11849076
C	-0.33932924	4.36746421	7.01225470
C	1.16943016	4.60971799	6.76256375
H	-0.51329108	3.29564338	7.24743862
C	1.50227400	6.05203328	6.30448068
H	2.57712627	6.14850794	6.04235347
H	-1.01344343	6.85205990	6.42844435
H	1.52541677	3.90207153	5.97943289
C	-1.24304097	4.80252593	5.83090246
H	-2.31574231	4.72581361	6.10822112
C	-0.87054776	6.24475747	5.49442718
C	0.61101170	6.34705740	5.09852028
H	2.41401821	8.59309321	5.02737418
O	4.31120774	7.07700584	4.57871353
N	0.62728641	7.65958441	4.44827292
H	-1.08066532	4.15430763	4.94120083
C	1.79402679	8.45689019	4.11751334
N	-1.52443861	6.95217898	4.38693496
H	0.81756304	5.55947788	4.32781263
C	-2.93553489	7.30136006	4.46515863
C	-0.62851786	7.92540644	3.90237253
C	3.87118655	7.26327923	3.44080823
H	1.39822629	9.43867123	3.78560625
N	2.69677498	7.93777828	3.10662431
O	-0.91725223	8.85724819	3.14666116
N	4.48745262	6.85059627	2.24337917
C	2.41004373	7.74811192	1.68241883
H	1.84955042	6.78596324	1.55193864
C	3.83028793	7.54760669	1.13115351
H	0.65655656	8.99573079	1.27729268
H	4.29959950	8.56322030	1.03105175
C	1.67671743	8.81913912	0.87548049
H	2.23155263	9.78242529	0.93564724
C	3.78688907	6.92968533	-0.26467968
H	3.28783910	5.93605304	-0.22095346
C	1.61768791	8.31324430	-0.58819682
H	0.93745371	7.43201655	-0.62733274
C	2.99695379	7.91158611	-1.16617601
H	3.61108898	8.83000732	-1.30722530
H	1.15159640	9.08719868	-1.23459570
H	2.86599396	7.47427708	-2.17907977
H	4.81282714	6.77093852	-0.65926506
H	-3.03395288	8.32151590	4.03072128
H	-3.25220341	7.31402636	5.53224604
H	6.39573175	7.40202869	1.55523333
H	6.27550280	6.85108753	3.28674313

cycHC[12] in concave octagon conformation (Figure S20)

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C	3.50899493	-7.53801965	1.59824113
C	3.58023000	-8.03390557	3.06427896
C	2.26147480	-8.67128732	3.56565090
H	4.39926338	-8.78488546	3.14191201
H	3.87075318	-7.19615277	3.73376456
C	3.01200090	-8.71370007	0.75888696
H	4.50402523	-7.18884995	1.24879965
H	2.80451344	-6.68229275	1.50063323
C	1.61901483	-9.16069796	1.22797473
C	1.69747474	-9.76801151	2.62757591
H	2.36179988	-10.66106462	2.61642657
H	0.69097247	-10.08492092	2.97053044
H	2.41010878	-9.08823428	4.58454956
H	1.49087795	-7.87434976	3.67152078
N	2.79503662	-8.57230524	-0.68305205
H	3.72177115	-9.56752177	0.92693056
N	1.18770591	-9.96875919	0.08066360
H	0.97134021	-8.24847407	1.29367344
C	1.80070007	-9.47840887	-1.07845698
O	1.52606608	-9.78999249	-2.24076982
C	-1.79645185	-9.76187540	-2.60672413
C	-2.34363902	-8.66343557	-3.55266374
C	-3.65280962	-8.00259283	-3.05642964
H	-2.49826616	-9.08521733	-4.56867439
H	-1.56103215	-7.87902412	-3.66382158
C	-1.70934819	-9.14588410	-1.21143445
H	-0.79471566	-10.09613461	-2.94711016
H	-2.47405535	-10.64479429	-2.58954129
C	-3.09596333	-8.67568908	-0.74609025
C	-3.57538534	-7.49849504	-1.59350538
H	-2.85890189	-6.65226248	-1.50061924
H	-4.56563525	-7.13307341	-1.24712342
H	-3.92973493	-7.16473626	-3.73152754
H	-4.48331436	-8.74129341	-3.13005264
N	-1.28977188	-9.95189518	-0.05840568
H	-1.04859978	-8.24355862	-1.28350594
N	-2.87793867	-8.52798170	0.69511208
H	-3.81790805	-9.52024980	-0.90903991
C	-1.89647655	-9.44538477	1.09702413
O	-1.62696634	-9.75320917	2.26152457
C	-0.05636034	-10.72104016	0.01392908
H	-0.13228416	-11.35685543	0.91801792
H	0.01062198	-11.36475179	-0.88525348
C	6.76184704	3.64816889	-1.07177988
C	6.38621931	3.81338779	-2.56554897
C	5.80321369	2.53231318	-3.20825164
H	7.27375987	4.15270323	-3.14122959
H	5.63776095	4.63398988	-2.64706187
C	5.53298237	3.08128118	-0.36406428
H	7.04260581	4.62920671	-0.63572598
H	7.62239440	2.95210926	-0.95346091
C	5.13618367	1.72501764	-0.97100462
C	4.63682253	1.90587351	-2.40328746
H	3.74609308	2.57369423	-2.41205733
H	4.34268891	0.92938169	-2.84098546
H	5.47012005	2.75004987	-4.24556946
H	6.61098361	1.77107980	-3.30125500
N	5.57932507	2.74469286	1.06478662
H	4.68527405	3.79314149	-0.54081494
N	4.25243859	1.20182100	0.07844192
H	6.05830850	1.08853236	-1.01549708
C	4.66497128	1.71412548	1.31404013
O	4.28749746	1.32765581	2.42515653
C	3.85856611	-8.20157321	-1.60112432
H	-0.01058260	11.36485965	-0.88528965
H	0.13225593	11.35700316	0.91798828
H	1.04874042	8.24374731	-1.28352452
H	-0.97126261	8.24865958	1.29374552
H	0.34866884	5.52409649	4.73002223
H	4.92790221	8.40124597	1.17387979
C	0.05638140	10.72116955	0.01390862
H	4.48353409	8.74159246	-3.12989009
H	3.03253890	4.19185637	2.18742376
H	0.79490896	10.09636764	-2.94709268
H	-3.87061892	7.19640783	3.73392528
O	-1.52605077	9.78995512	-2.24079142
H	-2.80439267	6.68245026	1.50080145
H	3.77718144	8.71423197	2.54914194
H	2.85906567	6.65248189	-1.50060799
O	1.62689615	9.75335593	2.26156041
C	1.70947058	9.14608228	-1.21140227
C	-1.80066521	9.47844170	-1.07846041
H	3.76331452	2.86554981	4.17953809
C	3.93827188	8.13986240	1.60983764
C	-1.61896019	9.16086359	1.22799328
N	-1.18767902	9.96887255	0.08063662
H	1.26939957	5.83703813	2.39862939
H	-0.69092624	10.08521466	2.97048633
C	1.44896762	5.51891100	4.57549404
N	1.28982235	9.95206478	-0.05838107
C	3.65303522	8.00287924	-3.05633473
C	1.89647777	9.44555162	1.09706952
C	3.70839171	4.66212168	2.94761909
N	-2.79497962	8.57233307	-0.68299251
C	1.79663326	9.76211441	-2.60666914
O	6.03242464	6.29163603	0.85343676
C	-3.50889537	7.53816565	1.59837401
C	-3.58012617	8.03412938	3.06438658
C	3.57554271	7.49872554	-1.59342945
C	3.48210485	3.93444077	4.27203211
C	5.12314811	5.96433369	1.62102335
N	5.05481405	4.78616337	2.37477288
H	1.77012276	3.61162930	5.60059367
H	1.88064208	6.07984697	5.43566126
N	2.87795794	8.52814930	0.69518812
C	1.80234967	6.27609850	3.27126041
C	-1.69742348	9.76825894	2.62755904
H	2.49855544	9.08553305	-4.56860793
C	-3.01194001	8.71381071	0.75894311
C	2.34388281	8.66371638	-3.55261818
C	1.97455972	4.06345132	4.60648763
C	3.09606735	8.67589059	-0.74599958
N	3.97354509	6.71679925	1.90254122
H	3.93000520	7.16504780	-3.73144550
C	3.31158150	6.14070089	3.07563964
C	-2.26138261	8.67157716	3.56570693
H	-4.39918092	8.78509026	3.14198515
H	2.47422370	10.64504265	-2.58942492
H	-1.49076165	7.87466836	3.67161660
H	-4.50392035	7.18895194	1.24896135
H	4.56578074	7.13330077	-1.24701439
H	4.10685656	4.39555031	5.06961900
H	-2.36177237	10.66129308	2.61636215
H	1.50339476	7.34381241	3.33917601
H	1.56129294	7.87929589	-3.66384151
H	1.40235955	3.45405454	3.87064054
H	3.81801867	9.52045658	-0.90888811
H	3.80578127	6.55113931	3.99670403
H	-2.41001679	9.08857962	4.58458253
C	5.95908891	3.67489097	2.11952747
H	6.05595372	3.07803379	3.04791116
H	6.94047977	4.11930151	1.86129554
C	-3.93831961	-8.13976936	1.60972122
H	-2.84856727	0.00176102	-0.90709017
H	-2.85252106	0.06195699	0.90477903
H	-6.05805931	-1.08888239	-1.01597962
H	-6.05599042	1.17073180	0.99885764
H	-1.40314396	-3.45389218	3.87125207

H	-6.94086775	-4.11951339	1.86092763
C	-3.48844338	0.03376589	-0.00261596
H	-5.63680803	-4.63460641	-2.64683753
H	-3.80627406	-6.55121664	3.99674004
H	-4.34176907	-0.93003858	-2.84097356
H	-5.62387857	4.71260661	2.63465423
O	-4.26862299	1.40112082	-2.43391872
H	-7.60930432	3.04296532	0.92999253
H	-6.05667541	-3.07818030	3.04774442
H	-7.62207627	-2.95254680	-0.95417731
O	-4.28826710	-1.32760934	2.42532889
C	-5.13592293	-1.72531348	-0.97106230
C	-4.64872129	1.78935065	-1.32429632
H	-1.26972987	-5.83674363	2.39908901
C	-5.95957032	-3.67502310	2.11937653
C	-5.13005032	1.80192079	0.95859827
N	-4.24477675	1.27402167	-0.08713533
H	-4.10772950	-4.39573545	5.06976109
H	-4.34851788	1.00141050	2.83157326
C	-1.97539630	-4.06339676	4.60696925
N	-4.25256522	-1.20192243	0.07862352
C	-6.38532172	-3.81401845	-2.56571948
C	-4.66541674	-1.71417486	1.31413570
C	-3.31198399	-6.14066257	3.07577457
N	-5.55797769	2.82539184	-1.07863569
C	-4.63604340	-1.90642626	-2.40314278
O	-6.03251477	-6.29171407	0.85320881
C	-6.74535445	3.73395267	1.05313435
C	-6.37606706	3.89587184	2.54886967
C	-6.76145737	-3.64858330	-1.07211109
C	-1.80276735	-6.27592725	3.27160392
C	-5.12337220	-5.96436873	1.62093160
N	-3.97372531	-6.71673759	1.90254164
H	-0.34937829	-5.52388857	4.73063671
H	-1.77115116	-3.61162654	5.60113912
N	-5.57962717	-2.74481777	1.06470751
C	-3.48290504	-3.93450448	4.27229984
C	-4.63587469	1.97953853	2.39308143
H	-5.46864618	-2.75094065	-4.24557766
C	-5.51635414	3.16075366	0.35069391
C	-5.80212685	-2.53303730	-3.20841917
C	-1.44965446	-5.51880260	4.57594804
C	-5.53284764	-3.08153249	-0.36408873
N	-5.05525177	-4.78623624	2.37475479
H	-7.27265131	-4.15345347	-3.14165405
C	-3.70892510	-4.66211073	2.94780295
C	-5.80260594	2.61131735	3.19326405
H	-7.26460904	4.23920948	3.12060401
H	-3.74531287	-2.57425686	-2.41144083
H	-5.47314825	2.82658072	4.23225611
H	-7.01825792	4.71702939	0.61674025
H	-7.04230686	-4.62956765	-0.63600325
H	-1.50371570	-7.34361710	3.33947698
H	-3.74197920	2.64304854	2.40586463
H	-3.76421116	-2.86563423	4.17984356
H	-4.66555994	3.86771764	0.53199878
H	-6.60987903	-1.77183702	-3.30184866
H	-1.88139793	-6.07984550	5.43601094
H	-4.68504546	-3.79336207	-0.54050448
H	-3.03300329	-4.19172911	2.18773932
H	-6.61467414	1.85415650	3.28196603
H	-2.99405767	4.24711771	-2.19138560
H	-3.73060215	2.93515868	-4.19035448
H	-0.28694742	5.56048900	-4.71942486
C	-3.66206870	4.72703606	-2.95244842
C	-3.43822213	4.00142810	-4.27842461
C	-1.38781687	5.56595647	-4.56891565
H	-1.72466208	3.66556982	-5.60174562
H	-1.21342433	5.87445909	-2.39024660
C	-1.92813526	4.11607999	-4.60684295
H	-4.05519315	4.47145357	-5.07686036
C	-1.73826090	6.32218728	-3.26337505
C	-3.24948288	6.20181204	-3.07390576
H	-1.81057683	6.13421550	-5.42870475
H	-1.36500334	3.49832002	-3.87097817
H	-1.42789178	7.38694597	-3.32628183
H	-3.73607751	6.62056293	-3.99527672
N	-5.00941339	4.86322114	-2.38440211
O	-5.97642942	6.37335551	-0.86077890
C	-5.06801120	6.03933266	-1.62643760
N	-3.90956425	6.78050893	-1.90112785
C	-5.92484909	3.75991140	-2.13422441
H	-6.02307203	3.16504805	-3.06371934
H	-6.90333116	4.21273553	-1.87969666
H	-4.92790664	-8.40115962	1.17367118
H	-3.77727447	-8.71420854	2.54899131
C	-3.85851202	8.20152387	-1.60104067
H	-4.84571535	8.47168914	-1.16504442
H	-3.68959270	8.77913763	-2.53697969
H	-3.72173194	9.56762421	0.92694343
H	7.26507200	-4.23868782	3.12010306
H	6.61496388	-1.85367279	3.28134225
H	7.60942760	-3.04259600	0.92935296
C	5.80294587	-2.61090556	3.19279359
C	6.37643943	-3.89546785	2.54843914
H	5.47362244	-2.82611002	4.23184037
C	6.74554787	-3.73364399	1.05264795
H	7.01848190	-4.71673683	0.61630909
H	6.05594572	-1.17048025	0.99823785
H	5.62432556	-4.71225544	2.63437432
C	4.63606923	-1.97929275	2.39269125
H	4.34866227	-1.00115468	2.83113363
C	5.13006221	-1.80176597	0.95814107
C	5.51642384	-3.16060464	0.35029499
H	6.90322139	-4.21265475	-1.88017288
O	5.97645731	-6.37326176	-0.86104625
N	5.55785817	-2.82534705	-1.07906249
H	3.74223267	-2.64287901	2.40563458
C	5.92469418	-3.75989613	-2.13464155
N	4.24461267	-1.27404299	-0.08751867
H	4.66570897	-3.86762679	0.53174691
C	3.48825866	-0.03380844	-0.00295419
C	4.64847941	-1.78941250	-1.32469513
C	5.06799531	-6.03933191	-1.62669459
H	6.02281083	-3.16505674	-3.06416189
N	5.00930935	-4.86327097	-2.38473099
O	4.26822211	-1.40130458	-2.43430190
N	3.90958103	-6.78058080	-1.90129705
C	3.66193266	-4.72719374	-2.95274094
H	2.99392739	-4.24727093	-2.19167788
C	3.24942548	-6.20199767	-3.07408534
H	3.73029763	-2.93539357	-4.19076198
H	3.73600944	-6.62078105	-3.99544719
C	3.43798371	-4.00168535	-4.27875333
H	4.05494834	-4.47172261	-5.07718682
C	1.73820317	-6.32247767	-3.26347910
H	1.21338239	-5.87472467	-2.39035485
C	1.92788792	-4.11645275	-4.60709744
H	1.36475365	-3.49867486	-3.87125090
C	1.38765477	-5.56635779	-4.56905124
H	1.81041190	-6.13464674	-5.42882200
H	1.72434510	-3.66602320	-5.60202232
H	0.28677662	-5.56097199	-4.71950973
H	1.42789362	-7.38725833	-3.32630491
H	2.84844592	-0.00175489	-0.90747218
H	2.85227871	-0.06202002	0.90440302
H	3.68963444	-8.77924173	-2.53702788
H	4.84577403	-8.47172256	-1.16512838

cycHC[12] in concave 12-gon conformation (Figure S21)

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C	7.66527812	4.68149841	3.29186764
C	8.81339029	3.65805190	3.47397930
C	9.18262448	2.90468991	2.17270624
H	9.71204173	4.20048695	3.84703251
H	8.54724492	2.92795967	4.26790651
C	8.06208288	5.58534581	2.12646401
H	7.49481003	5.26835055	4.21837980
H	6.70776500	4.16613776	3.05434276
C	8.22318982	4.75761042	0.84264123
C	9.43526413	3.83338883	0.95856451
H	10.35690770	4.43950458	1.10703123
H	9.56348890	3.23477139	0.03267455
H	10.07400209	2.26544656	2.34901610
H	8.35405876	2.20815961	1.91052395
N	7.18111804	6.66566590	1.66782088
H	9.06290128	6.02960959	2.37443316
N	8.17692772	5.80748754	-0.17948504
H	7.31357123	4.10987306	0.73778453
C	7.41756647	6.88245070	0.30224044
O	7.03892811	7.85866408	-0.35109985
C	5.29354940	6.28460322	-2.78114698
C	3.75063103	6.24440540	-2.64333809
C	3.10465262	4.94678960	-3.18744320
H	3.30502828	7.12694447	-3.15013609
H	3.49560055	6.35038901	-1.56432235
C	5.82982154	4.99453536	-2.16086380
H	5.70650637	7.17389251	-2.26079518
H	5.59499250	6.34121065	-3.85107248
C	5.25669968	3.77384335	-2.89691212
C	3.75561227	3.65345197	-2.63772046
H	3.57165623	3.54953412	-1.54497488
H	3.33284522	2.75105315	-3.12758276
H	2.01632025	4.94701521	-2.96431226
H	3.18819205	4.93799071	-4.29821078
N	7.26462271	4.69029546	-2.18128262
H	5.46719425	4.95490516	-1.10017804
N	6.18540775	2.71973913	-2.47693261
H	5.39283068	3.94250067	-3.99859522
C	7.43572377	3.29969096	-2.21657915
O	8.49707787	2.68897459	-2.06228676
C	8.28841746	5.55422186	-1.60947582
H	9.26020990	5.06615673	-1.82326077
H	8.25231694	6.54572717	-2.10319887
C	-3.50899900	4.95894392	0.82749822
C	-3.05926871	6.35785903	0.33554512
C	-2.53862657	7.27834262	1.46742695
H	-3.89588112	6.85694809	-0.19835395
H	-2.25236720	6.22246775	-0.42041615
C	-2.35066997	4.38078842	1.64013232
H	-3.76818642	4.30028901	-0.02847347
H	-4.41445415	5.03550808	1.46966891
C	-2.03366707	5.28668144	2.83840453
C	-1.45693122	6.61725801	2.35806045
H	-0.52428856	6.43244164	1.77965650
H	-1.18670046	7.27148657	3.21370333
H	-2.14512410	8.22156985	1.03219833
H	-3.39447576	7.57479667	2.11583712
N	-2.46618161	3.07375384	2.29208067
H	-1.44781197	4.36412692	0.97285560
N	-1.24973294	4.38103949	3.68393270
H	-3.00017894	5.51167122	3.36320281
C	-1.66404909	3.06593446	3.44062253
O	-1.37686970	2.07480005	4.11808550
C	6.80872820	7.78162864	2.52619496
H	-9.49911359	-3.66324990	-3.44051844
H	-10.07385415	-3.18907883	-1.78874934
H	-6.30515809	-3.01348325	-2.61927900
H	-7.23163329	-4.29320179	-0.38255204
H	-7.10501090	-1.86693121	4.34593852
H	-6.72893174	1.33731466	-1.25001028
C	-9.18942671	-3.47207201	-2.39375333
H	-5.29173475	-0.08166551	-5.02758241
H	-4.08545224	-0.55571546	2.21604930
H	-7.31234082	-3.45646421	-4.88159760
H	-6.95889376	-6.59344535	2.78284966
O	-8.01287498	-5.60107857	-3.98673185
H	-5.89303693	-6.04387568	0.55764449
H	-7.88229623	0.64390941	-0.02401328
H	-4.46087992	-1.49243385	-2.38663307
O	-9.03359006	-1.45962485	-0.29994991
C	-7.00974518	-2.26796124	-3.07306367
C	-7.96732488	-5.60619447	-2.75339011
H	-3.62678854	0.78580454	4.30931391
C	-6.91748401	0.48996743	-0.55455838
C	-8.15065437	-4.91940690	-0.52834411
N	-8.64234766	-4.72678908	-1.89596207
H	-6.07375341	-1.89722757	2.03882950
H	-9.39379685	-3.61955139	0.71123609
C	-6.71590188	-0.92158251	3.91135743
N	-8.28789615	-2.32875159	-2.35594432
C	-4.83654591	-0.94512138	-4.49082653
C	-8.21397473	-1.50925355	-1.22136022
C	-4.62390217	0.41331592	2.39442957
N	-7.24556534	-6.51148640	-1.96139428
C	-6.95300370	-2.44751318	-4.58998056
O	-4.38941040	1.88539952	-0.79652684
C	-6.78791283	-6.70435609	0.60021302
C	-7.60445934	-6.44644011	1.89076199
C	-5.02298519	-0.72822250	-2.96865717
C	-4.65198122	0.64951494	3.90429144
C	-4.72813000	1.32494190	0.24983912
N	-4.07289995	1.42089444	1.48452040
H	-5.45627771	-0.43056918	5.63376895
H	-7.44751161	-0.13098476	4.19512022
N	-7.04721121	-0.73769772	-1.32448867
C	-6.68404025	-1.02591511	2.36580886
C	-9.06625831	-4.67936862	0.67201417
H	-5.39088112	-2.30014612	-6.11906826
C	-7.71137027	-6.39049830	-0.57507605
C	-5.47432750	-2.25613770	-5.01210097
C	-5.34086222	-0.58444355	4.53966682
C	-6.51847846	-0.86463509	-2.68620216
N	-5.83482350	0.48359946	0.41558733
H	-3.75546431	-0.92619366	-4.74609690
C	-6.05139416	0.26519992	1.84918206
C	-8.25471245	-5.04224285	1.94095931
H	-8.40351845	-7.21939012	1.96159316
H	-7.60699056	-1.69369020	-5.08278937
H	-7.45532122	-4.27793182	2.07219876
H	-6.41956254	-7.75043585	0.55622565
H	-4.64249907	0.26671523	-2.65499222
H	-5.22000473	1.58016692	4.12644412
H	-9.97423503	-5.31725794	0.58527617
H	-7.70467363	-1.16803175	1.95195849
H	-4.88847722	-3.12145451	-4.62666771
H	-4.66546538	-1.46278110	4.42445811
H	-7.05071135	-0.12262103	-3.33951789
H	-6.66134974	1.11889592	2.24832625
H	-8.90431596	-4.96117191	2.83857559
C	-2.68519757	1.84730689	1.54450583
H	-2.07627070	1.05694566	2.03668263
H	-2.34594463	1.98841515	0.49444538
C	6.10846106	1.36536080	-3.00283756
H	2.02720286	-7.33454357	-2.14827487
H	2.09439858	-6.63372769	-0.46945821
H	2.93958264	-5.37118494	-3.62877930
H	0.15271307	-7.75986498	0.78060472
H	6.10286124	-1.82182053	1.84920683
H	1.98523782	-1.16041755	-2.06934573
C	1.54707862	-6.62695006	-1.43775842
H	0.82311260	-2.92674997	-5.84896533
H	6.72262984	-1.25789904	-1.98197581
H	0.89983222	-6.60730806	-4.47598182
H	-3.43576699	-6.39106342	1.53840644

O	0.18533486	-8.65250366	-2.98244203
H	-1.74495250	-8.99343199	1.61353405
H	2.43763790	-1.88400915	-0.45982987
H	3.67957139	-3.33963851	-4.69743676
O	2.31978269	-4.25032177	0.02915641
C	1.90921309	-4.99799391	-3.38543754
C	-0.28974276	-8.20896596	-1.93325280
H	6.65366404	0.57216163	0.49422020
C	2.68573397	-1.84645725	-1.54364952
C	-0.43963242	-7.08666797	0.10488115
N	0.18861453	-7.10009710	-1.21990171
H	5.95890779	-3.27031686	-0.89615727
H	0.28713773	-5.24297078	1.03909878
C	6.60545881	-2.30505542	0.98042688
N	1.63904783	-5.27801667	-1.97182827
C	1.80219499	-3.45807334	-5.85169339
C	2.17472511	-4.24252223	-1.19666092
C	6.17741272	-0.55135393	-1.30101517
N	-1.38726282	-8.72830807	-1.23323754
C	0.97313333	-5.49927623	-4.48387514
O	3.44243605	0.28573691	-3.35149672
C	-2.41920465	-8.26284199	1.11310837
C	-2.63700748	-7.01299195	2.00288977
C	2.63858728	-2.94941701	-4.65060364
C	7.17142664	-0.08685152	-0.23800944
C	4.21596579	-0.14966299	-2.49367996
N	5.44479990	0.41279824	-2.12767248
H	8.39427995	-1.07996203	1.28634621
H	7.06196728	-3.23843127	1.37344937
N	2.52037469	-3.19452042	-2.05990826
C	5.52797920	-2.65140858	-0.07801984
C	-0.66953640	-5.77642347	0.85673244
H	0.86378900	-5.26351155	-6.66055342
C	-1.78037550	-7.77731970	-0.18790997
C	1.54558449	-4.98542022	-5.82882371
C	7.71563142	-1.36204829	0.45339686
C	1.95419781	-3.46341444	-3.38424982
N	4.02010891	-1.29778449	-1.71517938
H	2.29916630	-3.17569507	-6.80423541
C	5.02377094	-1.32586497	-0.64815168
C	-1.36838440	-6.14508661	2.18882210
H	-3.02940710	-7.32202043	2.99526173
H	-0.05187756	-5.10197288	-4.31053332
H	-1.62453981	-5.22114414	2.75004491
H	-3.38614232	-8.76981572	0.91271587
H	2.70305519	-1.84059872	-4.65131733
H	7.99413792	0.50775828	-0.68828526
H	-1.30979333	-5.10157473	0.24567935
H	4.69903162	-3.23612719	0.37435320
H	-2.46788818	-7.01236564	-0.63548762
H	2.50395726	-5.51682836	-6.02868650
H	8.34513447	-1.91726012	-0.27890064
H	0.89592951	-3.08841394	-3.39861481
H	4.64182731	-0.71393315	0.21228747
H	-0.64104830	-6.69745140	2.82657644
H	-2.81810967	-7.19199046	-3.34581044
H	-1.46261016	-8.78822137	-4.73862836
H	-4.05858182	-5.99880359	-6.87043653
C	-3.28077913	-8.14566782	-3.71245222
C	-2.52536992	-8.56906614	-4.97217575
C	-4.07433734	-6.90183533	-6.22354498
H	-2.16094726	-7.68571344	-6.94360415
H	-4.41379771	-5.73549133	-4.38165375
C	-2.62741523	-7.39508055	-5.97809164
H	-2.98308753	-9.49273453	-5.39191123
C	-4.85579523	-6.60361953	-4.92001922
C	-4.75080911	-7.85320535	-4.04818955
H	-4.63036475	-7.67834795	-6.79697286
H	-2.01823951	-6.54873710	-5.58689358
H	-5.91458383	-6.34698866	-5.13216244
H	-5.14132104	-8.71527250	-4.65220608
N	-3.42618705	-9.06655216	-2.58105562
O	-4.99297315	-9.26371919	-0.83801572
C	-4.63176153	-8.79368668	-1.92052074
N	-5.36946600	-7.90675787	-2.71856851
C	-2.30417632	-9.66387590	-1.86991904
H	-1.69504144	-10.26164501	-2.57698737
H	-2.74432376	-10.32988596	-1.10123590
H	5.54316766	1.37918285	-3.96067224
H	7.15201911	1.02772093	-3.18460606
C	-6.80735933	-7.78057777	-2.52544147
H	-7.12476250	-8.59854781	-1.84296432
H	-7.30746512	-7.89719029	-3.51128461
H	-8.62983920	-7.02521413	-0.45654796
H	5.10904164	2.48801495	6.26978751
H	2.73442766	1.82909520	6.49369442
H	3.74561830	4.33229287	7.31488063
C	3.09488797	2.13727570	5.48575012
C	4.35642204	3.01984856	5.64930606
H	3.36051163	1.19692916	4.95712347
C	4.07202190	4.41783783	6.25424081
H	4.98675517	5.04602738	6.22634209
H	1.49380260	3.92642621	6.55236371
H	4.82933456	3.16320761	4.65113426
C	1.93372390	2.84775801	4.74712843
H	1.01775075	2.22008795	4.74037968
C	1.69506000	4.16998765	5.47493206
C	2.95611948	5.04576029	5.41932525
H	3.98429648	7.43826982	6.64277984
O	5.96489471	7.00276724	5.17555481
N	2.40471080	6.35956586	5.76787957
H	2.20154426	3.04790739	3.68555289
C	3.20033219	7.57517847	5.87154496
N	0.66782282	5.11165976	5.01879807
H	3.30676065	5.07215378	4.35420797
C	-0.74467598	4.76380174	4.99243405
C	1.06224191	6.41143022	5.36871954
C	5.18151914	7.51647937	4.37203170
H	2.50234993	8.37612813	6.18712137
N	3.89173947	7.98504238	4.65688404
O	0.34509594	7.41554123	5.34223097
N	5.43660774	7.75484422	3.01343119
C	3.21194165	8.31093231	3.39957776
H	2.73980491	7.37912683	2.99117355
C	4.40535442	8.66345785	2.49914280
H	1.29789938	9.17782536	3.99664457
H	4.71412606	9.71619902	2.73766444
C	2.16231784	9.42087645	3.34414004
H	2.60662438	10.37620420	3.70299973
C	3.98627557	8.63487916	1.03076717
H	3.60634764	7.62134095	0.77146670
C	1.70855495	9.54225953	1.86771310
H	1.12829680	8.62818821	1.60658359
C	2.87558033	9.70113204	0.86272380
H	3.33270579	10.70858059	0.99333097
H	1.00205928	10.39289346	1.76022017
H	2.48240126	9.67766530	-0.17604721
H	4.84756611	8.83789198	0.36081122
H	-1.30503643	5.65357854	5.35346621
H	-0.91982817	3.90369197	5.67560587
H	6.95737397	8.71545222	1.94187130
H	7.47758966	7.78225608	3.41399125

6.9 Optimised geometries of cycHC[12] uisng LC-TPSS/cc-pVTZ

cycHC[12] in regular 12-gon conformation (Figure S22)

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C	6.33010	-2.53940	-2.70090
C	6.55290	-1.79210	-4.00400
C	7.01420	-0.35910	-3.80390
H	7.30630	-2.32920	-4.58290
H	5.64400	-1.80310	-4.60190
C	7.59170	-2.39040	-1.91030
H	6.10750	-3.58810	-2.89050
H	5.49350	-2.11740	-2.14350
C	7.87000	-0.94200	-1.62520
C	8.22590	-0.23490	-2.89700
H	9.09740	-0.70940	-3.34990
H	8.47350	0.80940	-2.71830
H	7.22670	0.09300	-4.77020
H	6.19820	0.22030	-3.36760
N	7.70010	-2.97160	-0.59790
H	8.41940	-2.77220	-2.52460
N	8.83240	-1.06760	-0.56550
H	6.95380	-0.48460	-1.22810
C	8.60420	-2.22310	0.11730
O	9.11630	-2.54930	1.16300
C	8.22670	0.22700	2.89780
C	7.01510	0.35230	3.80480
C	6.55520	1.78570	4.00490
H	7.22730	-0.10000	4.77110
H	6.19860	-0.22630	3.36850
C	7.87140	0.93440	1.62610
H	8.47330	-0.81750	2.71900
H	9.09860	0.70070	3.35060
C	7.59440	2.38310	1.91120
C	6.33300	2.53320	2.70180
H	5.49600	2.11200	2.14450
H	6.11130	3.58210	2.89140
H	5.64630	1.79750	4.60280
H	7.30910	2.32210	4.58380
N	8.83380	1.05910	0.56620
H	6.95480	0.47790	1.22900
N	7.70320	2.96420	0.59870
H	8.42250	2.76410	2.52540
C	8.60660	2.21490	-0.11660
O	9.11880	2.54050	-1.16230
C	9.59530	-0.00460	0.00020
H	10.22190	0.44960	-0.76290
H	10.22170	-0.45960	0.76310
C	-3.34950	-7.16120	3.13600
C	-2.46840	-6.26140	3.98460
C	-0.99570	-6.62720	3.92580
H	-2.80680	-6.27960	5.01830
H	-2.59480	-5.23340	3.63940
C	-2.77020	-7.13120	1.75520
H	-4.38090	-6.81500	3.14310
H	-3.33780	-8.18310	3.51760
C	-1.36620	-7.66500	1.77940
C	-0.45650	-6.72850	2.50970
H	-0.45640	-5.75540	2.01790
H	0.56650	-7.10040	2.51360
H	-0.41670	-5.90350	4.49570
H	-0.85000	-7.59060	4.41760
N	-3.33430	-7.94220	0.71140
H	-2.73810	-6.08550	1.42260
N	-1.14300	-7.95850	0.38760
H	-1.38210	-8.61550	2.33160
C	-2.35680	-8.30050	-0.16370
O	-2.51660	-8.84160	-1.23310
C	7.74520	-4.39160	-0.44710
H	-10.22170	0.45960	0.76310
H	-10.22190	-0.44960	-0.76280
H	-6.95480	-0.47790	1.22910
H	-6.95380	0.48460	-1.22810
H	-5.47880	-3.94840	-4.35170
H	-8.03880	-4.84000	1.39510
C	-9.59530	0.00460	0.00030
H	-7.30910	-2.32210	4.58380
H	-4.16580	-5.53180	-1.09470
H	-8.47330	0.81750	2.71910
H	-5.64400	1.80300	-4.60190
O	-9.11630	2.54930	1.16300
H	-5.49350	2.11740	-2.14350
H	-8.50840	-4.59720	-0.30640
H	-5.49600	-2.11200	2.14460
O	-9.11880	-2.54050	-1.16230
C	-7.87140	-0.93440	1.62610
C	-8.60420	2.22310	0.11730
H	-4.05440	-7.55990	-2.53430
C	-7.74960	-4.38410	0.44810
C	-7.87000	0.94200	-1.62520
N	-8.83240	1.06750	-0.56540
H	-5.13940	-3.52770	-1.92900
H	-8.47350	-0.80940	-2.71820
C	-5.74130	-4.72190	-3.63300
N	-8.83380	-1.05910	0.56630
C	-6.55530	-1.78570	4.00500
C	-8.60660	-2.21490	-0.11650
C	-5.05930	-6.14700	-1.26300
N	-7.70010	2.97160	-0.59790
C	-8.22670	-0.22700	2.89790
O	-6.40650	-6.35860	1.90960
C	-6.33010	2.53930	-2.70090
C	-6.55290	1.79200	-4.00400
C	-6.33300	-2.53320	2.70190
C	-4.88980	-6.86390	-2.56720
C	-6.11590	-6.10720	0.76300
N	-5.36170	-6.87920	-0.06390
H	-4.57960	-6.24240	-4.59990
H	-6.67210	-5.16670	-3.98920
N	-7.70320	-2.96420	0.59880
C	-6.00080	-4.10240	-2.27080
C	-8.22590	0.23480	-2.89700
H	-7.22740	0.10000	4.77120
C	-7.59170	2.39040	-1.91030
C	-7.01520	-0.35230	3.80490
C	-4.66040	-5.78870	-3.61450
C	-7.59440	-2.38310	1.91120
N	-6.51480	-4.99130	0.06160
H	-5.64640	-1.79750	4.60300
C	-6.25470	-5.24010	-1.33310
C	-7.01420	0.35910	-3.80390
H	-7.30630	2.32910	-4.58290
H	-9.09870	-0.70070	3.35060
H	-6.19820	-0.22030	-3.36750
H	-6.10750	3.58810	-2.89050
H	-6.11140	-3.58210	2.89150
H	-5.79130	-7.43530	-2.79250
H	-9.09740	0.70940	-3.34980
H	-6.85760	-3.43230	-2.31080
H	-6.19860	0.22630	3.36860
H	-3.69670	-5.31610	-3.41530
H	-8.42250	-2.76410	2.52550
H	-7.09240	-5.82590	-1.73770
H	-7.22670	-0.09310	-4.77020
C	-4.71650	-8.06560	0.38910
H	-4.77660	-8.83010	-0.38130
H	-5.26850	-8.38970	1.26760
C	7.74960	4.38420	0.44800
H	-0.31280	9.35940	0.83090
H	0.32250	9.35860	-0.83330
H	1.38210	8.61550	2.33140
H	-1.37380	8.61620	-2.33310
H	3.69670	5.31610	-3.41550
H	5.26850	8.38970	1.26740
C	0.00450	8.72950	-0.00100
H	2.59470	5.23340	3.63930
H	7.09240	5.82590	-1.73780

H	-0.56650	7.10040	2.51330
H	-2.58990	5.23490	-3.63970
O	-2.50730	8.84430	1.23180
H	-3.33010	8.18520	-3.51860
H	4.77660	8.83000	-0.38140
H	3.33780	8.18310	3.51740
O	2.51660	8.84160	-1.23330
C	1.36610	7.66500	1.77920
C	-2.34820	8.30280	0.16250
H	5.13940	3.52770	-1.92920
C	4.71650	8.06550	0.38890
C	-1.35860	7.66580	-1.78060
N	-1.13490	7.95950	-0.38890
H	5.79140	7.43530	-2.79260
H	0.57340	7.09920	-2.51500
C	4.66050	5.78870	-3.61470
N	1.14300	7.95850	0.38740
C	2.46830	6.26140	3.98450
C	2.35680	8.30050	-0.16390
C	6.25470	5.24010	-1.33320
N	-3.32630	7.94520	-0.71230
C	0.45650	6.72850	2.50950
O	6.40650	6.35860	1.90940
C	-3.34260	7.16350	-3.13660
C	-2.46260	6.26260	-3.98520
C	3.34940	7.16120	3.13580
C	6.00090	4.10240	-2.27090
C	6.11590	6.10720	0.76290
N	6.51480	4.99130	0.06150
H	5.47890	3.94840	-4.35180
H	4.57970	6.24240	-4.60010
N	3.33430	7.94220	0.71120
C	4.88990	6.86380	-2.56730
C	-0.44990	6.72820	-2.51080
H	0.41660	5.90350	4.49550
C	-2.76310	7.13340	-1.75590
C	0.99560	6.62720	3.92560
C	5.74140	4.72190	-3.63310
C	2.77020	7.13120	1.75500
N	5.36180	6.87920	-0.06410
H	2.80670	6.27950	5.01820
C	5.05940	6.14700	-1.26310
C	-0.98950	6.62710	-3.92680
H	-2.80120	6.28080	-5.01880
H	0.45640	5.75540	2.01770
H	-0.41130	5.90260	-4.49660
H	-4.37440	6.81820	-3.14340
H	4.38080	6.81500	3.14290
H	6.85770	3.43230	-2.31090
H	-0.45070	5.75530	-2.01870
H	4.05440	7.55990	-2.53440
H	-2.73190	6.08770	-1.42310
H	0.85000	7.59060	4.41740
H	6.67220	5.16670	-3.98930
H	2.73810	6.08540	1.42240
H	4.16580	5.53180	-1.09490
H	-0.84310	7.59010	-4.41890
H	-4.15990	5.53580	1.09480
H	-4.04600	7.56430	2.53360
H	-5.47420	3.95490	4.35240
C	-5.05270	6.15210	1.26290
C	-4.88230	6.86920	2.56690
C	-5.73600	4.72860	3.63350
H	-4.57250	6.24810	4.59980
H	-5.13570	3.53310	1.92980
C	-4.65390	5.79410	3.61450
H	-5.78310	7.44170	2.79210
C	-5.99640	4.10890	2.27150
C	-6.24910	5.24660	1.33350
H	-6.66620	5.17440	3.98970
H	-3.69070	5.32040	3.41530
H	-6.85390	3.43970	2.31190
H	-7.08610	5.83340	1.73800
N	-5.35450	6.88420	0.06370
O	-6.40030	6.36420	-1.90950
C	-6.10970	6.11280	-0.76290
N	-6.50970	4.99760	-0.06100
C	-4.70820	8.06990	-0.38970
H	-4.76750	8.83460	0.38050
H	-5.26010	8.39430	-1.26820
H	8.03880	4.84000	1.39500
H	8.50850	4.59720	-0.30650
C	-7.74520	4.39160	-0.44710
H	-8.03430	4.84770	-1.39400
H	-8.50350	4.60530	0.30760
H	-8.41940	2.77210	-2.52460
H	2.80110	-6.28080	-5.01870
H	0.84300	-7.59020	-4.41870
H	3.33010	-8.18520	-3.51840
C	0.98940	-6.62710	-3.92660
C	2.46250	-6.26260	-3.98500
H	0.41120	-5.90270	-4.49640
C	3.34260	-7.16350	-3.13650
H	4.37430	-6.81820	-3.14330
H	1.37370	-8.61620	-2.33290
H	2.58980	-5.23490	-3.63950
C	0.44990	-6.72820	-2.51060
H	-0.57350	-7.09920	-2.51480
C	1.35850	-7.66580	-1.78040
C	2.76310	-7.13340	-1.75580
H	5.26010	-8.39430	-1.26800
O	6.40020	-6.36420	-1.90940
N	3.32620	-7.94520	-0.71210
H	0.45060	-5.75530	-2.01860
C	4.70820	-8.06990	-0.38960
N	1.13490	-7.95950	-0.38880
H	2.73190	-6.08770	-1.42290
C	-0.00450	-8.72950	-0.00080
C	2.34820	-8.30280	0.16270
C	6.10960	-6.11280	-0.76280
H	4.76750	-8.83460	0.38060
N	5.35450	-6.88420	0.06380
O	2.50730	-8.84430	1.23200
N	6.50970	-4.99760	-0.06100
C	5.05280	-6.15210	1.26310
H	4.15990	-5.53580	1.09490
C	6.24910	-5.24660	1.33360
H	4.04610	-7.56420	2.53380
H	7.08610	-5.83340	1.73810
C	4.88230	-6.86910	2.56700
H	5.78320	-7.44160	2.79220
C	5.99640	-4.10880	2.27160
H	5.13570	-3.53310	1.92990
C	4.65400	-5.79400	3.61460
H	3.69080	-5.32040	3.41540
C	5.73600	-4.72850	3.63360
H	6.66630	-5.17440	3.98980
H	4.57260	-6.24800	4.59990
H	5.47430	-3.95490	4.35250
H	6.85400	-3.43970	2.31190
H	0.31280	-9.35940	0.83110
H	-0.32250	-9.35860	-0.83310
H	8.50360	-4.60530	0.30760
H	8.03430	-4.84770	-1.39400

cycHC[12] in concave octagon conformation (Figure S23)

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C	-7.04200	3.37610	-1.23170
C	-7.51940	3.63420	-2.64990
C	-8.24980	2.45080	-3.25950
H	-8.18810	4.49660	-2.63510
H	-6.67940	3.91110	-3.28410
C	-8.24300	2.92050	-0.46430
H	-6.61530	4.27740	-0.79370
H	-6.27570	2.60000	-1.21170
C	-8.79310	1.65110	-1.04760
C	-9.38320	1.92530	-2.39610
H	-10.17960	2.66510	-2.30650
H	-9.79760	1.01900	-2.82970
H	-8.62800	2.72310	-4.24250
H	-7.53990	1.63740	-3.41970
N	-8.12270	2.55840	0.92080
H	-9.01470	3.69750	-0.55590
N	-9.63170	1.20500	0.03590
H	-7.96230	0.94510	-1.17710
C	-9.09760	1.64720	1.21480
O	-9.42920	1.29650	2.32410
C	-9.38340	-1.92770	2.39510
C	-8.25020	-2.45270	3.25910
C	-7.51880	-3.63570	2.64980
H	-8.62870	-2.72520	4.24190
H	-7.54070	-1.63900	3.41960
C	-8.79280	-1.65320	1.04690
H	-9.79850	-1.02160	2.82860
H	-10.17940	-2.66790	2.30520
C	-8.24190	-2.92230	0.46390
C	-7.04100	-3.37730	1.23190
H	-6.27500	-2.60090	1.21210
H	-6.61370	-4.27840	0.79400
H	-6.67900	-3.91230	3.28440
H	-8.18710	-4.49850	2.63470
N	-9.63110	-1.20740	-0.03690
H	-7.96240	-0.94680	1.17680
N	-8.12110	-2.56010	-0.92120
H	-9.01320	-3.69970	0.55520
C	-9.09630	-1.64940	-1.21560
O	-9.42750	-1.29890	-2.32510
C	-10.39690	-0.00140	-0.00070
H	-11.02350	0.00700	-0.88730
H	-11.02390	-0.01010	0.88560
C	3.30160	5.95800	0.66980
C	3.70740	5.61200	2.09140
C	2.64250	4.84880	2.85750
H	3.97030	6.51790	2.63350
H	4.61520	5.00810	2.04630
C	2.87440	4.67350	0.03020
H	4.13960	6.39810	0.13530
H	2.47250	6.66650	0.66260
C	1.69770	4.10000	0.76990
C	2.13170	3.62280	2.12140
H	2.92030	2.87710	2.01190
H	1.30280	3.17490	2.66280
H	3.02870	4.56270	3.83360
H	1.79370	5.50820	3.04670
N	2.37900	4.66740	-1.32170
H	3.70700	3.96160	0.11010
N	1.18590	3.17040	-0.20420
H	0.96340	4.90400	0.91510
C	1.48390	3.64370	-1.45280
O	1.03180	3.22590	-2.49510
C	-7.67140	3.48120	1.90920
H	11.02390	0.01010	0.88560
H	11.02350	-0.00700	-0.88730
H	7.96240	0.94680	1.17680
H	7.96230	-0.94510	-1.17710
H	5.26610	-0.53250	-4.40990
H	7.88060	4.50360	-1.59060
C	10.39690	0.00140	-0.00070
H	8.18710	4.49850	2.63470
H	3.84560	2.31870	-2.24900
H	9.79850	1.02160	2.82860
H	6.67940	-3.91110	-3.28410
O	9.42920	-1.29650	2.32410
H	6.27570	-2.60000	-1.21170
H	8.21910	3.26450	-2.82490
H	6.27500	2.60090	1.21210
O	9.42760	1.29890	-2.32510
C	8.79270	1.65320	1.04690
C	9.09760	-1.64710	1.21480
H	2.49110	2.71880	-4.28160
C	7.66910	3.48290	-1.90930
C	8.79310	-1.65110	-1.04760
N	9.63170	-1.20500	0.03590
H	5.54630	0.68090	-2.26090
H	9.79760	-1.01900	-2.82970
C	5.20370	0.55390	-4.39440
N	9.63110	1.20740	-0.03690
C	7.51880	3.63570	2.64980
C	9.09630	1.64940	-1.21560
C	4.25770	2.90070	-3.08380
N	8.12270	-2.55840	0.92080
C	9.38340	1.92770	2.39510
O	5.75360	5.50660	-1.38820
C	7.04200	-3.37610	-1.23170
C	7.51930	-3.63420	-2.64990
C	7.04100	3.37730	1.23190
C	3.55020	2.48200	-4.33550
C	5.47520	4.50980	-2.01430
N	4.31620	4.29080	-2.70840
H	3.29960	0.61910	-5.37630
H	5.71360	0.90200	-5.29450
N	8.12110	2.56010	-0.92120
C	5.94090	1.10320	-3.18590
C	9.38320	-1.92530	-2.39610
H	8.62870	2.72510	4.24190
C	8.24300	-2.92050	-0.46430
C	8.25020	2.45270	3.25910
C	3.74780	0.98090	-4.45350
C	8.24190	2.92230	0.46390
N	6.26640	3.40480	-2.15430
H	6.67900	3.91220	3.28430
C	5.72080	2.58360	-3.19900
C	8.24980	-2.45080	-3.25950
H	8.18810	-4.49660	-2.63510
H	10.17940	2.66790	2.30520
H	7.53990	-1.63740	-3.41970
H	6.61530	-4.27730	-0.79370
H	6.61370	4.27840	0.79400
H	3.98090	3.00050	-5.19300
H	10.17960	-2.66510	-2.30650
H	7.00250	0.86440	-3.23560
H	7.54070	1.63900	3.41960
H	3.19990	0.50190	-3.64030
H	9.01320	3.69970	0.55520
H	6.07500	2.96750	-4.16580
H	8.62800	-2.72300	-4.24250
C	3.15900	5.08660	-2.44520
H	2.50700	5.06180	-3.31290
H	3.50280	6.10260	-2.27740
C	-7.66910	-3.48290	-1.90930
H	-0.12370	-1.77480	0.87910
H	0.12670	-1.77500	-0.87950
H	-0.96340	-4.90400	0.91510
H	0.96630	-4.90430	-0.91480
H	-3.19990	-0.50190	-3.64020
H	-3.50280	-6.10260	-2.27730
C	0.00150	-2.39950	-0.00010
H	-4.61520	-5.00810	2.04630
H	-6.07500	-2.96750	-4.16580
H	-1.30290	-3.17490	2.66290
H	4.61820	-5.00890	-2.04580

O	1.03460	-3.22530	2.49490
H	2.47520	-6.66680	-0.66180
H	-2.50700	-5.06180	-3.31290
H	-2.47240	-6.66650	0.66270
O	-1.03180	-3.22590	-2.49500
C	-1.69770	-4.10000	0.77000
C	1.48670	-3.64340	1.45280
H	-5.54630	-0.68090	-2.26090
C	-3.15900	-5.08660	-2.44510
C	1.70060	-4.10030	-0.76980
N	1.18890	-3.17040	0.20400
H	-3.98080	-3.00050	-5.19290
H	1.30590	-3.17560	-2.66300
C	-3.74780	-0.98090	-4.45340
N	-1.18600	-3.17040	-0.20410
C	-3.70750	-5.61200	2.09140
C	-1.48390	-3.64370	-1.45280
C	-5.72080	-2.58360	-3.19900
N	2.38180	-4.66710	1.32200
C	-2.13170	-3.62280	2.12150
O	-5.75370	-5.50660	-1.38820
C	3.30440	-5.95840	-0.66910
C	3.71030	-5.61280	-2.09080
C	-3.30160	-5.95810	0.66990
C	-5.94090	-1.10320	-3.18580
C	-5.47520	-4.50980	-2.01420
N	-6.26640	-3.40480	-2.15430
H	-5.26600	0.53250	-4.40990
H	-3.29950	-0.61910	-5.37630
N	-2.37900	-4.66740	-1.32170
C	-3.55010	-2.48200	-4.33540
C	2.13470	-3.62350	-2.12140
H	-3.02870	-4.56270	3.83370
C	2.87730	-4.67370	-0.02990
C	-2.64260	-4.84890	2.85760
C	-5.20370	-0.55390	-4.39440
C	-2.87440	-4.67350	0.03030
N	-4.31620	-4.29080	-2.70840
H	-3.97030	-6.51790	2.63360
C	-4.25770	-2.90070	-3.08380
C	2.64550	-4.84980	-2.85710
H	3.97310	-6.51890	-2.63270
H	-2.92040	-2.87720	2.01190
H	3.03170	-4.56390	-3.83330
H	4.14230	-6.39830	-0.13450
H	-4.13950	-6.39810	0.13530
H	-7.00250	-0.86440	-3.23560
H	2.92340	-2.87780	-2.01200
H	-2.49110	-2.71880	-4.28150
H	3.70990	-3.96190	-0.11000
H	-1.79370	-5.50820	3.04680
H	-5.71350	-0.90200	-5.29450
H	-3.70700	-3.96170	0.11020
H	-3.84560	-2.31870	-2.24900
H	1.79660	-5.50910	-3.04620
H	3.84770	-2.31810	2.24950
H	2.49360	-2.71860	4.28220
H	5.26770	0.53340	4.41020
C	4.26010	-2.90010	3.08430
C	3.55250	-2.48150	4.33600
C	5.20560	-0.55300	4.39480
H	3.30160	-0.61870	5.37690
H	5.54800	-0.68000	2.26120
C	3.74980	-0.98040	4.45400
H	3.98350	-3.00000	5.19350
C	5.94280	-1.10220	3.18620
C	5.72310	-2.58260	3.19930
H	5.71560	-0.90100	5.29480
H	3.20170	-0.50150	3.64080
H	7.00430	-0.86310	3.23570
H	6.07750	-2.96640	4.16610
N	4.31880	-4.29020	2.70890
O	5.75640	-5.50560	1.38850
C	5.47780	-4.50890	2.01460
N	6.26880	-3.40370	2.15460
C	3.16170	-5.08610	2.44560
H	2.50970	-5.06130	3.31330
H	3.50570	-6.10210	2.27790
H	-7.88060	-4.50360	-1.59060
H	-8.21910	-3.26440	-2.82490
C	7.67140	-3.48120	1.90920
H	7.88320	-4.50190	1.59040
H	8.22160	-3.26260	2.82450
H	9.01470	-3.69750	-0.55590
H	-3.97310	6.51890	-2.63270
H	-1.79660	5.50910	-3.04620
H	-2.47520	6.66680	-0.66180
C	-2.64550	4.84980	-2.85720
C	-3.71030	5.61280	-2.09080
H	-3.03170	4.56390	-3.83340
C	-3.30440	5.95840	-0.66920
H	-4.14230	6.39830	-0.13450
H	-0.96630	4.90430	-0.91480
H	-4.61820	5.00900	-2.04580
C	-2.13470	3.62350	-2.12150
H	-1.30590	3.17570	-2.66300
C	-1.70070	4.10030	-0.76990
C	-2.87730	4.67370	-0.02990
H	-3.50570	6.10210	2.27790
O	-5.75640	5.50560	1.38850
N	-2.38180	4.66710	1.32200
H	-2.92340	2.87790	-2.01210
C	-3.16170	5.08610	2.44560
N	-1.18890	3.17040	0.20400
H	-3.70990	3.96190	-0.11000
C	-0.00150	2.39950	-0.00020
C	-1.48670	3.64340	1.45280
C	-5.47780	4.50890	2.01460
H	-2.50970	5.06130	3.31330
N	-4.31880	4.29020	2.70890
O	-1.03460	3.22530	2.49490
N	-6.26880	3.40370	2.15450
C	-4.26010	2.90010	3.08430
H	-3.84770	2.31820	2.24950
C	-5.72310	2.58260	3.19930
H	-2.49350	2.71860	4.28220
H	-6.07750	2.96640	4.16610
C	-3.55250	2.48150	4.33600
H	-3.98340	2.99990	5.19340
C	-5.94280	1.10220	3.18610
H	-5.54800	0.68000	2.26120
C	-3.74970	0.98040	4.45390
H	-3.20160	0.50150	3.64070
C	-5.20560	0.55300	4.39470
H	-5.71560	0.90100	5.29480
H	-3.30150	0.61870	5.37680
H	-5.26760	-0.53340	4.41020
H	-7.00430	0.86310	3.23570
H	0.12360	1.77480	0.87900
H	-0.12670	1.77500	-0.87960
H	-8.22160	3.26260	2.82450
H	-7.88320	4.50190	1.59040

cycHC[12] in concave 12-gon conformation (Figure S24)

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C	8.71680	2.07610	-1.91440
C	8.74630	3.43290	-2.59450
C	8.15410	4.54150	-1.74280
H	9.78410	3.67660	-2.82890
H	8.22260	3.38470	-3.54720
C	9.38000	2.26210	-0.58640
H	9.22440	1.32250	-2.51310
H	7.69070	1.73880	-1.76190
C	8.60520	3.24250	0.24590
C	8.73620	4.61450	-0.34160
H	9.78820	4.90030	-0.37110
H	8.19640	5.34680	0.25340
H	8.28120	5.49750	-2.24660
H	7.07860	4.38280	-1.65400
N	9.51230	1.15800	0.32670
H	10.37760	2.68670	-0.76500
N	9.13370	2.96440	1.55560
H	7.54490	2.95650	0.21530
C	9.54020	1.65870	1.59950
O	9.87860	1.05250	2.59000
C	7.20740	1.27390	4.45950
C	6.38610	-0.00360	4.48360
C	4.88660	0.23420	4.45160
H	6.64340	-0.59240	5.36160
H	6.66990	-0.60460	3.61840
C	6.73200	2.06210	3.27790
H	8.26600	1.04150	4.37350
H	7.05350	1.85260	5.37090
C	5.27390	2.38340	3.43700
C	4.44760	1.14160	3.31610
H	4.62790	0.67270	2.34810
H	3.38380	1.36300	3.38180
H	4.36630	-0.71940	4.39090
H	4.57760	0.69010	5.39380
N	7.26990	3.37300	3.02030
H	6.85020	1.43960	2.38040
N	5.12000	3.45770	2.49370
H	5.12690	2.78660	4.44870
C	6.30630	4.13240	2.41400
O	6.47090	5.21600	1.90210
C	8.65230	3.60730	2.73890
H	8.77870	4.68120	2.64150
H	9.25450	3.24300	3.56560
C	1.65190	-4.43650	1.99840
C	2.88860	-4.65260	2.85280
C	4.04520	-5.27660	2.09140
H	2.64290	-5.27030	3.71390
H	3.20480	-3.68640	3.25020
C	2.09970	-3.65310	0.80370
H	0.88130	-3.90690	2.55570
H	1.22990	-5.38880	1.67580
C	3.12530	-4.42600	0.02920
C	4.39470	-4.53410	0.81360
H	4.77310	-3.53460	1.03360
H	5.16230	-5.06290	0.25100
H	4.91800	-5.33790	2.73850
H	3.78620	-6.30450	1.83120
N	1.16860	-3.32070	-0.23980
H	2.56940	-2.72690	1.16300
N	3.10530	-3.72670	-1.22730
H	2.73760	-5.44210	-0.12840
C	1.84890	-3.21980	-1.42020
O	1.41690	-2.76580	-2.45460
C	10.28260	0.00010	-0.00000
H	-9.25460	-3.24330	3.56540
H	-8.77880	-4.68140	2.64120
H	-6.85020	-1.43980	2.38050
H	-7.54490	-2.95650	0.21510
H	-4.91790	-5.33740	-2.73890
H	-3.27640	-4.01100	3.23410
C	-8.65240	-3.60750	2.73870
H	-4.57760	-0.69070	5.39400
H	-2.56930	-2.72680	-1.16300
H	-8.26600	-1.04190	4.37360
H	-8.22250	-3.38440	-3.54740
O	-9.87870	-1.05270	2.59000
H	-7.69070	-1.73870	-1.76200
H	-4.12500	-5.21420	2.22970
H	-4.62790	-0.67290	2.34830
O	-6.47100	-5.21620	1.90170
C	-6.73200	-2.06240	3.27780
C	-9.54020	-1.65880	1.59950
H	-0.88130	-3.90660	-2.55580
C	-3.88500	-4.15680	2.34190
C	-8.60520	-3.24250	0.24570
N	-9.13370	-2.96450	1.55540
H	-4.77300	-3.53440	-1.03380
H	-8.19640	-5.34680	0.25300
C	-4.04520	-5.27620	-2.09170
N	-7.27000	-3.37330	3.02020
C	-4.88670	-0.23460	4.45180
C	-6.30640	-4.13260	2.41380
C	-2.09970	-3.65300	-0.80390
N	-9.51230	-1.15800	0.32670
C	-7.20740	-1.27440	4.45950
O	-1.41690	-2.76600	2.45460
C	-8.71670	-2.07590	-1.91450
C	-8.74630	-3.43260	-2.59470
C	-4.44760	-1.14190	3.31620
C	-1.65180	-4.43630	-1.99860
C	-1.84890	-3.21990	1.42010
N	-1.16850	-3.32070	0.23970
H	-2.64280	-5.26990	-3.71420
H	-3.78620	-6.30420	-1.83160
N	-5.12000	-3.45790	2.49360
C	-4.39460	-4.53390	-0.81390
C	-8.73620	-4.61440	-0.34190
H	-6.64350	0.59190	5.36190
C	-9.38000	-2.26200	-0.58650
C	-6.38610	0.00320	4.48390
C	-2.88850	-4.65220	-2.85310
C	-5.27390	-2.38370	3.43700
N	-3.10520	-3.72670	1.22720
H	-4.36640	0.71900	4.39130
C	-3.12530	-4.42590	-0.02940
C	-8.15410	-4.54130	-1.74310
H	-9.78410	-3.67630	-2.82920
H	-7.05350	-1.85310	5.37090
H	-7.07860	-4.38260	-1.65430
H	-9.22430	-1.32230	-2.51320
H	-3.38380	-1.36330	3.38190
H	-1.22990	-5.38870	-1.67610
H	-9.78820	-4.90030	-0.37140
H	-5.16230	-5.06270	-0.25130
H	-6.66990	0.60430	3.61870
H	-3.20470	-3.68600	-3.25040
H	-5.12700	-2.78700	4.44860
H	-2.73770	-5.44200	0.12800
H	-8.28110	-5.49730	-2.24700
C	0.00000	-2.54010	-0.00000
H	-0.15170	-1.91270	-0.87850
H	0.15180	-1.91280	0.87860
C	3.88490	4.15660	2.34210
H	-4.12510	5.21420	-2.22970
H	-3.27640	4.01110	-3.23420
H	-2.73770	5.44200	-0.12800
H	-5.12700	2.78710	-4.44870
H	3.20470	3.68640	-3.25020
H	-0.15180	1.91270	0.87850
C	-3.88500	4.15680	-2.34200
H	-3.20480	3.68590	3.25030
H	2.73760	5.44210	0.12840
H	-5.16240	5.06270	0.25130

H	-6.66980	-0.60420	-3.61890
O	-6.47100	5.21610	-1.90170
H	-7.05350	1.85320	-5.37100
H	0.15170	1.91290	-0.87860
H	-1.23000	5.38860	1.67620
O	-1.41690	2.76610	-2.45460
C	-3.12540	4.42590	0.02940
C	-6.30640	4.13260	-2.41380
H	4.77300	3.53460	-1.03360
C	-0.00000	2.54010	-0.00000
C	-5.27390	2.38370	-3.43710
N	-5.12000	3.45800	-2.49360
H	1.22990	5.38890	-1.67580
H	-3.38380	1.36340	-3.38200
C	2.88850	4.65270	-2.85280
N	-3.10530	3.72680	-1.22720
C	-2.88870	4.65220	2.85310
C	-1.84890	3.21990	-1.42010
C	3.12530	4.42600	-0.02920
N	-7.27000	3.37330	-3.02020
C	-4.39470	4.53390	0.81380
O	1.41680	2.76570	2.45460
C	-7.20740	1.27440	-4.45960
C	-6.38610	-0.00310	-4.48400
C	-1.65190	4.43620	1.99860
C	4.39460	4.53410	-0.81360
C	1.84890	3.21970	1.42020
N	3.10520	3.72660	1.22730
H	4.91790	5.33790	-2.73850
H	2.64280	5.27040	-3.71380
N	-1.16860	3.32080	-0.23970
C	1.65180	4.43660	-1.99840
C	-4.44760	1.14200	-3.31630
H	-4.91800	5.33740	2.73890
C	-6.73200	2.06240	-3.27790
C	-4.04530	5.27620	2.09170
C	4.04510	5.27660	-2.09130
C	-2.09980	3.65300	0.80390
N	1.16850	3.32070	0.23980
H	-2.64300	5.26980	3.71420
C	2.09970	3.65310	-0.80370
C	-4.88660	0.23470	-4.45190
H	-6.64340	-0.59170	-5.36210
H	-4.77310	3.53430	1.03370
H	-4.36630	-0.71890	-4.39140
H	-8.26600	1.04200	-4.37370
H	-0.88140	3.90650	2.55590
H	5.16230	5.06290	-0.25090
H	-4.62790	0.67290	-2.34840
H	0.88130	3.90700	-2.55570
H	-6.85020	1.43980	-2.38060
H	-3.78630	6.30410	1.83160
H	3.78620	6.30450	-1.83110
H	-2.56940	2.72670	1.16300
H	2.56940	2.72700	-1.16300
H	-4.57760	0.69080	-5.39410
H	-7.54490	2.95640	-0.21520
H	-8.19630	5.34670	-0.25300
H	-8.22230	3.38430	3.54740
C	-8.60510	3.24240	-0.24560
C	-8.73610	4.61430	0.34200
C	-8.74610	3.43250	2.59480
H	-8.28090	5.49720	2.24710
H	-7.69050	1.73860	1.76200
C	-8.15390	4.54120	1.74310
H	-9.78810	4.90020	0.37150
C	-8.71660	2.07580	1.91450
C	-9.37990	2.26200	0.58660
H	-9.78390	3.67620	2.82930
H	-7.07840	4.38250	1.65430
H	-9.22420	1.32220	2.51320
H	-10.37750	2.68650	0.76530
N	-9.13370	2.96450	-1.55530
O	-9.87880	1.05260	-2.58990
C	-9.54020	1.65870	-1.59940
N	-9.51240	1.15800	-0.32660
C	-8.65240	3.60750	-2.73870
H	-8.77890	4.68140	-2.64110
H	-9.25470	3.24320	-3.56530
H	3.27630	4.01070	3.23430
H	4.12500	5.21400	2.23010
C	-10.28260	-0.00000	0.00000
H	-10.91010	-0.22970	-0.86060
H	-10.91010	0.22960	0.86070
H	-10.37760	-2.68660	-0.76510
H	6.64340	0.59230	-5.36180
H	4.57760	-0.69020	-5.39390
H	7.05350	-1.85270	-5.37100
C	4.88660	-0.23430	-4.45170
C	6.38610	0.00350	-4.48370
H	4.36630	0.71930	-4.39100
C	7.20740	-1.27400	-4.45950
H	8.26600	-1.04160	-4.37360
H	5.12690	-2.78660	-4.44870
H	6.66990	0.60460	-3.61860
C	4.44760	-1.14160	-3.31610
H	3.38380	-1.36310	-3.38190
C	5.27390	-2.38340	-3.43710
C	6.73200	-2.06210	-3.27790
H	9.25460	-3.24300	-3.56560
O	9.87860	-1.05240	-2.59000
N	7.27000	-3.37310	-3.02030
H	4.62790	-0.67270	-2.34820
C	8.65240	-3.60730	-2.73890
N	5.12000	-3.45780	-2.49370
H	6.85020	-1.43960	-2.38050
C	3.88500	-4.15660	-2.34210
C	6.30640	-4.13240	-2.41400
C	9.54020	-1.65860	-1.59950
H	8.77880	-4.68120	-2.64150
N	9.13370	-2.96440	-1.55550
O	6.47100	-5.21600	-1.90200
N	9.51240	-1.15800	-0.32670
C	8.60530	-3.24250	-0.24580
H	7.54500	-2.95650	-0.21520
C	9.38000	-2.26200	0.58650
H	8.19660	-5.34680	-0.25330
H	10.37770	-2.68660	0.76500
C	8.73630	-4.61440	0.34170
H	9.78840	-4.90020	0.37110
C	8.71680	-2.07600	1.91440
H	7.69070	-1.73880	1.76200
C	8.15420	-4.54150	1.74280
H	7.07870	-4.38270	1.65410
C	8.74650	-3.43280	2.59460
H	9.78420	-3.67650	2.82890
H	8.28130	-5.49740	2.24670
H	8.22270	-3.38460	3.54720
H	9.22440	-1.32240	2.51310
H	4.12500	-5.21410	-2.23000
H	3.27640	-4.01080	-3.23430
H	10.91010	-0.22960	0.86060
H	10.91000	0.22980	-0.86070

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