

Supporting Information for:

Chiral, triformylphenol-derived salen-type [4 + 6] organic cages

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Experimental details

All liquid spectra were recorded at 298 K. The samples concentration was 0.01 M. The ^1H and ^{13}C NMR measurements were performed on a Bruker FOURIER 300 MHz, Bruker AVANCE III HD 400MHz or Agilent DD2 800 spectrometer, operating at frequencies 799.926 and 201.162 MHz, respectively, equipped with $^1\text{H}\{^{13}\text{C}/^{15}\text{N}\}$ triple resonance probe (90° pulse width: ^1H – 13.6; ^{13}C – 6.9) and standard one-pulse sequence (*s2pul*). The ^{13}C NMR spectra were recorded with broadband ^1H decoupling. Line broadening factor of 1 Hz was used for ^{13}C spectra. The internal TMS was used as a reference (0.00 ppm). ^{13}C CP MAS spectra were recorded at 295 K on Agilent 400 MHz spectrometer, operating at frequency 100.66 MHz, equipped with Wide Bore Triple Resonance T3 MAS XY{1H-19F}, 4 mm probe head, using standard cross polarization sequence (*tancpx*) with ^1H decoupling. The following parameters were used: sample rotation – 10 000 Hz, relaxation delay – 7s, acquisition time – 0.05 s, cross-polarization contact time – 0.9 ms. The spectra were referred to the methylene signal of external glycine (43.30 ppm).

Mass spectroscopy data was collected on a AB Sciex Triple TOF 5600+ coupled with an electrospray ionization (ESI) source of ion. Unless otherwise stated, infrared data was collected using a Nicolet iS50 FT-IR machine as a thin film. UV and ECD spectra were recorded on Jasco J-815 spectropolarimeter. The solution of **7** suitable for UV and ECD measurements were prepared by 60 minutes sonification of 1 mg of **7** in 10 ml of CHCl_3 and filtration of slightly opalescent mixture through the syringe filter.

XRPD's were recorded on a PANalytical X'Pert³ Powder diffractometer, CuK α 1 wavelength and PIXcel1D detector. SEM pictures were taken on Quanta 250 FEG microscope. TGA and DSC analyses were performed on NETZSCH thermogravimetric analyzer. The surface areas and porosities of cage compounds were characterized by nitrogen adsorption and desorption analysis at 77.35 K with an autosorb computer controlled surface analyzer (ASAP 2420 Accelerated Surface Area and Porosimetry System, Micromeritics). Each sample was degassed at 70 °C for 72 h before analyzed.

2-hydroxy-1,3,5-triformylbenzene (1) was prepared from phenol and urotropine (hexamethylenetetraamine, HMTA) according to the modified procedure:[1]

Phenol (5.93 g, 63 mmol) and HMTA (17.2 g, 123 mmol) were placed in a round-bottomed flask, and 60 mL of trifluoroacetic acid was added. The resulting mixture was stirred at 130 °C under argon atmosphere for about 16 h. Then the reaction mixture was then heated to 150°C and stirred for 3 h. The mixture was cooled to 120 °C, treated with 100 mL of 4M HCl, heated at 105 °C for 30 min and cooled to room temperature overnight. The precipitated yellowish solid was filtered off, washed with 10% HCl, water, methanol, dichloromethane and dried on air. Yield: 4.8 g (47%) The crude product was recrystallized from 70 mL of DMF. Yield of the recovered product: 3.36 g (33%). The product gave all spectra identical with those previously published.[1]

IR (film) $\nu_{\max}$ 3343, 3055, 3029, 2881, 2783, 2563, 2324, 2270, 1685, 1661, 1590, 1485, 1457, 1443, 1392, 1379, 1341, 1302, 1279, 1246, 1188, 1137, 1126, 1030, 971, 917, 821, 785, 752, 646, 599, 561, 533 cm^{-1} ; ^1H NMR (300 MHz, DMSO) δ 10.30 (s, 2H), 9.99 (s, 1H), 8.52 (s, 2H).

Cage 5. To 2-hydroxy-1,3,5-triformylbenzene (0.356 g, 2 mmol) dissolved in 70 mL of DMSO, 1,2-diaminoethane (**2**, 0.2 mL, 3 mmol) was added in one portion. The resulting mixture was stirred at room temperature for 2 weeks. The solvent was evaporated under vacuum and the orange solid product was obtained quantitatively (0.420 g). The crude product was further purified by one week solid-liquid extraction in Soxhlet apparatus using 300 mL of dry chloroform. After slow evaporation of the solvent, the microcrystalline product was obtained with 80% recovery.

IR (film) $\nu_{\max}$ 3412, 2910, 2831, 1634, 1601, 1521, 1456, 1434, 1366, 1335, 1292, 1258, 1241, 1210, 1153, 1115, 1049, 999, 917, 879, 753 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 14.17 (dd, J = 89.0, 28.8 Hz, 4H), 8.71 – 8.53 (m, 4H), 8.31 (d, J = 13.9 Hz, 4H), 8.09 (d, J = 12.5 Hz, 4H), 7.99 – 7.80 (m, 8H), 4.29 (d, J = 30.5 Hz, 12H), 3.89 – 3.63 (m, 12H); ESI-HR-MS calcd for $\text{C}_{48}\text{H}_{49}\text{N}_{12}\text{O}_4$ $[\text{M}+\text{H}]^+$: 857.4000 found 857.3991.

Cage 6. To *trans*-(1*R*,2*R*)-diaminocyclohexane (**3**, 0.171 g, 1.5 mmol) dissolved in 40 mL of chloroform and 30 mL of DMSO, finely pulverized 2-hydroxy-1,3,5-triformylbenzene (**1**, 0.178 g, 1 mmol) was added in small portion during 30 minutes. The aldehyde was dissolved slowly and the resulting mixture was stirred at room temperature for 2 weeks. The solvent was evaporated under vacuum and the orange solid product was obtained quantitatively (0.290 g). The analytically pure sample was obtained by slow diffusion of diethyl ether to diluted chloroform solution of the crude product. The orange microcrystalline solid was obtained with 15% recovery.

IR (film) $\nu_{\max}$ 3380, 2925, 2855, 1633, 1601, 1524, 1450, 1376, 1346, 1290, 1259, 1225, 1158, 1142, 1091, 1010, 947, 937, 866, 797, 766, 643 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 14.49 (d, J = 56.2 Hz, 3H), 14.03 (dd, J = 36.7, 19.6 Hz, 1H), 8.69 – 8.53 (m, 4H), 8.34 – 8.23 (m, 4H), 8.08 (dd, J = 9.5, 4.9 Hz, 4H), 7.89 (dt, J = 10.9, 9.9 Hz, 8H), 3.32 (d, J = 13.5 Hz, 12H), 1.84 (s, 12H), 1.69 (s, 24H), 1.46 (s, 12H); ^{13}C NMR (101 MHz, CDCl_3) δ ^{13}C NMR (101 MHz, CDCl_3) δ 165.03 – 161.88 (m), 160.16 – 157.35 (m), 154.52 (ddd, J = 71.0, 41.9, 20.2 Hz), 132.67 – 129.86 (m), 127.59 – 124.79 (m), 124.39 – 122.37 (m), 119.71 – 118.23 (m), 75.92 – 71.98 (m), 34.54 – 31.73 (m), 25.57 – 23.30 (m); ESI-HR-MS calcd for $\text{C}_{72}\text{H}_{85}\text{N}_{12}\text{O}_4$ $[\text{M}+\text{H}]^+$: 1181.6817 found 1181.6832

Cage 7. To (1*R*,2*R*)-diphenylethylenediamine (**4**, 0.318 g, 1.5 mmol) dissolved in 50 mL of chloroform and 20 mL of DMSO, finely pulverized 2-hydroxy-1,3,5-triformylbenzene (**1**, 0.178 g, 1 mmol) was added in one portion. The aldehyde was dissolved slowly within 30 minutes and the resulting mixture was further stirred at room temperature for 2 weeks. During the course of the reaction, the yellowish precipitate was formed. The microcrystalline phase was then filtered off, washed with chloroform and dichloromethane and dried under vacuum. Yield: 0.159 g (36%) The filtrate was evaporated under vacuum and the orange glassy solid product was obtained with yield: 0.276g (63%).

IR (film) $\nu_{\max}$ 3389, 3060, 3030, 2966, 2860, 1633, 1600, 1454, 1373, 1252, 1153, 1058, 1028, 1010, 755, 696 cm^{-1} ; ^1H NMR (300 MHz, CDCl_3) δ 14.35 (ddd, $J = 30.7, 27.7, 8.3$ Hz, 4H), 8.92 – 8.81 (m, 4H), 8.67 – 8.49 (m, 4H), 8.38 (dd, $J = 6.1, 2.9$ Hz, 4H), 8.31 – 8.10 (m, 8H), 7.20 – 7.05 (m, 60H), 4.85 – 4.67 (m, 12H); ESI-HR-MS calcd for $\text{C}_{120}\text{H}_{97}\text{N}_{12}\text{O}_4$ $[\text{M}+\text{H}]^+$: 1769.7756 found 1769.7777.

General procedure for synthesis of model compounds 8 and 9: to a solution of amine (1.5 mmol, 3 eq) in 50 mL of chloroform, finely pulverized 2-hydroxy-1,3,5-triformylbenzene (**1**, 0.089 g, 0.5 mmol, 1 eq) was added in one portion. The aldehyde was dissolved slowly within 30 minutes and the resulting mixture was further stirred at room temperature for 24 h. After evaporation of the solvent, the yellow solidified oil was obtained quantitatively.

Model compound 8: ^1H NMR (CDCl_3 , δ): 15.00 (bs; OH); 8.75 & 8.38 (bs; *ortho*-CH=N, *Z* and *E* isomers); 8.22 (s; *para*-CH=N); 8.09 & 7.89 (bs; Ar-H, *Z* and *E* isomers); 3.25 (bs; 4-Cy, CH-N=); 3.11 (tt, 4.1 & 10.7 Hz; 2,6-Cy, CH-N); 1.15-1.85 (m; CH_2). ^{13}C NMR (CDCl_3 , δ): 165.3 (Ar, $^1\text{C-OH}$); 162.2 (*ortho*-CH=N, *E*-isomer); 157.4 (*para*-CH=N); 153.8 (*ortho*-CH=N, *Z*-isomer); 131.6 (Ar, $^3\text{C-H}$); 126.3 (Ar, $^4\text{C-C=N}$); 124.9 (Ar, $^2\text{C-(E)C=N}$); 118.5 ($^2\text{C-(Z)C=N}$); 70.0 (2,6-CyN=C, $^1\text{CH-N}$, *E*-isomer); 69.6 (4-CyN=C, $^1\text{CH-N}$); 65.7 (2,6-CyN=C, $^1\text{CH-N}$, *Z*-isomer); 34.4 (4-Cy, $^2\text{CH}_2$); 34.2 (2,6-Cy, $^2\text{CH}_2$); 25.6 (4-Cy, $^4\text{CH}_2$); 25.4 (2,6-Cy, $^4\text{CH}_2$); 24.8 (4-Cy, $^3\text{CH}_2$); 24.5 (2,6-Cy, $^3\text{CH}_2$).

IR (film) $\nu_{\max}$ 2924, 2851, 1627, 1598, 1448, 1377, 1347, 1298, 1257, 1155, 1078, 964 cm^{-1} ; HR ESI MS Calcd for $\text{C}_{27}\text{H}_{39}\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$: 422.3166 found: 422.3206

Model compound 9: ^1H NMR (CDCl_3 , δ): 14.76 (bs; OH); 8.88 & 8.47 (bs; *ortho*-CH=N, *Z* and *E* isomers); 8.33 (s, *para*-CH=N); 8.24 & 8.04 (bs; Ar-H, *Z* and *E* isomers); 7.41 (*pseudodot*; 4-R-N=, $^2\text{C-H}$); 7.39 (bm; 2,6-R-N=, $^2\text{C-H}$); 7.36 (*pseudodot*; 2,6-R-N=, $^3\text{C-H}$); 7.34 (*pseudodot*; 4-R-N=, $^3\text{C-H}$); 7.26 (bm; 2,6-R-N=, $^4\text{C-H}$); 7.24 (tt, 1.5 & 7.3 Hz; 4-R-N=, $^4\text{C-H}$); 4.62 (q, 6.7 Hz; 2,6-R-N=, PhCH); 4.53 (q, 6.7 Hz; 4-R-N=, PhCH); 1.65 (d, 6.7 Hz; 2,6-R-N=, CH_3); 1.59 (d, 6.7 Hz; 4-R-N=, CH_3). ^{13}C NMR (CDCl_3 , δ): 163.7 (Ar, $^1\text{C-OH}$); 163.2 (*ortho*-CH=N, *E*-isomer); 158.3 (*para*-CH=N); 154.5 (*ortho*-CH=N, *Z*-isomer); 145.0 (4-R, $^1\text{C}_{\text{Ar-C}}$); 144.6 & 142.9 (2,6-R, $^1\text{C}_{\text{Ar-C}}$, *Z* and *E* isomers); 132.0 (Ar, $^3\text{C-H}$); 128.6 (2,6-R, $^2\text{C}_{\text{Ar-H}}$); 128.5 (Ar, $^4\text{C-C=N}$); 128.4 (4-R, $^2\text{C}_{\text{Ar-H}}$); 127.1 (Ar, $^2\text{C-(E)C=N}$); 127.0 (4-R, $^4\text{C}_{\text{Ar-H}}$); 126.8 (2,6-R, $^4\text{C}_{\text{Ar-H}}$); 126.6 (2,6-R, $^3\text{C}_{\text{Ar-H}}$); 126.5 (4-R, $^3\text{C}_{\text{Ar-H}}$); 119.3 ($^2\text{C-(Z)C=N}$); 69.7 (2,6-R, $^1\text{CH-N}$, *E*-isomer); 69.3 (4-R, $^1\text{CH-N}$); 67.4 (2,6-R, $^1\text{CH-N}$, *Z*-isomer); 24.6 (4-R, CH_3); 24.5 (2,6-R, CH_3).

IR (film) $\nu_{\max}$ 3027, 2969, 2926, 2864, 1632, 1599, 1492, 1450, 1373, 1299, 1253, 1152, 1119, 1106, 1082, 1018, 971, 908, 759, 696 cm^{-1} ; HR ESI MS Calcd for $\text{C}_{33}\text{H}_{33}\text{N}_3\text{O}$ $[\text{M}+\text{H}]^+$: 488.2696 found: 488.2719.

Syntheses of cage **7** under different reaction conditions

2-hydroxy-1,3,5-triformylbenzene (178 mg, 1 mmol) and (1*R*,2*R*)-diphenylethylenediamine (318 mg, 1.5 mmol) were dissolved in appropriate mixture of solvents (total volume = 50 mL). In each case, the resulting mixture was stirred under argon atmosphere at room temperature for 14 days. The formed yellow precipitate was filtered off, dried and then activated. The content of solvent in "raw" and activated material was estimated on the basis on thermogravimetric (TGA) analyses.

The percentage contents of solvents: DMSO (100); DMSO-CHCl₃ (75:25; 50:50; 25:75); DMSO-H₂O (90:10; 92.5:7.5; 95:5; 97.5:2.5).

General activation procedure for 5-7 and sorption experiments

The non-activated material obtained after processing of the crude **5** and **6** or by filtration of microcrystalline **7** was initially dried at room temperature under reduced pressure (20 mbar). Activation procedure requires drying of the initially dried material under high vacuum (0.5-2 mmHg) at 70 °C for 72 hours.

Before gas sorption measurements, the stabilities of **7** were investigated by TGA. The cage compound **7**, obtained in different conditions and dried showed no weight loss up to 200 °C with exception of materials synthesized in the mixture of DMSO and chloroform (50:50 and 25:75) where 4.6 and 2.55% weight loss was observed.

The surface areas and porosities of cage compounds were characterized by nitrogen adsorption and desorption analyses at 77.35 K.

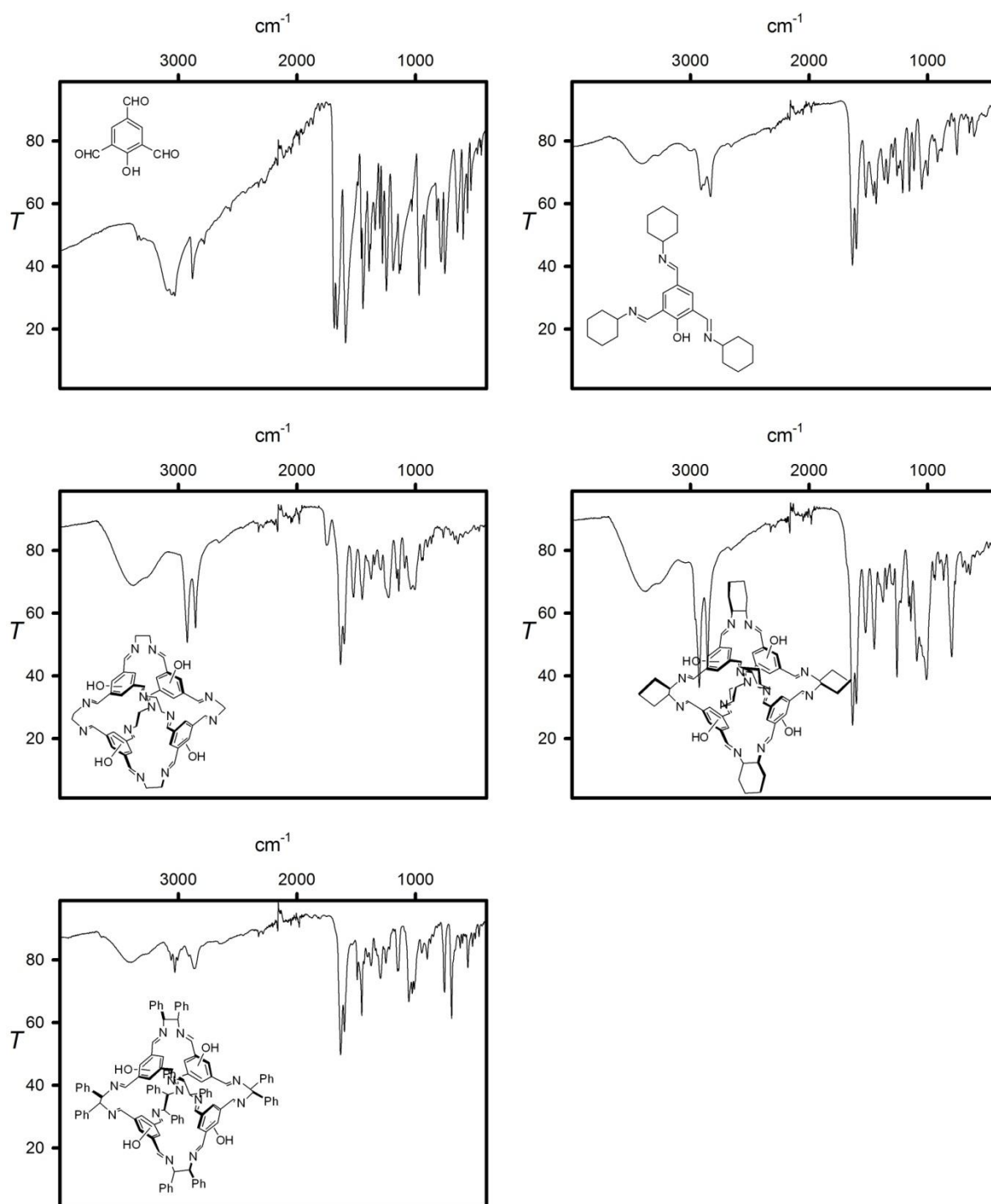


Figure SI_1. FT-IR spectra of **1**, **8**, **5-7**.

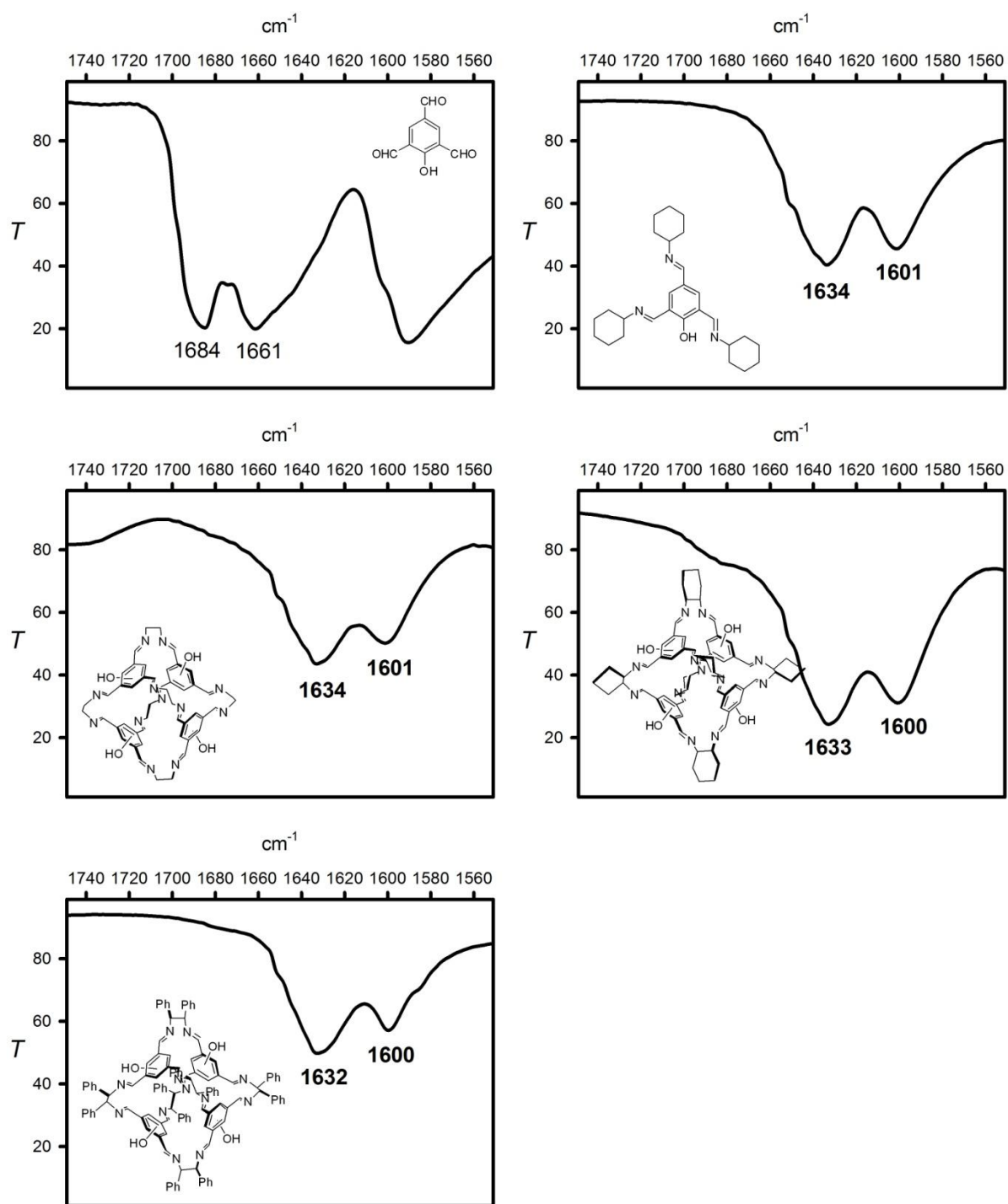


Figure SI_2. Diagnostic parts of FT-IR spectra of **1**, **8**, **5-7**.

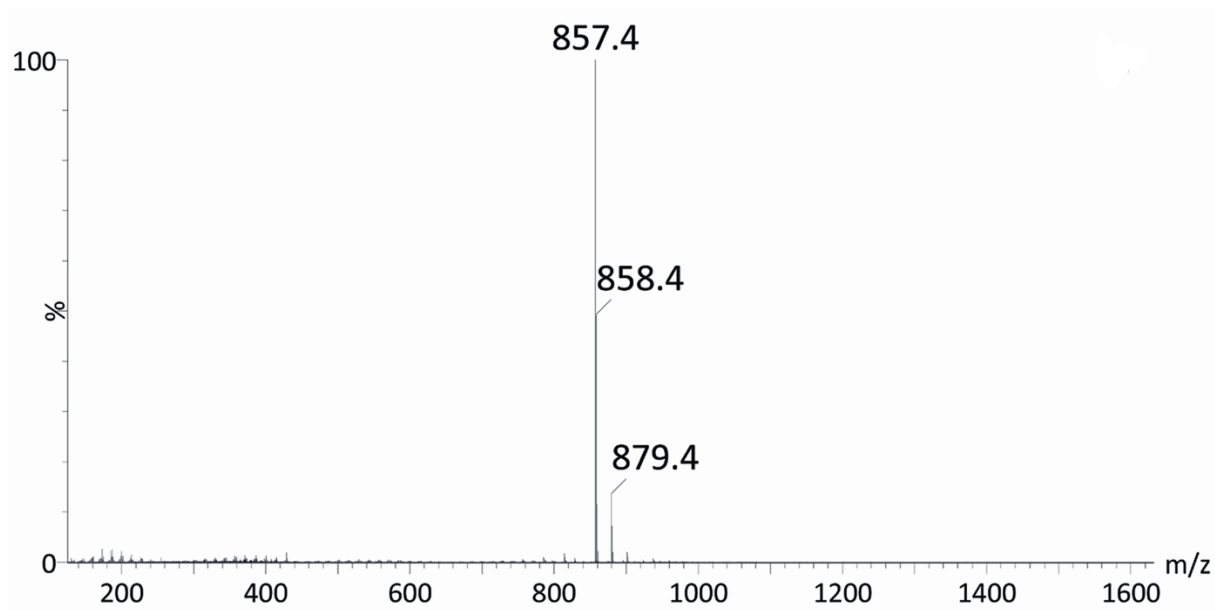


Figure SI_3. ESI-TOF mass spectrum of cage 5.

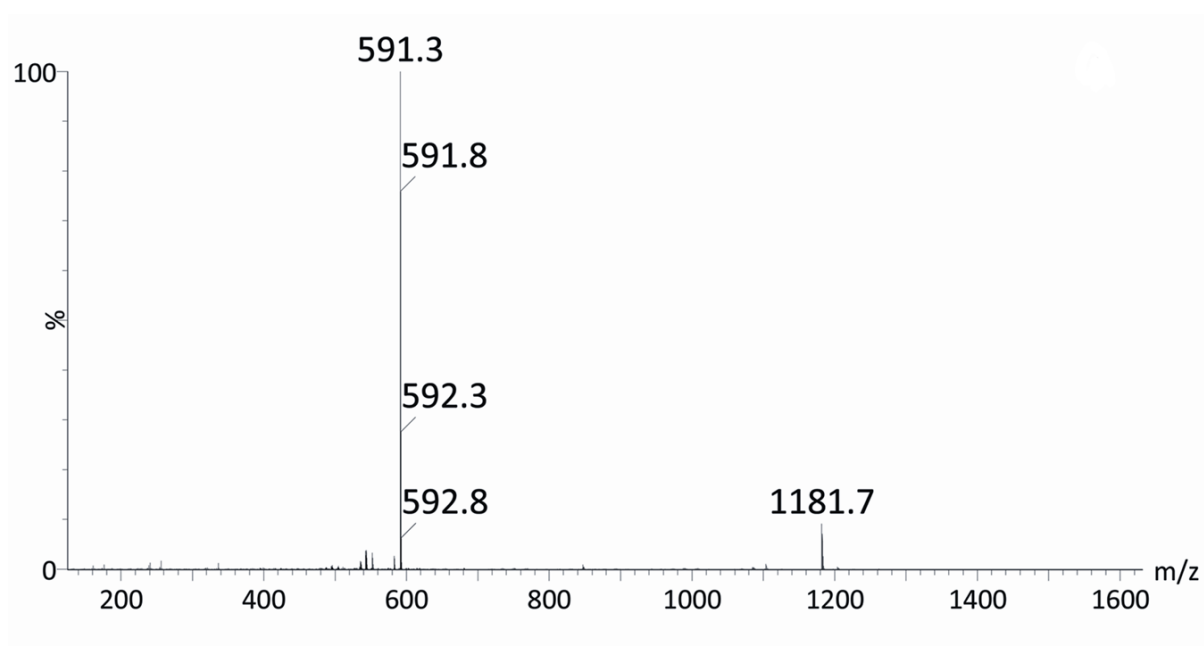


Figure SI_4. ESI-TOF mass spectrum of cage 6.

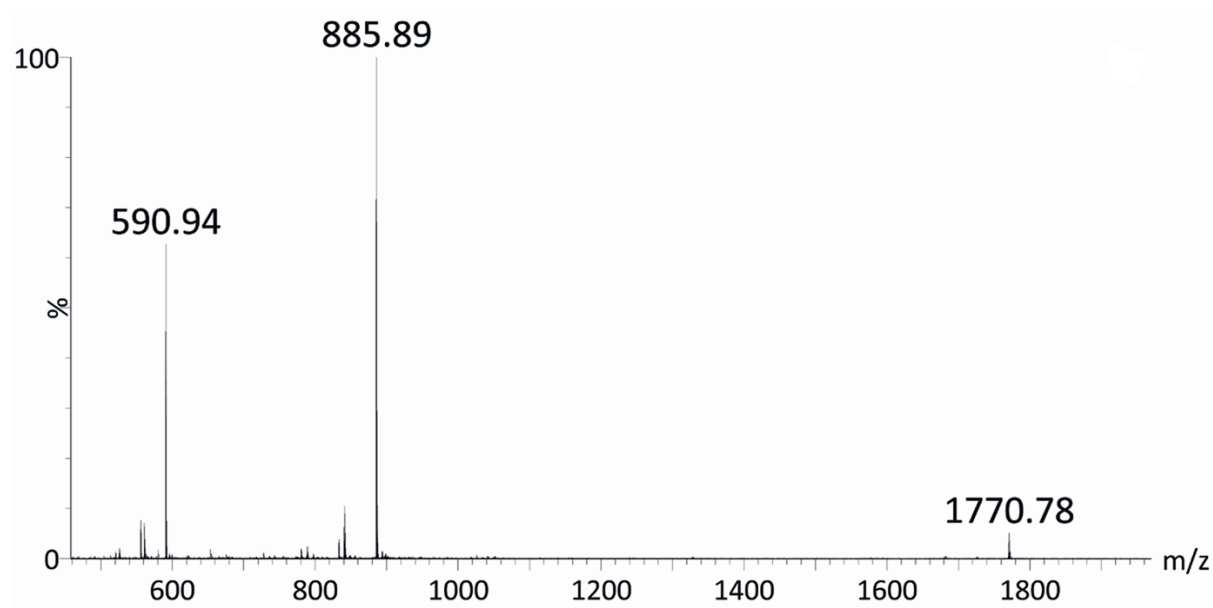


Figure SI_5. ESI-TOF mass spectrum of cage 7.

Interpretation of ^{13}C MAS NMR spectra

The ^{13}C MAS NMR spectra recorded for cages **5** and **7** were confronted with ^{13}C NMR spectra measured for model compounds **8** and **9**, respectively. Due to the solubility in CDCl_3 we were able to compare directly the ^{13}C NMR spectra measured for solid and dissolved samples of **6**.

The characteristic feature of ^{13}C NMR of **5-7** is the appearance of imine CHN signals within 152-163 ppm range, in good agreement with the values 153 and 163 ppm found for model compounds **8** and **9**. The imine carbon atom in *para* position to OH group is slightly deshielded comparing to these in *ortho* positions. In the spectral region between 163.5 and 165.0 ppm the signals corresponding to $\text{C}_{\text{ar}}\text{-OH}$ carbon atoms are observed. The 110-140 ppm regions of ^{13}C MAS NMR spectra of **5** and **6** are quite similar. The $\text{C}_{\text{ar}}\text{-2}$ carbon atoms give the signals between 118-124 ppm, $\text{C}_{\text{ar}}\text{-3}$ were observed at 129-131 ppm while $\text{C}_{\text{ar}}\text{-4}$ at 125 ppm, in very good agreement with chemical shift values obtained for **8**. The same region in ^{13}C MAS NMR spectrum of **7** is more complicated, due to overlapping of the signals originated from phenyl substituents and cage core aromatic rings. The characteristic signal assigned to *ipso* phenyl carbon atom is observed at 137.6 ppm, whereas the corresponding signal in **9** appeared at 144.9 ppm. This shielding is due to steric and electronic interactions with amine and aryl moieties in γ position. The similar tendency is observed in parent amines, methylbenzylamine and 1,2-diphenylethylenediamine. In aliphatic region of the ^{13}C NMR spectrum of cage **5** only one signal at the chemical shift characteristic for $\text{NCH}_2\text{CH}_2\text{N}$ moiety ($\delta = 60.2$) is observed. In the ^{13}C NMR spectrum of cage **6** the CH-N signal occurs at 72.4 ppm and is slightly deshielded in comparison to the model triimine **8** ($\delta = 69.5$) due to the inductive effect of the nitrogen atom bonded to the carbon atom in β position. The signals of the methylene carbon atoms of the cyclohexane moiety of the cage studied occur at 32.6 and 22.9 ppm and for model compound respective signals appeared at 34.3, 25.5 and 24.8 ppm. For **7** the aliphatic C^*H carbon atoms gave the broad signal at 80.2 ppm, while for the model compound **9** this particular signal appeared at 69.4 ppm.

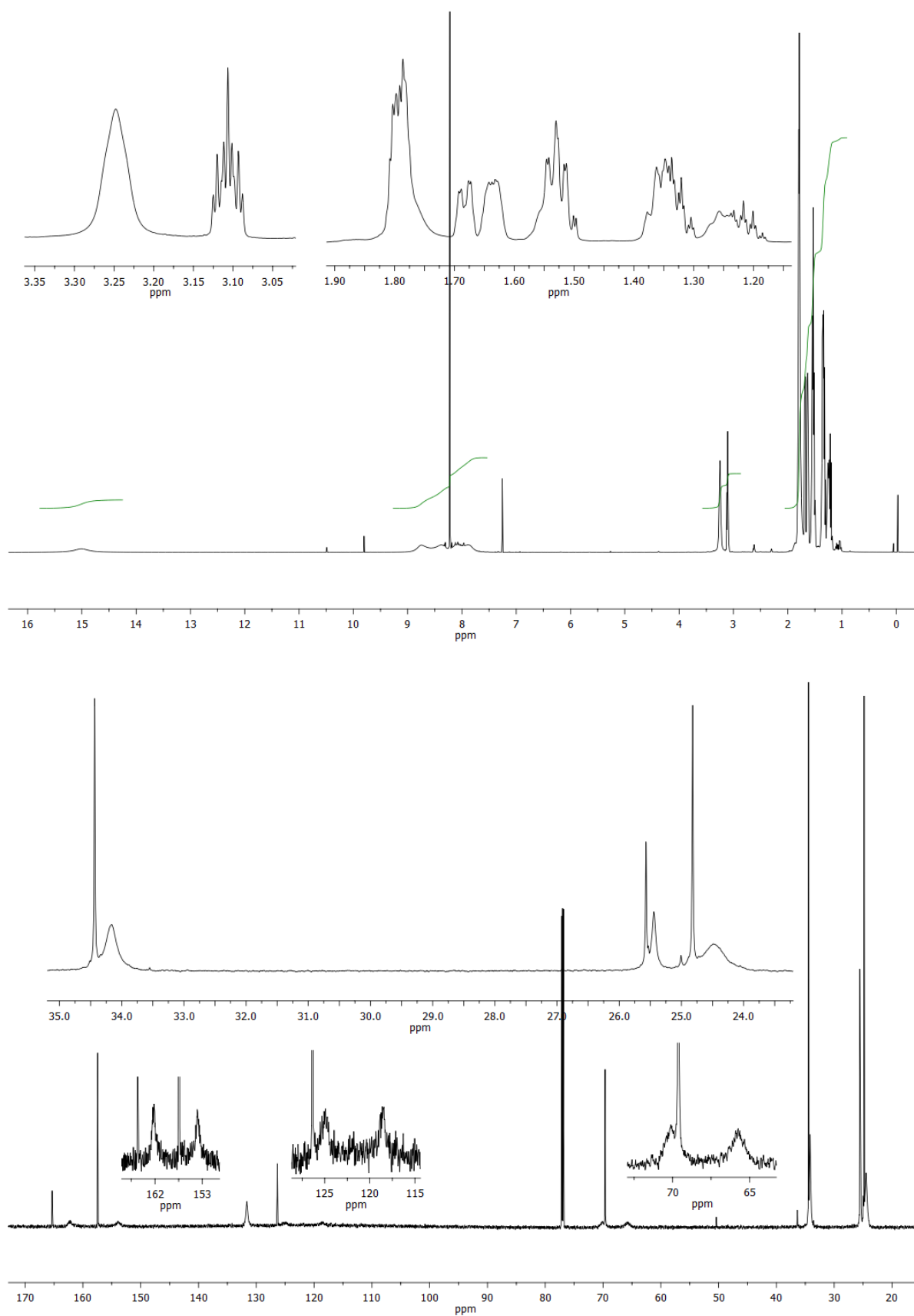


Figure SI_6. ^1H and ^{13}C NMR spectra of **8**.

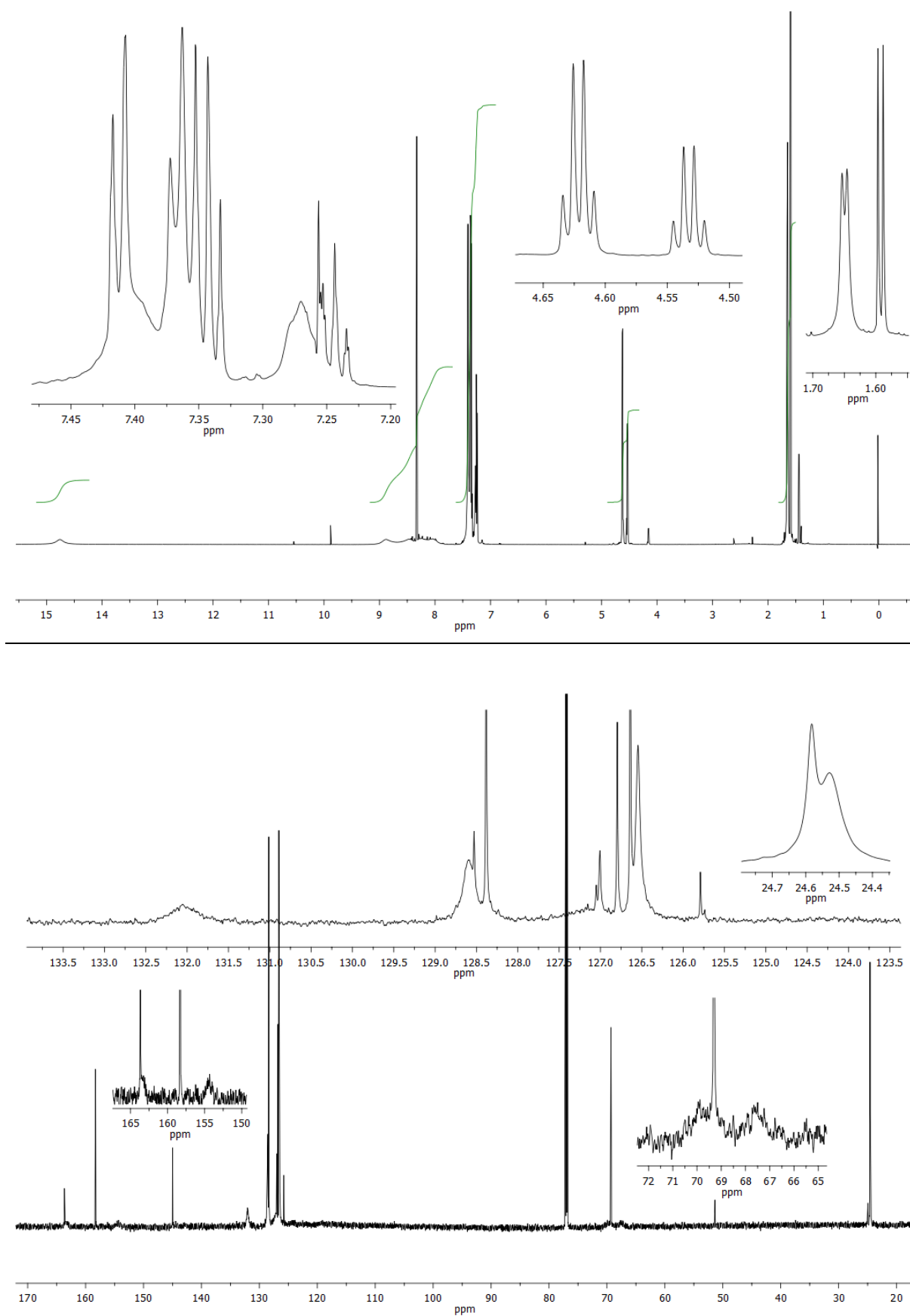


Figure SI_7. ^1H and ^{13}C NMR spectra of 9.

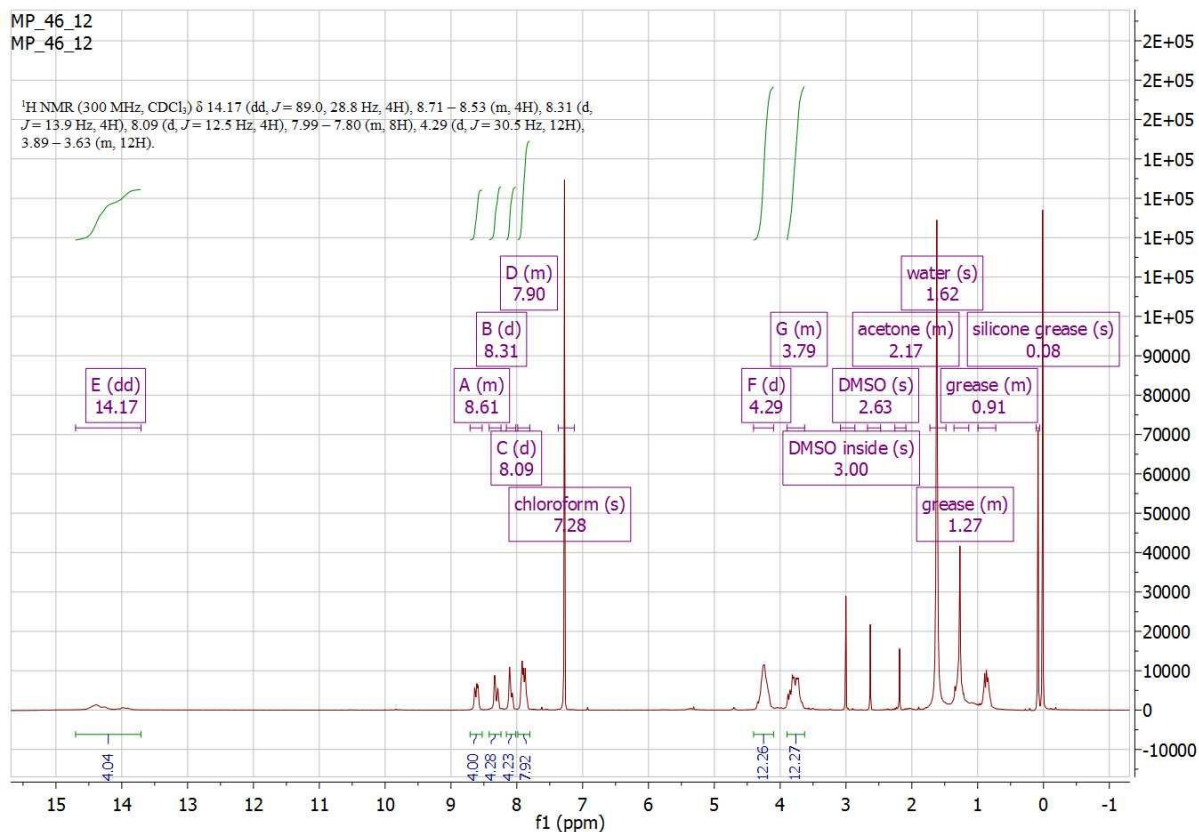


Figure SI_8. ^1H NMR spectrum of 5.

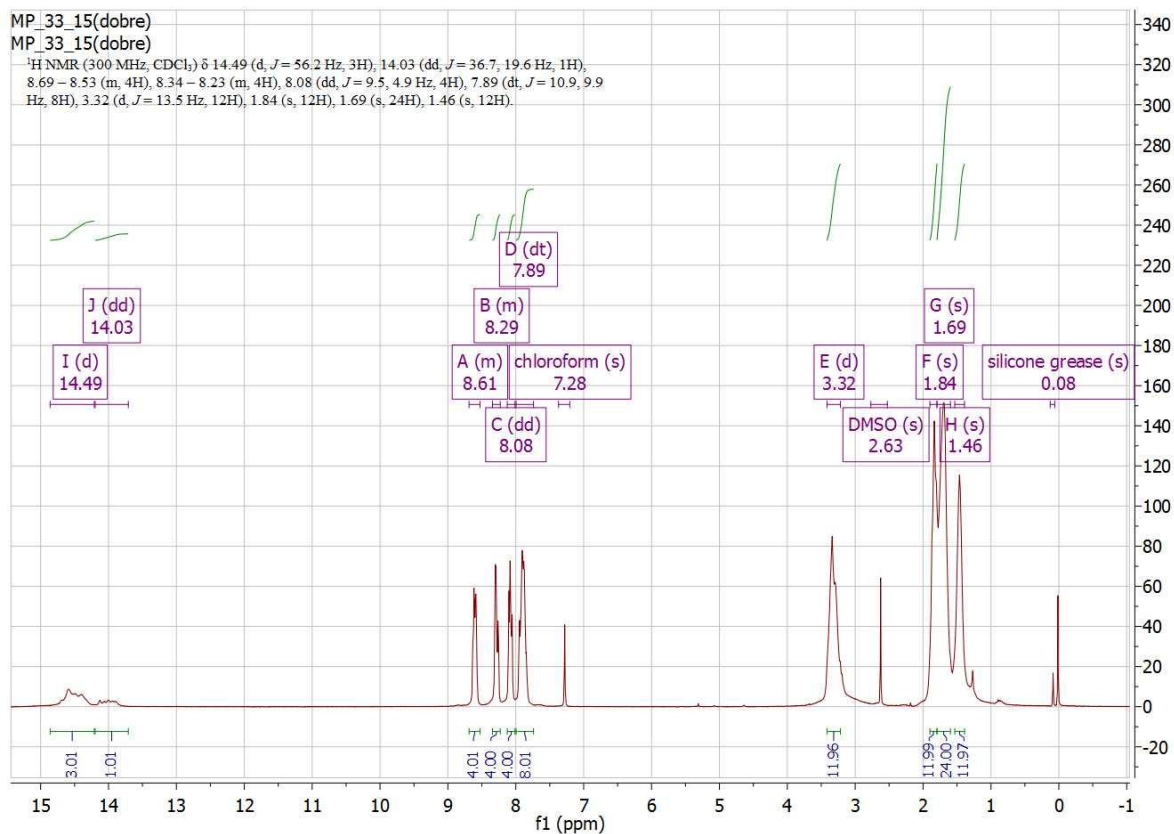


Figure SI_9. ^1H NMR spectrum of 6.

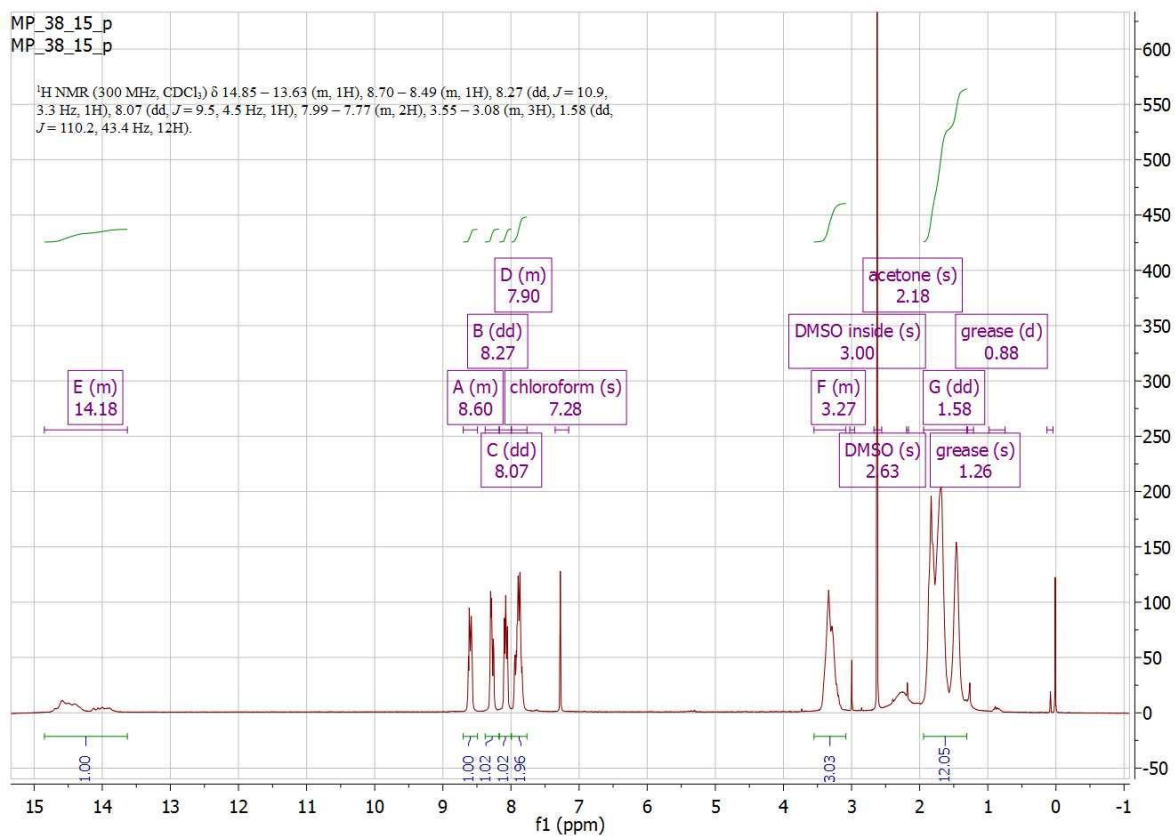


Figure SI_10. ¹H NMR spectrum of crude **6** measured after a month course of the reaction between **1** and **3**.

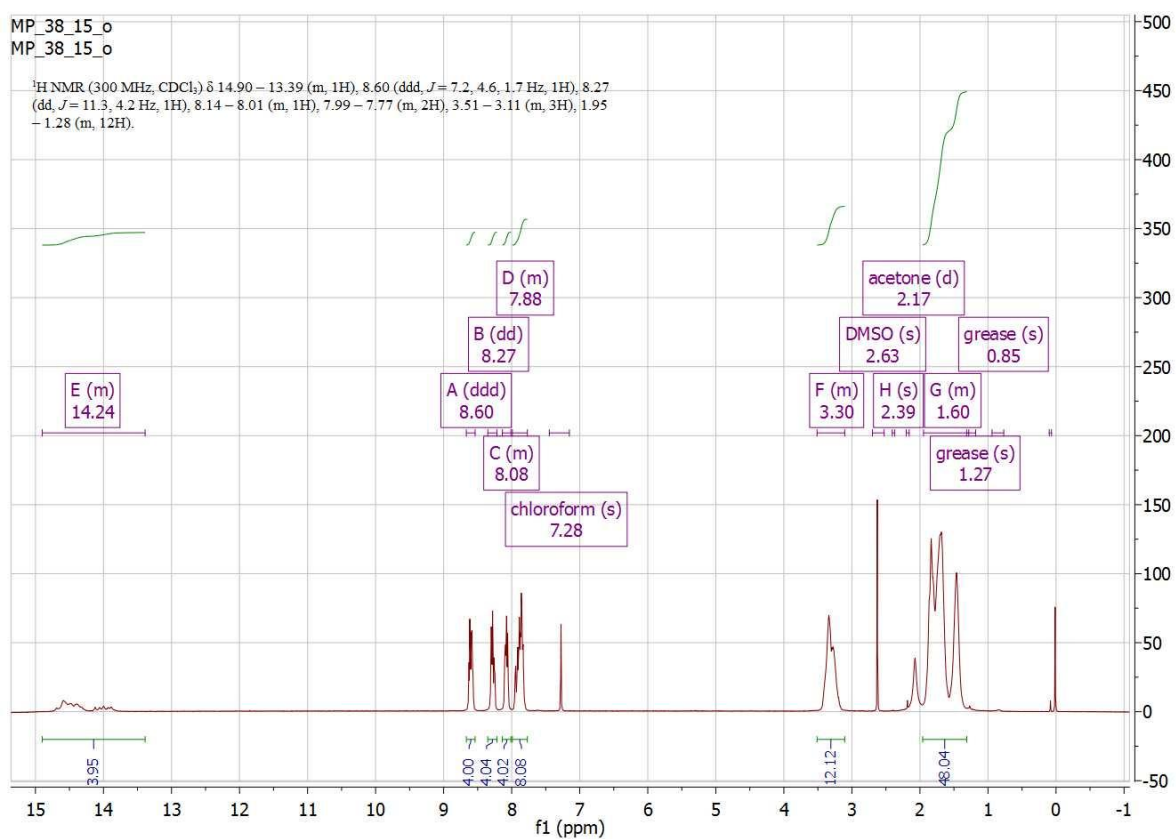


Figure SI_11. ¹H NMR spectrum of crude **6** measured after three months course of the reaction between **1** and **3**.

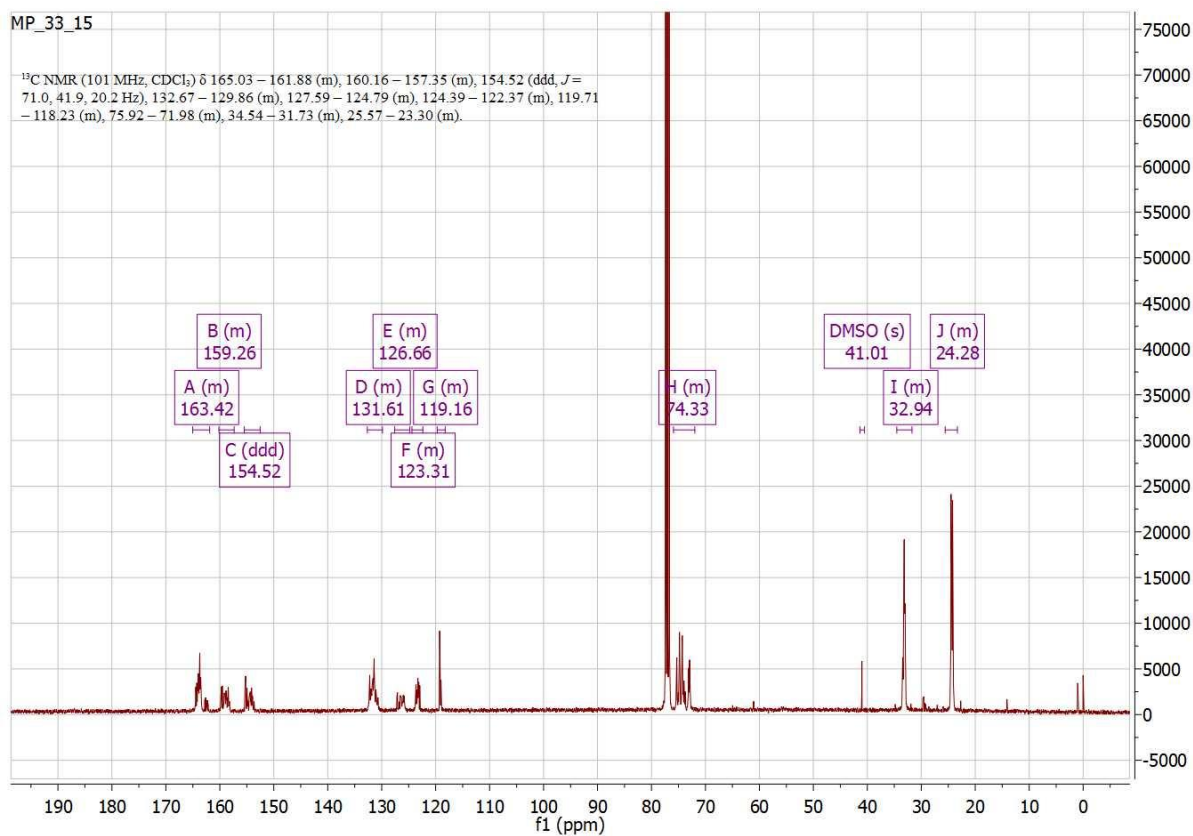


Figure SI_12. ^{13}C NMR spectrum of 6.

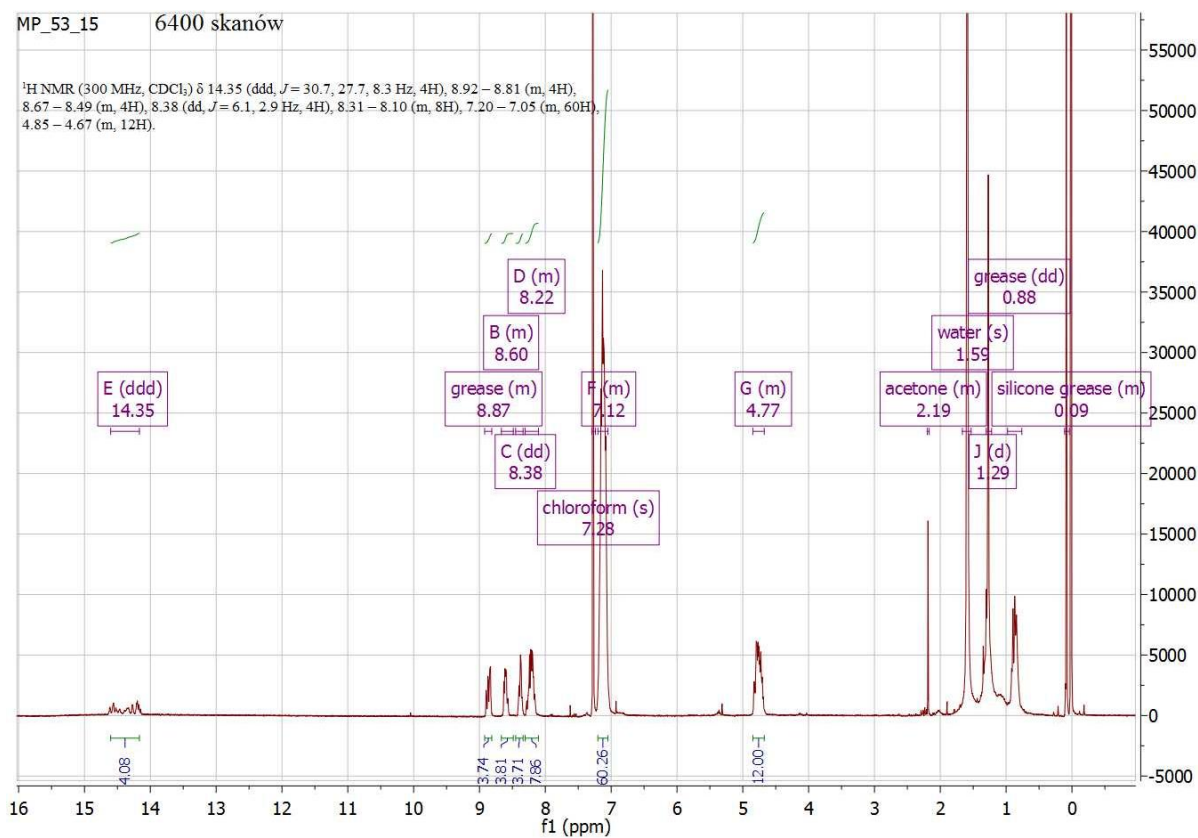


Figure SI_13. ^1H NMR spectrum of 7.

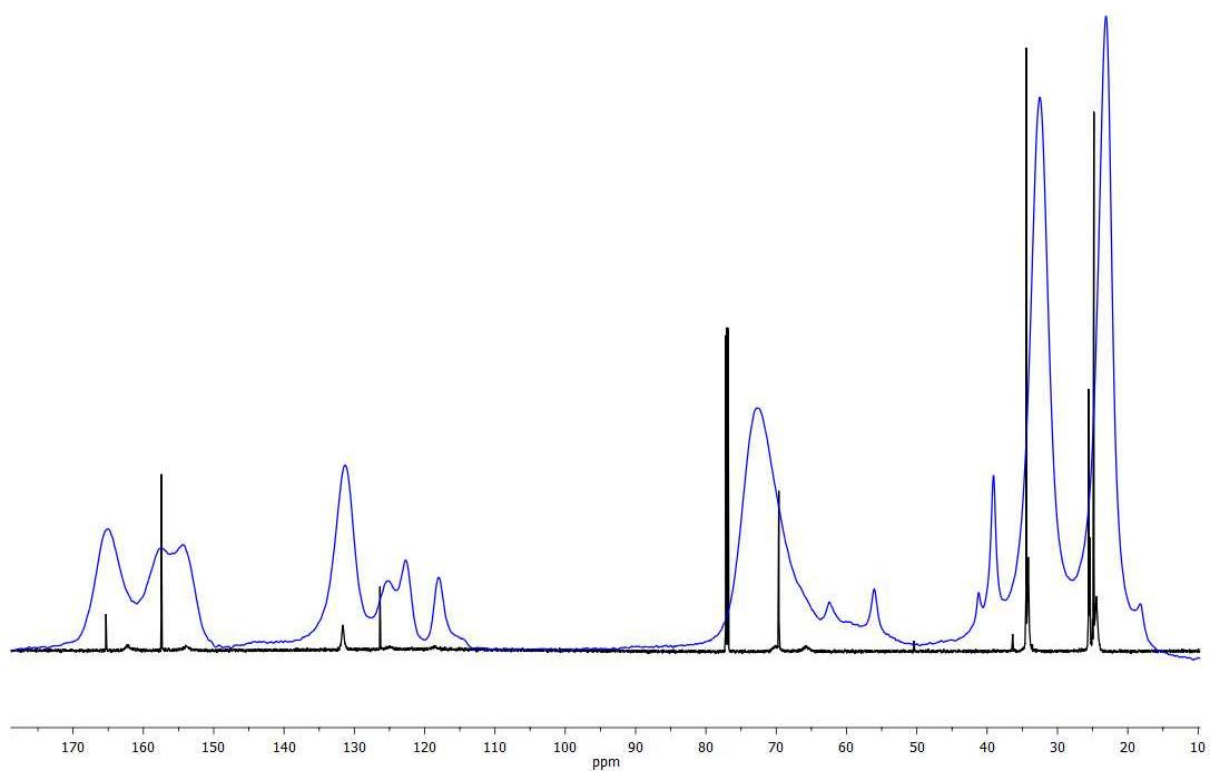


Figure SI_14. The comparison of ^{13}C NMR spectra measured for solid **5** (blue line) and solute of **8** (black line).

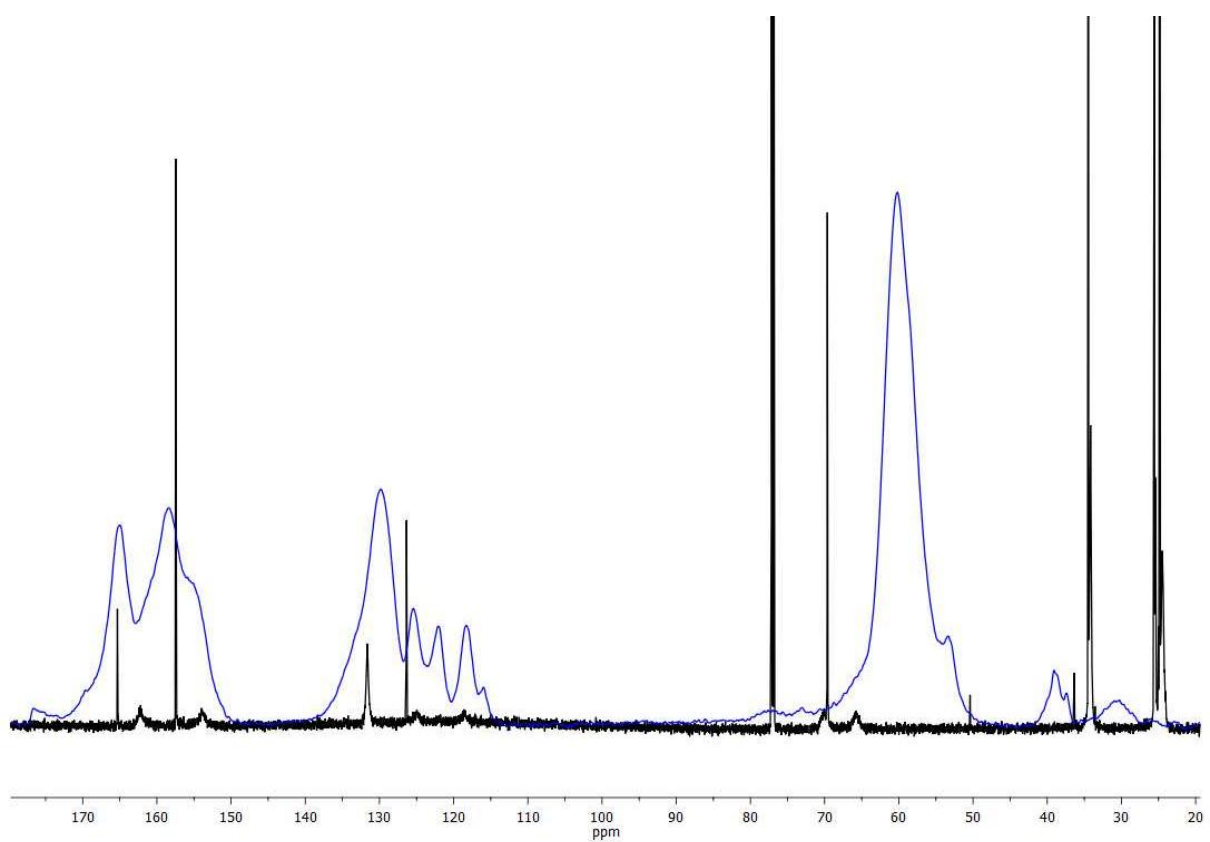


Figure SI_15. The comparison of ^{13}C NMR spectra measured for solid **6** (blue line) and solute of **8** (black line).

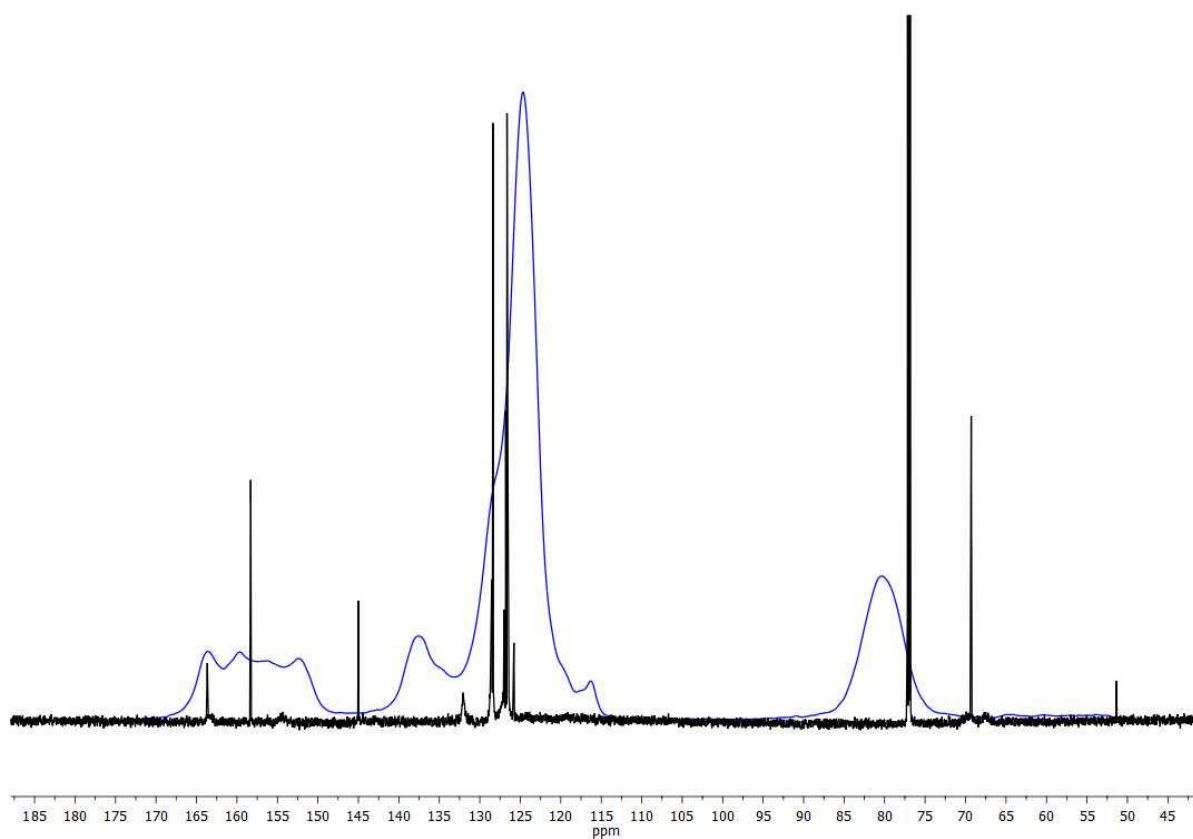


Figure SI_16. The comparison of ^{13}C NMR spectra measured for solid **7** (blue line) and solute of **9** (black line).

Generation of possible structures of cages 5-7

The truncated tetrahedron was taken as macroscopic representation of molecular cages **5-7** and its symmetry was systematically decreased by adding the hydroxyl groups (one for each triangular side). There are three possible hydroxyl groups positions {A , B , C } and four different aromatic rings (Figure SI_17). That gives us four-combinations with repetitions of three elements, what can be calculated as:

$$\bar{C}_n^k = \binom{n}{k}, \text{ where } k = 4 \text{ and } n = 3$$

$$\bar{C}_n^k = 15$$

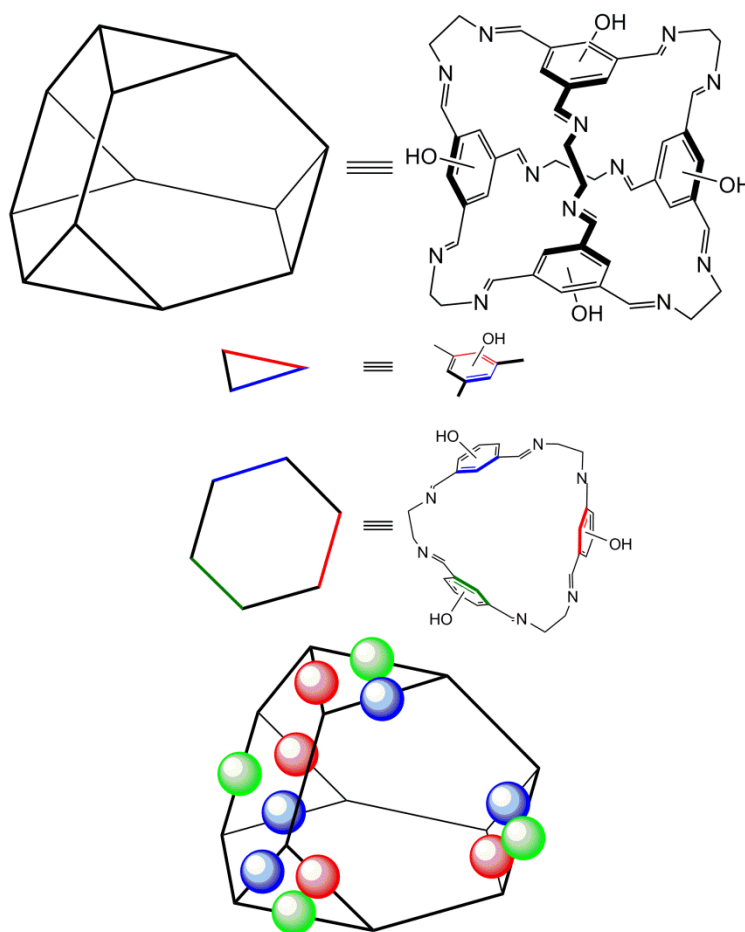


Figure SI_17. Cage's macroscopic representation - truncated tetrahedron and possible hydroxyl groups positions {A , B , C }.

This result can be verified by listing all the 4-multisubsets of the set {A,B,C}, displayed in Table SI_1. Because of cage's macroscopic representation - truncated tetrahedron, each combination has its own symmetry. There are three possible symmetries D_2 , C_2 and C_1 . However, some of combinations are equal through symmetry operations, what is displayed in Table SI_2.

Table SI_1. List of all possible 4-multisets.

No.	4-Multiset	No.	4-Multiset	No.	4-Multiset
1	{A,A,A,A}	6	{B,B,B,A}	11	{A,A,C,C}
2	{B,B,B,B}	7	{B,B,B,C}	12	{A,A,B,C}
3	{C,C,C,C}	8	{C,C,C,A}	13	{B,B,C,C}
4	{A,A,A,B}	9	{C,C,C,B}	14	{B,B,A,C}
5	{A,A,A,C}	10	{A,A,B,B}	15	{C,C,A,B}

Table SI_2. Symmetries of all possible isomers.

Symmetry	4-Multiset(s)
D_2	$\{A,A,A,A\} \xleftrightarrow{C_3} \{B,B,B,B\} \xleftrightarrow{C_3} \{C,C,C,C\}$ $\{A,A,B,B\}$
C_2	$\{A,A,C,C\}$ $\{B,B,C,C\}$ $\{A,A,A,B\} \xleftrightarrow{C_3} \{B,B,B,C\} \xleftrightarrow{C_3} \{C,C,C,A\}$ $\{A,A,A,C\} \xleftrightarrow{C_3} \{B,B,B,A\} \xleftrightarrow{C_3} \{C,C,C,B\}$
C_1	$\{A,A,B,C\}$ $\{B,B,A,C\}$ $\{C,C,A,B\}$

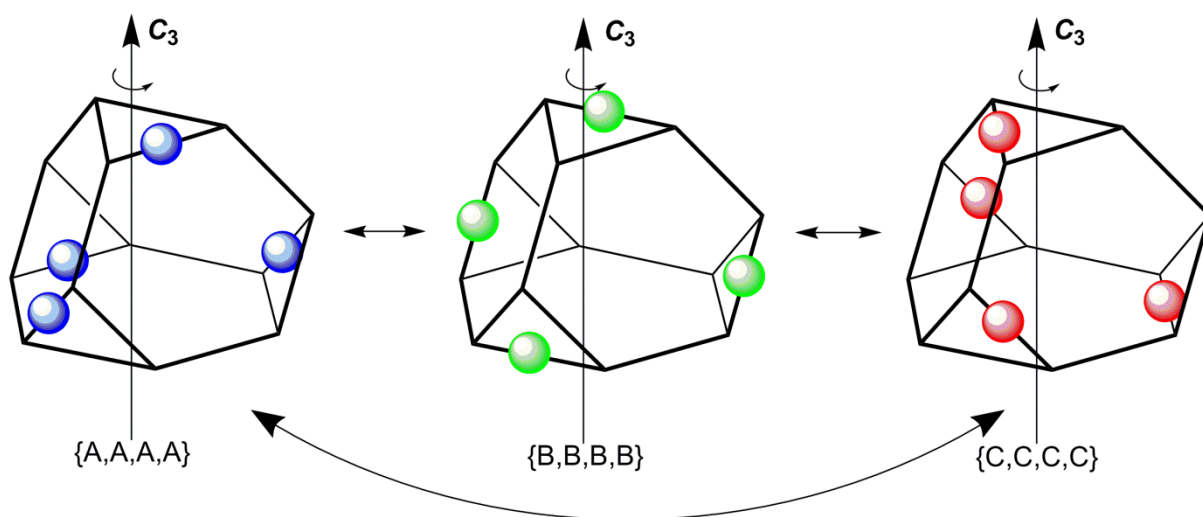


Figure SI_18. Isomer of D_2 symmetry. Arrows indicated isomers of the same symmetry.

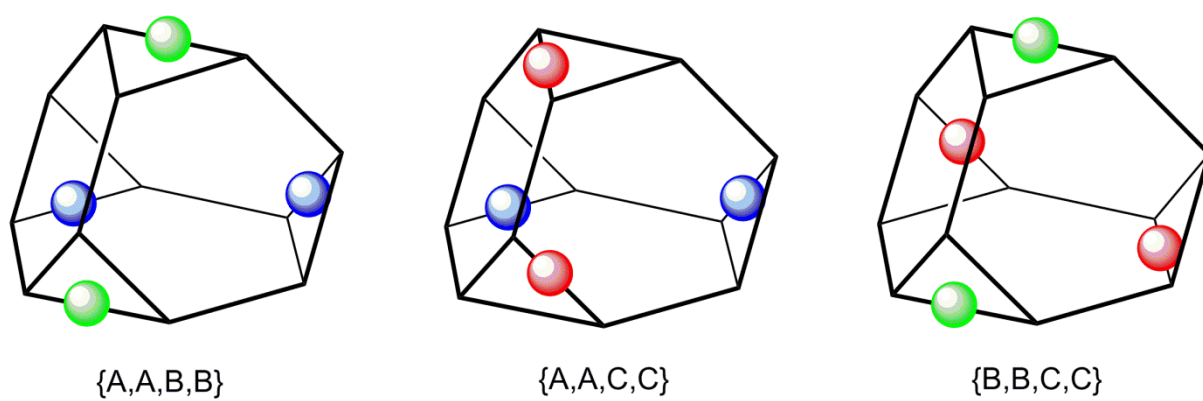


Figure SI_19. Isomers of C_2 symmetry.

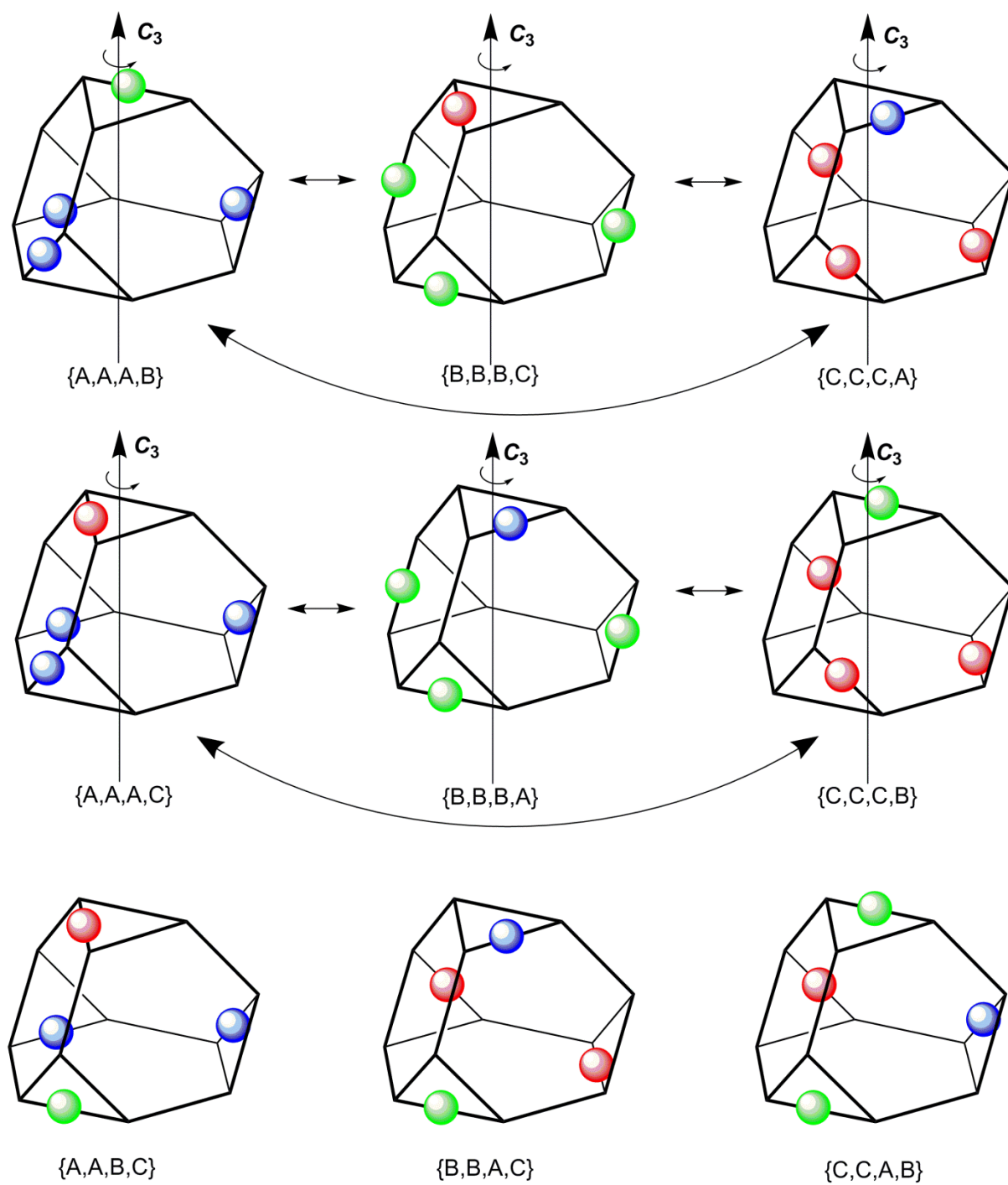


Figure SI_20. Isomers of C_1 symmetry. Arrows indicated isomers of the same symmetry.

Computational details

The initial molecular geometries of possible isomers of **5-7** were based on models generated on the basis on the carbon skeleton of known molecular cage of *T*-symmetry, where respective protons were replaced by hydroxyl groups, according to the procedure described above. The structure of individual isomers of **5** and **6** were fully optimized at IEFPCM/B3LYP/6-311G(d,p) level. Due to the size of **7** the calculations were performed with the use of smaller double- ζ basis set 6-31G(d,p). Since the synthesis of **5-7** were done in DMSO as the solvent we used the IEFPCM solvent model to estimate influence of polar environment on isomer energies.[2] The structures thus obtained were the real minimum energy structures (no imaginary frequencies have been found). The total and free energy values were used to obtain the Boltzmann population of isomers at 298.15 K.

ECD spectra for all structures optimized at the DFT level were calculated employing CAM-B3LYP, [3] B2LYP,[4] LC-wPBE [5] and M06-2X [6] hybrid functional, all in conjunction with 6-311G(d,p) basis set.[2] The calculated ECD spectra were Boltzmann averaged by taking into account isomers of **6** and **7** ranging from 0 to 2.0 kcal mol⁻¹ in relative energies, following a generally accepted protocol.[7] Rotatory strengths were calculated using both length and velocity representations. In the present study, the differences between the length and velocity calculated values of rotatory strengths were quite small, and for this reason, only the velocity representations were further used. The ECD spectra were simulated by overlapping Gaussian functions for each transition, according to the procedure previously described by Harada and Stephens.[8]

The solvent effect on structure and ECD spectra was simulated with the use of IEFPCM solvent model of chloroform.

The comparison between measured and calculated ECD spectra provide conclusion that all the methods satisfactorily reproduce experiment. However the best match between experiment and theory was achieved for spectra calculated at the IEFPCM/CAM-B3LYP/6-311G(d,p) level of theory and these results were discussed in the main text.

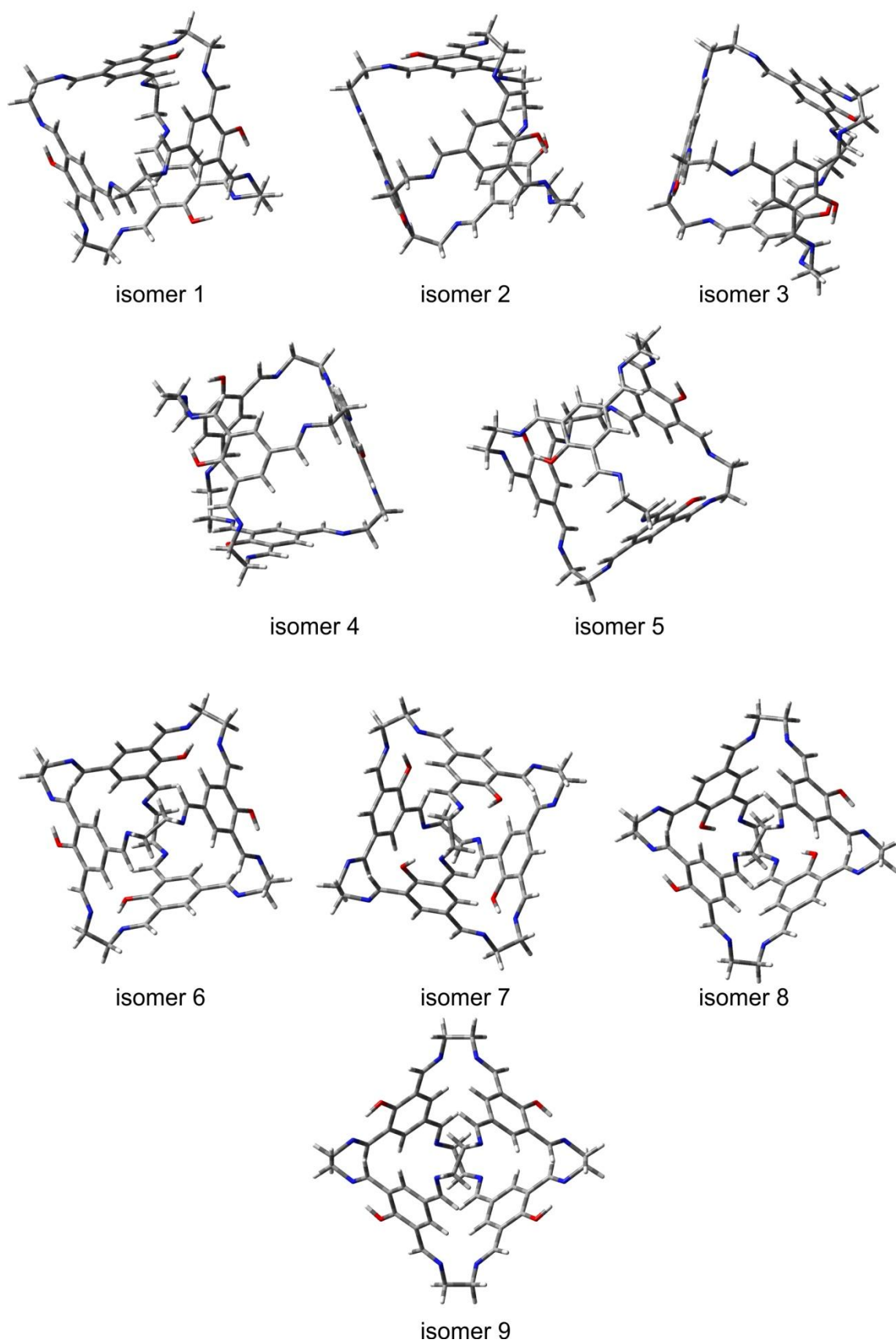


Figure SI_21. Structures of possible isomers of cage **5** calculated at the IEFPCM/B3LYP/6-311G(d,p) level.

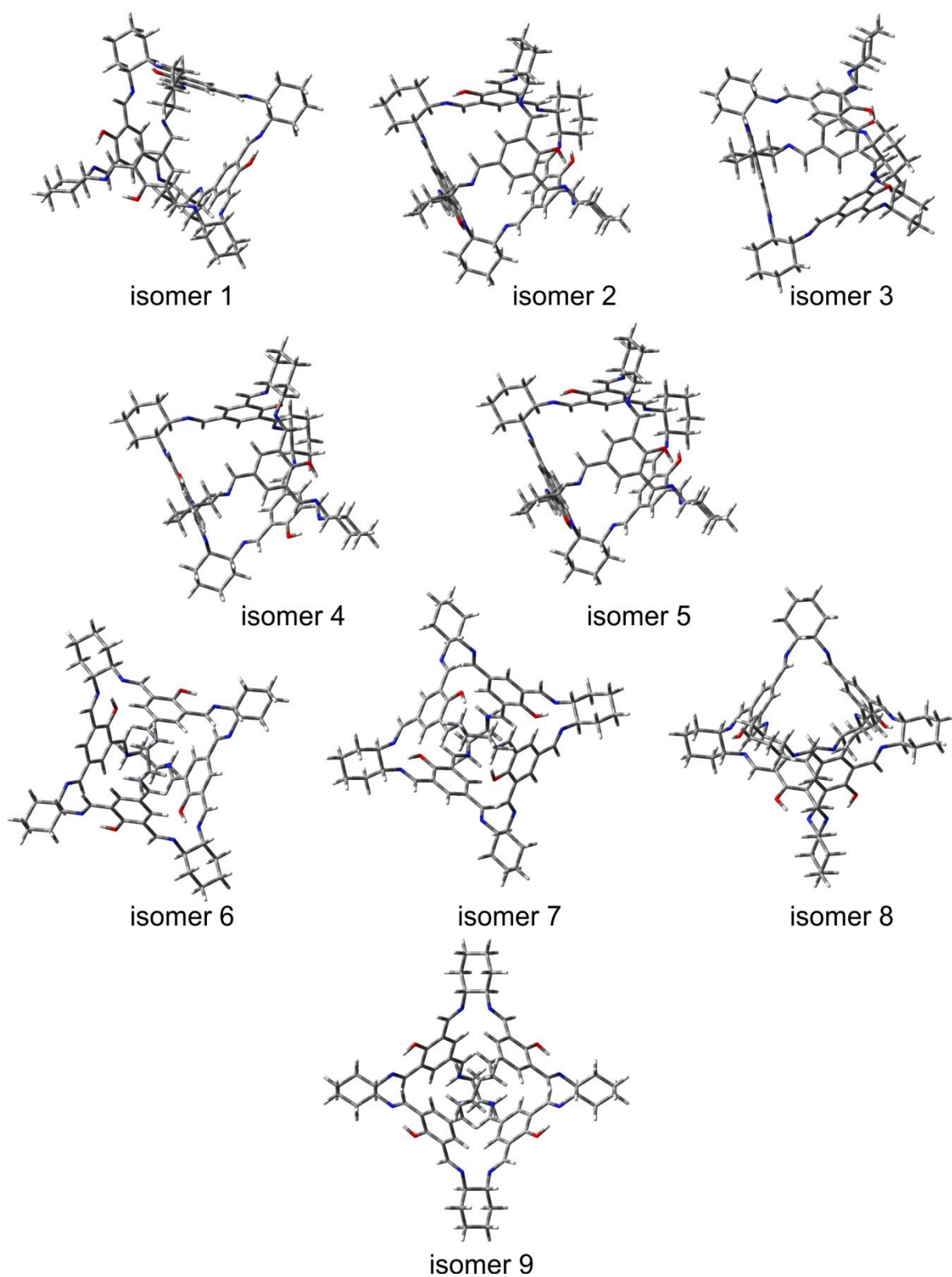


Figure SI_22. Structures of possible isomers of cage **6** calculated at the IEFPCM/B3LYP/6-311G(d,p) level.

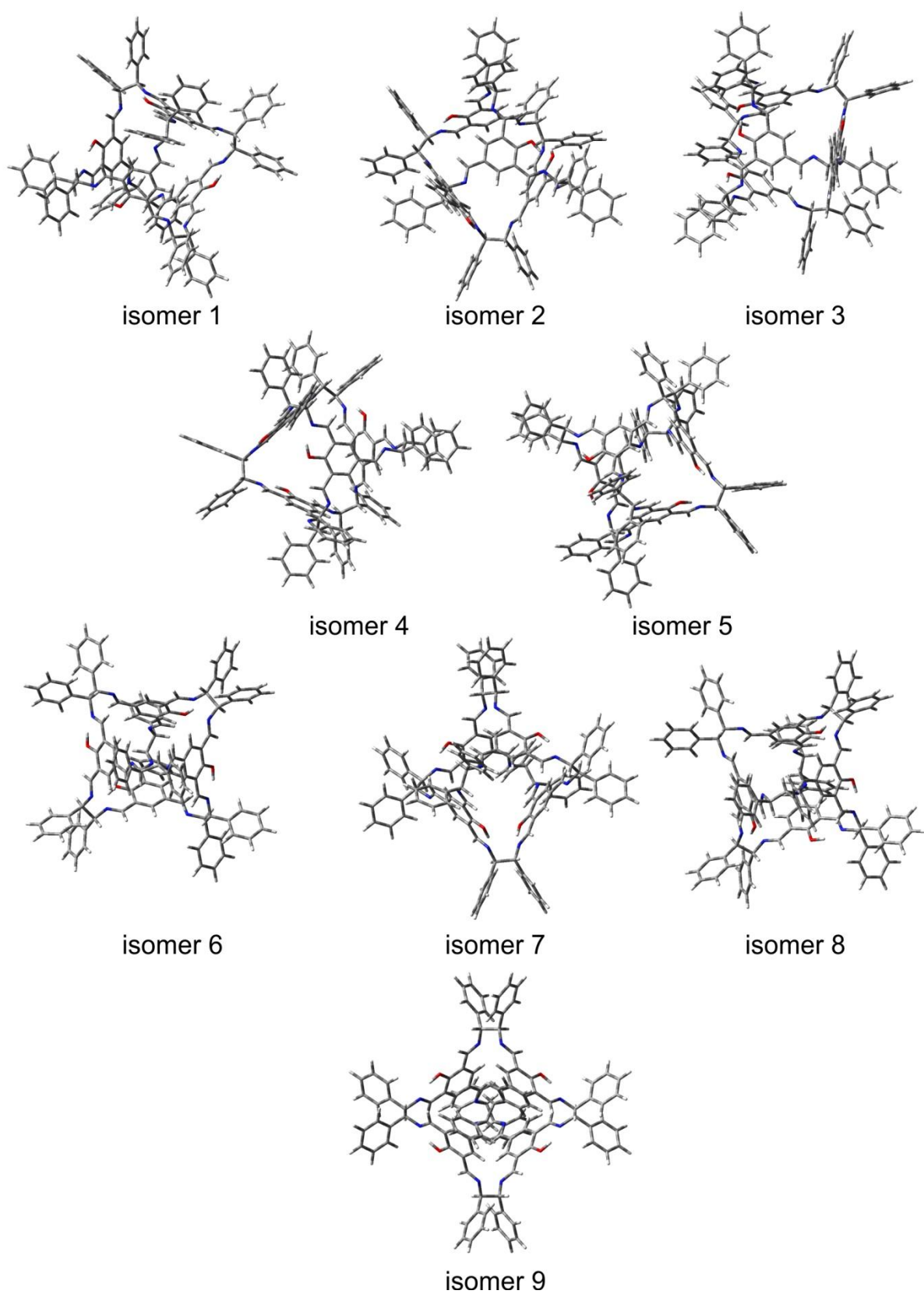


Figure SI_23. Structures of possible isomers of cage **7** calculated at the IEFPCM/B3LYP/6-311G(d,p) level.

Table SI_3. Total energies (E , in Hartree), relative energies (ΔE and $\Delta\Delta G$, in kcal mol⁻¹) and percentage populations calculated at the IEFPCM/B3LYP/6-311G(d,p) level of individual isomers of **5**.

Isomer no	E	ΔE	Pop.	$\Delta\Delta G$	Pop
1	-2816.594344	0.33	9.16	0.10	15.07
2	-2816.594821	0.03	15.2	0.00	17.78
3	-2816.594864	0.00	15.9	0.03	16.88
4	-2816.594515	0.22	10.99	0.29	10.88
5	-2816.594	0.33	9.13	0.17	13.42
6	-2816.594733	0.08	13.84	0.27	11.32
7	-2816.594313	0.35	8.87	0.45	8.37
8	-2816.59442	0.28	9.94	0.85	4.26
9	-2816.594087	0.49	6.98	1.29	2.02

Table SI_4. Total energies (E , in Hartree), relative energies (ΔE and $\Delta\Delta G$, in kcal mol⁻¹) and percentage populations calculated at the IEFPCM/B3LYP/6-311G(d,p) level of individual isomers of **6**.

Isomer no	E	ΔE	Pop.	$\Delta\Delta G$	Pop
1	-3753.162238	0.33	9.32	0.26	14.07
2	-3753.162556	0.13	13.06	0.00	21.75
3	-3753.162635	0.08	14.2	0.45	10.25
4	-3753.16217	0.37	8.68	0.50	9.34
5	-3753.163	0.13	13.11	0.01	21.36
6	-3753.162764	0.00	16.28	1.32	2.35
7	-3753.162016	0.47	7.37	0.33	12.38
8	-3753.162254	0.32	9.49	0.56	8.5
9	-3753.16215	0.39	8.49	3.62	

Table SI_3. Total energies (E , in Hartree), relative energies (ΔE and $\Delta\Delta G$, in kcal mol⁻¹) and percentage populations calculated at the IEFPCM/B3LYP/6-31G(d,p) level of individual isomers of **7**.

Isomer no	E	ΔE	Pop.	$\Delta\Delta G$	Pop
1	-5588.504199	0.18	11.54	1.69	2.13
2	-5588.504307	0.11	12.94	0.00	37.19
3	-5588.504412	0.04	14.47	0.62	13.12
4	-5588.503983	0.31	9.18	0.57	14.13
5	-5588.504028	0.28	9.63	1.47	3.09
6	-5588.504479	0.00	15.52	0.78	9.9
7	-5588.503973	0.22	10.64	1.06	6.2
8	-5588.504034	0.28	9.69	0.69	11.53
9	-5588.50364	0.53	6.38	1.55	2.72

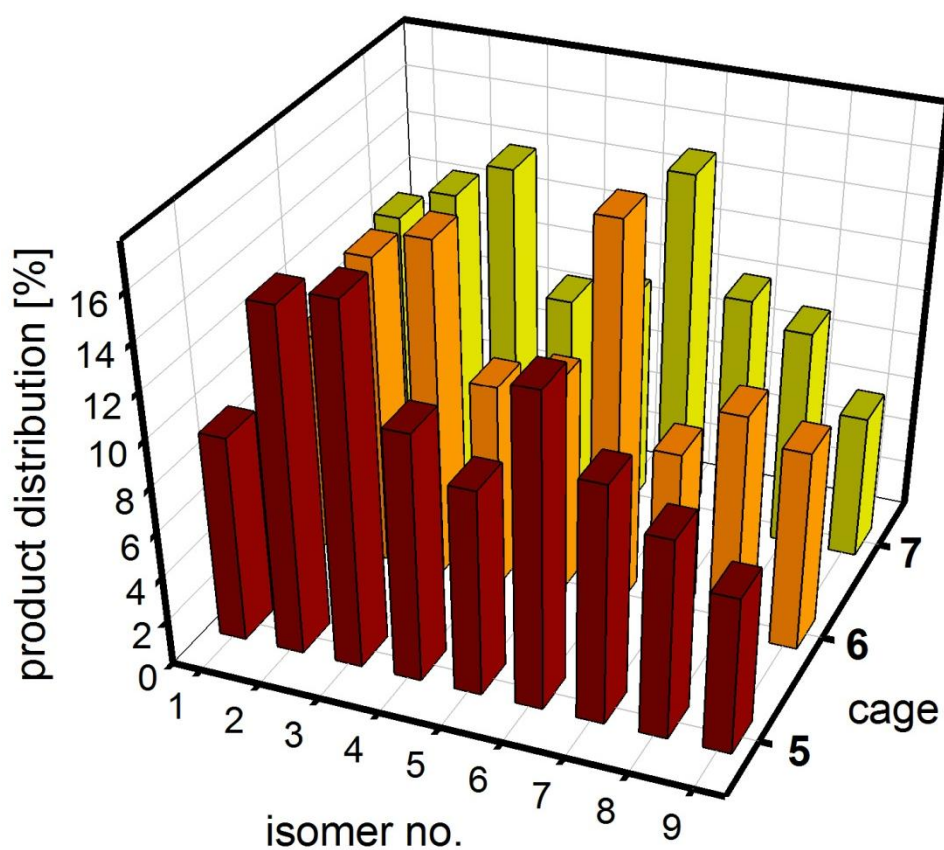


Figure SI_24. ΔE -Based product distributions calculated for **5-7** at the DFT level.

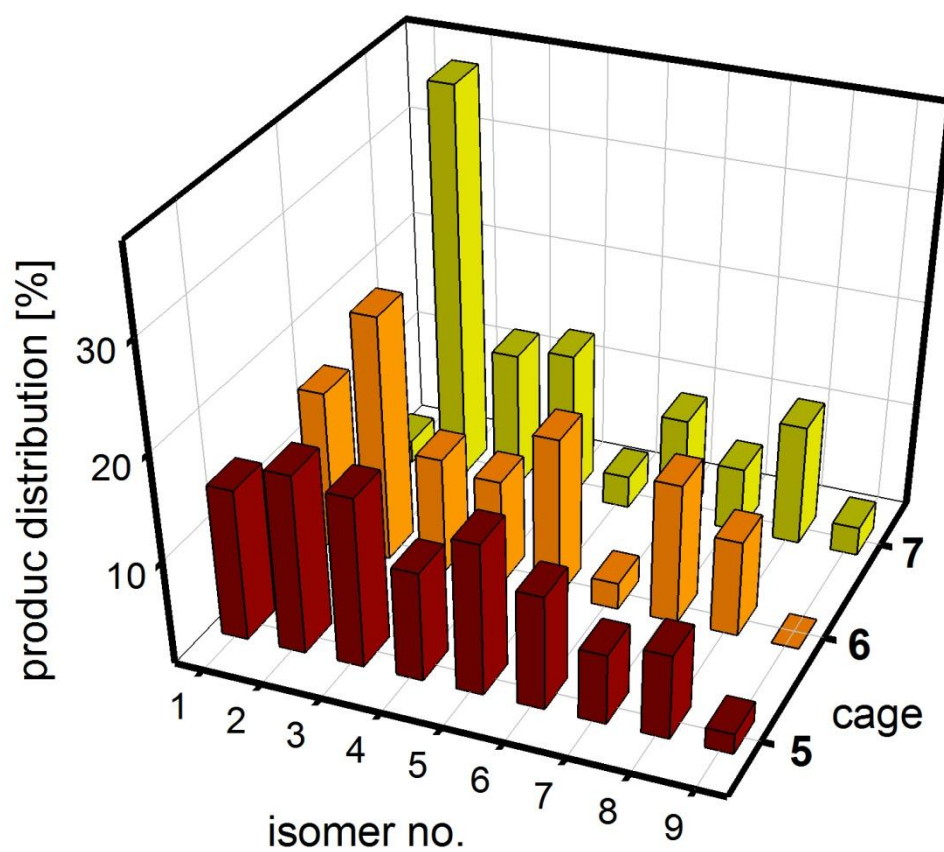


Figure SI_25. $\Delta\Delta G$ -Based product distributions calculated for 5-7 at the DFT level.

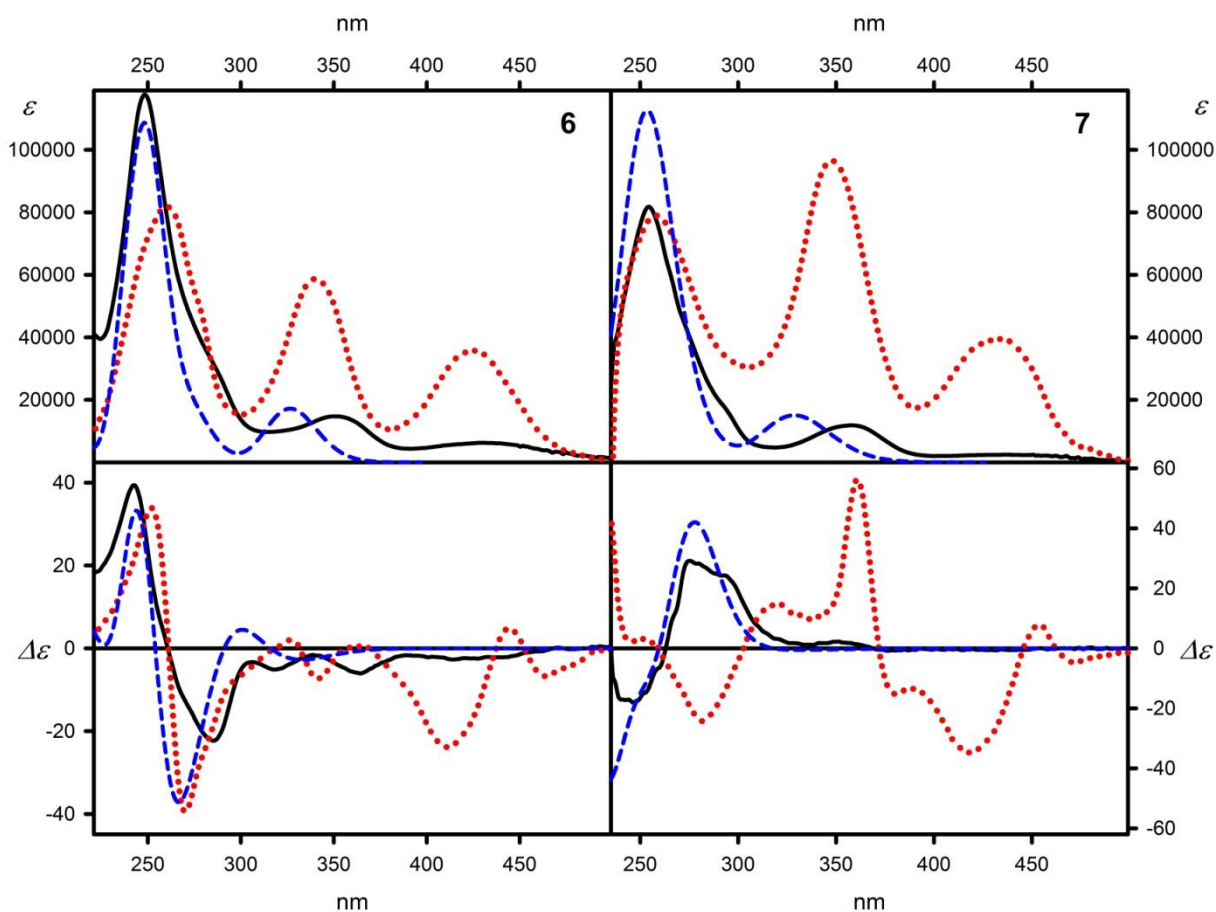


Figure SI_26. UV (upper panel) and ECD spectra (lower panel) of cages **6** (left column) and **7** (right column) measured in chloroform (solid black lines) and in acidified chloroform solutions (dotted red lines) and calculated UV and ECD spectra (blue dashed lines) for neutral **6** and **7**. The calculated spectra were wavelength corrected to match the short-wavelength UV absorption maxima.

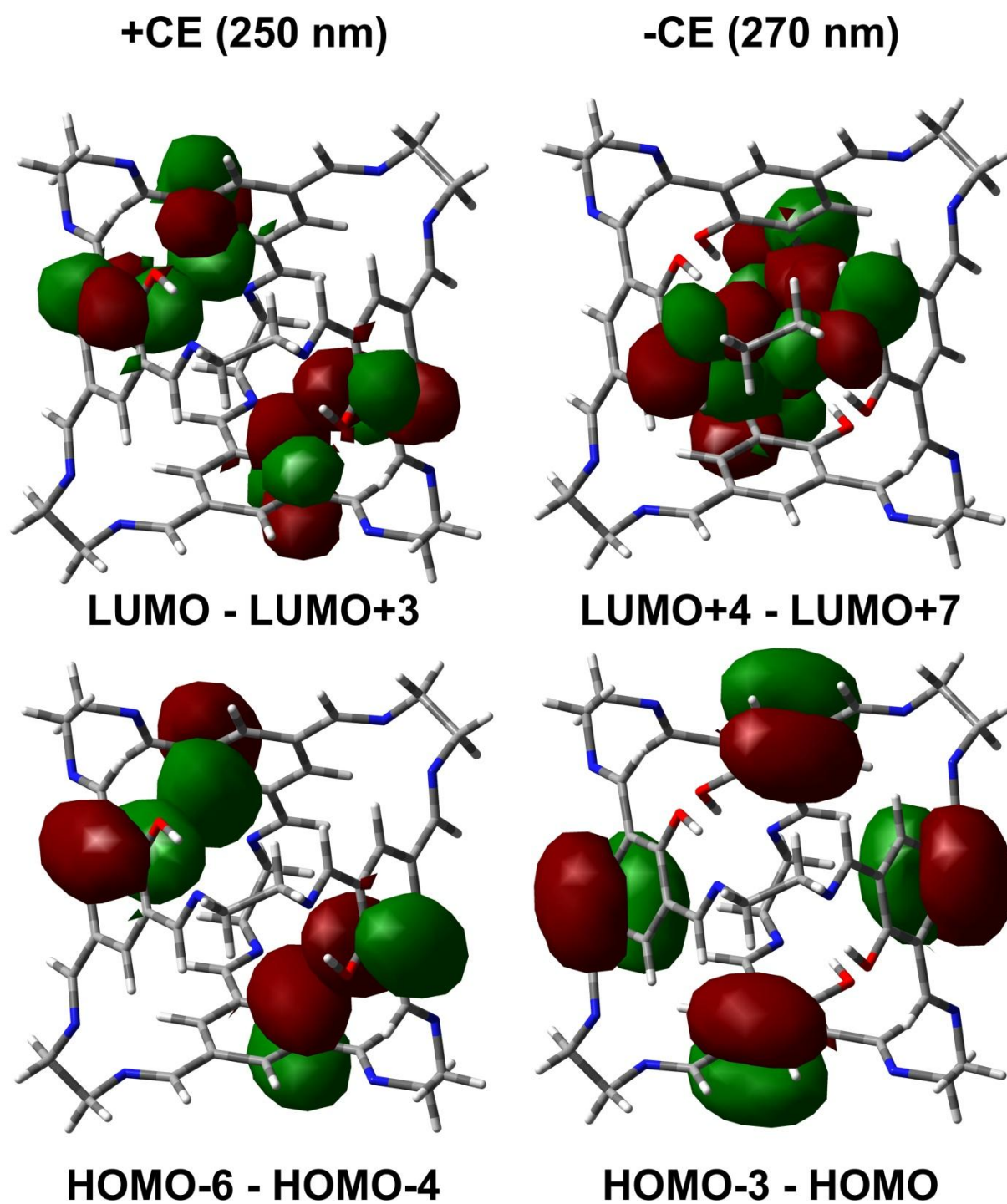


Figure SI_27. Calculated with NBO method orbitals involved in electronic transitions responsible for the highest intensity Cotton effects in ECD spectrum of **6** (the tetramethylene chains of cyclohexane units were replaced by hydrogen atoms).

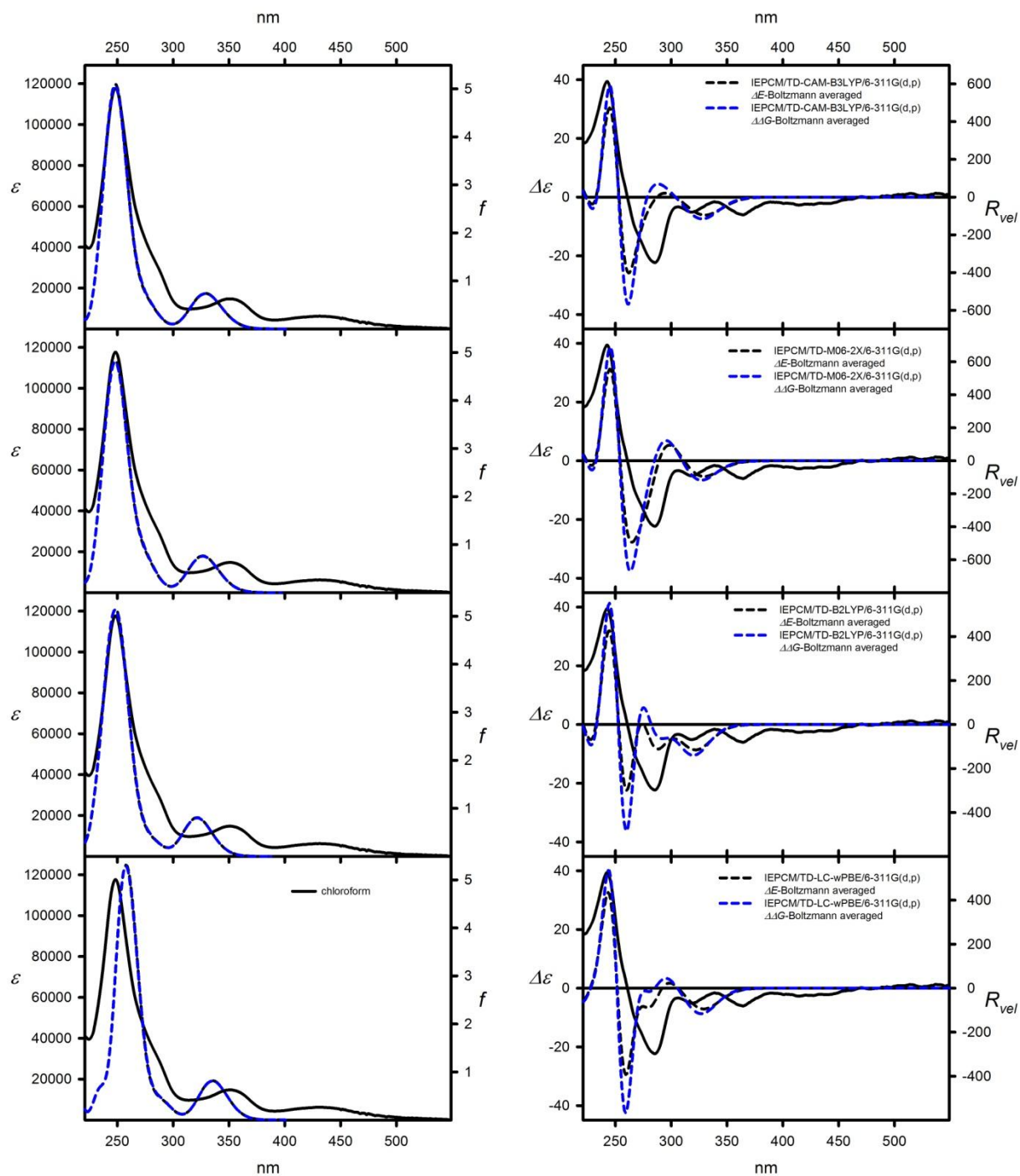


Figure SI_28. Experimental (solid black lines) and ΔE and $\Delta\Delta G^\circ$ Boltzmann averaged (dashed lines) calculated at the TD-DFT/6-311G(d,p) level for structures optimized at the DFT/6-311G(2d,2p) levels UV (left column) and ECD (right column) spectra of cage **6**. All calculated spectra were wavelength corrected.

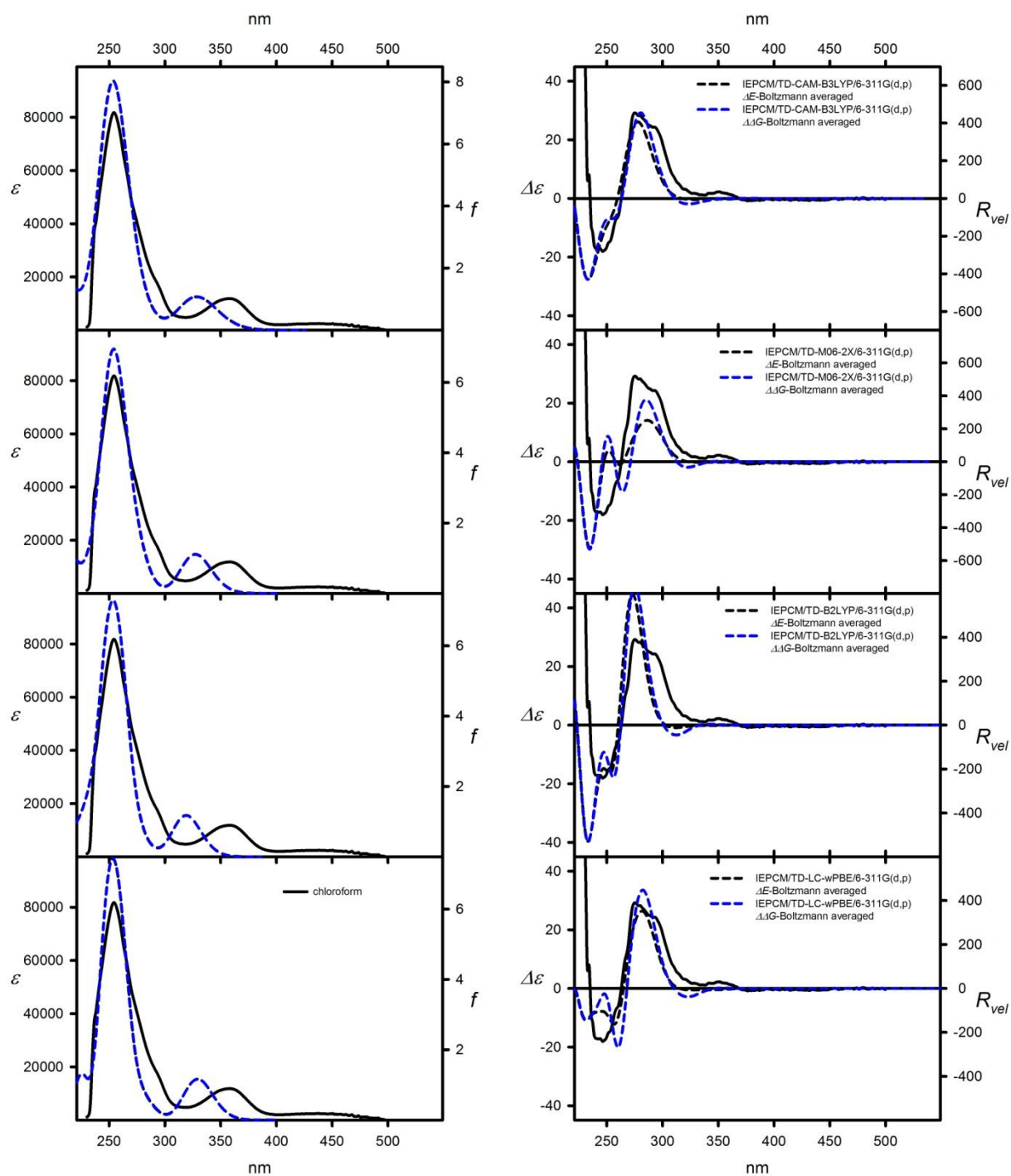
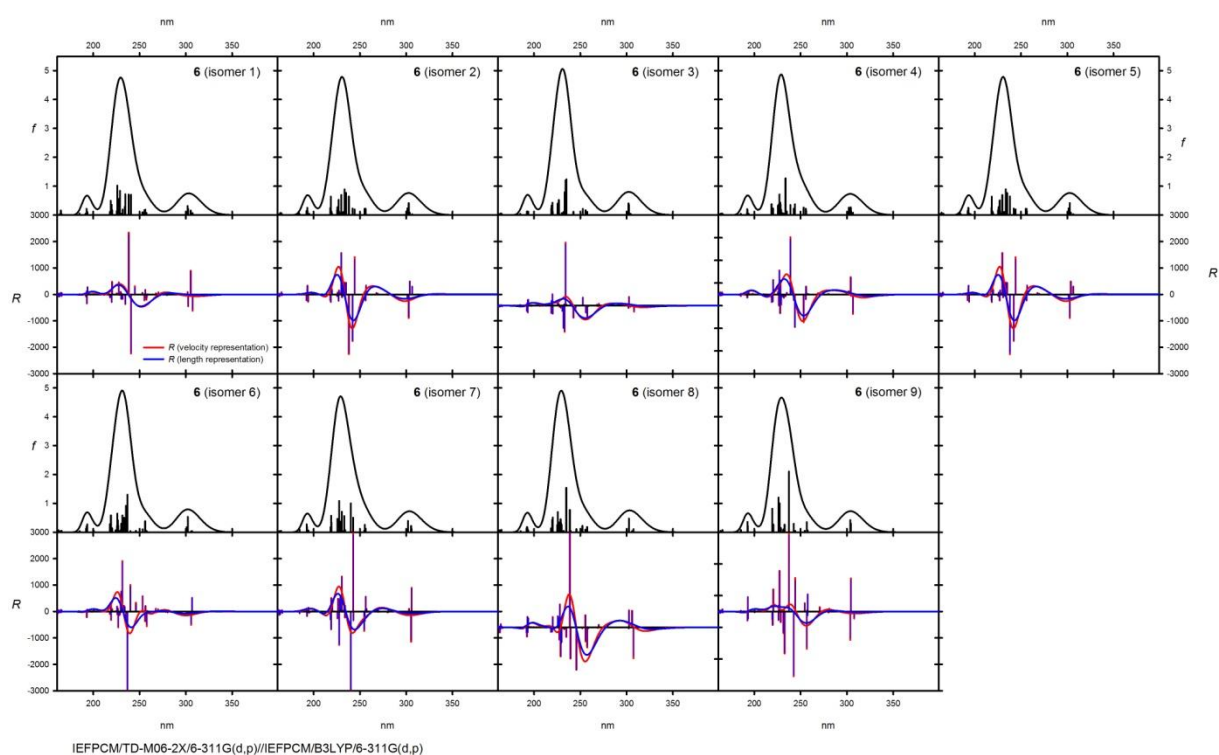
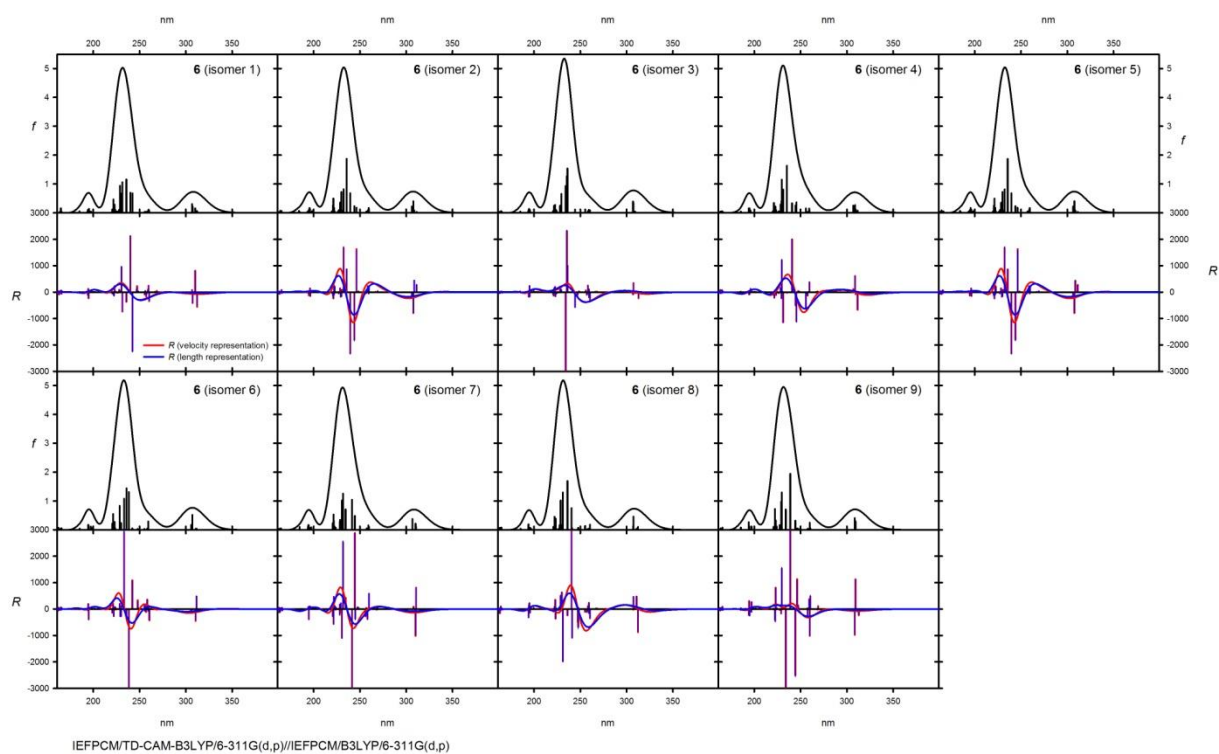


Figure SI_29. Experimental (solid black lines) and ΔE and $\Delta \Delta G^\circ$ Boltzmann averaged (dashed lines) calculated at the TD-DFT/6-311G(d,p) level for structures optimized at the DFT/6-311G(2d,2p) levels UV (left column) and ECD (right column) spectra of cage 7. All calculated spectra were wavelength corrected.



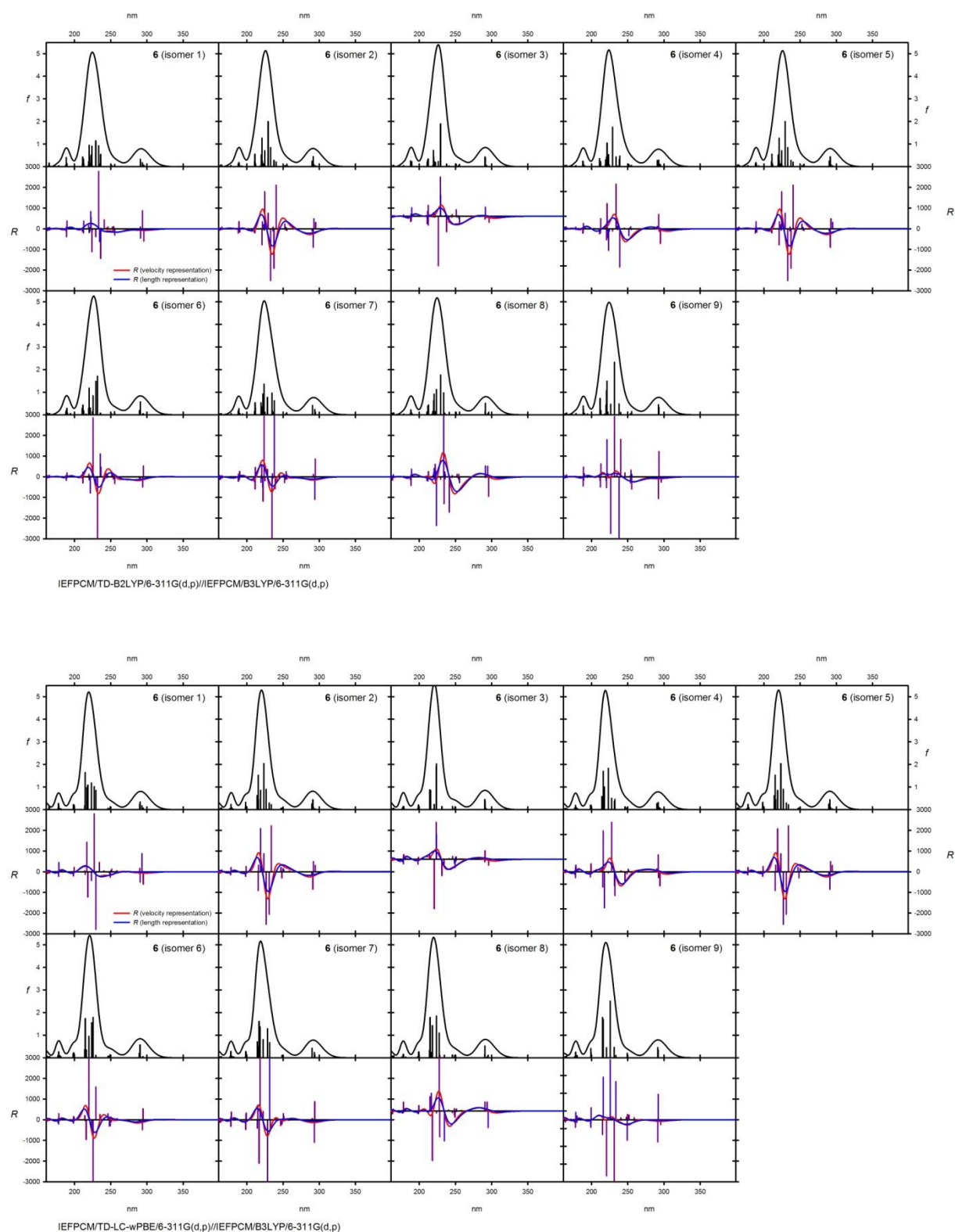
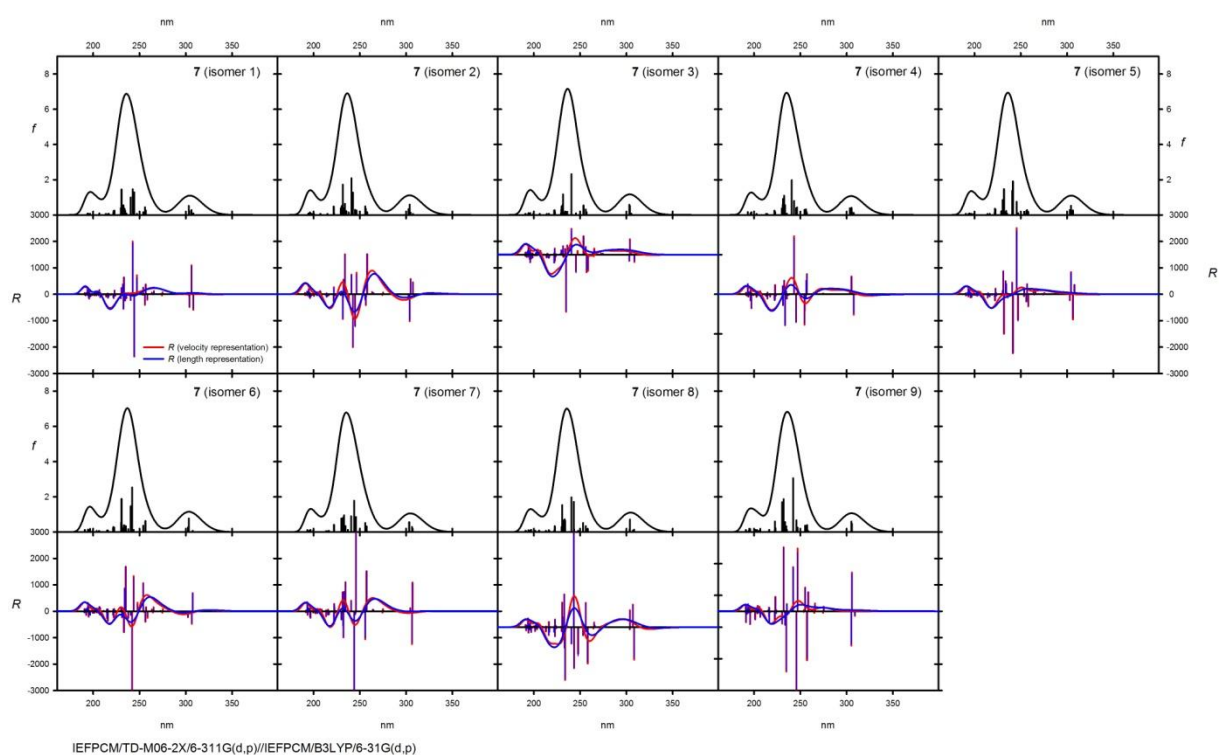
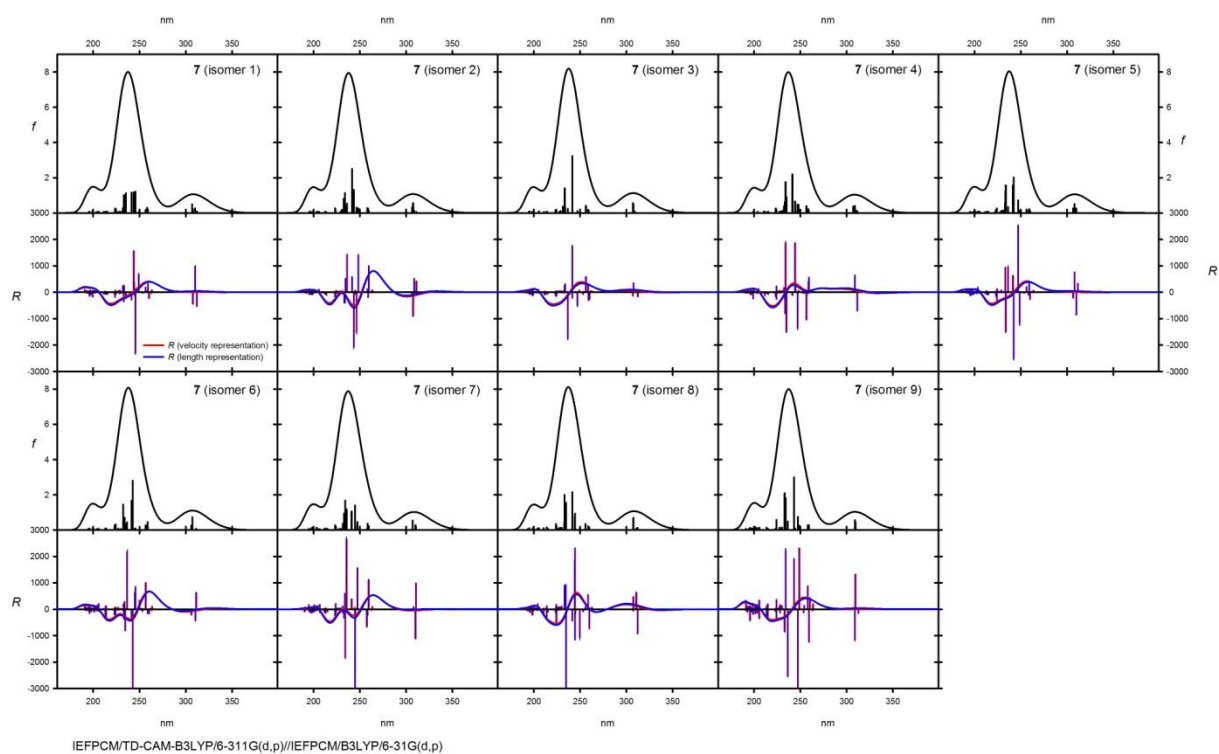


Figure SI_30. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual isomers of **6** optimized at the IEFPCM/B3LYP/6-311G(d,p) level. Wavelengths were not corrected.



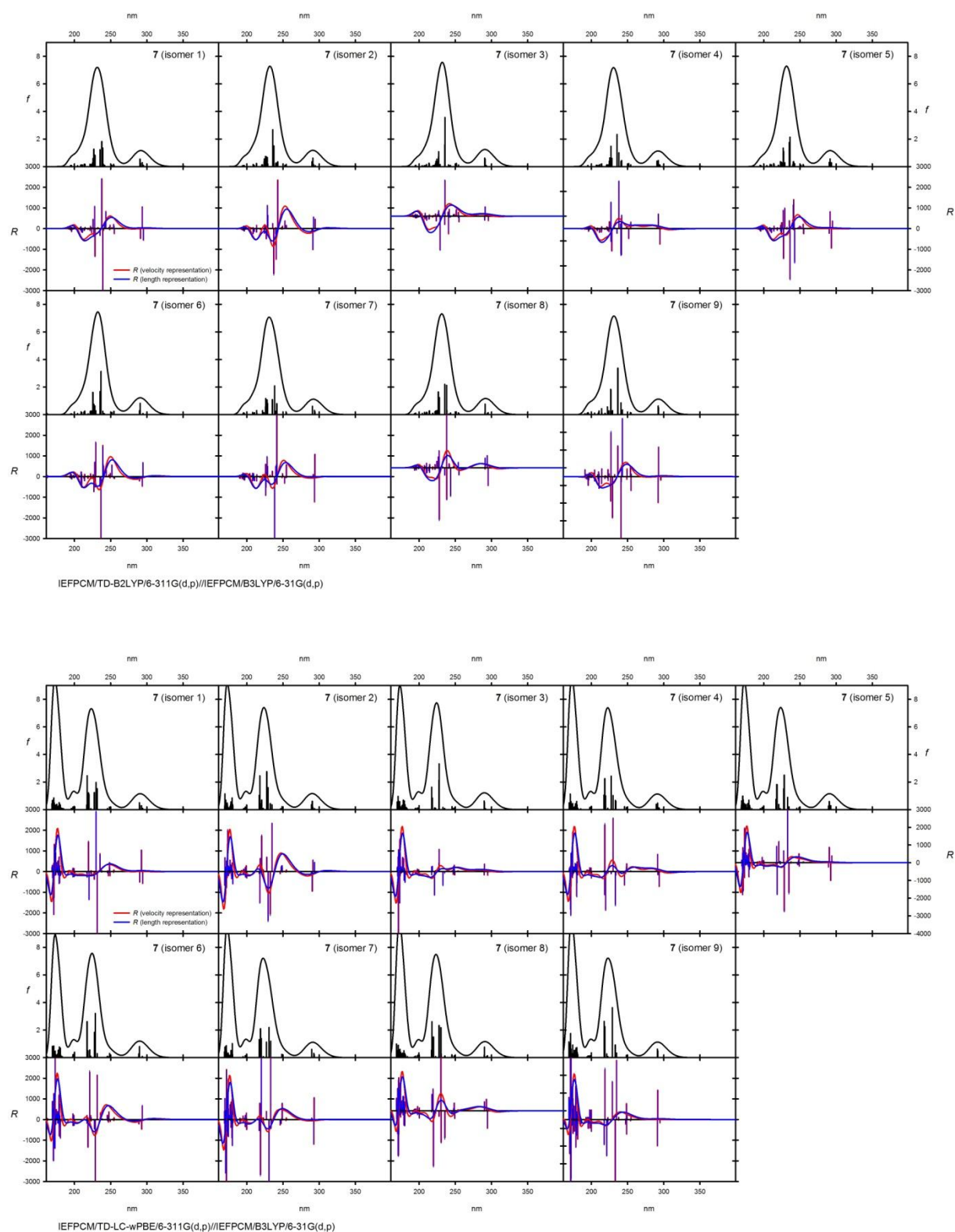
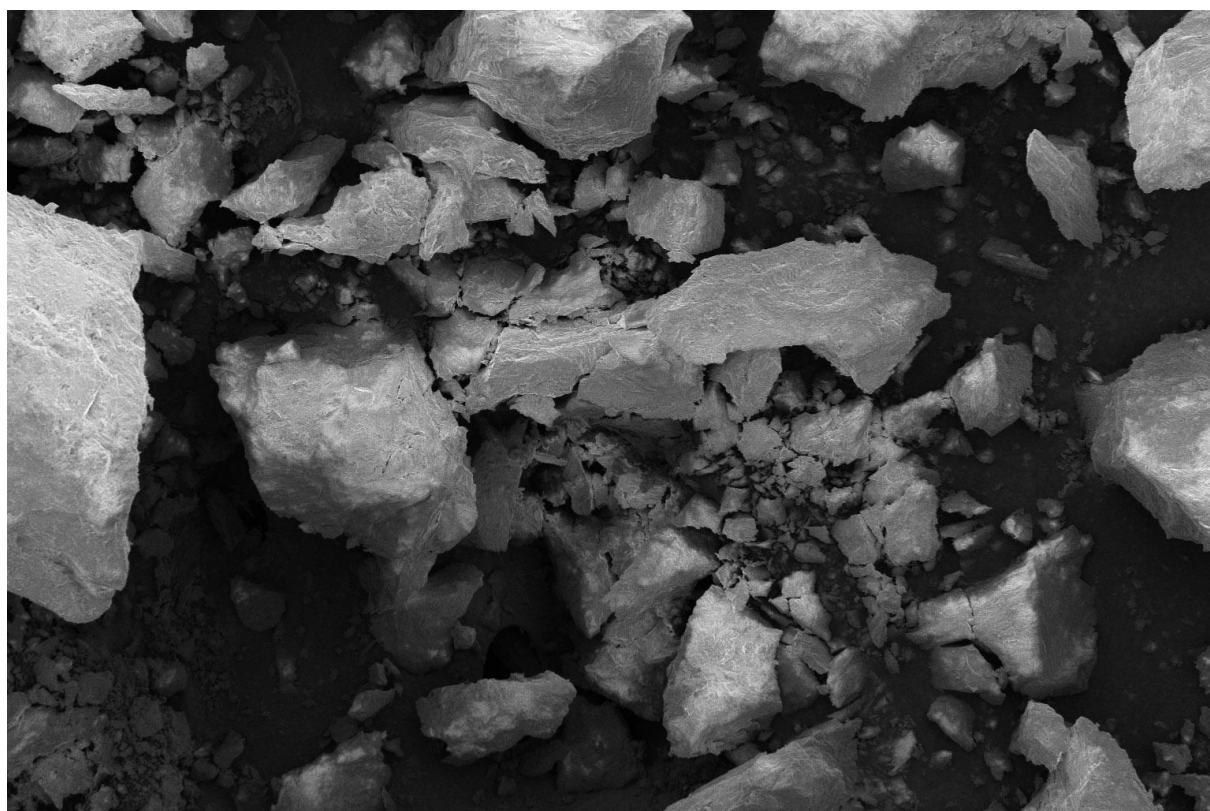
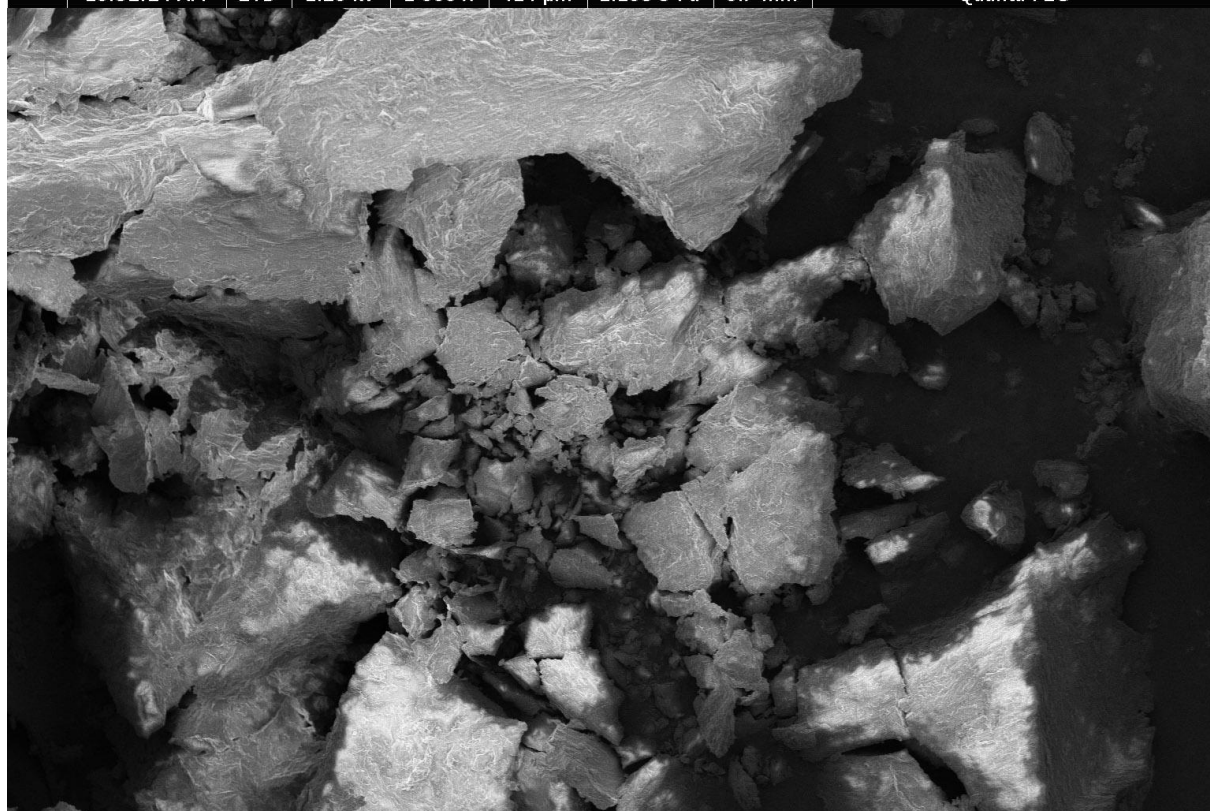


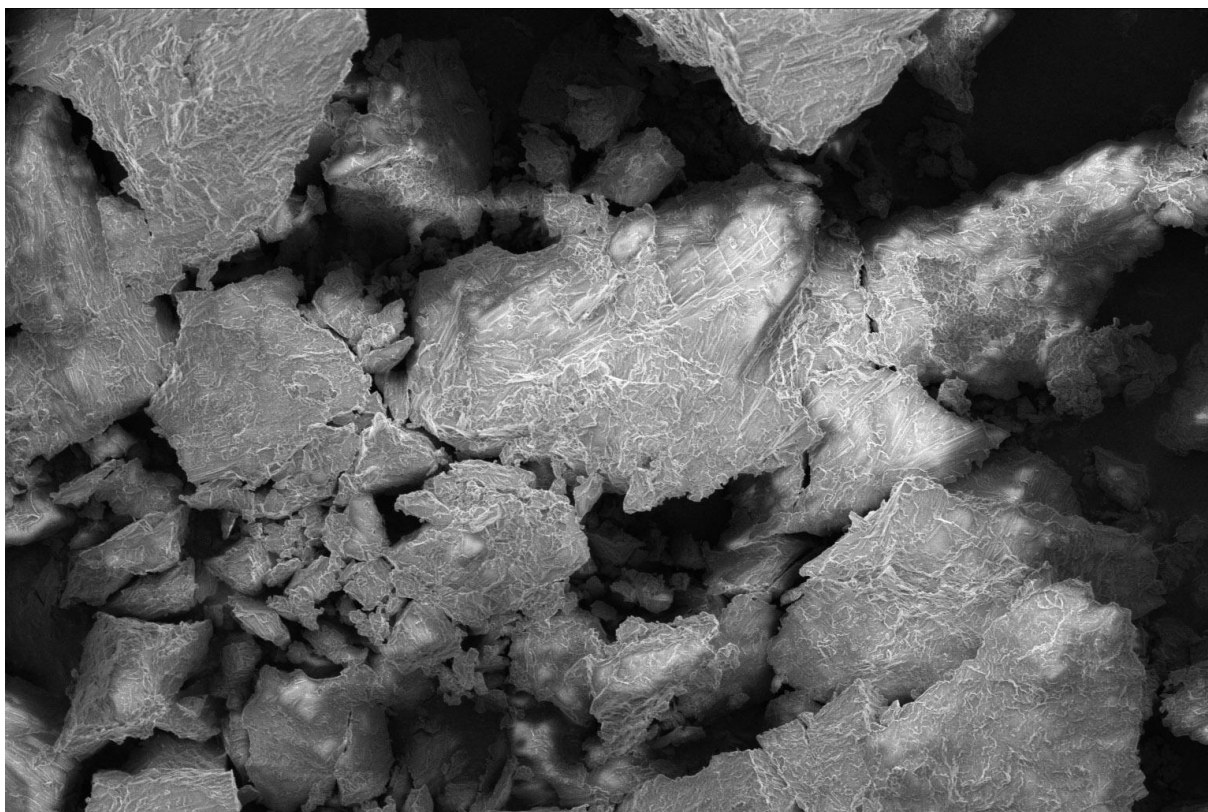
Figure SI_31. UV (upper panels) and CD (lower panels) spectra calculated at various levels of theory for individual isomers of **7** optimized at the IEFCM/B3LYP/6-311G(d,p) level. Wavelengths were not corrected.



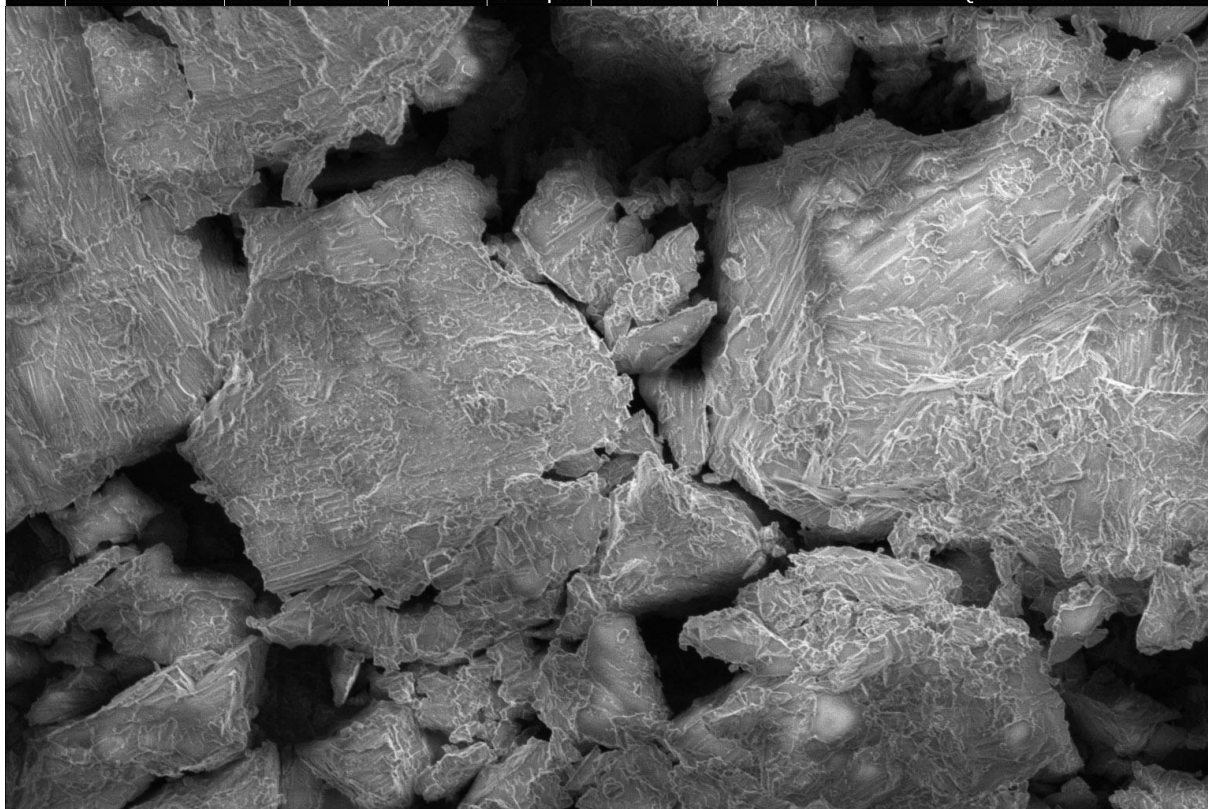
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								Quanta FEG



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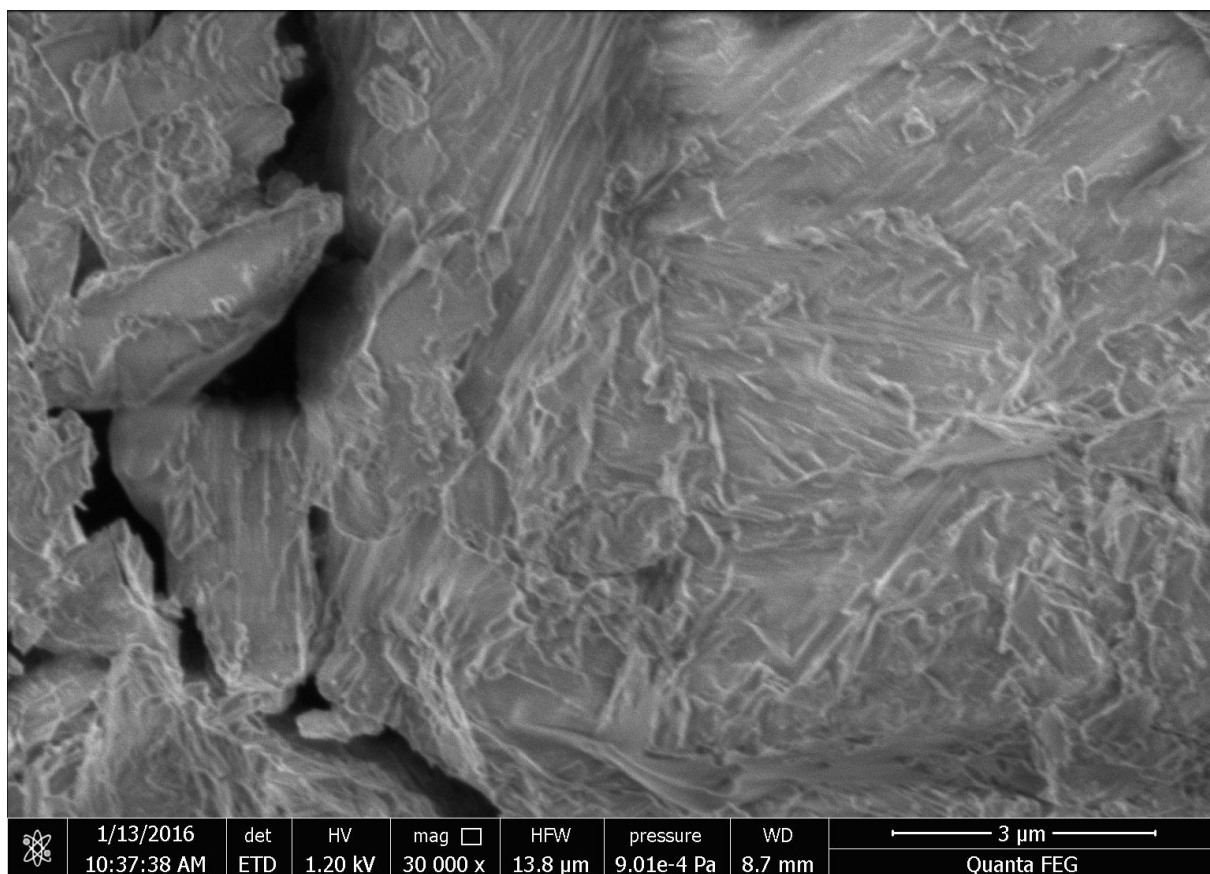
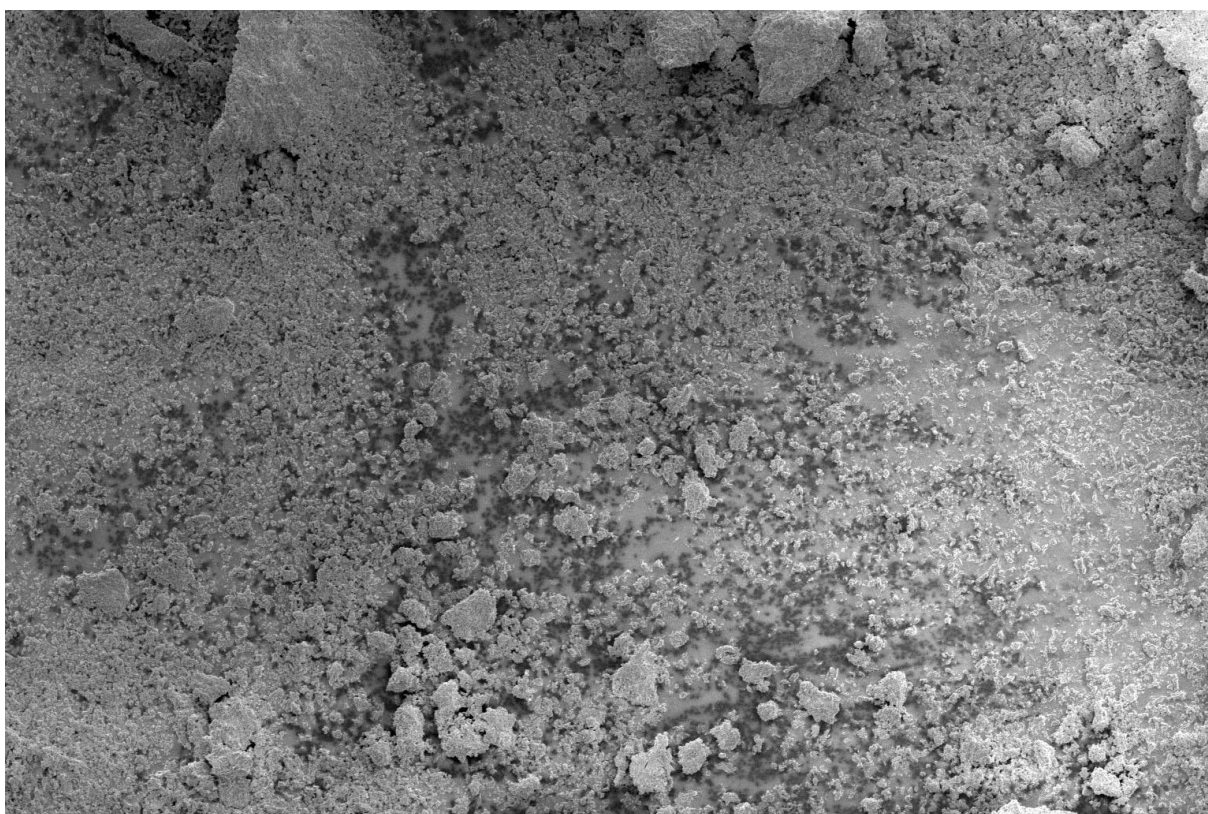
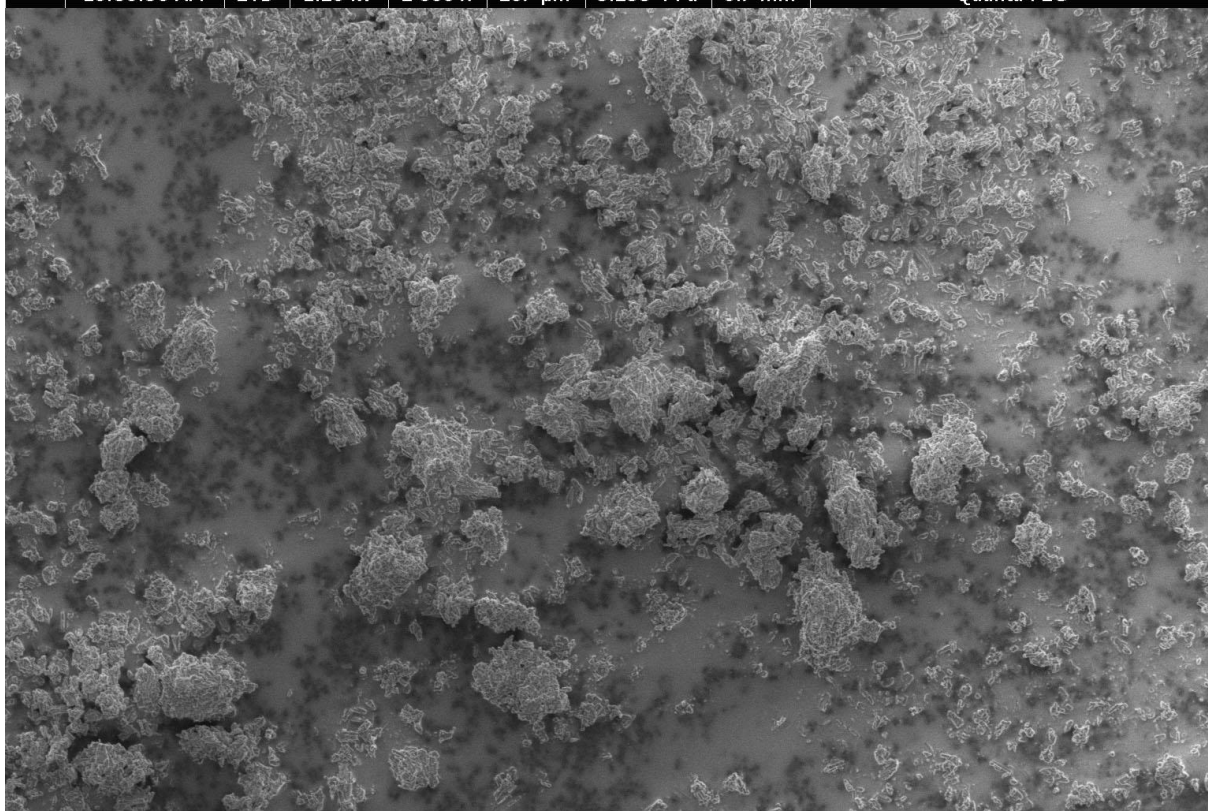


Figure SI_32. SEM images of material derived from **7**, characterizing by value of Brunauer-Emmett-Teller surface area (SA_{BET}) estimated as $12.5 \text{ m}^2 \text{ g}^{-1}$.



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	Quanta FEG							



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	Quanta FEG							

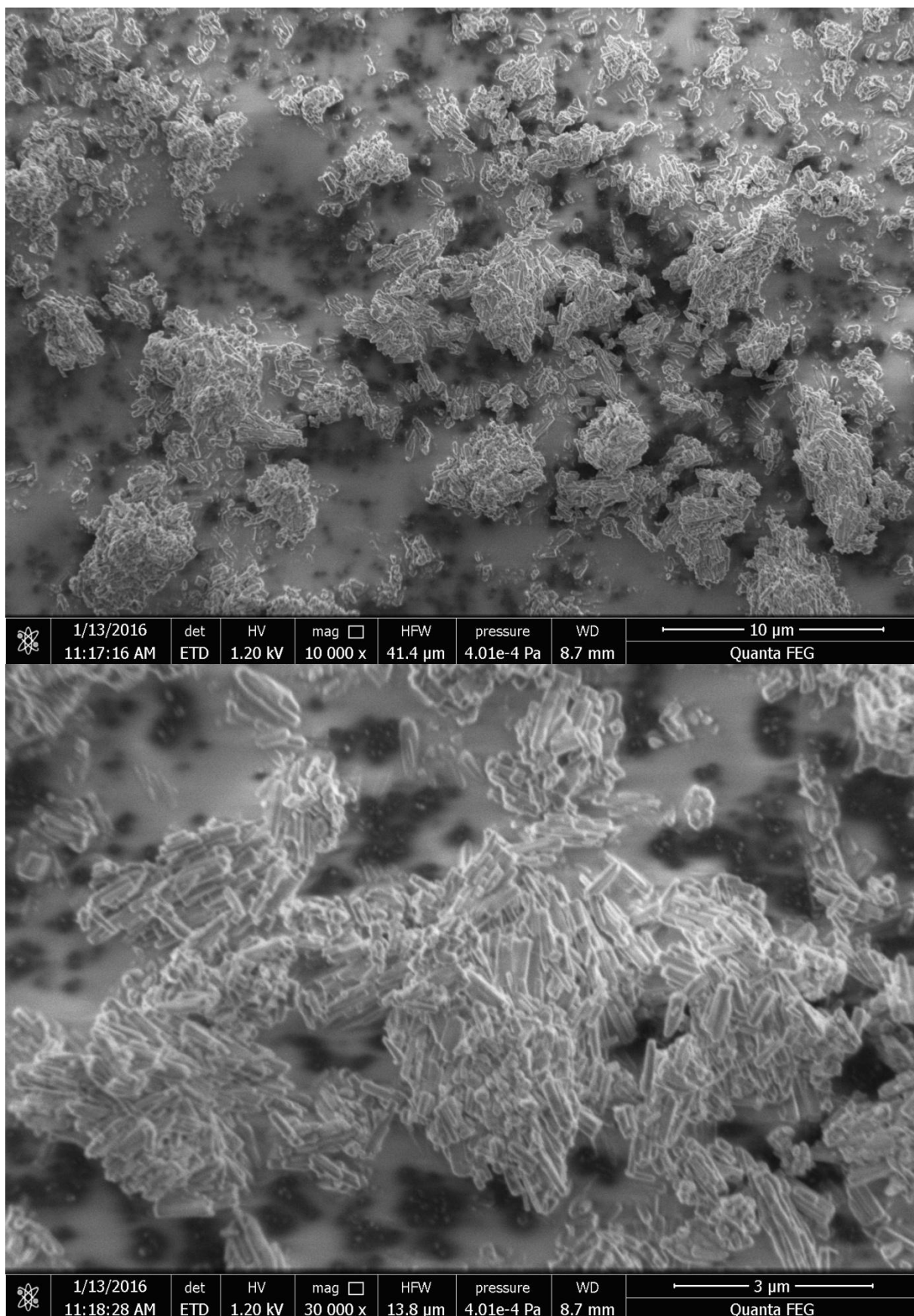


Figure SI_33. SEM images of material derived from **7**, characterizing by value of Brunauer-Emmett-Teller surface area (SA_{BET}) estimated as $577.8 \text{ m}^2 \text{ g}^{-1}$.

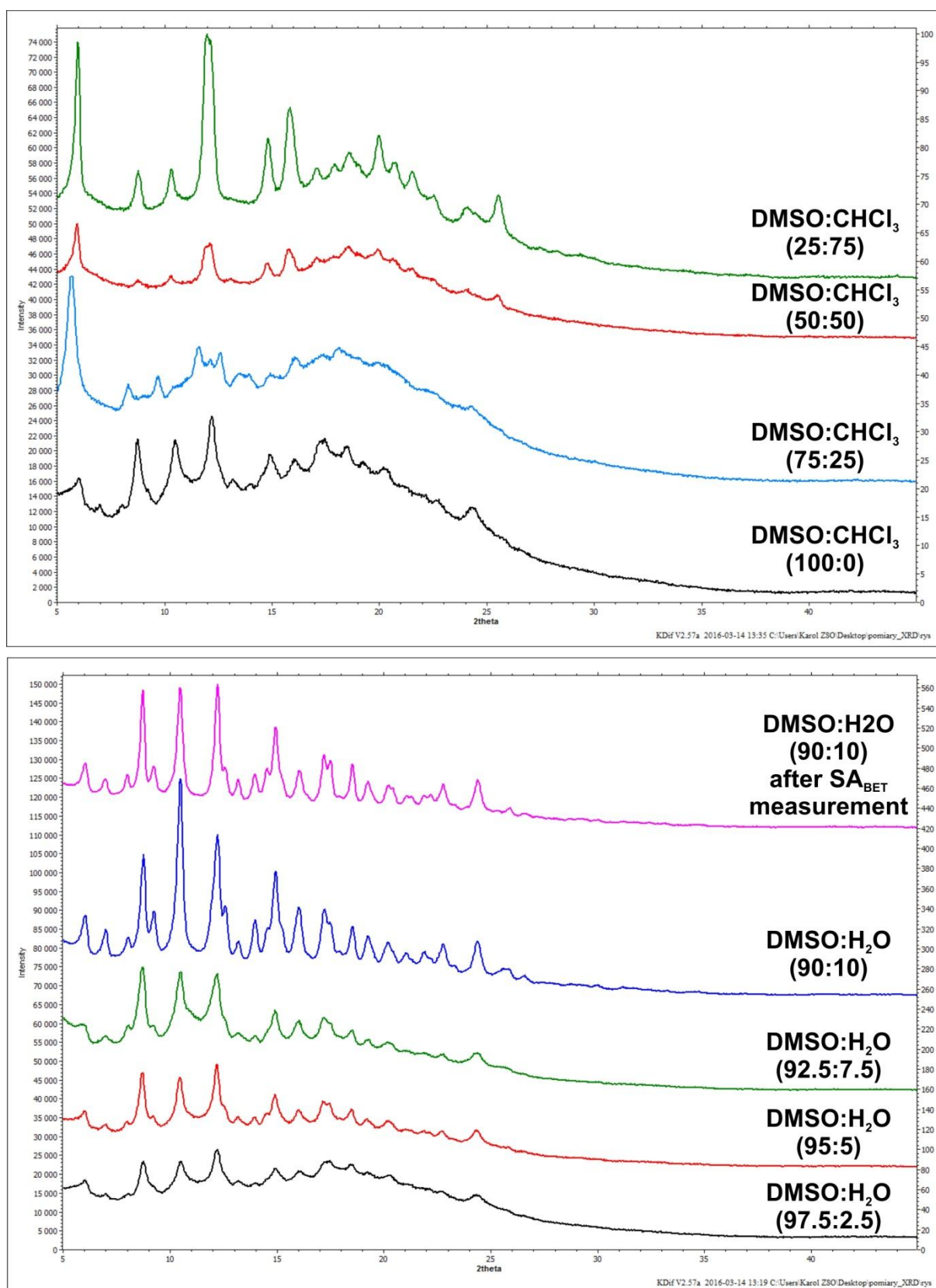
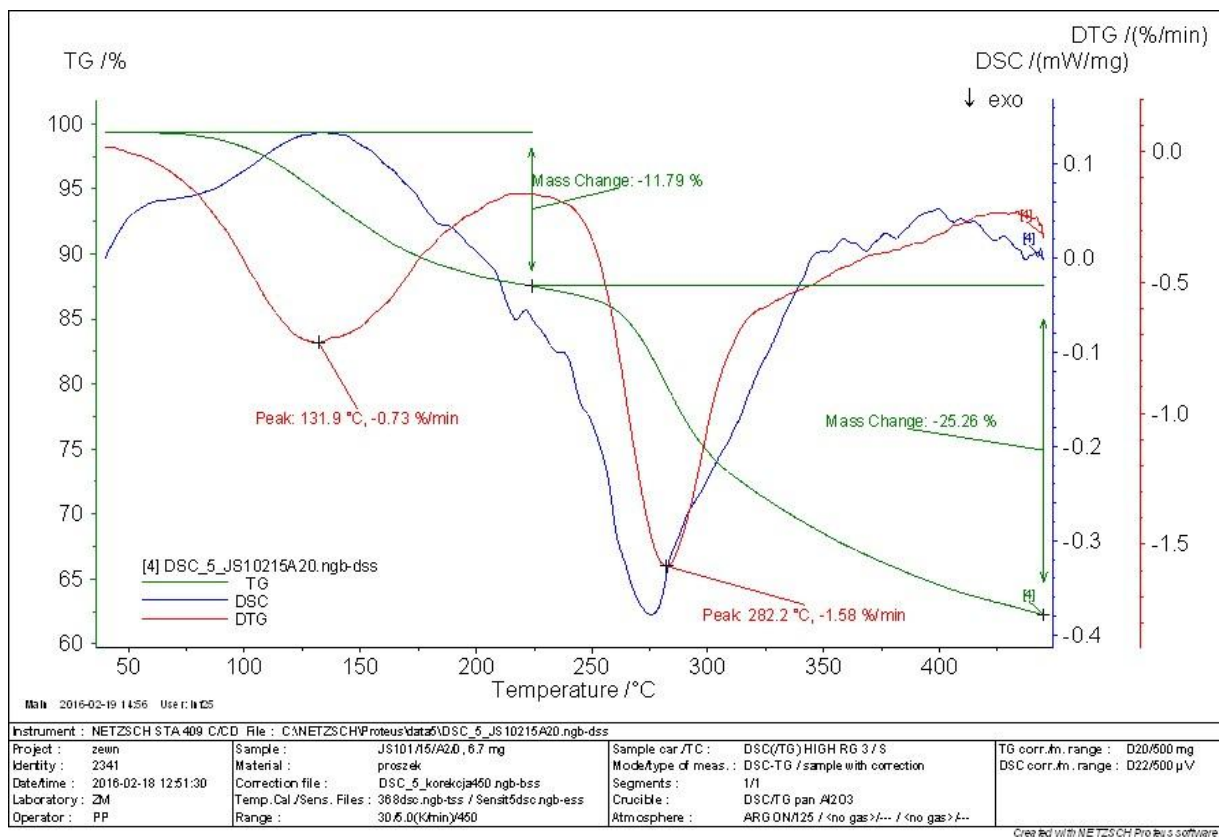
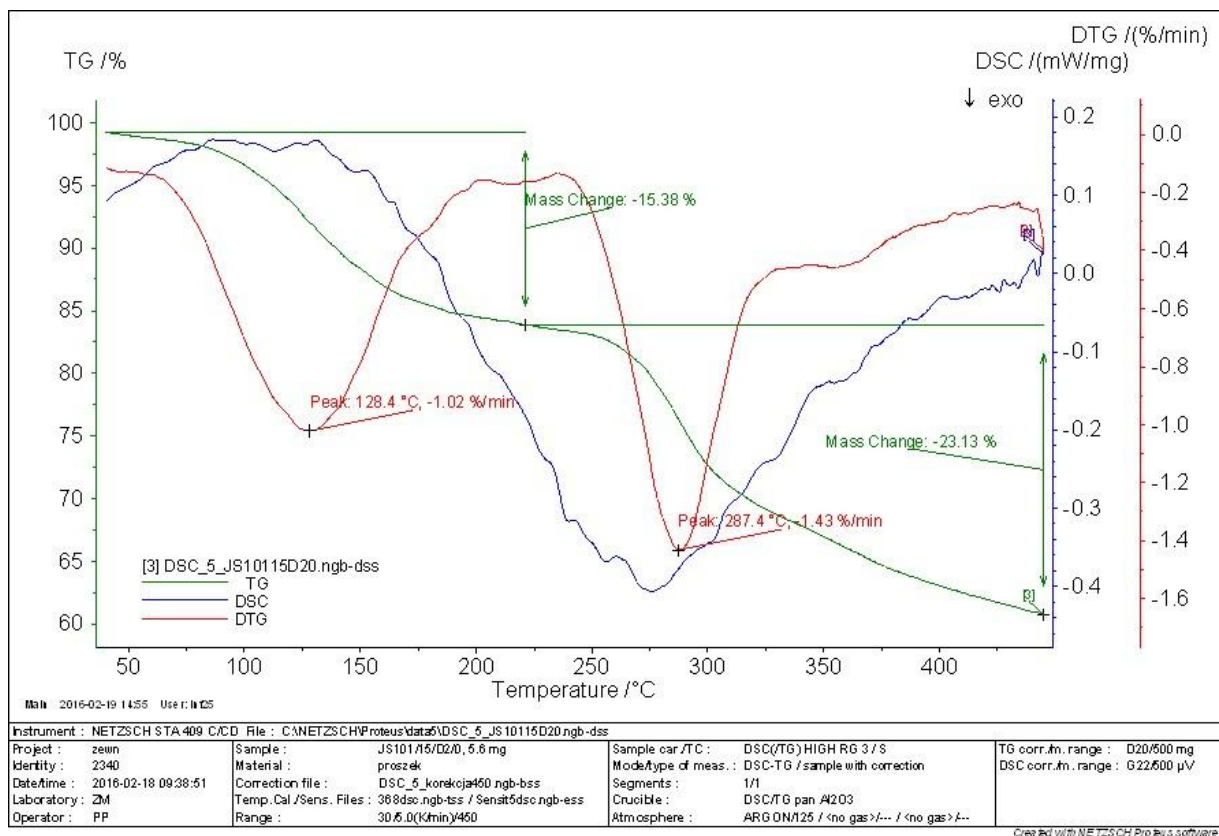
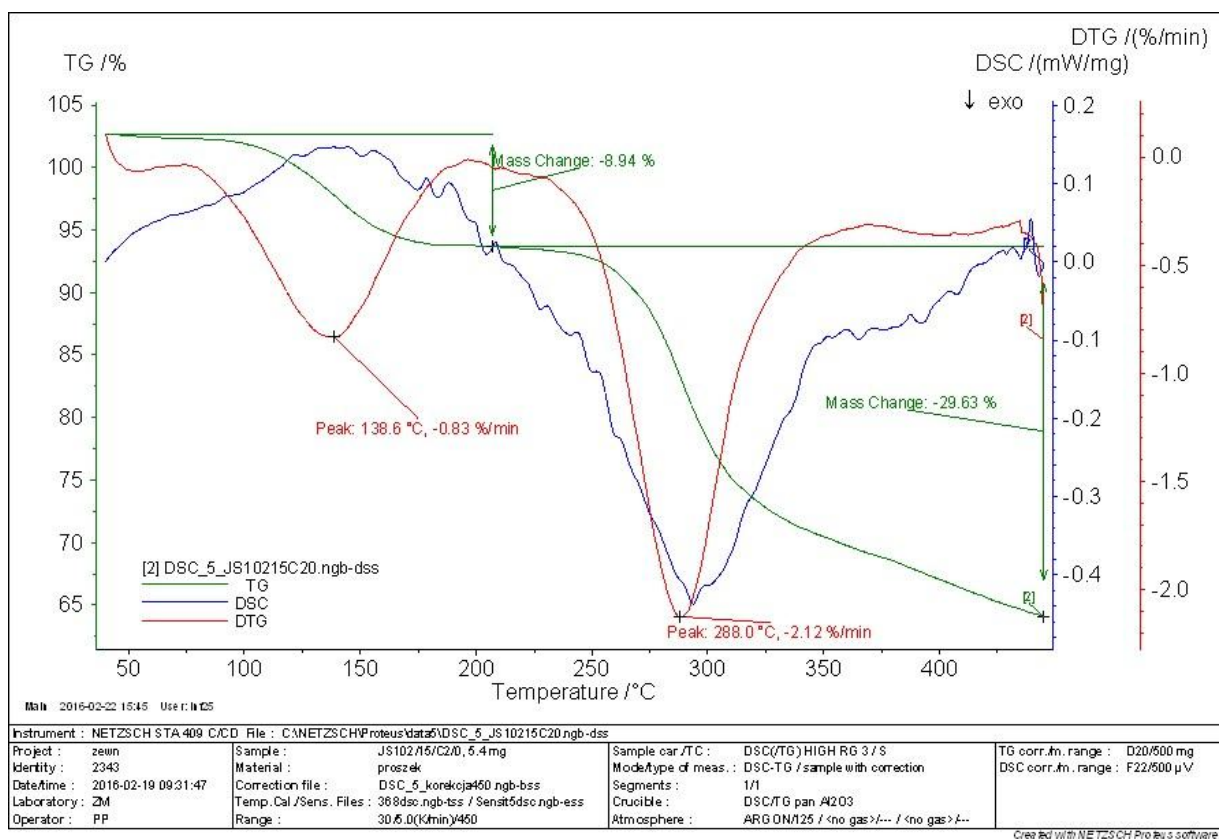
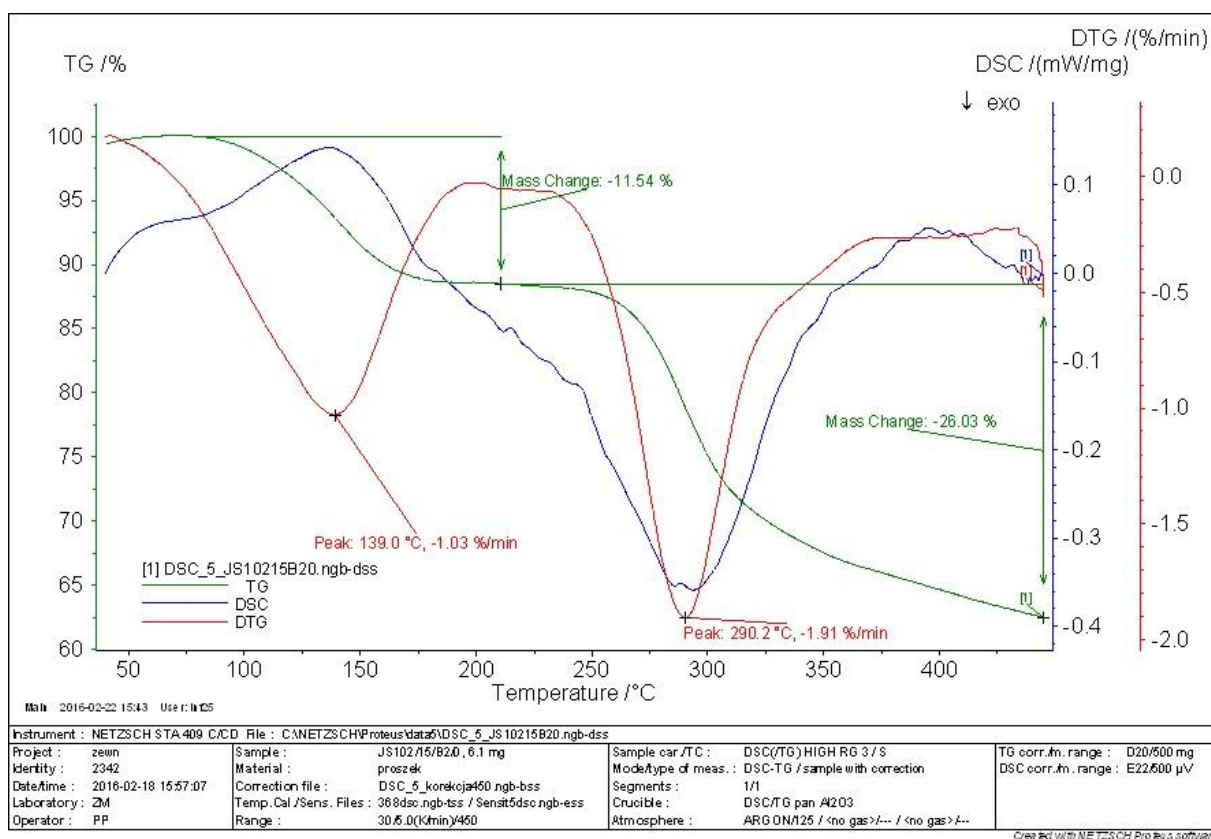
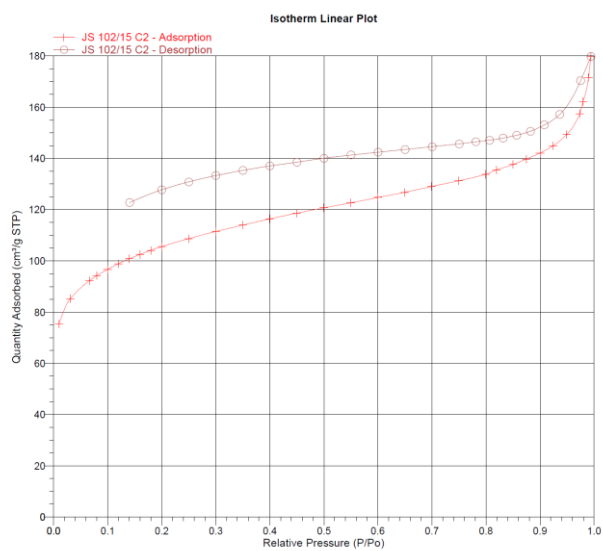
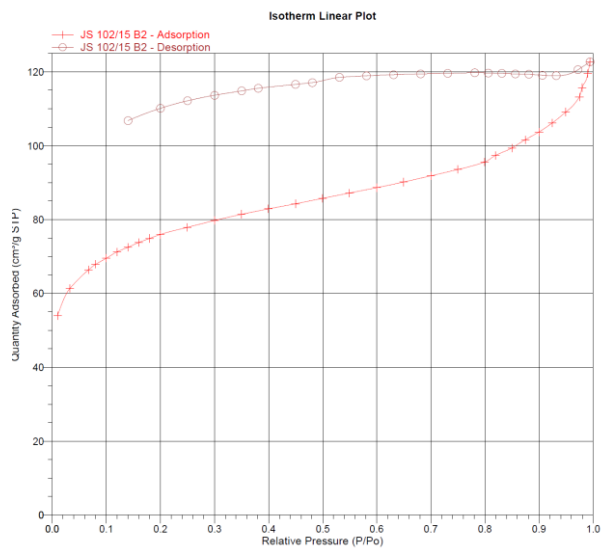
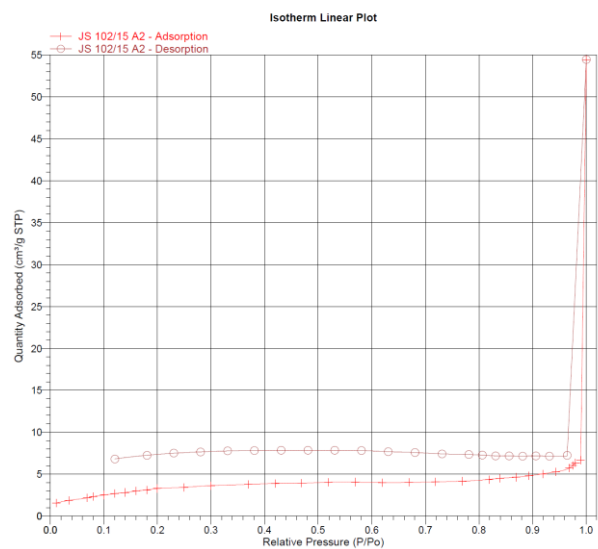


Figure SI_34. X-Ray powder diffraction (XRPD) data for materials derived from **7** and obtained under different reaction conditions.







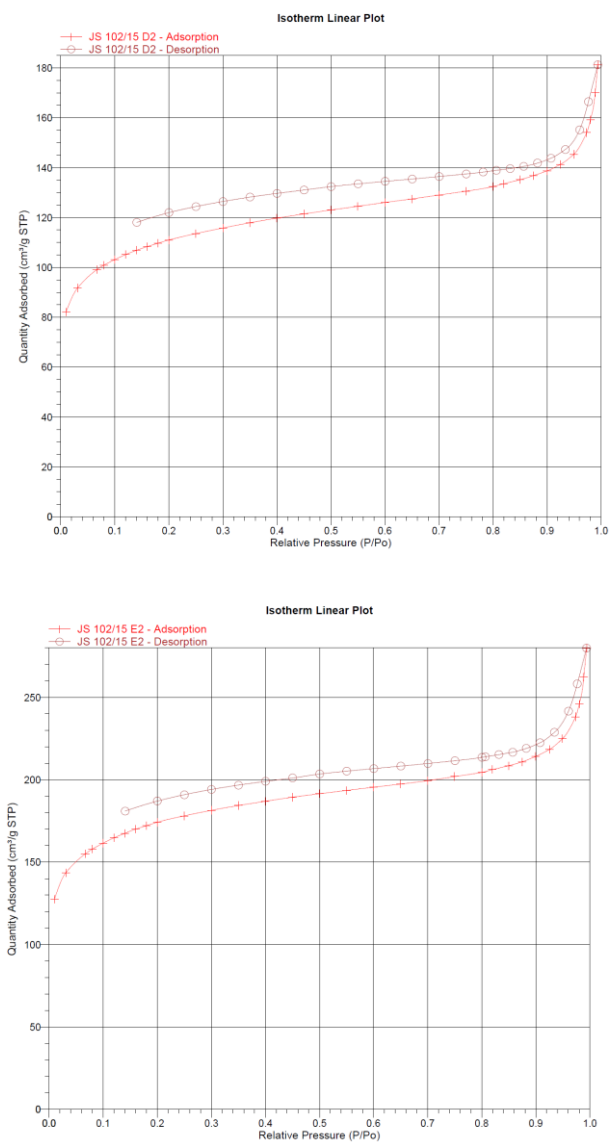


Figure SI_36. Nitrogen adsorption (crosses, raw data) and desorption isotherms (open symbols, raw data) of cage compound **7** obtained in mixture of solvents DMSO and H₂O (from top to bottom: 100; 97.5:2.5; 95:5; 92.5:7.5; 90:10) and measured at 77.35 K.

Single- Crystal X-ray Diffraction

Owing to the poor solubility of all cages investigated in most organic solvents we were able to obtain crystals only for cage **6**. Those crystals were obtained by slow evaporation of xylenes commercial mixture under ambient conditions.

Reflection intensities for cage **6** were measured on a SuperNova diffractometer equipped with a Cu microfocus source ($\lambda = 1.54178 \text{ \AA}$) and 135 mm Atlas CCD detector at 150 K. The low temperature was controlled with an Oxford Instruments Cryosystem cold nitrogen-gas blower. Data reduction and analysis were carried out with CrysAlisPro program.[9] The crystal structure of **6** was solved by direct methods using SHELXT,[10] and refined by the full-matrix least-squares technique with SHELXL-2014.[10] All heavy atoms were refined anisotropically. The hydrogen atoms attached to carbon atoms were placed in their idealized positions and refined using the riding model, and their isotropic displacement parameters were assigned a value 20% higher than the isotropic equivalent for the atom to which they were attached. The position of the hydroxyl H atom was constrained to an ideal geometry [O-H=0.84 $\text{\AA}$ and $U_{\text{iso}}(\text{H})=1.2U_{\text{eq}}(\text{O})$] using first AFIX 147 and then AFIX 3 command integrated in SHELXL.[10] Where necessary, restraints for the 1,2- and 1,3-distances were applied. Owing to the Flack parameter[11] was meaningless, the correct absolute structure of the crystal investigated was assumed from the known absolute configuration of the (*R,R*)-1,2-diaminecyclohexane which was used as a starting material in the syntheses of cage **6**.

Crystals of **6** were small and weakly diffracting, and gave no detectable diffraction above resolution of 0.96 $\text{\AA}$ ($\theta = 53.4^\circ$) well below the required limit (0.837 $\text{\AA}$, $\theta = 67^\circ$). That led to collection of a poor quality data; in the crystal structure of **6** the bond precision on C-C bonds was low. There was not also possible to properly determine the position of solvent molecules that were located in both internal and external cavities and therefore their contribution was subtracted from the diffraction data using the SQUEEZE as implemented in PLATON.[12] The estimated electron count is 248 in an accessible void volume of 2467 $\text{\AA}^3$ and can indicate squeezing of approximately 4 molecules of xylenes per unit cell.

Graphical images were produced in Platon[12] and Mercury[13] programs. The relevant crystal data The relevant crystal data and refinement parameters are listed in Table SI_5.

Table SI_5. Crystal data, data collection and refinement procedures for cage **6**.

cage6_squeezed	
<i>Crystal data</i>	
Chemical formula	C ₇₂ H ₈₀ N ₁₂ O ₄
M_r	1177.48
Crystal system, space group	Cubic, $F4_132$
Temperature (K)	150
a (Å)	24.8942(5)
V (Å ³)	15427.5(9)
Z	8
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	0.51
Crystal size (mm)	0.15 × 0.15 × 0.15
<i>Data collection</i>	
Diffractometer	SuperNova, Single source at offset, Atlas detector
Absorption correction	<i>Multi-scan</i> (CrysAlis PRO 1.171.38.41 (Rigaku Oxford Diffraction, 2015))
$T_{\min}$, $T_{\max}$	0.848, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	14070, 772, 748
R_{int}	0.097
$\theta_{\max}$ (°)	53.4
$(\sin\theta/\lambda)_{\max}$ (Å ⁻¹)	0.521
<i>Refinement</i>	
$R[F^2 > 2\sigma(F^2)]$,	0.110,
$wR(F^2)$,	0.292,
S	1.43
No. of reflections	772
No. of parameters	73
No. of restraints	3
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.48, -0.63
Absolute structure parameter	0.0(4) (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259)

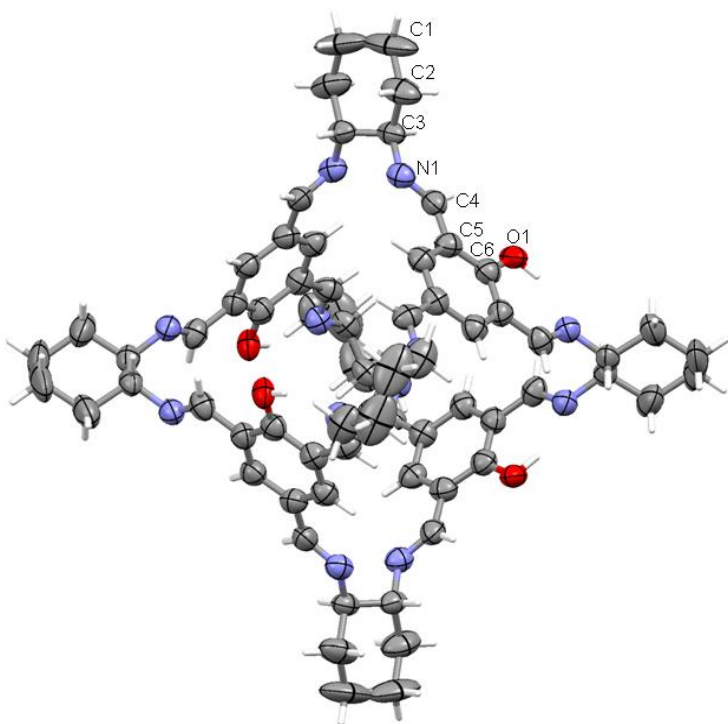


Figure SI_37. Perspective view of the cage **6**. Labels mark the symmetry independent part of molecules. Displacement ellipsoids are drawn at 30% probability level and the H-atoms are drawn in arbitrary scale. The disorder of the hydroxyl group is not displayed.

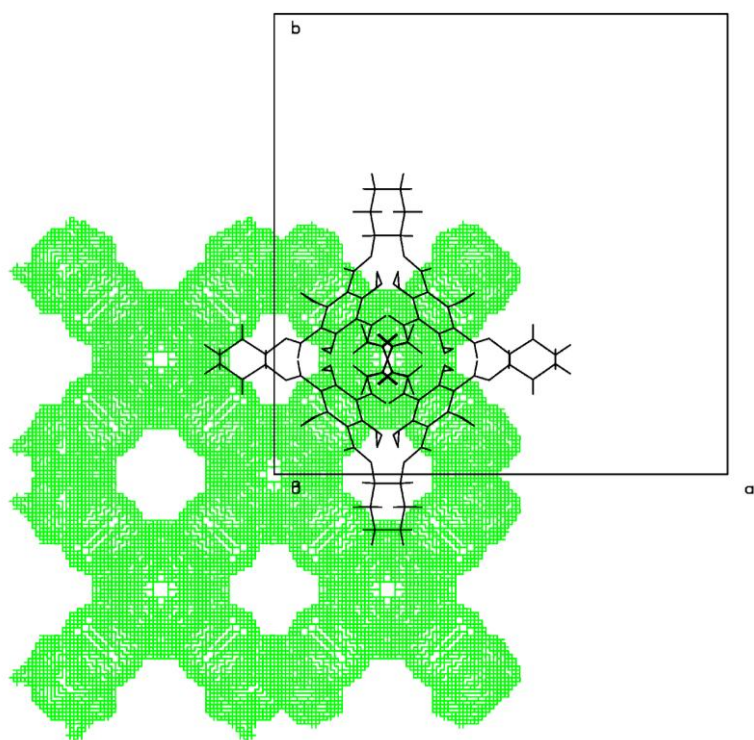


Figure SI_38. The diagram shows the void (in green) from which xylene guest molecules were removed as viewed along c lattice direction.

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Cartesian coordinates

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H	-4.47126100	-0.74106700	-2.39754300
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H	4.50172700	-0.55805400	3.01805900
H	0.72977200	-2.56483100	4.30677900

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C	2.59920700	-6.09088500	0.72599400
H	3.61937000	-5.70464400	0.58607300
C	2.07892300	-4.60566900	-1.00056300
H	3.14314600	-4.35479700	-1.06173600
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C	1.30076800	0.08488700	4.38921800
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H	-3.00960300	1.10064500	6.13965900
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C	-0.46196700	-2.56204700	-3.77295900
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C	1.46712700	-1.40457500	-4.79294000
H	0.75242200	-0.90247600	-5.45468900
N	-3.30288500	-3.17087600	-3.60871900
C	-1.02854100	-3.44283300	-2.84345300
C	-0.18138900	-4.09658500	-1.94621600
C	-4.70973300	-3.50469800	-3.46135700
H	-4.90005900	-4.14744500	-2.58942300
C	-2.47639400	-3.69270000	-2.79464200
H	-2.80627900	-4.37629200	-1.99917700
N	3.30093200	1.70892900	-4.37574000
C	2.96480900	2.73430200	-2.22058600
C	3.46705600	2.90245000	-0.91226200
C	4.09520100	0.83604400	-5.22432500
H	4.92844200	0.36715200	-4.68089100
C	3.68122100	1.86918000	-3.17109800
H	4.57315200	1.36958700	-2.77857800
N	-5.31498800	-1.51830400	-2.12957700
C	-4.68742900	0.47845800	-0.96182700
C	-4.32695600	1.81978600	-1.05660000
C	-5.57181800	-2.24020400	-3.36598700
H	-5.39475200	-1.60446100	-4.24258000
C	-4.96111000	-0.28996400	-2.17361200
H	-4.85149700	0.23966200	-3.12665200
N	-4.39700700	0.63759000	3.88611900
C	-4.50983900	0.62622100	1.47926500
C	-4.78465700	-0.13307800	0.32188200
C	-4.51937300	-0.08675900	5.14077600
H	-4.75511500	-1.15001500	4.98802400
C	-4.60574900	-0.00345800	2.80646500
H	-4.87399900	-1.06518900	2.80986200
N	-3.59403800	4.63672300	-1.10292400
C	-4.05544100	2.58447200	0.08433200
C	-4.15094900	1.96861400	1.33404400
C	-3.21249300	6.03896500	-1.05699300
H	-3.00568800	6.38182500	-0.03258500
C	-3.67747800	4.00287300	-0.00360700
H	-3.47266500	4.49228800	0.95961800
N	-0.79302200	5.69638900	-1.39124200
C	1.10065600	4.22927200	-1.69569600
C	1.79210300	3.40197200	-2.58298900
C	-1.98967900	6.31132300	-1.94240200
H	-2.19773800	5.97365400	-2.96822400
C	-0.12752200	4.90847700	-2.13507400
H	-0.43759000	4.69273000	-3.16781100
H	3.35126300	-3.28672500	2.65268200

5 (4)

H	-0.76067200	-2.59256800	4.24136500
H	1.32753700	1.12149900	4.70649300
H	1.42482800	3.25942400	-3.59324500
O	4.58964800	2.27383800	-0.55080200
H	4.77608600	2.53231100	0.40522900
H	1.07742700	5.02700000	0.29567600
H	-0.58991000	-4.78486200	-1.21464300
H	-4.25342000	2.28858400	-2.03144100
H	5.76174700	4.11639600	3.09866500
H	5.45251200	2.49363100	4.84936800
H	4.51846700	1.44021700	-6.03461100
H	3.85214900	-0.80540000	-6.57849600
H	-4.04599800	6.63108900	-1.45161500
H	-1.83347300	7.39580600	-1.96714900
H	-6.62330700	-2.54513000	-3.36905400
H	-5.02809000	-4.04937800	-4.35735500
H	-5.33741000	0.36406200	5.71418300
H	-3.44264500	-0.41592700	6.95789200
H	2.87891900	-6.51985500	2.80607600
H	2.61109400	-7.16398700	0.50444300
O	3.08372000	-2.82170600	-2.91521900
H	3.27315800	-2.16629500	-3.65714900
H	-1.11190600	-2.04937500	-4.47303700
H	-3.94486500	2.53358300	2.23639400
O	-5.13417700	-1.41760700	0.44321900
H	-5.29017000	-1.76838900	-0.48844600
N	-4.67831900	3.34667000	0.27375100
C	-3.60823900	2.38203700	-1.64218400
C	-3.59885600	1.34644500	-2.57285200
C	-5.70782400	3.31773900	1.30009400
H	-6.31799700	2.40842500	1.22965000
C	-4.61852400	2.40298800	-0.58825000
H	-5.32896300	1.56884000	-0.57332400
N	-4.29280600	2.26434500	3.02348800
C	-2.22596200	1.28357100	3.73972300
C	-0.92204000	1.50286600	4.17504200
C	-5.09961100	3.43067400	2.70229100
H	-4.51561600	4.35609000	2.78360900
C	-3.08028600	2.41854700	3.40120100
H	-2.63175000	3.41426800	3.49057400
N	-3.49387900	-0.72536400	-4.61230300
C	-2.64492100	1.29400000	-3.59592300
C	-1.68866000	2.30961700	-3.66444700
C	-3.37178800	-1.74223200	-5.64449300
H	-2.48591300	-1.58877400	-6.27782500
C	-2.63003600	0.20753800	-4.58698900
H	-1.81373500	0.25599500	-5.32222600
N	0.22857700	4.47047800	-3.77069800
C	-1.65884400	3.36917200	-2.75444400
C	-2.62854100	3.41302600	-1.73001700
C	1.17853800	5.57137200	-3.76134700
H	1.03470400	6.23876600	-2.89918100

C	-0.64479700	4.43261900	-2.84553900
H	-0.69010000	5.19951800	-2.06512800
O	-2.61673000	4.42371900	-0.85490700
N	2.96371600	4.40310700	-2.52322800
C	3.80896600	2.44997000	-1.38099100
C	4.33053100	1.16231000	-1.52361300
C	2.62413000	5.05867200	-3.77592000
H	2.77075700	4.40003500	-4.64445300
C	3.42414500	3.21873900	-2.57398300
H	3.56602300	2.69722100	-3.53165400
N	1.79956500	1.81542800	5.15922700
C	-0.07550600	0.43887100	4.50858000
C	-0.56735900	-0.86287000	4.39077200
C	3.16854400	1.89877800	5.64051600
H	3.63947900	0.90982900	5.73932200
C	1.29940400	0.65963900	4.97993500
H	1.87744800	-0.25410100	5.17959200
N	-1.66688900	-3.52426400	4.16414100
C	-1.86840600	-1.13226100	3.95890500
C	-2.71417500	-0.05095700	3.63098600
C	-2.26560000	-4.83961500	4.00994700
H	-3.26734900	-4.79477400	3.55822900
C	-2.36816200	-2.51163800	3.84224900
H	-3.38956000	-2.61624700	3.46155700
N	4.21294500	2.17385100	3.42311000
C	4.03497700	2.23580700	1.03395700
C	3.66813900	2.97163200	-0.08944200
C	4.02344600	2.78665800	4.72840800
H	3.56311000	3.77876100	4.63983100
C	3.87099100	2.80970500	2.36722500
H	3.44215400	3.81668800	2.41965200
N	-1.28138800	-5.31582500	1.79791900
C	0.00520900	-4.64789300	-0.11108500
C	1.27316100	-4.44948100	-0.65061800
C	-1.36665000	-5.76309300	3.17951400
H	-0.37255000	-5.82532800	3.63972300
C	-0.13620300	-5.09801100	1.27137100
H	0.79061800	-5.24491000	1.83723500
N	-2.08906100	-3.36686600	-4.30409900
C	-0.98591700	-3.97092600	-2.24913600
C	-1.14562700	-4.40817900	-0.91688900
C	-3.32728600	-3.14917800	-5.03436900
H	-4.21598700	-3.30301100	-4.40511100
C	-2.17227000	-3.72273900	-3.08480500
H	-3.13945400	-3.86862300	-2.59218900
N	3.85965200	-4.02196700	-1.91845100
C	1.44462800	-4.01612100	-1.97083100
C	0.30638700	-3.78406300	-2.74591400
C	5.11695000	-3.77134500	-2.60451700
H	4.96719300	-3.35444200	-3.61115400
C	2.77870800	-3.80075400	-2.55072300
H	2.78353200	-3.43296500	-3.58705500

5 (5)

N	5.46575900	-1.48700600	-1.74295400
C	4.71443400	0.38687400	-0.42674100
C	4.56837600	0.92429900	0.87004400
C	6.01587000	-2.83208500	-1.79030800
H	6.17253500	-3.25430100	-0.78701300
C	5.26675300	-0.96689000	-0.59831700
H	5.50391500	-1.50366900	0.32640000
H	-3.38390700	4.27397900	-0.22143900
H	-4.34298500	0.56056600	-2.50998600
H	-0.93527100	2.29656900	-4.44424700
H	4.45163100	0.73050400	-2.51098300
H	2.15071600	-4.63278800	-0.04093000
H	3.28185500	5.92736900	-3.89403800
H	1.02618400	6.15798300	-4.67451400
H	5.00701800	2.90440000	5.19450700
H	3.15538700	2.36653500	6.63132600
H	5.64423100	-4.72661300	-2.70793000
H	6.98767100	-2.78352800	-2.29467300
H	-1.81131300	-6.76357300	3.18552100
H	-2.36365500	-5.28937000	5.00440500
H	-3.36556800	-3.86952500	-5.85945300
H	-4.26039200	-1.68651000	-6.28352900
H	-6.36429600	4.18100100	1.15131300
H	-5.92473200	3.48407300	3.41972800
H	0.06437200	-1.70825200	4.64014300
H	0.40553400	-3.44778700	-3.77204000
O	-2.37518300	-4.59453900	-0.42681600
H	-2.26741700	-4.91229100	0.52317600
O	4.93445300	0.19722800	1.93024500
H	4.75621600	0.75978200	2.74713900
O	-3.96383400	-0.29206700	3.22358900
H	-4.39549300	0.60080200	3.05295100
H	-0.54861700	2.51689400	4.26157300
H	3.26440600	3.97064100	0.03027600
N	1.74475900	-3.26549300	4.38351100
C	2.44556400	-3.31806400	2.07865800
C	3.42753800	-2.92935100	1.14243900
C	1.96788000	-2.79635900	5.74154500
H	2.83708500	-2.12660800	5.81444400
C	2.57069800	-2.90247300	3.48553800
H	3.42735800	-2.26065100	3.71711000
N	0.50216600	-0.81712400	5.61948200
C	-0.97743700	0.63533900	4.39351500
C	-2.27945100	0.82389800	3.88279300
C	0.72647500	-2.08486400	6.29488800
H	-0.14256500	-2.75520000	6.22540800
C	-0.64165000	-0.61203000	5.10042200
H	-1.44214000	-1.35732900	5.15607500
N	5.33359800	-2.24991300	-0.88824100
C	3.30168600	-3.33150600	-0.21898500
C	2.21303600	-4.10771100	-0.60647000
C	6.29742500	-1.88086800	-1.91347600

H	5.97518300	-2.22525200	-2.90419700
C	4.30224800	-2.93600200	-1.20684400
H	4.12803300	-3.26029500	-2.23889800
N	-0.08605000	-5.76084700	-1.26944200
C	1.23468600	-4.50327000	0.31338900
C	1.37069300	-4.09704900	1.64253100
C	-1.26139100	-6.57305200	-1.53856600
H	-1.89815100	-6.69291500	-0.64991600
C	0.08475000	-5.32838200	-0.08576300
H	-0.62837800	-5.55833900	0.71915000
N	-2.72394500	-4.73598300	-2.28832200
C	-3.07615700	-2.38096200	-2.68869200
C	-2.81135400	-1.29795300	-3.52985600
C	-2.09229300	-5.98350700	-2.68586000
H	-1.45572400	-5.86491400	-3.57493300
C	-2.49730900	-3.69924600	-2.98893200
H	-1.84887400	-3.73447600	-3.87630900
N	-4.87278000	1.38553600	2.79429400
C	-2.59783300	2.02903700	3.19180300
C	-1.62108000	3.00875200	3.03608300
C	-6.18853800	1.65660500	2.23746400
H	-6.19848100	2.59839200	1.67453400
C	-3.93598600	2.24458700	2.64868600
H	-4.10130700	3.18489500	2.11089000
N	0.50299500	4.98586200	2.82262200
C	-0.32817800	2.83621200	3.54399900
C	-0.03102500	1.64697200	4.21347600
C	1.61053300	5.92303100	2.73844300
H	2.54384900	5.50776800	3.14604500
C	0.70931500	3.86624100	3.39020000
H	1.69245500	3.60582000	3.80793400
N	-5.83031600	0.38523100	0.15512500
C	-4.44114700	-0.92024700	-1.29895000
C	-3.89413400	-2.17098100	-1.57239100
C	-6.66207100	0.50724700	1.34156400
H	-6.68257900	-0.42866700	1.91414000
C	-5.28591800	-0.73893700	-0.12192500
H	-5.43359900	-1.61809000	0.51519900
N	2.31992800	5.28459400	0.46457000
C	2.12015000	3.86225700	-1.45364000
C	1.40492500	3.55381100	-2.60720300
C	1.83899500	6.37935000	1.29230500
H	0.91303800	6.80775100	0.88848500
C	1.67835200	4.95612600	-0.59197200
H	0.76979900	5.48669000	-0.89787200
N	5.33718500	0.34011100	-2.38012800
C	3.68986700	2.05103500	-1.97022200
C	3.28123900	3.10407600	-1.12400500
C	6.52953200	-0.36552600	-1.94101900
H	6.87841100	-0.02744400	-0.95426100
C	4.88773700	1.26655300	-1.63123000
H	5.37728400	1.53195200	-0.68831500

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N	0.02486100	2.82406500	-5.06152300
C	1.80054300	2.51205400	-3.45504700
C	2.93991800	1.77866600	-3.11740900
C	-0.62670200	2.40583100	-6.29209600
H	-0.16388700	1.50764100	-6.72666600
C	1.05156500	2.18003300	-4.67667200
H	1.44547900	1.32809700	-5.24951600
N	-2.34388000	0.97316700	-5.25107900
C	-3.33766800	-0.02493500	-3.29659400
C	-4.16559200	0.17247400	-2.17114800
C	-2.12339600	2.15391800	-6.07042900
H	-2.58573100	3.05375300	-5.63918400
C	-3.04693900	1.10238000	-4.19799600
H	-3.47958900	2.06613700	-3.90917100
H	2.11500800	-4.41773900	-1.64072600
H	-2.17903100	-1.42687200	-4.40136500
H	-2.88272100	-6.70312600	-2.92715200
H	-0.92299900	-7.56754700	-1.85082000
H	-7.68424100	0.73336900	1.02156400
H	-6.89851000	1.74746100	3.06579700
H	-0.53291400	3.22074700	-7.01905100
H	-2.57800300	1.97452500	-7.05141300
H	2.60515100	7.16124900	1.29954000
H	1.35272800	6.81231000	3.32436900
H	7.32842600	-0.17213400	-2.66568400
H	7.24999900	-2.36490400	-1.67447800
H	2.15806600	-3.67063200	6.37461300
H	0.91031300	-1.87540400	7.35490700
H	-1.86078600	3.92742100	2.51279000
H	3.27272900	0.96621800	-3.75382700
O	-4.68273800	1.38286000	-1.93693700
H	-5.24156100	1.30807700	-1.10374200
H	-4.10224400	-3.00395400	-0.91046700
O	-3.19945000	-0.13033200	4.05479500
H	-4.05057300	0.20157400	3.63320500
H	0.96233900	1.48226500	4.61605200
O	4.46622400	-2.18981400	1.54376600
H	5.04616600	-2.03476700	0.73474400
H	0.62891800	-4.38615100	2.37881600
H	0.52168500	4.12894600	-2.86111100
O	3.98904700	3.38038000	-0.02485900
H	3.53817200	4.16190000	0.42495400
N	-4.47773700	3.62756000	-0.86641400
C	-2.44065300	3.27196900	-2.11529900
C	-1.85381900	2.63253200	-3.20951600
C	-5.88770200	3.32699100	-0.68264400
H	-6.25185600	2.56976500	-1.39240300
C	-3.86382700	3.05201200	-1.82042700
H	-4.37617600	2.34792900	-2.49184100
N	-5.55898800	1.57450500	1.02213200
C	-4.10500300	0.17719600	2.31775000
C	-3.25007000	0.08234900	3.41199400

C	-6.17164200	2.86580000	0.75193000
H	-5.82394600	3.62733100	1.46126800
C	-4.74869700	1.45033800	2.00401300
H	-4.50653500	2.29664100	2.65654800
N	-0.58913300	1.38525900	-5.48561800
C	-0.50797900	2.80550900	-3.54141100
C	0.28568200	3.65532300	-2.74157000
C	0.10350900	0.76007000	-6.60063700
H	1.18029900	0.98337600	-6.60187700
C	0.08938200	2.12345000	-4.70149100
H	1.16039200	2.29409000	-4.85388200
O	1.57394700	3.83557900	-3.04782500
N	1.74162500	5.42247700	-1.01784000
C	-0.29602400	4.31218700	-1.61827800
C	-1.64248600	4.11052200	-1.32794200
C	2.49785700	6.30597800	-0.14388400
H	1.88796300	6.64642300	0.70243200
C	0.50797900	5.19091700	-0.77231700
H	-0.00031800	5.64671200	0.08481600
N	3.45002100	4.52175300	1.26479500
C	3.71174900	2.19417400	1.83417800
C	4.34529000	0.97440200	1.51343400
C	3.76989600	5.62428900	0.37323700
H	4.39198400	5.30870500	-0.47697100
C	3.95782000	3.38364800	1.00358400
H	4.61332000	3.23173300	0.13956000
O	5.16500300	0.91381800	0.45970200
N	-1.48078900	-0.26784200	5.69314600
C	-2.61807000	-1.12261000	3.74232800
C	-2.86210100	-2.24086900	2.94238400
C	-0.57871900	-0.50340600	6.80856800
H	-0.17385200	-1.52599100	6.80949200
C	-1.71957700	-1.23367100	4.90115100
H	-1.26467400	-2.22414400	5.04701900
N	-3.45002100	-4.52175300	1.26479500
C	-3.71174900	-2.19417400	1.83417800
C	-4.34529000	-0.97440200	1.51343400
C	-3.76989600	-5.62428900	0.37323700
H	-4.39198400	-5.30870500	-0.47697100
C	-3.95782000	-3.38364800	1.00358400
H	-4.61332000	-3.23173300	0.13956000
O	-5.16500300	-0.91381800	0.45970200
N	1.48078900	0.26784200	5.69314600
C	2.61807000	1.12261000	3.74232800
C	2.86210100	2.24086900	2.94238400
C	0.57871900	0.50340600	6.80856800
H	0.17385200	1.52599100	6.80949200
C	1.71957700	1.23367100	4.90115100
H	1.26467400	2.22414400	5.04701900
N	-1.74162500	-5.42247700	-1.01784000
C	0.29602400	-4.31218700	-1.61827800
C	1.64248600	-4.11052200	-1.32794200

C	-2.49785700	-6.30597800	-0.14388400
H	-1.88796300	-6.64642300	0.70243200
C	-0.50797900	-5.19091700	-0.77231700
H	0.00031800	-5.64671200	0.08481600
N	0.58913300	-1.38525900	-5.48561800
C	0.50797900	-2.80550900	-3.54141100
C	-0.28568200	-3.65532300	-2.74157000
C	-0.10350900	-0.76007000	-6.60063700
H	-1.18029900	-0.98337600	-6.60187700
C	-0.08938200	-2.12345000	-4.70149100
H	-1.16039200	-2.29409000	-4.85388200
O	-1.57394700	-3.83557900	-3.04782500
N	4.47773700	-3.62756000	-0.86641400
C	2.44065300	-3.27196900	-2.11529900
C	1.85381900	-2.63253200	-3.20951600
C	5.88770200	-3.32699100	-0.68264400
H	6.25185600	-2.56976500	-1.39240300
C	3.86382700	-3.05201200	-1.82042700
H	4.37617600	-2.34792900	-2.49184100
N	5.55898800	-1.57450500	1.02213200
C	4.10500300	-0.17719600	2.31775000
C	3.25007000	-0.08234900	3.41199400
C	6.17164200	-2.86580000	0.75193000
H	5.82394600	-3.62733100	1.46126800
C	4.74869700	-1.45033800	2.00401300
H	4.50653500	-2.29664100	2.65654800
H	-2.08848200	4.61051200	-0.47564900
H	-2.44536300	1.97594400	-3.83778300
H	2.44536300	-1.97594400	-3.83778300
H	2.08848200	-4.61051200	-0.47564900
H	2.38804400	3.18866300	3.17231500
H	3.06628600	-0.95590100	4.02723800
H	-2.38804400	-3.18866300	3.17231500
H	-3.06628600	0.95590100	4.02723800
H	-1.95105500	-4.47521000	-2.36681300
H	-5.51336400	0.03064100	0.41267800
H	5.51336400	-0.03064100	0.41267800
H	1.95105500	4.47521000	-2.36681300
H	7.25508000	-2.75802900	0.86615600
H	6.45934000	-4.24698600	-0.84849100
H	1.14245400	0.36017000	7.73736600
H	-1.14245400	-0.36017000	7.73736600
H	2.79720000	7.18383000	-0.72585600
H	4.33154700	6.37336000	0.94266800
H	-6.45934000	4.24698600	-0.84849100
H	-7.25508000	2.75802900	0.86615600
H	-4.33154700	-6.37336000	0.94266800
H	-2.79720000	-7.18383000	-0.72585600
H	0.32643500	-1.15259300	-7.52922200
H	-0.32643500	1.15259300	-7.52922200
N	1.46781200	-0.32131700	-5.64285000
C	2.58543000	-1.22148700	-3.70684500

C	2.82718000	-2.36915400	-2.92198600
C	0.56137800	-0.52248900	-6.76174300
H	0.12318800	-1.53116500	-6.76848300
C	1.68763400	-1.30875600	-4.87039100
H	1.21822900	-2.28437100	-5.03496100
N	-1.46781200	0.32131700	-5.64285000
C	-2.58543000	1.22148700	-3.70684500
C	-2.82718000	2.36915400	-2.92198600
C	-0.56137800	0.52248900	-6.76174300
H	-0.12318800	1.53116500	-6.76848300
C	-1.68763400	1.30875600	-4.87039100
H	-1.21822900	2.28437100	-5.03496100
N	3.43754600	-4.59608100	-1.22601700
C	3.69114900	-2.28127600	-1.79195000
C	4.29002800	-1.06389700	-1.48046000
C	3.71901700	-5.73315500	-0.36414900
H	4.36778500	-5.44807600	0.47362600
C	3.94942300	-3.45442500	-0.96069600
H	4.60864200	-3.30931700	-0.09751100
N	5.50483800	1.52858600	-0.96841900
C	4.06164700	0.08071100	-2.25358900
C	3.20893800	-0.02172600	-3.35482100
C	6.06754700	2.85215900	-0.75575500
H	5.66876300	3.59442300	-1.46267400
C	4.69256400	1.37017800	-1.93403900
H	4.41739800	2.20289500	-2.59743100
N	4.41884500	3.61513000	0.91166100
C	2.42504200	3.24073400	2.21026800
C	1.85871600	2.59856900	3.33204600
C	5.82645100	3.33396200	0.68067200
H	6.22631900	2.59238000	1.38752900
C	3.84590900	3.03021600	1.88607700
H	4.38529000	2.33733900	2.54047200
O	2.62208200	1.80876200	4.09356400
N	-3.43754600	4.59608100	-1.22601700
C	-3.69114900	2.28127600	-1.79195000
C	-4.29002800	1.06389700	-1.48046000
C	-3.71901700	5.73315500	-0.36414900
H	-4.36778500	5.44807600	0.47362600
C	-3.94942300	3.45442500	-0.96069600
H	-4.60864200	3.30931700	-0.09751100
N	-5.50483800	-1.52858600	-0.96841900
C	-4.06164700	-0.08071100	-2.25358900
C	-3.20893800	0.02172600	-3.35482100
C	-6.06754700	-2.85215900	-0.75575500
H	-5.66876300	-3.59442300	-1.46267400
C	-4.69256400	-1.37017800	-1.93403900
H	-4.41739800	-2.20289500	-2.59743100
N	-1.75088500	5.45403300	1.09179400
C	0.26643900	4.28337900	1.72064800
C	1.61543100	4.06878100	1.42939200
C	-2.42504200	6.35637300	0.17323600

H	-1.78243300	6.65561200	-0.66767000
C	-0.53075100	5.17437000	0.86520500
H	0.00526700	5.59757700	0.00349500
N	-4.41884500	-3.61513000	0.91166100
C	-2.42504200	-3.24073400	2.21026800
C	-1.85871600	-2.59856900	3.33204600
C	-5.82645100	-3.33396200	0.68067200
H	-6.22631900	-2.59238000	1.38752900
C	-3.84590900	-3.03021600	1.88607700
H	-4.38529000	-2.33733900	2.54047200
N	1.75088500	-5.45403300	1.09179400
C	-0.26643900	-4.28337900	1.72064800
C	-1.61543100	-4.06878100	1.42939200
C	2.42504200	-6.35637300	0.17323600
H	1.78243300	-6.65561200	-0.66767000
C	0.53075100	-5.17437000	0.86520500
H	-0.00526700	-5.59757700	0.00349500
N	-0.54644300	-1.38765300	5.57490000
C	-0.48169300	-2.80036000	3.63952600
C	0.28540600	-3.63635000	2.83258000
C	0.10995700	-0.75834000	6.70945900
H	1.18450800	-0.97994500	6.72446600
C	0.12817300	-2.14040900	4.79067300
H	1.19595300	-2.32498200	4.95334600
N	0.54644300	1.38765300	5.57490000
C	0.48169300	2.80036000	3.63952600
C	-0.28540600	3.63635000	2.83258000
C	-0.10995700	0.75834000	6.70945900
H	-1.18450800	0.97994500	6.72446600
C	-0.12817300	2.14040900	4.79067300
H	-1.19595300	2.32498200	4.95334600
H	3.00967500	0.84729800	-3.97200100
H	2.07185200	4.55298400	0.57331500
H	-1.33245800	3.79428200	3.06455400
H	-4.94813500	0.99277500	-0.62201300
H	0.33362900	1.15911500	7.62642300
H	-0.33362900	-1.15911500	7.62642300
H	-2.70327600	7.26174600	0.72417100
H	-4.23903500	6.49044900	-0.95959800
H	7.15126700	2.78819800	-0.90600500
H	6.38432300	4.26767900	0.81505200
H	1.13273000	-0.39397700	-7.68826900
H	-1.13273000	0.39397700	-7.68826900
H	-7.15126700	-2.78819800	-0.90600500
H	-6.38432300	-4.26767900	0.81505200
H	2.70327600	-7.26174600	0.72417100
H	4.23903500	-6.49044900	-0.95959800
O	2.24351400	-3.52635700	-3.24844000
H	2.54974500	-4.20983700	-2.57427800
H	-2.07185200	-4.55298400	0.57331500
H	4.94813500	-0.99277500	-0.62201300
H	2.03817800	1.46128800	4.83582900

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H	1.33245800	-3.79428200	3.06455400
O	-2.62208200	-1.80876200	4.09356400
H	-2.03817800	-1.46128800	4.83582900
O	-2.24351400	3.52635700	-3.24844000
H	-2.54974500	4.20983700	-2.57427800
H	-3.00967500	-0.84729800	-3.97200100
N	-5.43544000	1.76549800	-0.84898300
C	-3.43328000	2.13525800	-2.13821500
C	-2.67530400	1.74435900	-3.26266600
C	-6.65427400	1.00213600	-0.63871500
H	-6.74618200	0.15624000	-1.33548500
C	-4.68813800	1.43328500	-1.82475300
H	-4.94540500	0.60178800	-2.48932800
N	-5.72160700	-0.49979800	1.08347500
C	-3.87511700	-1.28876500	2.39318100
C	-3.04997300	-1.07203400	3.49335200
C	-6.74701000	0.49387200	0.80472400
H	-6.67969600	1.33952500	1.50058100
C	-4.92354900	-0.32531700	2.06780300
H	-4.99693900	0.55695500	2.71358000
N	-1.01284000	1.09290800	-5.50611300
C	-1.45870800	2.42309400	-3.56224900
C	-1.03610900	3.46650500	-2.74334900
C	-0.17271300	0.74659700	-6.64122400
H	0.74825900	1.34299300	-6.65471000
C	-0.65316600	2.03266700	-4.71596000
H	0.27751400	2.58860700	-4.87489800
N	-0.30132800	5.66341500	-0.98976900
C	-1.78067400	3.86597800	-1.62722800
C	-2.96818600	3.18762800	-1.34494200
C	0.02898000	6.73552900	-0.06519600
H	-0.67376300	6.79180400	0.77902400
C	-1.34323300	4.97152800	-0.76099700
H	-1.98821400	5.16976500	0.10712900
N	1.57030600	5.43857300	1.35650200
C	2.66158200	3.36618700	1.92007300
C	3.68604800	2.45240800	1.59256800
C	1.45870800	6.58591100	0.47055900
H	2.16290000	6.53242100	-0.37240000
C	2.45902000	4.56643100	1.09206100
H	3.12560000	4.66707000	0.22893700
O	4.46815000	2.68957100	0.53469400
N	-1.28852100	-0.77622500	5.79231900
C	-2.03387200	-1.97391700	3.83171800
C	-1.85787700	-3.10561000	3.03269400
C	-0.36187900	-0.67634200	6.90825400
H	0.38028900	-1.48793700	6.90778200
C	-1.16095000	-1.75894800	4.99535500
H	-0.38013000	-2.51958000	5.14062100
N	-1.57030600	-5.43857300	1.35650200
C	-2.66158200	-3.36618700	1.92007300
C	-3.68604800	-2.45240800	1.59256800

C	-1.45870800	-6.58591100	0.47055900
H	-2.16290000	-6.53242100	-0.37240000
C	-2.45902000	-4.56643100	1.09206100
H	-3.12560000	-4.66707000	0.22893700
O	-4.46815000	-2.68957100	0.53469400
N	1.28852100	0.77622500	5.79231900
C	2.03387200	1.97391700	3.83171800
C	1.85787700	3.10561000	3.03269400
C	0.36187900	0.67634200	6.90825400
H	-0.38028900	1.48793700	6.90778200
C	1.16095000	1.75894800	4.99535500
H	0.38013000	2.51958000	5.14062100
N	0.30132800	-5.66341500	-0.98976900
C	1.78067400	-3.86597800	-1.62722800
C	2.96818600	-3.18762800	-1.34494200
C	-0.02898000	-6.73552900	-0.06519600
H	0.67376300	-6.79180400	0.77902400
C	1.34323300	-4.97152800	-0.76099700
H	1.98821400	-5.16976500	0.10712900
N	1.01284000	-1.09290800	-5.50611300
C	1.45870800	-2.42309400	-3.56224900
C	1.03610900	-3.46650500	-2.74334900
C	0.17271300	-0.74659700	-6.64122400
H	-0.74825900	-1.34299300	-6.65471000
C	0.65316600	-2.03266700	-4.71596000
H	-0.27751400	-2.58860700	-4.87489800
N	5.43544000	-1.76549800	-0.84898300
C	3.43328000	-2.13525800	-2.13821500
C	2.67530400	-1.74435900	-3.26266600
C	6.65427400	-1.00213600	-0.63871500
H	6.74618200	-0.15624000	-1.33548500
C	4.68813800	-1.43328500	-1.82475300
H	4.94540500	-0.60178800	-2.48932800
N	5.72160700	0.49979800	1.08347500
C	3.87511700	1.28876500	2.39318100
C	3.04997300	1.07203400	3.49335200
C	6.74701000	-0.49387200	0.80472400
H	6.67969600	-1.33952500	1.50058100
C	4.92354900	0.32531700	2.06780300
H	4.99693900	-0.55695500	2.71358000
H	-3.56663900	3.47267800	-0.48671700
H	3.56663900	-3.47267800	-0.48671700
H	1.07782300	3.82173600	3.26639800
H	3.19216100	0.18889800	4.10599100
H	-1.07782300	-3.82173600	3.26639800
H	-3.19216100	-0.18889800	4.10599100
H	-5.12973800	-1.93176800	0.48261500
H	7.72477500	-0.01871900	0.93465600
H	7.50806200	-1.66896600	-0.80405700
H	0.93948500	0.74408000	7.83707400
H	-0.93948500	-0.74408000	7.83707400
H	-0.02194700	7.68335800	-0.61304700

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H	1.69064300	7.48607500	1.05118300
H	-7.50806200	1.66896600	-0.80405700
H	-7.72477500	0.01871900	0.93465600
H	-1.69064300	-7.48607500	1.05118300
H	0.02194700	-7.68335800	-0.61304700
H	0.73080600	-0.96024400	-7.55838600
H	-0.73080600	0.96024400	-7.55838600
O	-3.10792000	0.74239400	-4.03425600
H	-2.43536600	0.62961600	-4.77441900
O	3.10792000	-0.74239400	-4.03425600
H	2.43536600	-0.62961600	-4.77441900
H	0.11099600	-3.98485500	-2.96873900
H	-0.11099600	3.98485500	-2.96873900
H	5.12973800	1.93176800	0.48261500
N	5.67036800	-1.12204500	-0.97628000
C	3.72996400	-1.70335400	-2.25878100
C	2.92728800	-1.40322300	-3.35595400
C	6.80961500	-0.25481600	-0.72263400
H	6.82988200	0.59375700	-1.41810000
C	4.88809200	-0.86714000	-1.95594800
H	5.05751800	-0.00769100	-2.61422100
N	5.67036800	1.12204500	0.97628000
C	3.72996400	1.70335400	2.25878100
C	2.92728800	1.40322300	3.35595400
C	6.80961500	0.25481600	0.72263400
H	6.82988200	-0.59375700	1.41810000
C	4.88809200	0.86714000	1.95594800
H	5.05751800	0.00769100	2.61422100
N	1.19445500	-0.91587600	-5.63801100
C	1.80881600	-2.18136800	-3.67615000
C	1.50600200	-3.27441100	-2.86138300
C	0.28288800	-0.71313800	-6.75217600
H	-0.54664800	-1.43529800	-6.75019100
C	0.95942100	-1.87536300	-4.83720100
H	0.09681000	-2.54310700	-4.97558000
N	0.96387700	-5.54282600	-1.15788800
C	2.28100600	-3.61436800	-1.74972200
C	3.41021100	-2.82609700	-1.44160300
C	0.72305100	-6.65731200	-0.25566900
H	1.41438300	-6.65996900	0.59962600
C	1.94306200	-4.77061900	-0.90308000
H	2.59238000	-4.93013500	-0.03577100
O	4.16744100	-3.14307000	-0.38627300
N	-0.96387700	-5.54282600	1.15788800
C	-2.28100600	-3.61436800	1.74972200
C	-3.41021100	-2.82609700	1.44160300
C	-0.72305100	-6.65731200	0.25566900
H	-1.41438300	-6.65996900	-0.59962600
C	-1.94306200	-4.77061900	0.90308000
H	-2.59238000	-4.93013500	0.03577100
O	-4.16744100	-3.14307000	0.38627300
N	1.19445500	0.91587600	5.63801100

C	1.80881600	2.18136800	3.67615000
C	1.50600200	3.27441100	2.86138300
C	0.28288800	0.71313800	6.75217600
H	-0.54664800	1.43529800	6.75019100
C	0.95942100	1.87536300	4.83720100
H	0.09681000	2.54310700	4.97558000
N	0.96387700	5.54282600	1.15788800
C	2.28100600	3.61436800	1.74972200
C	3.41021100	2.82609700	1.44160300
C	0.72305100	6.65731200	0.25566900
H	1.41438300	6.65996900	-0.59962600
C	1.94306200	4.77061900	0.90308000
H	2.59238000	4.93013500	0.03577100
O	4.16744100	3.14307000	0.38627300
N	-1.19445500	-0.91587600	5.63801100
C	-1.80881600	-2.18136800	3.67615000
C	-1.50600200	-3.27441100	2.86138300
C	-0.28288800	-0.71313800	6.75217600
H	0.54664800	-1.43529800	6.75019100
C	-0.95942100	-1.87536300	4.83720100
H	-0.09681000	-2.54310700	4.97558000
N	-0.96387700	5.54282600	-1.15788800
C	-2.28100600	3.61436800	-1.74972200
C	-3.41021100	2.82609700	-1.44160300
C	-0.72305100	6.65731200	-0.25566900
H	-1.41438300	6.65996900	0.59962600
C	-1.94306200	4.77061900	-0.90308000
H	-2.59238000	4.93013500	-0.03577100
O	-4.16744100	3.14307000	-0.38627300
N	-1.19445500	0.91587600	-5.63801100
C	-1.80881600	2.18136800	-3.67615000
C	-1.50600200	3.27441100	-2.86138300
C	-0.28288800	0.71313800	-6.75217600
H	0.54664800	1.43529800	-6.75019100
C	-0.95942100	1.87536300	-4.83720100
H	-0.09681000	2.54310700	-4.97558000
N	-5.67036800	1.12204500	-0.97628000
C	-3.72996400	1.70335400	-2.25878100
C	-2.92728800	1.40322300	-3.35595400
C	-6.80961500	0.25481600	-0.72263400
H	-6.82988200	-0.59375700	-1.41810000
C	-4.88809200	0.86714000	-1.95594800
H	-5.05751800	0.00769100	-2.61422100
N	-5.67036800	-1.12204500	0.97628000
C	-3.72996400	-1.70335400	2.25878100
C	-2.92728800	-1.40322300	3.35595400
C	-6.80961500	-0.25481600	0.72263400
H	-6.82988200	0.59375700	1.41810000
C	-4.88809200	-0.86714000	1.95594800
H	-5.05751800	-0.00769100	2.61422100
H	4.91627900	-2.47236300	-0.34851300
H	4.91627900	2.47236300	0.34851300

6 (1)

H	-4.91627900	2.47236300	-0.34851300
H	-4.91627900	-2.47236300	0.34851300
H	3.16765600	-0.55044700	-3.98055700
H	0.64433100	-3.89505400	-3.08060400
H	-0.64433100	-3.89505400	3.08060400
H	-3.16765600	-0.55044700	3.98055700
H	3.16765600	0.55044700	3.98055700
H	0.64433100	3.89505400	3.08060400
H	-0.64433100	3.89505400	-3.08060400
H	-3.16765600	0.55044700	-3.98055700
H	0.87452300	-7.58596000	-0.81786500
H	-0.87452300	-7.58596000	0.81786500
H	-0.84775600	0.84631600	-7.68174600
H	0.84775600	-0.84631600	-7.68174600
H	-0.87452300	7.58596000	-0.81786500
H	0.87452300	7.58596000	0.81786500
H	7.72410300	0.83815400	0.87035000
H	7.72410300	-0.83815400	-0.87035000
H	0.84775600	0.84631600	7.68174600
H	-0.84775600	-0.84631600	7.68174600
H	-7.72410300	-0.83815400	0.87035000
H	-7.72410300	0.83815400	-0.87035000
N	5.73864700	0.57772100	-1.16315500
C	4.19989400	-1.16734900	-1.74619900
C	3.38836900	-1.72145600	-2.73186200
C	6.50331600	1.76920100	-1.51141000
H	6.21083300	2.12199900	-2.51122500
C	4.96083200	0.04714400	-2.02915600
H	4.83867500	0.47939500	-3.02870600
C	8.87053500	2.65679600	-1.80601800
H	9.92831700	2.38083700	-1.76213700
H	8.67851700	3.00504100	-2.82830300
C	8.00438800	1.42563700	-1.51538600
H	8.26952500	1.00440800	-0.53867800
H	8.18357200	0.64255200	-2.25796600
N	4.79571500	3.28066900	-0.59881200
C	2.68986300	3.68723600	0.51672300
C	2.02055200	3.70724500	1.74228600
C	6.19890700	2.90136200	-0.50423600
H	6.44097300	2.52851900	0.50426000
C	4.10154100	3.27986600	0.46753200
H	4.53296400	2.97940300	1.43319800
C	8.57034800	3.78957700	-0.81753900
H	9.15050900	4.68169000	-1.07204500
H	8.88518000	3.48687000	0.18870900
C	7.07593500	4.13198900	-0.80385100
H	6.77603200	4.54275400	-1.77494400
H	6.86323000	4.90150000	-0.05586000
N	1.70578200	-3.00474300	-4.71866600
C	2.65707700	-2.89318600	-2.50305400
C	2.75539800	-3.50152400	-1.24971100
C	0.87459400	-3.70219200	-5.69064600

H	0.35456900	-4.55583900	-5.22665900
C	1.81477000	-3.49372100	-3.54950000
H	1.28507400	-4.41160800	-3.25660100
C	0.95934800	-4.87773800	-7.95539700
H	1.63153900	-5.19691800	-8.75780400
H	0.47239400	-5.78397100	-7.57433700
C	1.77033000	-4.22114200	-6.83189400
H	2.34570100	-3.37786700	-7.23157300
H	2.49436300	-4.92733200	-6.41410300
N	3.05698200	-4.73710600	1.34848300
C	3.55797700	-2.98367500	-0.22914500
C	4.29133600	-1.80283700	-0.47422000
C	3.25282400	-5.32269500	2.66845600
H	3.85071300	-4.65601200	3.31056100
C	3.66146400	-3.64895100	1.08071600
H	4.30134600	-3.15030800	1.81623600
C	4.14945200	-7.39413800	3.85890900
H	4.64347800	-8.35752200	3.69981700
H	4.80466700	-6.80941200	4.51638300
O	5.06918100	-1.29636500	0.48855500
C	3.99054600	-6.66693900	2.51835400
H	3.42891200	-7.29504400	1.81691400
H	4.96761000	-6.48017200	2.06247400
N	1.24868100	-4.23964700	3.59974800
C	-0.70822400	-2.84036700	3.42843700
C	-2.04139000	-2.74398800	2.97583200
C	1.88275900	-5.52867000	3.35445000
H	1.26508600	-6.15040500	2.68662400
C	0.05542800	-4.07593700	3.18704300
H	-0.47452700	-4.86004000	2.63615200
C	2.79235600	-7.59355200	4.54350700
H	2.92371000	-8.06049800	5.52444900
H	2.18176700	-8.28220200	3.94647600
O	-2.59076100	-3.77198800	2.32057000
C	2.05337500	-6.25996700	4.69967600
H	2.60500400	-5.60494600	5.38420700
H	1.06393700	-6.41625000	5.14001700
N	0.59199100	3.81851400	4.24926100
C	0.68838600	4.11059900	1.85926700
C	-0.00530900	4.50850100	0.69641900
C	-0.15912200	3.92924700	5.49234200
H	-1.21177100	4.18861400	5.29527000
C	0.00943100	4.14569100	3.16551900
H	-1.03266400	4.48152600	3.15022400
C	-0.20369700	5.14892400	7.73216400
H	0.29863400	5.91696000	8.32825900
H	-1.24076900	5.48159300	7.60043600
C	0.47366400	5.03196700	6.36228100
H	1.53865600	4.80541000	6.49016400
H	0.41548600	5.98105500	5.82080600
N	-1.24543400	5.32646200	-1.75251900
C	0.66078900	4.49041300	-0.56382100

C	1.99012100	4.08174300	-0.63028800
C	-1.88898600	5.77390700	-2.98187600
H	-1.23205800	5.57792900	-3.84176200
C	-0.03463100	4.91416400	-1.77731300
H	0.53610600	4.87019300	-2.71163000
C	-2.91942400	7.80795100	-4.11643300
H	-3.12972300	8.87441200	-3.99229900
H	-2.28092100	7.71453700	-5.00343900
C	-2.16535900	7.28603000	-2.88735700
H	-2.75152900	7.47731100	-1.98095400
H	-1.21295500	7.81036200	-2.76615900
N	-0.85284700	1.57375400	5.44843600
C	-0.87086800	-0.59097200	4.37852900
C	-0.15238700	-1.76031000	4.11911800
C	-0.14201100	2.57266400	6.23519200
H	0.91214000	2.28530600	6.37880200
C	-0.24213000	0.50300700	5.13514200
H	0.80337900	0.32925700	5.42786700
C	-0.19166500	3.80481000	8.46976100
H	-0.72844200	3.88469700	9.42005600
H	0.84285500	3.53452000	8.71526600
C	-0.81959000	2.69966800	7.61253200
H	-1.88471800	2.90777400	7.45722600
H	-0.75802100	1.73344500	8.12254600
N	-2.89934300	3.57544700	-3.39964000
C	-3.31604900	1.27396200	-2.81697600
C	-4.06387100	0.38627400	-2.01422200
C	-3.20057000	4.98620500	-3.19875400
H	-3.83203600	5.13365900	-2.30782000
C	-3.50593400	2.72606200	-2.66993000
H	-4.21422500	3.03566800	-1.89440400
C	-4.21933200	7.02736200	-4.34088400
H	-4.71701100	7.37000800	-5.25304400
H	-4.91060100	7.22541000	-3.51254000
O	-4.93100800	0.87540000	-1.12183300
C	-3.95014500	5.52116700	-4.43427200
H	-3.35068800	5.30300100	-5.32574100
H	-4.88722200	4.96651300	-4.53930800
N	-1.11913200	-2.36421000	-5.16770700
C	-2.24297300	-0.62879900	-3.91950200
C	-2.42194200	0.74599400	-3.75222200
C	-0.20348100	-2.73830800	-6.23752800
H	0.31484800	-1.85316900	-6.64039600
C	-1.30564500	-1.12723900	-4.93804800
H	-0.77588300	-0.34965100	-5.50695900
C	-0.10639900	-3.91937900	-8.49768700
H	-0.71502800	-4.41557900	-9.25986100
H	0.38406100	-3.07089800	-8.99076300
C	-1.00822400	-3.40476900	-7.37007200
H	-1.58424700	-4.23481000	-6.94440100
H	-1.73389300	-2.68169100	-7.75490700
N	-5.53137300	-1.56027100	-0.50669500

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C	-3.89166100	-1.01978000	-2.16983600
C	-2.98806300	-1.49877300	-3.11452000
C	-6.29949500	-2.53615200	0.25547100
H	-5.91060900	-3.54837500	0.07130300
C	-4.66382900	-1.95780200	-1.35929100
H	-4.46778400	-3.02361200	-1.52106600
C	-8.65007400	-3.42717100	0.65296300
H	-9.69451200	-3.32946900	0.34280000
H	-8.35690100	-4.46408200	0.44912800
C	-7.77668400	-2.47770600	-0.17584500
H	-8.13320800	-1.44715700	-0.06514500
H	-7.84033100	-2.72324900	-1.23975900
N	-4.76848000	-2.39187300	2.16732700
C	-2.78767500	-1.55639000	3.22756700
C	-2.19099300	-0.50645200	3.92052300
C	-6.16077000	-2.23980700	1.76557300
H	-6.49316100	-1.20595800	1.93940900
C	-4.17212800	-1.43822300	2.77757200
H	-4.67952000	-0.49154600	2.99418900
C	-8.50855700	-3.14478800	2.15312300
H	-9.09048300	-3.86648100	2.73376100
H	-8.92133300	-2.15396400	2.37840900
C	-7.03994200	-3.19778100	2.59084200
H	-6.65084400	-4.21606300	2.47584300
H	-6.94178100	-2.93803600	3.64872200
H	5.51001900	-0.47474100	0.10835300
H	-5.37055000	0.08664000	-0.67657900
H	-3.53883300	-3.51045300	2.10595900
H	3.32050500	-1.24343500	-3.70246200
H	2.20211600	-4.41054500	-1.04109400
H	0.87109300	-1.85759800	4.46395600
H	-2.75719300	0.39664000	4.11890000
H	2.53649100	3.41078000	2.64876700
H	-1.86311100	1.44588000	-4.36360800
H	-2.85884200	-2.56773000	-3.24037200
O	-1.27875400	4.90361400	0.79125600
H	-1.57602400	5.15924500	-0.13764600
H	2.50172800	4.07257400	-1.58618300
N	3.82921400	0.74907300	-4.26240300
C	2.94486200	-1.24132000	-3.26278700
C	2.03548400	-2.29074900	-3.35955400
C	3.85837300	1.73569900	-5.33465100
H	3.03068200	1.55286900	-6.03545000
C	2.98677800	-0.21283400	-4.30001500
H	2.26529800	-0.31077500	-5.11886600
C	5.32577600	2.69541500	-7.18007400
H	6.30151800	2.60697800	-7.66697800
H	4.57029300	2.52056400	-7.95593000
C	5.19577800	1.62525900	-6.09023700
H	6.01461200	1.72559100	-5.36822600
H	5.27401700	0.62276400	-6.52110300
N	2.35185400	3.26010500	-4.13870100

C	0.99532900	3.84456700	-2.22736300
C	0.99137100	4.32480400	-0.91604600
C	3.67265600	3.15171700	-4.74281000
H	4.46547000	3.30831300	-3.99340000
C	2.27201500	3.65146500	-2.93060900
H	3.17043000	3.88150700	-2.34002000
C	5.14143500	4.10220400	-6.59938300
H	5.18093700	4.85185200	-7.39536600
H	5.97025300	4.32486300	-5.91611900
C	3.81165200	4.21827800	-5.84515600
H	2.97400300	4.10745200	-6.54369500
H	3.71216100	5.20667700	-5.38685300
N	0.24644000	-4.58829500	-3.47518500
C	1.98269700	-3.30261800	-2.39272800
C	2.86756800	-3.23695900	-1.31438400
C	-0.58627700	-5.78348700	-3.49730100
H	-0.50338100	-6.34090500	-2.55026600
C	1.04840700	-4.43285300	-2.49968200
H	1.09673200	-5.15814500	-1.67467500
C	-1.01967600	-7.92579900	-4.81731800
H	-0.67960900	-8.51625300	-5.67343700
H	-0.92305100	-8.56895000	-3.93396100
C	-0.12544300	-6.69139300	-4.65342600
H	-0.12785200	-6.10217800	-5.57790600
H	0.91183600	-6.98705700	-4.47021800
N	4.78206300	-3.07648500	0.84489200
C	3.79788000	-2.20420200	-1.17460900
C	3.84227500	-1.19129100	-2.15655000
C	5.78063500	-2.95679200	1.89842200
H	6.30051500	-1.98679900	1.84224600
C	4.73848200	-2.16480100	-0.04323200
H	5.41131100	-1.30137200	-0.01521400
C	7.84606000	-4.09318600	2.87603500
H	8.53227600	-4.93548600	2.74636000
H	8.45378300	-3.18156000	2.82221000
O	4.73160600	-0.20052500	-2.04124300
C	6.81386200	-4.08828500	1.74224400
H	6.27903600	-5.04493400	1.71861300
H	7.30658500	-3.97773200	0.77173200
N	4.18460000	-1.91733200	3.45207800
C	2.00750400	-1.03795300	3.94351100
C	0.68769900	-1.32090900	4.28467800
C	5.09199900	-3.04510200	3.27950600
H	4.52664000	-3.98799100	3.31252100
C	2.95374700	-2.13013100	3.72844500
H	2.55727300	-3.14714000	3.82411700
C	7.16180300	-4.16686800	4.24596600
H	7.90377500	-4.10886100	5.04791500
H	6.66079300	-5.13700500	4.35096400
C	6.13443300	-3.04145000	4.41323700
H	6.64168300	-2.06961100	4.42008200
H	5.61274100	-3.13366800	5.37036800

N	0.90649000	5.38824000	1.76706600
C	-0.19135700	4.55041000	-0.20716200
C	-1.42414700	4.28114700	-0.83950500
C	0.81284400	5.93096200	3.11555700
H	-0.22447900	5.89310900	3.48540200
C	-0.17280100	5.07583500	1.16855800
H	-1.15119100	5.19008300	1.64684700
C	1.30968200	8.01377600	4.50244700
H	1.68492300	9.04034600	4.44845200
H	0.28650400	8.07352700	4.89357600
C	1.28528100	7.39755200	3.09914500
H	2.28777900	7.43440900	2.65690000
H	0.62712200	7.96921600	2.43771800
N	-3.83212100	3.72712300	-2.29277900
C	-1.43841300	3.78797600	-2.17663400
C	-0.23411200	3.58003100	-2.84290800
C	-5.06762400	3.48501900	-3.02764800
H	-4.84129500	3.02118800	-3.99874700
C	-2.70309500	3.52073900	-2.85770900
H	-2.63749400	3.14252800	-3.88413000
C	-7.13779500	4.63667300	-3.96257900
H	-7.63200300	5.60618100	-4.07570600
H	-6.97316200	4.24751900	-4.97487900
C	-5.78726200	4.82616000	-3.26188900
H	-5.93518900	5.31745200	-2.29310100
H	-5.13420900	5.47686600	-3.85084400
N	1.14409900	3.73842700	4.17258400
C	1.49716600	1.35798800	4.04844900
C	2.42557200	0.31912400	3.82421100
C	1.68342900	5.08850400	4.07652800
H	2.70890600	5.07542800	3.67361300
C	1.92756700	2.76215600	3.94001300
H	2.97292800	2.91881400	3.65377700
C	2.17007000	7.17831600	5.45723800
H	2.13376000	7.59486600	6.46855400
H	3.21803500	7.22444200	5.13607800
C	1.70588600	5.71735600	5.48262300
H	0.69748500	5.65380700	5.90814700
H	2.35766900	5.11599200	6.12369200
N	-5.30748300	1.21227100	-2.13135900
C	-4.54283500	-0.61099200	-0.74268300
C	-4.45430700	-1.11483800	0.55684600
C	-5.96538300	2.50739400	-2.23557200
H	-6.14001200	2.94421600	-1.23887500
C	-5.15173400	0.70727600	-0.97387400
H	-5.47972200	1.23565800	-0.06720200
C	-8.03244800	3.66562000	-3.18382000
H	-8.96934600	3.49386800	-3.72221500
H	-8.30153600	4.11327800	-2.21924400
C	-7.32061100	2.32889800	-2.94650900
H	-7.14601900	1.82240700	-3.90293700
H	-7.94350200	1.66078500	-2.34439400

N	-2.51542100	-4.61533700	-2.52649100
C	-3.50162400	-2.65219300	-1.56647100
C	-4.05863400	-1.39720200	-1.79530400
C	-2.06764100	-5.38353000	-3.68154300
H	-2.13804200	-4.76890900	-4.59085700
C	-3.01487000	-3.44905800	-2.69026200
H	-3.10326000	-2.99916000	-3.68545800
C	-2.48819400	-7.52357300	-4.99442800
H	-3.12431000	-8.41176300	-5.05347600
H	-2.60681500	-6.98824900	-5.94448900
C	-2.95916500	-6.62912300	-3.84197100
H	-2.94541000	-7.19303800	-2.90196100
H	-3.99138400	-6.30394700	-4.00179400
N	-4.28884100	-2.24003400	3.21140500
C	-3.90646500	-2.36949800	0.83586500
C	-3.42200100	-3.15215600	-0.23406700
C	-4.20939800	-2.86149900	4.52658000
H	-3.64907600	-3.80932100	4.48166400
C	-3.84139700	-2.88966600	2.21218500
H	-3.38854500	-3.88026200	2.32494000
C	-5.64571600	-3.71292900	6.45568800
H	-6.67768800	-3.86588300	6.78613700
H	-5.16500900	-4.69899700	6.45939000
C	-5.63690500	-3.14592800	5.03142100
H	-6.20957900	-2.21165900	4.99733100
H	-6.12174300	-3.83885500	4.33700300
N	-2.07918900	-1.76550400	5.07381900
C	-0.24188900	-0.29959600	4.51502000
C	0.18370100	1.02450700	4.38918200
C	-3.46304300	-1.92235400	5.50217100
H	-3.98869600	-0.95390700	5.49978200
C	-1.63180200	-0.58735900	4.90136200
H	-2.26932200	0.29686500	5.04557800
C	-4.90463400	-2.78372100	7.42381800
H	-4.86708600	-3.22522000	8.42446100
H	-5.45758200	-1.84079100	7.51739500
C	-3.48154100	-2.49684000	6.93156100
H	-2.88974900	-3.41966400	6.94293500
H	-2.97748300	-1.79049700	7.59823800
H	4.61176900	0.39625000	-2.84520500
H	1.35578900	-2.33568300	-4.20294300
H	2.85506500	-4.00828000	-0.55238100
H	-0.51070800	1.83878200	4.56414700
H	1.92712400	4.54393900	-0.41379000
H	-4.12619800	-1.01700800	-2.80829800
O	3.68975100	0.62022700	3.50854100
H	4.18468100	-0.25152100	3.41357900
H	0.36791100	-2.35223800	4.38219300
H	-0.24154000	3.21259800	-3.86283400
O	-2.56590100	4.49883800	-0.17908000
H	-3.31775200	4.26411700	-0.80769300
O	-2.89765200	-4.35656400	0.01375900

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H	-2.62798600	-4.74762200	-0.87509500
H	-4.82357000	-0.53136100	1.39291200
N	-5.14798900	1.77968600	2.19036100
C	-4.57175200	-0.28061500	1.11021300
C	-4.23467400	-1.62289900	1.26191100
C	-5.40714700	2.56629300	3.38987200
H	-5.16162800	1.97808400	4.28606900
C	-4.81219300	0.54929400	2.28881300
H	-4.69677100	0.06359200	3.26431200
C	-7.22130100	3.86510600	4.61810800
H	-8.27853900	4.14509500	4.58879400
H	-7.06744900	3.31429000	5.55413200
C	-6.89742600	2.95291800	3.42894200
H	-7.15231600	3.45874400	2.49033000
H	-7.49606300	2.03809500	3.46829800
N	-3.10943600	3.42040600	3.48229600
C	-0.85264600	3.57501300	2.63621600
C	-0.01109500	4.16246400	1.68940800
C	-4.50649300	3.82212500	3.38770100
H	-4.69858100	4.37075500	2.45141800
C	-2.29260500	3.87218700	2.61781100
H	-2.62420500	4.52964800	1.80135500
C	-6.33452300	5.11502200	4.61244800
H	-6.53830600	5.73172800	5.49294300
H	-6.57657800	5.72843800	3.73591700
C	-4.84926600	4.73669900	4.57942800
H	-4.57422700	4.21849600	5.50550200
H	-4.22327500	5.63207100	4.52086200
N	-3.58808700	-4.45855000	1.42782600
C	-4.01133500	-2.44932500	0.15383500
C	-4.13016200	-1.89408800	-1.12209100
C	-3.30434300	-5.88745900	1.44449400
H	-3.10044200	-6.26060000	0.42777000
C	-3.68156600	-3.87531900	0.30130900
H	-3.53038400	-4.41923700	-0.64228700
C	-4.27738500	-8.13676500	2.15574200
H	-5.15652200	-8.61745500	2.59579500
H	-4.14153500	-8.58011700	1.16146600
C	-4.52735700	-6.63096600	2.01427600
H	-4.77083000	-6.19924200	2.99211400
H	-5.38603800	-6.44141700	1.36298400
N	-4.45813100	-0.69468900	-3.73120600
C	-4.46710000	-0.55333300	-1.32499500
C	-4.69263600	0.26818400	-0.19981100
C	-4.65314100	-0.04672900	-5.02141900
H	-4.82390000	1.03482500	-4.89763100
C	-4.60751300	0.00714800	-2.67949600
H	-4.85915800	1.07173200	-2.72872300
C	-6.09600100	-0.10678400	-7.12436300
H	-6.95198600	-0.60241200	-7.59260200
H	-6.34803200	0.95883300	-7.05761000
O	-5.02352400	1.55154100	-0.37613600

C	-5.87893800	-0.67052600	-5.71546700
H	-5.73505500	-1.75615200	-5.76620700
H	-6.76016600	-0.49755900	-5.09025300
N	-2.26656200	0.48050200	-5.27784400
C	0.01566500	0.44062100	-4.48691700
C	1.16547500	-0.33274600	-4.31425900
C	-3.38618400	-0.22248200	-5.89042300
H	-3.17964400	-1.30237200	-5.96562900
C	-1.19673100	-0.16976100	-5.05367400
H	-1.11436900	-1.24077800	-5.28869500
C	-4.84009800	-0.27808000	-7.98657200
H	-4.98639500	0.17791300	-8.97058400
H	-4.66089700	-1.34655800	-8.15887500
C	-3.61503600	0.34234500	-7.30545500
H	-3.74009300	1.42886400	-7.22945900
H	-2.71317200	0.16926900	-7.90050700
N	1.80393400	5.41837500	-0.17485500
C	1.36707200	3.93304700	1.67165700
C	1.92633800	3.07475300	2.64260500
C	2.76073800	6.02059200	-1.09282500
H	3.75732700	5.56338200	-0.98185000
C	2.23983100	4.57849400	0.67749500
H	3.29714600	4.29678800	0.71953900
C	3.78701200	8.24918300	-1.78936600
H	3.80508300	9.31982500	-1.56460000
H	4.81473600	7.88520000	-1.66824900
C	2.86835900	7.52814800	-0.79608300
H	1.86265900	7.96298400	-0.83242700
H	3.23075300	7.65562500	0.22830600
N	2.89551500	1.34565500	4.71175600
C	1.08154900	2.46494300	3.61521200
C	-0.28558700	2.72573300	3.59452300
C	3.41394600	0.49458100	5.77605000
H	2.58121100	0.05291000	6.34249200
C	1.64120100	1.58625500	4.64002600
H	0.93259900	1.14919600	5.35249000
C	4.92620200	0.49416200	7.82610400
H	5.56175000	1.12683800	8.45283700
H	4.14511100	0.08712300	8.47979000
C	4.27903000	1.34397600	6.72600500
H	5.05473800	1.84657600	6.13655500
H	3.65390500	2.12896100	7.16161800
N	2.30656800	4.36168600	-2.84442300
C	1.22540100	2.36983800	-3.62243700
C	0.06474300	1.79447500	-4.13224600
C	2.29759600	5.78891700	-2.54939800
H	1.27655900	6.18589200	-2.64621900
C	1.24869300	3.79062300	-3.28190200
H	0.31600400	4.34699400	-3.42727300
C	3.33143200	8.01369200	-3.23397900
H	4.02642400	8.48371700	-3.93615500
H	2.35609500	8.49073600	-3.39013300

C	3.22253600	6.51606400	-3.54300000
H	4.21489000	6.05206800	-3.49940600
H	2.84272900	6.35689200	-4.55652200
N	3.37252500	-1.51398000	4.36115400
C	2.95747600	-2.63838300	2.26844800
C	3.42680800	-2.88832000	0.96090900
C	4.23779900	-0.66172100	5.16539700
H	5.03655600	-0.21639000	4.55056400
C	3.72431600	-1.75439000	3.16079800
H	4.63113200	-1.31754000	2.72961700
C	5.73984500	-0.65885500	7.22723900
H	6.14756900	-1.29115000	8.02165800
H	6.59743100	-0.25156600	6.67794200
O	4.55818800	-2.31108400	0.54430700
C	4.88278700	-1.50686400	6.28061700
H	4.08618100	-2.00784100	6.84288800
H	5.48442600	-2.29375500	5.81622400
N	-0.88026000	-5.55728900	1.68039700
C	1.04538800	-4.11009600	1.86186500
C	1.77656300	-3.25569600	2.68972600
C	-2.04929600	-6.16294100	2.30477300
H	-2.22973400	-5.73341900	3.30346800
C	-0.17975000	-4.74831900	2.36787000
H	-0.45147100	-4.48582700	3.40050100
C	-3.03315000	-8.41114100	3.00797400
H	-2.83063100	-9.48557200	3.05472300
H	-3.21804400	-8.08150000	4.03785000
C	-1.80918000	-7.67831000	2.44709500
H	-1.55232300	-8.08268200	1.46100000
H	-0.93725200	-7.83491800	3.08944400
N	4.24882900	-3.53295200	-1.70703600
C	2.69213700	-3.75650200	0.10202300
C	1.52028500	-4.34747700	0.56603800
C	4.68833600	-3.85033500	-3.06040300
H	3.92024300	-4.44730500	-3.57328600
C	3.16314700	-4.03470500	-1.25300900
H	2.54050100	-4.69904200	-1.86263500
C	6.55778200	-4.94790100	-4.39607800
H	7.50658500	-5.48534700	-4.30728300
H	5.86926700	-5.61200300	-4.93288700
C	5.99913500	-4.65596000	-2.99775600
H	6.73205100	-4.08657200	-2.41435200
H	5.81400900	-5.58647300	-2.45315900
N	3.61109500	-1.84874300	-3.99797000
C	2.35351600	0.20015200	-3.80730800
C	2.39071000	1.56639500	-3.45535900
C	4.88449300	-2.54204200	-3.85955800
H	5.61412300	-1.92218700	-3.31386500
C	3.56490600	-0.62164700	-3.65973100
H	4.43902500	-0.10618400	-3.24833600
C	6.74611500	-3.65532200	-5.19874400
H	7.08863200	-3.88295300	-6.21267400

6 (4)

H	7.53047200	-3.04781000	-4.73101700
C	5.44444100	-2.84893200	-5.26157400
H	4.68590300	-3.40392800	-5.82570000
H	5.60140500	-1.90293200	-5.78814500
H	-5.15272700	1.94922600	0.54103600
H	4.71923200	-2.62899000	-0.39876900
H	-4.14737600	-2.04500800	2.25671300
H	-3.96650400	-2.50928200	-1.99990100
H	-0.82189600	2.40353700	-4.26789100
H	-0.41914000	4.82882400	0.93756700
H	1.43732700	-3.05506900	3.69994600
H	0.96063000	-5.01157500	-0.08286500
O	3.24377900	2.85009400	2.64364900
H	3.43542000	2.23340200	3.41762200
H	-0.93006000	2.26845900	4.33673300
H	1.16063200	-1.38264700	-4.58575100
O	3.52219000	2.09307200	-2.97699100
H	3.34300600	3.07174200	-2.81225900
N	-3.81386400	-2.01096400	3.87500100
C	-3.76329100	-2.23756200	1.48870100
C	-3.44140300	-3.04507400	0.40128700
C	-3.57993000	-2.54350800	5.21155600
H	-3.04586400	-3.50263100	5.14434700
C	-3.50705400	-2.70895400	2.84769700
H	-3.04765800	-3.69893500	2.94534200
C	-4.75701100	-3.25494500	7.35339700
H	-5.73719700	-3.36630600	7.82646300
H	-4.29584200	-4.25022300	7.34683900
C	-4.93347900	-2.76530600	5.91158800
H	-5.49092200	-1.82139000	5.90280500
H	-5.51689300	-3.48347400	5.32798300
N	-1.38083000	-1.47153800	5.39467200
C	0.38380300	-0.09047600	4.49250600
C	0.81464900	1.21265900	4.23430600
C	-2.69379400	-1.56667700	6.01780300
H	-3.19790800	-0.58671800	6.03004800
C	-0.94071100	-0.31730800	5.08991800
H	-1.53473500	0.59037100	5.26901200
C	-3.87818200	-2.29205700	8.15979200
H	-3.71225300	-2.68067700	9.16904500
H	-4.39941500	-1.33359100	8.27388000
C	-2.52978000	-2.06287100	7.46703700
H	-1.95411600	-2.99573200	7.45076400
H	-1.93115000	-1.33204600	8.01880000
N	-2.87335000	-4.65130200	-1.95991200
C	-3.69529800	-2.63479400	-0.91310500
C	-4.28205200	-1.38362400	-1.11550300
C	-2.65785700	-5.42690400	-3.17444800
H	-2.85763700	-4.81899100	-4.07153200
C	-3.38271900	-3.49075500	-2.06787100
H	-3.63224700	-3.06066900	-3.04865600
C	-3.38588600	-7.56343100	-4.36659700

H	-4.05537000	-8.42635300	-4.29783000
H	-3.64793000	-7.03531300	-5.29170700
C	-3.61223600	-6.63644200	-3.16663800
H	-3.46088000	-7.19079800	-2.23302400
H	-4.64266600	-6.26849000	-3.15207300
N	-5.54818300	1.19502700	-1.45447900
C	-4.62291200	-0.53818500	-0.05646200
C	-4.36274700	-0.96434400	1.26363000
C	-6.21047200	2.48811100	-1.56506700
H	-6.27900400	2.98005800	-0.58135700
C	-5.25913400	0.76919900	-0.28985300
H	-5.47894300	1.35629200	0.60801500
C	-8.36530600	3.60240100	-2.35537400
H	-9.35371000	3.40697500	-2.78245800
H	-8.53176400	4.10402100	-1.39398900
O	-4.68880200	-0.17117100	2.28952100
C	-7.63223400	2.27685100	-2.11968900
H	-7.55879100	1.71755100	-3.05986000
H	-8.18990400	1.64638100	-1.42042700
N	-4.09773700	3.69986000	-1.89631600
C	-1.69032500	3.74195000	-2.10331300
C	-0.59804100	3.48707000	-2.93544500
C	-5.39462700	3.41454300	-2.49629100
H	-5.27603600	2.89619600	-3.46153900
C	-3.05268800	3.45819500	-2.57994300
H	-3.11327400	3.02562200	-3.58902200
C	-7.55635500	4.52418900	-3.27501900
H	-8.06048600	5.48872600	-3.38944100
H	-7.49891000	4.07911600	-4.27617200
C	-6.14026200	4.74200300	-2.72994600
H	-6.18548100	5.28709500	-1.77973600
H	-5.55218000	5.35648200	-3.41844800
N	1.80988200	3.88431500	3.75029400
C	2.07026400	1.48866500	3.68695200
C	2.92992000	0.41213700	3.38003600
C	2.37367300	5.20580100	3.51019500
H	3.32122500	5.13551700	2.95184700
C	2.51724000	2.87019700	3.44544500
H	3.50918300	2.97544200	2.99393400
C	3.14937300	7.32890700	4.69256200
H	3.29102800	7.78882200	5.67519900
H	4.13320500	7.31426400	4.20761600
C	2.64189600	5.89252500	4.86302600
H	1.71245300	5.88974100	5.44433300
H	3.36550200	5.29075700	5.42081700
N	4.55907100	-1.88933800	2.86160100
C	2.50592000	-0.92408000	3.63659100
C	1.24641000	-1.14955800	4.18510400
C	5.41559900	-3.04517500	2.62902300
H	4.84486400	-3.97353300	2.77727000
C	3.38541000	-2.05316500	3.34461100
H	2.99222300	-3.05138300	3.56747200

C	7.57845800	-4.16354800	3.37315200
H	8.41851700	-4.08281500	4.06909100
H	7.08404100	-5.11908800	3.58586700
C	6.59458100	-3.01380900	3.61997000
H	7.10966800	-2.05151300	3.51917800
H	6.19683400	-3.05644900	4.63787200
N	1.22881000	5.43990900	1.35000000
C	-0.15537900	4.56530200	-0.40122400
C	-1.44788300	4.28224400	-0.83447700
C	1.39074300	6.04746300	2.66520900
H	0.42468200	6.06626100	3.19044500
C	0.05960800	5.14433400	0.92292100
H	-0.83361500	5.32094600	1.53268500
C	2.17831400	8.16124500	3.84760000
H	2.57775100	9.16646500	3.68352700
H	1.23420200	8.28288700	4.39274600
C	1.90505500	7.48926600	2.49689300
H	2.82380700	7.46496300	1.89924000
H	1.16860000	8.05945200	1.92308300
N	4.80654000	-3.14452700	0.25135800
C	3.56035800	-2.35518100	-1.63992500
C	3.44962800	-1.39390100	-2.64101100
C	5.92995100	-3.02874400	1.17248300
H	6.45360100	-2.07521400	1.00994100
C	4.64585600	-2.26776200	-0.66673400
H	5.32466900	-1.41343600	-0.76605300
C	8.08108500	-4.16163300	1.92488600
H	8.73484200	-5.02024000	1.74624500
H	8.68600400	-3.26361900	1.75038200
C	6.91247800	-4.18987900	0.93223700
H	6.36594500	-5.13557900	1.02378800
H	7.27767000	-4.13192800	-0.09704300
N	-0.30580900	-4.74216700	-3.36417400
C	1.58623400	-3.49335400	-2.54479700
C	2.61941600	-3.42392200	-1.58599200
C	-1.18641100	-5.89640100	-3.24344500
H	-0.97330800	-6.45973700	-2.32069500
C	0.61907400	-4.60307100	-2.50033700
H	0.74801900	-5.31278400	-1.67641700
C	-1.92529700	-8.02277100	-4.44075200
H	-1.76162400	-8.63584200	-5.33229100
H	-1.69996300	-8.65887300	-3.57590000
C	-0.97001200	-6.82369100	-4.45470500
H	-1.11615100	-6.24011000	-5.37117000
H	0.07138000	-7.15969500	-4.45641000
N	3.14606300	0.50321500	-4.82236500
C	2.43211600	-1.45328100	-3.60054400
C	1.51604600	-2.50513700	-3.53060100
C	2.96649000	1.40559300	-5.95182400
H	2.02662500	1.18984700	-6.48518500
C	2.32270100	-0.45498500	-4.67596300
H	1.47656100	-0.59824700	-5.36322700

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C	4.08411000	2.20966400	-8.09959700
H	4.95754600	2.07167800	-8.74425000
H	3.20202000	1.99034300	-8.71379200
C	4.14650100	1.22552000	-6.92550000
H	5.08057700	1.36700400	-6.36934100
H	4.14711900	0.19264400	-7.28681400
N	1.70391300	3.04363000	-4.62627100
C	0.71662600	3.75539300	-2.54569400
C	0.94751500	4.29874900	-1.26374200
C	2.89378000	2.86548300	-5.44778500
H	3.80816500	3.06304200	-4.86551900
C	1.85284200	3.49951800	-3.44685700
H	2.84231000	3.73526500	-3.04122600
C	4.00835800	3.65738900	-7.60155700
H	3.90663900	4.34722100	-8.44495000
H	4.94599200	3.91678800	-7.09462000
C	2.83443700	3.84706000	-6.63418200
H	1.88637300	3.69556000	-7.16341200
H	2.81803500	4.86858900	-6.24228800
H	-4.44178900	-0.66535800	3.13227100
H	-2.99149300	-4.01694300	0.56941700
H	-4.49553000	-1.03907600	-2.12128000
H	-2.28941600	4.48705300	-0.18231800
H	0.17127700	2.05430200	4.46577200
H	0.71793400	-2.58036600	-4.26075900
O	4.13570100	0.65971900	2.85908500
H	4.59012700	-0.22976700	2.73350200
H	0.92237800	-2.16445200	4.38562800
H	-0.75337100	3.07320700	-3.92563800
O	2.19930600	4.56298700	-0.87520100
H	2.14233300	4.95409900	0.05175400
O	2.70735800	-4.36590400	-0.64068400
H	3.51209200	-4.14441000	-0.07911700
H	4.16686300	-0.58231600	-2.68669400
N	-4.29526400	-2.23483400	3.20787900
C	-3.91103900	-2.36360100	0.83258600
C	-3.42719300	-3.14660300	-0.23737200
C	-4.21728200	-2.85684700	4.52287100
H	-3.65858100	-3.80562100	4.47783400
C	-3.84757600	-2.88442100	2.20874000
H	-3.39572700	-3.87547900	2.32143600
C	-5.65543600	-3.70658700	6.45129200
H	-6.68772400	-3.85796100	6.78147800
H	-5.17639000	-4.69346300	6.45462300
C	-5.64538300	-3.13895100	5.02728400
H	-6.21636700	-2.20363600	4.99353900
H	-6.13134600	-3.83068100	4.33245800
N	-2.08532700	-1.76459500	5.07106200
C	-0.24521900	-0.30148000	4.51416100
C	0.18262600	1.02198200	4.38917800
C	-3.46955700	-1.91931100	5.49898000
H	-3.99359200	-0.94999300	5.49688400

C	-1.63578300	-0.58710500	4.89974800
H	-2.27182000	0.29812300	5.04434700
C	-4.91297400	-2.77907300	7.42000400
H	-4.87633200	-3.22111400	8.42044000
H	-5.46437300	-1.83527200	7.51394500
C	-3.48931400	-2.49432200	6.92815300
H	-2.89903800	-3.41811500	6.93929000
H	-2.98424100	-1.78905600	7.59520000
N	-2.52146600	-4.61028200	-2.52983600
C	-3.50529800	-2.64602200	-1.56963700
C	-4.06022600	-1.39008200	-1.79830800
C	-2.07422100	-5.37875100	-3.68491000
H	-2.14336700	-4.76379300	-4.59409000
C	-3.01917100	-3.44324000	-2.69346100
H	-3.10646400	-2.99292100	-3.68855900
C	-2.49722700	-7.51796100	-4.99846100
H	-3.13454600	-8.40526200	-5.05791500
H	-2.61471600	-6.98232300	-5.94848500
C	-2.96743500	-6.62306200	-3.84603800
H	-2.95490400	-7.18717000	-2.90612900
H	-3.99911600	-6.29639100	-4.00626900
N	-5.30436200	1.22178200	-2.13397300
C	-4.54373100	-0.60348100	-0.74565400
C	-4.45674700	-1.10797100	0.55373300
C	-5.96002000	2.51806900	-2.23794300
H	-6.13461200	2.95462500	-1.24112600
C	-5.15028400	0.71591700	-0.97664100
H	-5.47804400	1.24438000	-0.06993700
C	-8.02446700	3.68030100	-3.18701100
H	-8.96126600	3.51040400	-3.72617000
H	-8.29349700	4.12786900	-2.22238200
C	-7.31505100	2.34225100	-2.94992700
H	-7.14064300	1.83598500	-3.90650600
H	-7.93949200	1.67486800	-2.34860900
N	-3.82467400	3.73426100	-2.29300200
C	-1.43091000	3.79139700	-2.17533900
C	-0.22658900	3.58189300	-2.84107200
C	-5.06007200	3.49460700	-3.02885800
H	-4.83384800	3.03093500	-4.00005500
C	-2.69560500	3.52654400	-2.85734600
H	-2.62993200	3.14888300	-3.88396500
C	-7.12764200	4.65029900	-3.96459000
H	-7.62013600	5.62070600	-4.07747400
H	-6.96297400	4.26147400	-4.97701000
C	-5.77727100	4.83709700	-3.26285400
H	-5.92504500	5.32809100	-2.29389000
H	-5.12270600	5.48703100	-3.85098300
N	1.14781500	3.73442300	4.17486100
C	1.49682500	1.35345500	4.04928800
C	2.42360600	0.31315900	3.82503600
C	1.68952200	5.08361600	4.08000000
H	2.71521500	5.06902200	3.67768400

C	1.92969200	2.75695800	3.94197900
H	2.97542300	2.91202000	3.65623500
C	2.17895200	7.17161200	5.46249600
H	2.14270100	7.58750100	6.47408700
H	3.22720600	7.21616100	5.14205700
C	1.71220400	5.71145100	5.48654200
H	0.70341000	5.64937300	5.91135400
H	2.36251000	5.10849400	6.12761400
N	4.17923800	-1.92579700	3.45296300
C	2.00326000	-1.04326400	3.94352900
C	0.68281900	-1.32422100	4.28388800
C	5.08506500	-3.05485900	3.28058800
H	4.51829100	-3.99692700	3.31272200
C	2.94791700	-2.13683600	3.72857800
H	2.54982900	-3.15326600	3.82370200
C	7.15243100	-4.18005500	4.24828100
H	7.89380900	-4.12348000	5.05088300
H	6.64993400	-5.14951600	4.35241800
C	6.12655000	-3.05323000	4.41518400
H	6.63518400	-2.08212200	4.42288600
H	5.60392800	-3.14512800	5.37183900
N	0.91444000	5.38625200	1.77029800
C	-0.18367100	4.55087500	-0.20483000
C	-1.41656000	4.28388600	-0.83794700
C	0.82096200	5.92825400	3.11908500
H	-0.21663000	5.89194700	3.48833800
C	-0.16500500	5.07553600	1.17117800
H	-1.14344800	5.19085600	1.64909800
C	1.32062400	8.00922600	4.50773400
H	1.69770400	9.03517100	4.45466200
H	0.29731300	8.07052500	4.89827600
C	1.29600300	7.39402000	3.10399000
H	2.29884300	7.42939900	2.66239900
H	0.63927500	7.96731500	2.44255200
N	4.77709000	-3.08472000	0.84574000
C	3.79529800	-2.20977300	-1.17377400
C	3.84184900	-1.19638400	-2.15516700
C	5.77500500	-2.96695800	1.90011300
H	6.29629800	-1.99767500	1.84478100
C	4.73524600	-2.17237700	-0.04179700
H	5.40921500	-1.30986600	-0.01281000
C	7.83796700	-4.10674400	2.87897200
H	8.52310600	-4.94995900	2.74952200
H	8.44702400	-3.19595600	2.82607100
C	6.80674400	-4.09986300	1.74430500
H	6.27057200	-5.05573600	1.71977600
H	7.30045500	-3.98957800	0.77426400
N	0.24101700	-4.58697400	-3.47719700
C	1.97884500	-3.30453900	-2.39332800
C	2.86335500	-3.24090800	-1.31456000
C	-0.59350900	-5.78089700	-3.50011300
H	-0.51185500	-6.33874900	-2.55322500

C	1.04273200	-4.43317000	-2.50122500
H	1.08944100	-5.15884500	-1.67646300
C	-1.02934200	-7.92225500	-4.82081100
H	-0.68974200	-8.51303600	-5.67689100
H	-0.93397200	-8.56567400	-3.93751700
C	-0.13347700	-6.68911500	-4.65630500
H	-0.13471600	-6.09967900	-5.58064400
H	0.90332000	-6.98626400	-4.47277200
N	3.83311200	0.74496500	-4.26025100
C	2.94486500	-1.24437900	-3.26185600
C	2.03376900	-2.29223100	-3.35958000
C	3.86413600	1.73218300	-5.33190300
H	3.03634300	1.55107800	-6.03303400
C	2.98890300	-0.21536400	-4.29849800
H	2.26742900	-0.31151800	-5.11756800
C	5.33358900	2.69084800	-7.17625700
H	6.30933200	2.60120600	-7.66293100
H	4.57805900	2.51774300	-7.95245800
C	5.20157500	1.62013700	-6.08721200
H	6.02038100	1.71864000	-5.36491600
H	5.27832200	0.61782100	-6.51876100
N	2.35950200	3.25810000	-4.13558700
C	1.00295200	3.84417000	-2.22476800
C	0.99907000	4.32378300	-0.91322500
C	3.68039500	3.14809800	-4.73921300
H	4.47313200	3.30300300	-3.98937300
C	2.27968400	3.64938600	-2.92746600
H	3.17816200	3.87800400	-2.33642200
C	5.15130500	4.09752400	-6.59463700
H	5.19228800	4.84767700	-7.39007300
H	5.98023400	4.31836700	-5.91092000
C	3.82145400	4.21519900	-5.84077400
H	2.98386300	4.10620200	-6.53966900
H	3.72339700	5.20343800	-5.38181600
H	-4.12659900	-1.00940000	-2.81119500
H	-0.51051800	1.83731700	4.56424100
H	1.35437700	-2.33552700	-4.20330300
O	3.68846700	0.61226600	3.51015000
H	4.18195700	-0.26027500	3.41518500
H	0.36133300	-2.35507000	4.38085300
H	-0.23408700	3.21507800	-3.86121600
O	-2.55829600	4.50306900	-0.17796900
H	-3.31021000	4.26982100	-0.80704800
O	-2.90486600	-4.35192700	0.01028100
H	-2.63536300	-4.74305800	-0.87860600
H	-4.82556600	-0.52422100	1.38980300
H	1.93491000	4.54124400	-0.41041000
O	4.73268200	-0.20709300	-2.03888400
H	4.61403100	0.39032200	-2.84253800
H	2.84918400	-4.01257100	-0.55293400
N	5.49132700	1.60265200	-0.85081400
C	4.00965600	0.14096400	-2.07987800

C	3.15177800	0.02558400	-3.17575000
C	6.10675100	2.91510700	-0.71057800
H	5.65119400	3.64141800	-1.40309200
C	4.66207800	1.42816400	-1.80003700
H	4.39255300	2.24529700	-2.48448400
C	8.34698200	4.13140500	-0.80706800
H	9.41489300	3.99726000	-1.00389100
H	7.98501000	4.87272100	-1.53000100
C	7.61096400	2.80432000	-1.02369600
H	8.04271200	2.02684000	-0.38267500
H	7.72703700	2.46275100	-2.05654100
N	4.47228300	3.63396500	0.97597300
C	2.49111300	3.22425300	2.26205200
C	1.92415100	2.57577300	3.35560800
C	5.89547300	3.44108100	0.72770400
H	6.29915400	2.69018000	1.42247600
C	3.90834200	3.03885800	1.95804500
H	4.46875700	2.36831100	2.61904500
C	8.12792300	4.65990700	0.61537500
H	8.60767500	5.63529800	0.73974300
H	8.60485200	3.98094900	1.33283200
C	6.63352800	4.77590700	0.93831800
H	6.17085700	5.53605500	0.29806800
H	6.48542200	5.09978100	1.97267900
N	1.43222000	-0.30100100	-5.47044400
C	2.52392600	-1.17680900	-3.50959700
C	2.76399700	-2.31342700	-2.70811300
C	0.57267000	-0.51943000	-6.62621300
H	0.11490800	-1.52110500	-6.59339200
C	1.64211800	-1.28035100	-4.68448800
H	1.18180000	-2.26030900	-4.84868100
C	0.56823000	-0.51431700	-9.17777800
H	1.20224700	-0.38376300	-10.06011000
H	0.14428300	-1.52405900	-9.24230800
O	2.17813000	-3.47448400	-3.01757900
C	1.41878600	-0.39646000	-7.90788100
H	1.93408400	0.57107000	-7.89216700
H	2.19443300	-1.16804700	-7.88964400
N	3.40093900	-4.52743700	-1.00198800
C	3.63351300	-2.21273000	-1.58321300
C	4.23813400	-0.99322600	-1.29122400
C	3.73874100	-5.67018700	-0.16237200
H	4.32792800	-5.33654500	0.70430400
C	3.90834200	-3.38055100	-0.74939100
H	4.58017400	-3.22807400	0.10274300
C	4.89531800	-7.93796600	-0.17815900
H	5.45069400	-8.64042300	-0.80675500
H	5.55364000	-7.67830200	0.65998100
C	4.57037700	-6.67404900	-0.98261200
H	4.00756900	-6.93972100	-1.88515200
H	5.48848500	-6.18069500	-1.31487400
N	1.73284500	-5.39426600	1.22621400

C	-0.31973900	-4.25626200	1.77837400
C	-1.68248500	-4.07803300	1.45680500
C	2.44643300	-6.33065400	0.36871000
H	1.83310300	-6.61661600	-0.50115800
C	0.51109300	-5.15324800	0.95909200
H	0.00832700	-5.61285200	0.10176500
C	3.61956800	-8.59486000	0.36139700
H	3.86928200	-9.46076800	0.98189500
H	3.02156200	-8.97123000	-0.47765800
O	-2.20128200	-4.71802800	0.40420500
C	2.78634800	-7.59806000	1.17567300
H	3.33434000	-7.29989300	2.07708400
H	1.85207000	-8.05809200	1.51082400
N	0.62501000	1.32844100	5.64261300
C	0.57372700	2.74436300	3.68557100
C	-0.20420200	3.58436900	2.88611900
C	-0.06792700	0.77012700	6.79633700
H	-1.14312300	1.00989900	6.76437500
C	-0.02784800	2.08335500	4.85408600
H	-1.09460700	2.29676800	5.01388600
C	-0.06699100	0.76345000	9.34917300
H	0.41958800	1.19076100	10.23133400
H	-1.12799000	1.03510800	9.41295000
C	0.54089700	1.36887700	8.07887200
H	1.62300900	1.19367200	8.06285000
H	0.39650700	2.45341200	8.06052500
N	-1.73284500	5.39426600	1.22621400
C	0.31973900	4.25626200	1.77837400
C	1.68248500	4.07803300	1.45680500
C	-2.44643300	6.33065400	0.36871000
H	-1.83310300	6.61661600	-0.50115800
C	-0.51109300	5.15324800	0.95909200
H	-0.00832700	5.61285200	0.10176500
C	-3.61956800	8.59486000	0.36139700
H	-3.86928200	9.46076800	0.98189500
H	-3.02156200	8.97123000	-0.47765800
O	2.20128200	4.71802800	0.40420500
C	-2.78634800	7.59806000	1.17567300
H	-3.33434000	7.29989300	2.07708400
H	-1.85207000	8.05809200	1.51082400
N	-0.62501000	-1.32844100	5.64261300
C	-0.57372700	-2.74436300	3.68557100
C	0.20420200	-3.58436900	2.88611900
C	0.06792700	-0.77012700	6.79633700
H	1.14312300	-1.00989900	6.76437500
C	0.02784800	-2.08335500	4.85408600
H	1.09460700	-2.29676800	5.01388600
C	0.06699100	-0.76345000	9.34917300
H	-0.41958800	-1.19076100	10.23133400
H	1.12799000	-1.03510800	9.41295000
C	-0.54089700	-1.36887700	8.07887200
H	-1.62300900	-1.19367200	8.06285000

H	-0.39650700	-2.45341200	8.06052500
N	-3.40093900	4.52743700	-1.00198800
C	-3.63351300	2.21273000	-1.58321300
C	-4.23813400	0.99322600	-1.29122400
C	-3.73874100	5.67018700	-0.16237200
H	-4.32792800	5.33654500	0.70430400
C	-3.90834200	3.38055100	-0.74939100
H	-4.58017400	3.22807400	0.10274300
C	-4.89531800	7.93796600	-0.17815900
H	-5.45069400	8.64042300	-0.80675500
H	-5.55364000	7.67830200	0.65998100
C	-4.57037700	6.67404900	-0.98261200
H	-4.00756900	6.93972100	-1.88515200
H	-5.48848500	6.18069500	-1.31487400
N	-1.43222000	0.30100100	-5.47044400
C	-2.52392600	1.17680900	-3.50959700
C	-2.76399700	2.31342700	-2.70811300
C	-0.57267000	0.51943000	-6.62621300
H	-0.11490800	1.52110500	-6.59339200
C	-1.64211800	1.28035100	-4.68448800
H	-1.18180000	2.26030900	-4.84868100
C	-0.56823000	0.51431700	-9.17777800
H	-1.20224700	0.38376300	-10.06011000
H	-0.14428300	1.52405900	-9.24230800
O	-2.17813000	3.47448400	-3.01757900
C	-1.41878600	0.39646000	-7.90788100
H	-1.93408400	-0.57107000	-7.89216700
H	-2.19443300	1.16804700	-7.88964400
N	-5.49132700	-1.60265200	-0.85081400
C	-4.00965600	-0.14096400	-2.07987800
C	-3.15177800	-0.02558400	-3.17575000
C	-6.10675100	-2.91510700	-0.71057800
H	-5.65119400	-3.64141800	-1.40309200
C	-4.66207800	-1.42816400	-1.80003700
H	-4.39255300	-2.24529700	-2.48448400
C	-8.34698200	-4.13140500	-0.80706800
H	-9.41489300	-3.99726000	-1.00389100
H	-7.98501000	-4.87272100	-1.53000100
C	-7.61096400	-2.80432000	-1.02369600
H	-8.04271200	-2.02684000	-0.38267500
H	-7.72703700	-2.46275100	-2.05654100
N	-4.47228300	-3.63396500	0.97597300
C	-2.49111300	-3.22425300	2.26205200
C	-1.92415100	-2.57577300	3.35560800
C	-5.89547300	-3.44108100	0.72770400
H	-6.29915400	-2.69018000	1.42247600
C	-3.90834200	-3.03885800	1.95804500
H	-4.46875700	-2.36831100	2.61904500
C	-8.12792300	-4.65990700	0.61537500
H	-8.60767500	-5.63529800	0.73974300
H	-8.60485200	-3.98094900	1.33283200
C	-6.63352800	-4.77590700	0.93831800

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H	-6.17085700	-5.53605500	0.29806800
H	-6.48542200	-5.09978100	1.97267900
H	4.90557800	-0.91524200	-0.44039600
H	2.95885800	0.88487300	-3.80834300
H	-2.95885800	-0.88487300	-3.80834300
H	-4.90557800	0.91524200	-0.44039600
H	1.25181800	-3.74000700	3.11882100
H	-2.53729300	-1.92960200	3.97344800
H	-1.25181800	3.74000700	3.11882100
H	2.53729300	1.92960200	3.97344800
H	-2.49284200	4.15148300	-2.34079100
H	3.17685500	4.46781300	0.36101400
H	-3.17685500	-4.46781300	0.36101400
H	2.49284200	-4.15148300	-2.34079100
N	0.24652900	-5.68202200	-0.91828000
C	-0.81604300	-3.92417800	-2.18891100
C	-0.71941700	-3.07272400	-3.29176300
C	1.37558000	-6.58489100	-0.73746000
H	2.19670100	-6.33393000	-1.42824400
C	0.28358200	-4.85180700	-1.88120400
H	1.15015700	-4.78982200	-2.55516300
C	2.01415100	-9.05587100	-0.74998400
H	1.62870800	-10.06506700	-0.92465000
H	2.83425100	-8.90494700	-1.46281900
C	0.90960100	-8.02681200	-1.01608200
H	0.04075400	-8.23907600	-0.38206000
H	0.56605900	-8.08832800	-2.05319200
N	2.47259800	-5.12282700	0.90292600
C	2.55145500	-3.08834300	2.19157400
C	2.05323000	-2.38750400	3.31062800
C	1.92068100	-6.45631900	0.70386300
H	1.08321600	-6.64357600	1.39503100
C	2.03422800	-4.43124800	1.87773900
H	1.24990100	-4.80653200	2.54338700
C	2.55429500	-8.92776800	0.67878700
H	3.37983200	-9.62782700	0.83988100
H	1.76639300	-9.20170600	1.39134300
C	3.02663800	-7.49730600	0.96279900
H	3.88699800	-7.25524000	0.32782400
H	3.36224800	-7.39979700	1.99975700
N	-0.61983600	-1.32607200	-5.59714800
C	-1.74164500	-2.18727800	-3.64377400
C	-2.91182500	-2.15276500	-2.85546000
C	-0.63438700	-0.44183200	-6.75526400
H	-1.50838500	0.22863000	-6.72791100
C	-1.62898000	-1.30984400	-4.82094300
H	-2.47836800	-0.64122500	-4.99624100
C	-0.62683400	-0.44106200	-9.30681400
H	-0.63867300	-1.08908700	-10.18858400
H	-1.51856700	0.19457000	-9.37207300
O	-3.90348500	-1.31747500	-3.18196400
C	-0.69997300	-1.29564000	-8.03610800

H	0.12977700	-2.01192600	-8.01943300
H	-1.62366000	-1.88210600	-8.01814000
N	-5.23091100	-2.24897800	-1.17405200
C	-3.02663800	-3.01335300	-1.72537600
C	-1.98112600	-3.87797000	-1.41378400
C	-6.43151400	-2.30402700	-0.34946200
H	-6.26758700	-2.97277300	0.50801800
C	-4.23594600	-3.00684400	-0.90537400
H	-4.25313200	-3.69223200	-0.05055700
C	-8.91879300	-2.84723800	-0.40991400
H	-9.72973300	-3.19583900	-1.05633700
H	-8.84662300	-3.56337800	0.41769600
C	-7.60182700	-2.83994100	-1.19501300
H	-7.70283100	-2.21263900	-2.08826000
H	-7.35288700	-3.84733200	-1.54135800
N	-5.67659600	-0.46267100	1.08733400
C	-4.06360000	1.22711800	1.70322900
C	-3.54474300	2.49067900	1.41170600
C	-6.75008100	-0.89618200	0.20383800
H	-6.85613100	-0.21385400	-0.65498800
C	-5.12649500	0.66166500	0.85889100
H	-5.42951000	1.28738200	0.00710900
C	-9.23822200	-1.45553000	0.14823200
H	-10.14831600	-1.48743000	0.75479000
H	-9.43803000	-0.76756900	-0.68233100
C	-8.07512300	-0.91714800	0.98954200
H	-7.93946600	-1.53826200	1.88252400
H	-8.28820900	0.09734400	1.33925800
N	1.18902400	-0.83849500	5.56569300
C	2.56833400	-1.09528900	3.62049200
C	3.55942200	-0.54123600	2.81458800
C	0.76843400	-0.07688700	6.73501900
H	1.21016000	0.93004400	6.70646600
C	2.07849100	-0.35710600	4.78164100
H	2.51799200	0.63162400	4.95461000
C	0.76174700	-0.08469500	9.28151700
H	1.08336300	-0.64844100	10.16205500
H	1.23798700	0.90106000	9.34790900
C	1.24041400	-0.79816100	8.01151800
H	0.86026800	-1.82617900	7.99302100
H	2.33202500	-0.86311900	7.99261200
N	5.67659600	0.46267100	1.08733400
C	4.06360000	-1.22711800	1.70322900
C	3.54474300	-2.49067900	1.41170600
C	6.75008100	0.89618200	0.20383800
H	6.85613100	0.21385400	-0.65498800
C	5.12649500	-0.66166500	0.85889100
H	5.42951000	-1.28738200	0.00710900
C	9.23822200	1.45553000	0.14823200
H	10.14831600	1.48743000	0.75479000
H	9.43803000	0.76756900	-0.68233100
C	8.07512300	0.91714800	0.98954200

H	7.93946600	1.53826200	1.88252400
H	8.28820900	-0.09734400	1.33925800
N	-1.18902400	0.83849500	5.56569300
C	-2.56833400	1.09528900	3.62049200
C	-3.55942200	0.54123600	2.81458800
C	-0.76843400	0.07688700	6.73501900
H	-1.21016000	-0.93004400	6.70646600
C	-2.07849100	0.35710600	4.78164100
H	-2.51799200	-0.63162400	4.95461000
C	-0.76174700	0.08469500	9.28151700
H	-1.08336300	0.64844100	10.16205500
H	-1.23798700	-0.90106000	9.34790900
C	-1.24041400	0.79816100	8.01151800
H	-0.86026800	1.82617900	7.99302100
H	-2.33202500	0.86311900	7.99261200
N	5.23091100	2.24897800	-1.17405200
C	3.02663800	3.01335300	-1.72537600
C	1.98112600	3.87797000	-1.41378400
C	6.43151400	2.30402700	-0.34946200
H	6.26758700	2.97277300	0.50801800
C	4.23594600	3.00684400	-0.90537400
H	4.25313200	3.69223200	-0.05055700
C	8.91879300	2.84723800	-0.40991400
H	9.72973300	3.19583900	-1.05633700
H	8.84662300	3.56337800	0.41769600
C	7.60182700	2.83994100	-1.19501300
H	7.70283100	2.21263900	-2.08826000
H	7.35288700	3.84733200	-1.54135800
N	0.61983600	1.32607200	-5.59714800
C	1.74164500	2.18727800	-3.64377400
C	2.91182500	2.15276500	-2.85546000
C	0.63438700	0.44183200	-6.75526400
H	1.50838500	-0.22863000	-6.72791100
C	1.62898000	1.30984400	-4.82094300
H	2.47836800	0.64122500	-4.99624100
C	0.62683400	0.44106200	-9.30681400
H	0.63867300	1.08908700	-10.18858400
H	1.51856700	-0.19457000	-9.37207300
O	3.90348500	1.31747500	-3.18196400
C	0.69997300	1.29564000	-8.03610800
H	-0.12977700	2.01192600	-8.01943300
H	1.62366000	1.88210600	-8.01814000
N	-0.24652900	5.68202200	-0.91828000
C	0.81604300	3.92417800	-2.18891100
C	0.71941700	3.07272400	-3.29176300
C	-1.37558000	6.58489100	-0.73746000
H	-2.19670100	6.33393000	-1.42824400
C	-0.28358200	4.85180700	-1.88120400
H	-1.15015700	4.78982200	-2.55516300
C	-2.01415100	9.05587100	-0.74998400
H	-1.62870800	10.06506700	-0.92465000
H	-2.83425100	8.90494700	-1.46281900

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C	-0.90960100	8.02681200	-1.01608200
H	-0.04075400	8.23907600	-0.38206000
H	-0.56605900	8.08832800	-2.05319200
N	-2.47259800	5.12282700	0.90292600
C	-2.55145500	3.08834300	2.19157400
C	-2.05323000	2.38750400	3.31062800
C	-1.92068100	6.45631900	0.70386300
H	-1.08321600	6.64357600	1.39503100
C	-2.03422800	4.43124800	1.87773900
H	-1.24990100	4.80653200	2.54338700
C	-2.55429500	8.92776800	0.67878700
H	-3.37983200	9.62782700	0.83988100
H	-1.76639300	9.20170600	1.39134300
C	-3.02663800	7.49730600	0.96279900
H	-3.88699800	7.25524000	0.32782400
H	-3.36224800	7.39979700	1.99975700
H	-2.06737700	-4.53659500	-0.55703600
H	0.16831900	-3.08827900	-3.91424400
H	-0.16831900	3.08827900	-3.91424400
H	2.06737700	4.53659500	-0.55703600
H	-3.95725000	-0.43938600	3.05007600
H	3.95725000	0.43938600	3.05007600
H	4.64193000	1.46357800	-2.51190000
H	-4.64193000	-1.46357800	-2.51190000
O	-1.10682600	2.94753300	4.07126300
H	-0.90701300	2.30129600	4.81612700
O	1.10682600	-2.94753300	4.07126300
H	0.90701300	-2.30129600	4.81612700
H	-3.91627100	3.04784100	0.55886600
H	3.91627100	-3.04784100	0.55886600
N	2.96460900	1.57226700	-4.70035500
C	3.34601600	2.09164100	-2.37936900
C	4.07603800	1.78564700	-1.21106100
C	3.28828200	0.77227700	-5.87372400
H	3.97028300	-0.05304700	-5.61278600
C	3.57178300	1.31621000	-3.61100700
H	4.30446300	0.50583400	-3.53598300
C	4.25518800	0.93294700	-8.22976400
H	4.70575200	1.61976000	-8.95283600
H	4.99105100	0.13954900	-8.04922000
C	3.97112900	1.67488100	-6.91902800
H	3.32171500	2.53705500	-7.11115600
H	4.89755900	2.06770300	-6.48900600
N	1.44001500	-0.80020200	-5.49417600
C	-0.44917700	-1.57358900	-4.20502100
C	-1.79774600	-1.38242200	-3.89669600
C	1.99613900	0.14819100	-6.45034500
H	1.28829300	0.96941400	-6.64750000
C	0.22965000	-0.65431600	-5.13182600
H	-0.38813700	0.17441200	-5.50673300
C	2.97403500	0.31608800	-8.80215600
H	3.19674000	-0.25821500	-9.70669400

H	2.28672400	1.11755100	-9.10048300
C	2.28962600	-0.58847600	-7.77110000
H	2.92684400	-1.45334700	-7.55183400
H	1.34887700	-0.98273000	-8.16739400
N	5.50157700	1.33526700	1.23686600
C	3.86747200	2.55250700	-0.02798300
C	2.94530100	3.59554100	-0.04095000
C	6.25472100	1.11425900	2.46540300
H	5.85572500	1.75057700	3.26878300
C	4.62419800	2.26507800	1.18831700
H	4.40834200	2.89333700	2.05976500
C	8.59609900	1.18724100	3.46160500
H	9.64260900	1.41612800	3.23933400
H	8.29440800	1.85561500	4.27732900
C	7.73367300	1.46946900	2.22566800
H	8.10008400	0.88640100	1.37272100
H	7.79993600	2.52364700	1.94094500
N	1.03407600	5.78729500	-0.23472500
C	2.21553600	3.90978600	-1.19373300
C	2.43095800	3.14685400	-2.34323000
C	0.10479100	6.89500800	-0.41357800
H	-0.38374300	6.84277900	-1.39999400
C	1.25923300	5.02644900	-1.22890400
H	0.75039000	5.17391100	-2.19248700
C	-0.03605300	9.44216700	-0.40112800
H	0.55278800	10.35744900	-0.28676900
H	-0.49250700	9.48496900	-1.39781900
C	0.88417200	8.22000400	-0.31182800
H	1.42866300	8.23062600	0.63969200
H	1.63626200	8.24459700	-1.10625700
N	-1.80464300	5.62829900	0.46465000
C	-2.70622700	3.57216900	1.35430500
C	-2.81146200	2.74278600	2.47283100
C	-1.00594500	6.83073200	0.66070100
H	-0.51537200	6.82185400	1.64751900
C	-1.90698900	4.80506500	1.42875300
H	-1.40191400	4.97802900	2.38998100
C	-1.14025200	9.37961500	0.66060600
H	-1.82560500	10.22568300	0.55075900
H	-0.69077900	9.46711000	1.65753400
C	-1.92300800	8.06455100	0.56591800
H	-2.46508400	8.02081500	-0.38602500
H	-2.67388500	8.00413700	1.35962600
N	-4.60841400	-1.09779800	-3.26828500
C	-2.49580800	-2.23798600	-3.03996100
C	-1.81232400	-3.33068700	-2.46474700
C	-6.02206400	-1.01452800	-2.92690000
H	-6.27852700	-1.72855900	-2.12759900
C	-3.92257300	-2.03286100	-2.74169000
H	-4.36650600	-2.74473500	-2.03804000
C	-8.36775000	-1.17904700	-3.91816100
H	-8.92248300	-1.38081000	-4.83945100

H	-8.69416500	-1.92648600	-3.18467100
C	-6.86461800	-1.33824400	-4.17545400
H	-6.55061300	-0.67253700	-4.98781400
H	-6.63402100	-2.35851800	-4.49596100
N	-0.27966700	-5.52016600	-1.42523200
C	-0.43541100	-3.53909500	-2.76677500
C	0.21723200	-2.66088600	-3.62754600
C	0.47828500	-6.65378800	-0.91128200
H	1.53978600	-6.55026700	-1.18013800
C	0.28897700	-4.67149200	-2.19586600
H	1.34657800	-4.76399900	-2.46692700
C	0.63389700	-9.19485600	-0.95815700
H	0.18955700	-10.09753000	-1.38745200
H	1.68700800	-9.18589800	-1.26459700
C	-0.07218700	-7.95598700	-1.52190900
H	-1.14736500	-8.01113000	-1.31582300
H	0.04088000	-7.90731100	-2.60867100
N	-5.62108000	0.67251700	-1.18144300
C	-4.16169400	2.04884400	0.13268900
C	-3.38987200	3.20597400	0.18863000
C	-6.35146300	0.40598200	-2.41437400
H	-6.04775300	1.12224200	-3.19171000
C	-4.87752900	1.70999700	-1.09500900
H	-4.75403000	2.39709200	-1.93968000
C	-8.69416700	0.22398400	-3.39318400
H	-9.75890200	0.30557100	-3.15518800
H	-8.48950900	0.96278300	-4.17771800
C	-7.86119900	0.55630300	-2.15006200
H	-8.13970200	-0.10871300	-1.32423700
H	-8.05902900	1.57854900	-1.81447900
N	0.98659400	-5.49249100	1.19250600
C	0.88934600	-3.56611000	2.61697800
C	0.13129100	-2.81693100	3.51280400
C	0.37907200	-6.69180400	0.63021000
H	-0.68639900	-6.73573200	0.89976600
C	0.31578000	-4.75797000	1.99755900
H	-0.71998300	-4.99829500	2.26226300
C	0.54931300	-9.23183400	0.57207200
H	1.10682300	-10.08704300	0.96499900
H	-0.49529800	-9.37071700	0.87595300
C	1.09261000	-7.93729600	1.18848900
H	2.16566300	-7.84645300	0.98380300
H	0.97655000	-7.94826900	2.27597200
N	4.71503600	-0.63464500	3.23863200
C	2.76532900	-2.02274100	2.94920400
C	2.22648400	-3.16865700	2.32607000
C	6.10727300	-0.35785000	2.91220400
H	6.45452600	-0.99688700	2.08438900
C	4.15329800	-1.62350400	2.66549400
H	4.68318000	-2.23967900	1.93166900
C	8.45072200	-0.26922100	3.91752100
H	9.02332100	-0.44118300	4.83388300

H	8.87326400	-0.93335700	3.15362800
O	2.98044400	-3.87279500	1.47556300
C	6.97959100	-0.63073500	4.15253500
H	6.58024500	-0.04991200	4.99207300
H	6.87943500	-1.68622400	4.42237500
N	-1.31557400	-1.19894100	5.45159800
C	0.65437900	-1.67896500	4.13849300
C	1.96608500	-1.30300000	3.84137500
C	-1.97841000	-0.37020400	6.44983300
H	-1.37340600	0.51920700	6.68930000
C	-0.13111300	-0.89358600	5.10328600
H	0.38386200	-0.01584100	5.51959800
C	-2.96007100	-0.42802000	8.80468800
H	-3.11116600	-1.06548000	9.68124300
H	-2.36793500	0.43237900	9.14026300
C	-2.18014800	-1.19857600	7.73300100
H	-2.71533000	-2.11908800	7.47166500
H	-1.19895700	-1.50049700	8.11185600
N	-3.11567100	1.00604100	4.76286500
C	-3.57594700	1.57293000	2.46582400
C	-4.26214200	1.21669100	1.28507200
C	-3.33674000	0.12290300	5.90038400
H	-3.91840400	-0.76488000	5.60420600
C	-3.69506300	0.72568100	3.66439200
H	-4.32543500	-0.16305000	3.55617600
C	-4.30615600	0.06320100	8.26031000
H	-4.82877700	0.66044900	9.01378200
H	-4.94739100	-0.80020200	8.04354600
C	-4.11476000	0.89222500	6.98513600
H	-3.56728700	1.81319600	7.21780900
H	-5.08175600	1.19542500	6.57234100
H	1.88526200	3.36867500	-3.25361300
H	2.40143900	-0.42958600	4.31405100
H	-0.88487800	-3.11882200	3.73978600
H	-3.31665000	3.84537100	-0.68381700
H	2.42285700	-4.65019600	1.16273500
O	-5.00442900	0.10465800	1.26280600
H	-5.41745800	0.04581900	0.34601200
H	-2.29717100	3.00105000	3.39195800
H	1.26294000	-2.81931400	-3.86565600
O	4.96044700	0.78285600	-1.22924300
H	5.37895800	0.74375300	-0.31399600
O	-2.46755000	-4.16199700	-1.64789300
H	-1.81370900	-4.87333500	-1.36579200
H	-2.34280300	-0.55186300	-4.33145900
H	2.78926500	4.18563000	0.85509600
N	5.62849300	-1.09467200	-0.95513200
C	3.67512700	-1.66722200	-2.22314900
C	2.87108000	-1.36858900	-3.31967000
C	6.79831800	-0.25544300	-0.72894700
H	6.76819600	0.62034900	-1.39377600
C	4.84112700	-0.83780000	-1.93050000

H	5.01351500	0.01630500	-2.59496700
C	9.34393500	-0.25909500	-0.72141600
H	10.22521900	-0.88090700	-0.90384900
H	9.40902100	0.58963200	-1.41312700
C	8.07486700	-1.06593400	-1.02037500
H	8.05803100	-1.97643500	-0.41012100
H	8.05598900	-1.38416800	-2.06659400
N	5.62849300	1.09467200	0.95513200
C	3.67512700	1.66722200	2.22314900
C	2.87108000	1.36858900	3.31967000
C	6.79831800	0.25544300	0.72894700
H	6.76819600	-0.62034900	1.39377600
C	4.84112700	0.83780000	1.93050000
H	5.01351500	-0.01630500	2.59496700
C	9.34393500	0.25909500	0.72141600
H	10.22521900	0.88090700	0.90384900
H	9.40902100	-0.58963200	1.41312700
C	8.07486700	1.06593400	1.02037500
H	8.05803100	1.97643500	0.41012100
H	8.05598900	1.38416800	2.06659400
N	1.15693200	-0.89816600	-5.61623300
C	1.75426500	-2.14911300	-3.64042500
C	1.45404300	-3.24291400	-2.82569300
C	0.28369700	-0.71942100	-6.76839100
H	-0.57117500	-1.41375700	-6.72820000
C	0.91548900	-1.85403500	-4.81283300
H	0.05947500	-2.52840000	-4.95902600
C	0.27507900	-0.71534300	-9.32050600
H	0.89762700	-0.88637700	-10.20409500
H	-0.55936300	-1.42506200	-9.38175900
C	1.09046900	-0.99066400	-8.05221600
H	1.98549500	-0.35750100	-8.04007600
H	1.43799400	-2.02813500	-8.03350800
N	0.93042800	-5.52655700	-1.13306100
C	2.23075700	-3.58229300	-1.71463700
C	3.35745100	-2.79056000	-1.40612600
C	0.72546700	-6.68041900	-0.26703200
H	1.40092100	-6.64617900	0.60294300
C	1.90813000	-4.75169000	-0.87928400
H	2.57092100	-4.92132200	-0.02433700
C	0.71994300	-9.23221000	-0.26279700
H	0.90103800	-10.11511500	-0.88347000
H	1.41536300	-9.29473000	0.58344300
O	4.11774100	-3.10758500	-0.35246300
C	1.01041700	-7.96307600	-1.07173500
H	0.39341700	-7.94923000	-1.97793100
H	2.05406500	-7.94449700	-1.40012600
N	-0.93042800	-5.52655700	1.13306100
C	-2.23075700	-3.58229300	1.71463700
C	-3.35745100	-2.79056000	1.40612600
C	-0.72546700	-6.68041900	0.26703200
H	-1.40092100	-6.64617900	-0.60294300

C	-1.90813000	-4.75169000	0.87928400
H	-2.57092100	-4.92132200	0.02433700
C	-0.71994300	-9.23221000	0.26279700
H	-0.90103800	-10.11511500	0.88347000
H	-1.41536300	-9.29473000	-0.58344300
O	-4.11774100	-3.10758500	0.35246300
C	-1.01041700	-7.96307600	1.07173500
H	-0.39341700	-7.94923000	1.97793100
H	-2.05406500	-7.94449700	1.40012600
N	1.15693200	0.89816600	5.61623300
C	1.75426500	2.14911300	3.64042500
C	1.45404300	3.24291400	2.82569300
C	0.28369700	0.71942100	6.76839100
H	-0.57117500	1.41375700	6.72820000
C	0.91548900	1.85403500	4.81283300
H	0.05947500	2.52840000	4.95902600
C	0.27507900	0.71534300	9.32050600
H	0.89762700	0.88637700	10.20409500
H	-0.55936300	1.42506200	9.38175900
C	1.09046900	0.99066400	8.05221600
H	1.98549500	0.35750100	8.04007600
H	1.43799400	2.02813500	8.03350800
N	0.93042800	5.52655700	1.13306100
C	2.23075700	3.58229300	1.71463700
C	3.35745100	2.79056000	1.40612600
C	0.72546700	6.68041900	0.26703200
H	1.40092100	6.64617900	-0.60294300
C	1.90813000	4.75169000	0.87928400
H	2.57092100	4.92132200	0.02433700
C	0.71994300	9.23221000	0.26279700
H	0.90103800	10.11511500	0.88347000
H	1.41536300	9.29473000	-0.58344300
O	4.11774100	3.10758500	0.35246300
C	1.01041700	7.96307600	1.07173500
H	0.39341700	7.94923000	1.97793100
H	2.05406500	7.94449700	1.40012600
N	-1.15693200	-0.89816600	5.61623300
C	-1.75426500	-2.14911300	3.64042500
C	-1.45404300	-3.24291400	2.82569300
C	-0.28369700	-0.71942100	6.76839100
H	0.57117500	-1.41375700	6.72820000
C	-0.91548900	-1.85403500	4.81283300
H	-0.05947500	-2.52840000	4.95902600
C	-0.27507900	-0.71534300	9.32050600
H	-0.89762700	-0.88637700	10.20409500
H	0.55936300	-1.42506200	9.38175900
C	-1.09046900	-0.99066400	8.05221600
H	-1.98549500	-0.35750100	8.04007600
H	-1.43799400	-2.02813500	8.03350800
N	-0.93042800	5.52655700	-1.13306100
C	-2.23075700	3.58229300	-1.71463700
C	-3.35745100	2.79056000	-1.40612600

C	-0.72546700	6.68041900	-0.26703200
H	-1.40092100	6.64617900	0.60294300
C	-1.90813000	4.75169000	-0.87928400
H	-2.57092100	4.92132200	-0.02433700
C	-0.71994300	9.23221000	-0.26279700
H	-0.90103800	10.11511500	-0.88347000
H	-1.41536300	9.29473000	0.58344300
O	-4.11774100	3.10758500	-0.35246300
C	-1.01041700	7.96307600	-1.07173500
H	-0.39341700	7.94923000	-1.97793100
H	-2.05406500	7.94449700	-1.40012600
N	-1.15693200	0.89816600	-5.61623300
C	-1.75426500	2.14911300	-3.64042500
C	-1.45404300	3.24291400	-2.82569300
C	-0.28369700	0.71942100	-6.76839100
H	0.57117500	1.41375700	-6.72820000
C	-0.91548900	1.85403500	-4.81283300
H	-0.05947500	2.52840000	-4.95902600
C	-0.27507900	0.71534300	-9.32050600
H	-0.89762700	0.88637700	-10.20409500
H	0.55936300	1.42506200	-9.38175900
C	-1.09046900	0.99066400	-8.05221600
H	-1.98549500	0.35750100	-8.04007600
H	-1.43799400	2.02813500	-8.03350800
N	-5.62849300	1.09467200	-0.95513200
C	-3.67512700	1.66722200	-2.22314900
C	-2.87108000	1.36858900	-3.31967000
C	-6.79831800	0.25544300	-0.72894700
H	-6.76819600	-0.62034900	-1.39377600
C	-4.84112700	0.83780000	-1.93050000
H	-5.01351500	-0.01630500	-2.59496700
C	-9.34393500	0.25909500	-0.72141600
H	-10.22521900	0.88090700	-0.90384900
H	-9.40902100	-0.58963200	-1.41312700
C	-8.07486700	1.06593400	-1.02037500
H	-8.05803100	1.97643500	-0.41012100
H	-8.05598900	1.38416800	-2.06659400
N	-5.62849300	-1.09467200	0.95513200
C	-3.67512700	-1.66722200	2.22314900
C	-2.87108000	-1.36858900	3.31967000
C	-6.79831800	-0.25544300	0.72894700
H	-6.76819600	0.62034900	1.39377600
C	-4.84112700	-0.83780000	1.93050000
H	-5.01351500	0.01630500	2.59496700
C	-9.34393500	-0.25909500	0.72141600
H	-10.22521900	-0.88090700	0.90384900
H	-9.40902100	0.58963200	1.41312700
C	-8.07486700	-1.06593400	1.02037500
H	-8.05803100	-1.97643500	0.41012100
H	-8.05598900	-1.38416800	2.06659400
H	4.86901600	-2.43949600	-0.32008200
H	4.86901600	2.43949600	0.32008200

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H	-4.86901600	2.43949600	-0.32008200
H	-4.86901600	-2.43949600	0.32008200
H	3.11224400	-0.51782200	-3.94660900
H	0.59647100	-3.86811600	-3.04793900
H	-0.59647100	-3.86811600	3.04793900
H	-3.11224400	-0.51782200	3.94660900
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H	-0.59647100	3.86811600	-3.04793900
H	-3.11224400	0.51782200	-3.94660900
N	5.51187000	-0.00599200	-1.80336100
C	3.63755200	-1.42644700	-2.29606200
C	2.64291100	-1.76437800	-3.21409200
C	6.43116400	1.06180600	-2.19219400
H	6.09099200	1.52782300	-3.12790500
C	4.54908300	-0.32345700	-2.59091600
H	4.38458500	0.20807200	-3.53666100
N	5.06106800	2.68359400	-0.95824700
C	3.17315400	3.16738600	0.46943600
C	2.66359200	3.12998300	1.77231700
C	6.42050600	2.17020300	-1.09023300
H	6.76768700	1.70693800	-0.15297100
C	4.51131500	2.62615500	0.19300000
H	5.02658500	2.18334300	1.05900200
N	0.61493900	-2.64699600	-5.10038900
C	1.78131800	-2.84863500	-2.99390300
C	1.93851400	-3.59545000	-1.82068300
C	-0.37901000	-3.17859300	-6.02805000
H	-0.93697500	-4.01625400	-5.58045900
C	0.76675300	-3.24406000	-3.98202900
H	0.15586500	-4.11663800	-3.70375000
N	2.41112400	-5.17267900	0.55639600
C	2.92231300	-3.29672100	-0.87138000
C	3.78170400	-2.19818400	-1.10468100
C	2.74328600	-5.95881200	1.74148000
H	3.53049100	-5.46996300	2.33685200
C	3.11308400	-4.12972400	0.32671800
H	3.91754100	-3.81460300	1.00179700
O	4.73135000	-1.90774400	-0.20533400
N	1.07253300	-4.71798100	3.05249500
C	-0.66195900	-3.04735600	3.18588000
C	-2.01373100	-2.73365500	2.91452200
C	1.47506700	-6.06294300	2.65031700
H	0.68821600	-6.55474400	2.05692100
C	-0.11920500	-4.35155600	2.77259100
H	-0.81224600	-5.00434700	2.22889300
O	-2.76876400	-3.61774600	2.24859300
N	1.61552500	3.20098900	4.45754400
C	1.41825800	3.67546700	2.10333300
C	0.64729700	4.27914500	1.08319900
C	1.06745800	3.32231700	5.80521000
H	0.05505800	3.75592400	5.78945700

C	0.92873300	3.67850200	3.49163700
H	-0.05243600	4.14113800	3.65134800
N	-0.72522700	5.56756700	-1.09623400
C	1.15101800	4.32690700	-0.25126300
C	2.39918800	3.77110000	-0.53205000
C	-1.38992600	6.27813000	-2.18698200
H	-0.84736700	6.11477700	-3.12885400
C	0.40178900	4.99328600	-1.31406500
H	0.86455200	4.99955800	-2.30903800
N	0.02341300	1.10595000	5.61552100
C	-0.39917500	-0.89811400	4.33463600
C	0.11628000	-2.12024200	3.88785000
C	0.94597800	1.89278500	6.42833300
H	1.95544700	1.45209900	6.42908100
C	0.45186400	0.01250900	5.11495400
H	1.48859600	-0.32630200	5.26388700
N	-2.71549300	4.27245700	-2.68796800
C	-3.34799300	2.00025800	-2.18665700
C	-4.10891600	1.14933200	-1.35234300
C	-2.82697700	5.69305400	-2.36998100
H	-3.36851700	5.85100300	-1.42376200
C	-3.33151000	3.44860800	-1.92925800
H	-3.90359700	3.78358000	-1.05599100
O	-4.77295300	1.67503400	-0.31448500
N	-2.09006000	-1.66839700	-5.11413100
C	-2.71212000	0.07530900	-3.56366000
C	-2.66303100	1.44318400	-3.27251900
C	-1.41818100	-2.05452700	-6.35082200
H	-0.85930000	-1.21000700	-6.78413200
C	-2.01942000	-0.44655400	-4.75130400
H	-1.45181100	0.29841600	-5.32972200
N	-5.69356600	-0.71571800	0.16434100
C	-4.17102500	-0.24805800	-1.63422500
C	-3.47291700	-0.75657700	-2.72989500
C	-6.55108600	-1.64977600	0.89100200
H	-6.37859000	-2.67593400	0.53638100
C	-4.99334600	-1.14258400	-0.82362100
H	-5.00159900	-2.19998900	-1.11656900
N	-4.76538300	-1.97024900	2.54666800
C	-2.55693300	-1.49256900	3.36264500
C	-1.74153400	-0.60068500	4.06017900
C	-6.17386200	-1.60883600	2.40543500
H	-6.33920800	-0.58185400	2.76122100
C	-3.96254000	-1.16303400	3.14037600
H	-4.30558900	-0.19478600	3.52614800
H	5.25563000	-1.12616100	-0.56936500
H	-5.27741800	0.92236400	0.12754900
H	-3.69656600	-3.22835500	2.18702600
H	2.53775500	-1.18800400	-4.12884500
H	1.29617500	-4.45062800	-1.62966300
H	1.14927500	-2.38348300	4.09736000
H	-2.15283300	0.34097100	4.41244300

H	3.24650700	2.68164800	2.57201600
H	-2.09303500	2.11492500	-3.90828600
H	-3.52714300	-1.81747100	-2.95675400
O	-0.54318100	4.81100600	1.39033400
H	-0.91221700	5.22011000	0.54512100
H	2.79219700	3.81679400	-1.54365400
C	-2.46199900	-2.51765900	-7.35965300
C	-2.45872300	-2.01103600	-8.66481200
C	-3.44357700	-3.45388700	-7.00259600
C	-3.40714800	-2.43585400	-9.59877300
H	-1.70743700	-1.28001500	-8.95341700
C	-4.39216600	-3.87974100	-7.93341500
H	-3.47124900	-3.83697400	-5.98690800
C	-4.37645800	-3.37300600	-9.23609400
H	-3.38931500	-2.03106400	-10.60728200
H	-5.14665200	-4.60524700	-7.64048200
H	-5.11648900	-3.70295300	-9.96024800
C	0.32748500	-3.67719700	-7.28224700
C	0.06583200	-4.95950000	-7.77948600
C	1.25068300	-2.86724300	-7.96008600
C	0.70163200	-5.42215200	-8.93452100
H	-0.64201800	-5.60111900	-7.26046000
C	1.88708900	-3.32681900	-9.11387900
H	1.48009300	-1.87887800	-7.57302000
C	1.61341100	-4.60605400	-9.60657900
H	0.48569900	-6.42070500	-9.30532900
H	2.59997800	-2.68674100	-9.62721800
H	2.11054600	-4.96422000	-10.50405500
C	3.24350500	-7.32976900	1.30418200
C	4.44515000	-7.83938300	1.81076800
C	2.51762000	-8.10283300	0.38585300
C	4.90931000	-9.09781700	1.41934200
H	5.02197700	-7.24805500	2.51764800
C	2.97901000	-9.36001400	-0.00675600
H	1.59592700	-7.70994900	-0.03299800
C	4.17645900	-9.86298700	0.51018900
H	5.84459000	-9.47676100	1.82296500
H	2.40496400	-9.94621800	-0.71966500
H	4.53659200	-10.84116500	0.20295600
C	1.73856100	-6.89771500	3.89736400
C	1.16463700	-8.16749800	4.03374800
C	2.55471200	-6.41252000	4.92995300
C	1.40768600	-8.94336400	5.17003100
H	0.52417600	-8.55332600	3.24440600
C	2.79835400	-7.18512500	6.06626200
H	2.98750900	-5.42003400	4.84716700
C	2.22679500	-8.45480100	6.18969600
H	0.95354800	-9.92684200	5.25825200
H	3.43262100	-6.79432700	6.85771500
H	2.41533200	-9.05566900	7.07531300
C	-7.03245200	-2.55820600	3.23165500
C	-7.97064800	-2.04761700	4.13657900

C	-6.90296000	-3.94890200	3.10451300
C	-8.77101700	-2.90569400	4.89462000
H	-8.07807000	-0.97165900	4.24827100
C	-7.70059000	-4.80760100	3.86188400
H	-6.16993400	-4.36452900	2.41892400
C	-8.63856500	-4.28876400	4.75877700
H	-9.49412000	-2.49158100	5.59203300
H	-7.58762400	-5.88289100	3.75298900
H	-9.25830100	-4.95824900	5.34894400
C	-8.01167500	-1.28768800	0.65295700
C	-8.90682500	-2.25578000	0.18290900
C	-8.48339800	0.01164000	0.89047200
C	-10.24942000	-1.93816000	-0.03738600
H	-8.55242100	-3.26500300	-0.01128500
C	-9.82365200	0.33106000	0.66964300
H	-7.80061800	0.78070400	1.24044700
C	-10.71169100	-0.64369000	0.20630000
H	-10.93067400	-2.70207400	-0.40219400
H	-10.17393800	1.34246500	0.85730400
H	-11.75494800	-0.39406300	0.03345300
C	7.36072200	3.31567700	-1.44563100
C	8.55982600	3.49190300	-0.74496900
C	7.04328100	4.21128900	-2.47724900
C	9.43088200	4.53428300	-1.07198300
H	8.81494400	2.80835300	0.06101500
C	7.91164600	5.25319900	-2.80542300
H	6.10541000	4.09854300	-3.01279300
C	9.10991000	5.41741800	-2.10466600
H	10.35722500	4.65637200	-0.51691800
H	7.65100600	5.93962400	-3.60679200
H	9.78507800	6.22996800	-2.35911200
C	7.81926600	0.47466600	-2.41262500
C	8.48529900	0.68336100	-3.62612200
C	8.45051900	-0.28687900	-1.41806300
C	9.75970600	0.15276000	-3.84132500
H	8.00487600	1.26609600	-4.40805000
C	9.72268200	-0.81911500	-1.63135700
H	7.94355900	-0.47264800	-0.47528800
C	10.38248400	-0.59949900	-2.84382800
H	10.26209800	0.32548200	-4.78931700
H	10.19799800	-1.40741500	-0.85102300
H	11.37269200	-1.01490600	-3.00995600
C	-1.40413700	7.77063700	-1.88266900
C	-0.91802000	8.68301500	-2.82668500
C	-1.89618500	8.25854400	-0.66313600
C	-0.92921300	10.05525700	-2.56512500
H	-0.52923200	8.31796800	-3.77400700
C	-1.90660800	9.62874800	-0.39900500
H	-2.26444100	7.56549500	0.08797200
C	-1.42417400	10.53224000	-1.35003800
H	-0.54802700	10.74874700	-3.30988800
H	-2.29008400	9.99080200	0.55119500

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H	-1.43133900	11.59892300	-1.14319300
C	-3.58211400	6.40180600	-3.48761300
C	-4.65200700	7.25348400	-3.18794400
C	-3.22395600	6.21432400	-4.83076000
C	-5.34484100	7.91473600	-4.20517900
H	-4.94477100	7.40179500	-2.15152000
C	-3.91511200	6.87315800	-5.84848200
H	-2.41069400	5.53865000	-5.07852200
C	-4.97734300	7.72740300	-5.53899000
H	-6.17298400	8.57209100	-3.95387000
H	-3.62603000	6.71699600	-6.88449900
H	-5.51628300	8.23889600	-6.33192000
C	0.43207800	1.93926800	7.86202900
C	1.28778800	1.64796300	8.93115700
C	-0.90227100	2.27234300	8.13809400
C	0.82686000	1.69660900	10.24931900
H	2.32295100	1.38214400	8.73151500
C	-1.36510200	2.32163500	9.45372900
H	-1.58177600	2.47924000	7.31671200
C	-0.50138800	2.03504000	10.51475600
H	1.50557700	1.46646300	11.06639500
H	-2.40216200	2.58072300	9.65074600
H	-0.86260700	2.07131800	11.53901800
C	1.97414200	4.22916200	6.62762300
C	1.43559300	5.29921200	7.35224900
C	3.36008300	4.01638900	6.66964000
C	2.25880600	6.13390400	8.11242500
H	0.36401800	5.48075800	7.32272000
C	4.18451900	4.84872600	7.42785200
H	3.79368000	3.20445100	6.09342500
C	3.63630400	5.91015900	8.15374300
H	1.82279300	6.95984700	8.66826800
H	5.25655900	4.67072100	7.44928400
H	4.27867800	6.55937000	8.74263300
N	4.02054400	1.03747700	-3.95504600
C	3.39845700	-0.95315800	-2.76340400
C	2.72849600	-2.17576000	-2.80846300
C	4.01932900	1.84092200	-5.17612300
H	3.33312100	1.40264200	-5.91460900
C	3.37530500	-0.07171000	-3.92879200
H	2.79615300	-0.41779900	-4.79409600
N	2.12233200	3.14715800	-4.33349400
C	0.51842200	3.63002100	-2.59353300
C	0.29602400	4.24775200	-1.35753500
C	3.48543800	3.27049400	-4.83978700
H	4.15884300	3.70299900	-4.08254100
C	1.86499000	3.63708600	-3.18256900
H	2.64323300	4.11815300	-2.57057300
N	1.49290400	-4.80706200	-2.82495100
C	2.76871300	-3.07248400	-1.73062200
C	3.49984400	-2.71300400	-0.59295000
C	0.94181500	-6.15767700	-2.79000900

H	1.05242300	-6.61254400	-1.79267700
C	2.11164200	-4.38601100	-1.79038400
H	2.21042800	-5.00194700	-0.88348400
N	5.12956500	-1.96506300	1.66818400
C	4.18989800	-1.49914600	-0.50173100
C	4.14013700	-0.60384900	-1.59509300
C	6.00478600	-1.55307600	2.76112400
H	6.37567300	-0.52631400	2.61399700
C	4.99744600	-1.16345400	0.68143200
H	5.50018300	-0.18945300	0.65541000
O	4.80423000	0.55664000	-1.52094600
N	4.06538500	-0.62969900	3.96318300
C	1.71390400	-0.15467300	4.09952800
C	0.43930300	-0.65594600	4.36442800
C	5.18173200	-1.56488600	4.08945000
H	4.80269200	-2.58712900	4.23015400
C	2.86663500	-1.05137800	4.14471900
H	2.65793800	-2.10581300	4.36581500
N	-0.25618800	5.61784500	1.12322000
C	-0.97345600	4.31258300	-0.77274300
C	-2.06642200	3.72694600	-1.45263800
C	-0.60833200	6.33759200	2.34421800
H	-1.66557600	6.17993400	2.60972100
C	-1.19597700	5.01520100	0.50140000
H	-2.22712000	5.01181100	0.87412600
N	-4.18482500	2.58042000	-3.03045500
C	-1.85869300	3.09313800	-2.71427700
C	-0.57486500	3.05604100	-3.25832700
C	-5.26804600	2.05478800	-3.85955400
H	-4.85447400	1.56744400	-4.75373500
C	-2.97777900	2.52660600	-3.46378100
H	-2.73712900	2.07000900	-4.43214600
N	-0.04990900	4.36048900	3.69588700
C	0.74942000	2.09089100	3.84360000
C	1.87707700	1.23782600	3.83383600
C	0.25218500	5.77875600	3.52445200
H	1.30983200	5.93256300	3.25811300
C	0.92343800	3.53572400	3.62314900
H	1.94809900	3.86653300	3.41618600
N	-5.10949800	-0.11188300	-2.71563600
C	-4.11942800	-1.51861500	-1.01816900
C	-4.08013200	-1.83687400	0.34402800
C	-6.03881500	0.96234200	-3.05120900
H	-6.43899800	1.44493600	-2.14521700
C	-4.96762700	-0.41200900	-1.48239900
H	-5.50206700	0.13297100	-0.68922400
N	-1.23229500	-5.25340000	-2.07628600
C	-2.61814800	-3.38953000	-1.46341600
C	-3.37804300	-2.30793900	-1.90918500
C	-0.58826500	-6.07696000	-3.09783800
H	-0.69667400	-5.60569900	-4.08510800
C	-1.89959200	-4.21591400	-2.43089600

H	-1.97742900	-3.91749000	-3.48393400
N	-4.06690500	-2.62945200	3.11674600
C	-3.33512200	-2.91281300	0.83861900
C	-2.59195600	-3.70034900	-0.07068500
C	-4.05677500	-3.09984800	4.49858100
H	-3.33383200	-3.91906500	4.63848900
C	-3.35191300	-3.26306400	2.26829600
H	-2.73036800	-4.11855600	2.55806600
N	-2.23939800	-1.54491400	5.05057700
C	-0.68772400	0.17833700	4.37657200
C	-0.50925600	1.54064500	4.11083900
C	-3.59950700	-1.92261700	5.42182900
H	-4.30498200	-1.09166900	5.26213500
C	-2.02560600	-0.33367600	4.70879900
H	-2.83675900	0.40954200	4.66883700
H	4.67623500	1.02823200	-2.40435800
H	2.17340200	-2.45151100	-3.70058200
H	3.55957000	-3.39203600	0.25297100
H	-1.36161600	2.21419900	4.12451700
H	1.12103200	4.71221200	-0.82474400
H	-3.41148900	-2.07554900	-2.96977000
O	3.08782800	1.75570300	3.58665300
H	3.75351500	1.00115900	3.66037000
H	0.31175100	-1.71278000	4.58056500
H	-0.41410000	2.58583900	-4.22424200
O	-3.28722200	3.78861700	-0.90476200
H	-3.92558100	3.35179600	-1.55284200
O	-1.88245200	-4.73827800	0.39139800
H	-1.45914600	-5.18706100	-0.40738300
H	-4.65374700	-1.25047400	1.05626900
C	-7.20188800	0.38819000	-3.85124100
C	-8.52223100	0.67648800	-3.48630500
C	-6.97312000	-0.43859500	-4.96104700
C	-9.59433800	0.15996000	-4.21830300
H	-8.71408900	1.30970600	-2.62367100
C	-8.04236900	-0.95529200	-5.69385400
H	-5.95399300	-0.68889000	-5.24065300
C	-9.35736800	-0.65633300	-5.32585600
H	-10.61288900	0.39361400	-3.91985100
H	-7.84891300	-1.59481200	-6.55111200
H	-10.18970500	-1.06054800	-5.89563100
C	-6.16968600	3.20103300	-4.29846800
C	-6.45511900	3.38713500	-5.65639300
C	-6.72380700	4.08866200	-3.36440100
C	-7.28442300	4.43030200	-6.07539900
H	-6.02706200	2.71058600	-6.39185400
C	-7.55125600	5.13238200	-3.78086600
H	-6.50161200	3.97047500	-2.30760700
C	-7.83576400	5.30588300	-5.13821800
H	-7.49530600	4.55897600	-7.13364400
H	-7.97215400	5.81201500	-3.04470400
H	-8.47906500	6.11952900	-5.46194000

C	-5.44574100	-3.60869700	4.86265900
C	-5.60251100	-4.86240700	5.46595100
C	-6.58877900	-2.83845700	4.60203000
C	-6.87045400	-5.33483800	5.81402300
H	-4.72576300	-5.47315300	5.66697200
C	-7.85653500	-3.30839900	4.94809100
H	-6.48319200	-1.87447500	4.11330800
C	-8.00181600	-4.55801900	5.55756100
H	-6.97243700	-6.31060500	6.28170400
H	-8.73236900	-2.69957300	4.73912400
H	-8.98923600	-4.92419500	5.82556300
C	-3.62647800	-2.30816700	6.89545000
C	-4.60368500	-1.77845900	7.74676100
C	-2.67830100	-3.19448500	7.42746100
C	-4.64200800	-2.13090900	9.09819800
H	-5.34154600	-1.08598800	7.34921000
C	-2.71379500	-3.54744800	8.77725600
H	-1.90213800	-3.59623600	6.78300200
C	-3.69708200	-3.01776900	9.61779400
H	-5.40784600	-1.70880700	9.74362200
H	-1.97084100	-4.23450800	9.17404200
H	-3.72321400	-3.29132600	10.66916500
C	-0.37705600	7.82766000	2.12688500
C	-1.38642300	8.75122200	2.42399700
C	0.84300100	8.30213900	1.62238400
C	-1.18183400	10.12027000	2.23318400
H	-2.33966800	8.39750600	2.80915700
C	1.04976100	9.66885500	1.43045200
H	1.62759800	7.59576700	1.36769300
C	0.03805700	10.58352700	1.73684600
H	-1.97727100	10.82210400	2.46966700
H	2.00080900	10.02005500	1.03854700
H	0.19884100	11.64759600	1.58583200
C	-0.03224000	6.51003100	4.83054600
C	0.92530400	7.36900800	5.38337000
C	-1.24961900	6.33487900	5.50517600
C	0.67226900	8.04820100	6.57791200
H	1.87606500	7.50867500	4.87485000
C	-1.50449200	7.01121300	6.69905100
H	-1.99264700	5.65464100	5.09981100
C	-0.54469100	7.87211500	7.23910200
H	1.42795500	8.71073800	6.99167700
H	-2.45247400	6.86374800	7.20995000
H	-0.74304400	8.39743000	8.16948900
C	5.42390000	1.86296200	-5.76499300
C	5.62870800	1.49943800	-7.10134300
C	6.53132800	2.23643600	-4.98940100
C	6.91016000	1.51616600	-7.65739100
H	4.77990600	1.20215900	-7.71207700
C	7.81257500	2.25198800	-5.54228000
H	6.39440000	2.50811000	-3.94649100
C	8.00613600	1.89288500	-6.87910500

H	7.05021200	1.23105500	-8.69662600
H	8.66052100	2.54264700	-4.92789600
H	9.00414000	1.90374200	-7.30864700
C	3.48789900	4.17405700	-6.06668200
C	4.40993300	5.22236000	-6.17125600
C	2.56778200	3.97801700	-7.10699600
C	4.42185500	6.05346100	-7.29425800
H	5.12387700	5.39054400	-5.36880100
C	2.57757200	4.80723900	-8.22941600
H	1.83207700	3.18317600	-7.02802600
C	3.50598000	5.84754100	-8.32769800
H	5.14412400	6.86302700	-7.35771900
H	1.85728200	4.64312800	-9.02662600
H	3.51192100	6.49430600	-9.20090000
C	1.67395200	-7.02616500	-3.80599700
C	2.15647100	-8.28861100	-3.44068800
C	1.87978100	-6.57862800	-5.11926300
C	2.82243900	-9.09409900	-4.36787300
H	2.00918400	-8.64543500	-2.42440900
C	2.54532900	-7.38125100	-6.04682600
H	1.53068200	-5.59191700	-5.40835600
C	3.01769700	-8.64310600	-5.67470500
H	3.19077900	-10.07110100	-4.06639800
H	2.69832000	-7.01972500	-7.06033600
H	3.53736600	-9.26709000	-6.39679600
C	-1.25094300	-7.44789400	-3.13235000
C	-1.74218700	-7.95903100	-4.33947800
C	-1.38796200	-8.21754000	-1.96763000
C	-2.34945000	-9.21627900	-4.38826100
H	-1.64854900	-7.37041900	-5.24858900
C	-1.99551000	-9.47301100	-2.01378800
H	-1.02644000	-7.83197300	-1.01846800
C	-2.47721100	-9.97738500	-3.22501700
H	-2.72452800	-9.59701000	-5.33444100
H	-2.09480200	-10.05680200	-1.10257500
H	-2.95133800	-10.95444600	-3.25986000
C	7.19829500	-2.49757200	2.83296400
C	8.50053000	-1.98833000	2.90150200
C	7.01639500	-3.88834200	2.82707400
C	9.60006600	-2.84731300	2.97374700
H	8.65630100	-0.91243000	2.89917200
C	8.11316600	-4.74820600	2.89865200
H	6.01276500	-4.29577400	2.75072800
C	9.40935100	-4.23036100	2.97396200
H	10.60395700	-2.43432800	3.02588400
H	7.95598000	-5.82361800	2.89231800
H	10.26328300	-4.90023300	3.02787200
C	6.02505500	-1.18259800	5.29899900
C	6.31289200	-2.13584000	6.28298100
C	6.52253900	0.11967700	5.45460300
C	7.08890100	-1.80168600	7.39559400
H	5.92888200	-3.14742700	6.17801100

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C	7.29677000	0.45599300	6.56582600
H	6.29755300	0.87749800	4.70937200
C	7.58383500	-0.50439300	7.53980600
H	7.30265200	-2.55497100	8.14910700
H	7.67413800	1.46954000	6.67210400
H	8.18567600	-0.24160600	8.40547900
N	-2.44697400	3.28873100	3.95416800
C	-1.22436300	1.22634800	4.09743500
C	-0.01195000	0.60993200	4.40779200
C	-2.51856800	4.73983700	4.11366000
H	-1.51823500	5.14773600	4.31693000
C	-1.33878800	2.68100100	4.17831700
H	-0.43184800	3.22917300	4.46290600
N	-2.05991800	5.03392400	1.72003500
C	-1.65001800	4.09654900	-0.46225500
C	-2.21583400	3.49498000	-1.61015300
C	-3.01406200	5.37001700	2.77232100
H	-4.00992700	4.94949700	2.56039500
C	-2.50677500	4.42770200	0.68723800
H	-3.56166700	4.14368600	0.59402500
N	2.41248300	-0.80875300	5.17040200
C	0.12727200	-0.78546600	4.38447400
C	-0.98587700	-1.55901200	4.03730700
C	3.58012200	-1.58580600	5.57591600
H	3.43356400	-2.66003200	5.38074800
C	1.38555500	-1.44677700	4.76035600
H	1.37698300	-2.54523900	4.68848800
N	-3.35638500	-3.09680600	3.44370700
C	-2.22362300	-0.98723200	3.72239800
C	-2.34959200	0.42092900	3.74783000
C	-4.59920600	-3.81800900	3.18561500
H	-5.40862100	-3.13136300	2.89079200
C	-3.39713900	-1.81949900	3.41474900
H	-4.31974400	-1.27517100	3.18106500
O	-3.53195400	0.97683400	3.45338700
N	-3.97887900	-4.03069500	0.81405900
C	-2.46006600	-3.61304400	-1.00032700
C	-1.27589800	-3.98617900	-1.63629100
C	-4.36605100	-4.80161200	1.99417600
H	-3.55126100	-5.47987500	2.28438400
C	-2.87237200	-4.29989300	0.22168000
H	-2.19702800	-5.07889200	0.59738300
N	-3.21251000	2.38024900	-4.07013000
C	-1.39441200	3.22404700	-2.74539200
C	-0.03983000	3.55418700	-2.70415200
C	-3.73154300	1.87834500	-5.34115200
H	-2.90379700	1.70107800	-6.04222900
C	-1.96267100	2.65270800	-3.96441300
H	-1.26861400	2.49055900	-4.79876200
N	2.73581600	4.40655300	-2.53351600
C	0.53487000	4.14792900	-1.57088700
C	-0.28539600	4.40602000	-0.46692100

C	4.10136100	4.90376700	-2.39802000
H	4.30073700	5.25659700	-1.37358100
C	1.94967100	4.54444900	-1.53656900
H	2.28685600	4.99836000	-0.59212100
N	-3.46441500	-0.42970600	-4.54047600
C	-2.87695100	-1.98333900	-2.79181400
C	-3.27565400	-2.59628900	-1.58121800
C	-4.43756100	0.50635500	-5.09605000
H	-5.26736200	0.68487500	-4.39410700
C	-3.74533600	-0.97474100	-3.41865100
H	-4.66641600	-0.73477100	-2.87435500
N	4.84730400	2.66112300	-1.71576200
C	4.37076700	0.35968300	-1.21716400
C	4.10815800	-0.91150200	-1.72828000
C	5.08924900	3.72758400	-2.68540800
H	4.88006900	3.36710500	-3.70258100
C	4.55555500	1.48289200	-2.13330100
H	4.45545200	1.26302900	-3.20371200
N	4.52835800	-1.39900300	3.31569900
C	4.37541700	-0.58220700	1.05259400
C	4.50462900	0.53306900	0.19296800
C	4.80808200	-1.12574700	4.72244500
H	4.94069200	-0.04718200	4.90253500
C	4.57294900	-0.41510300	2.50154900
H	4.78720400	0.60584200	2.83897200
N	3.69037100	-3.62779000	-2.67271000
C	3.97393100	-2.02556500	-0.88726000
C	4.10922600	-1.83683200	0.49280400
C	3.53639100	-5.01980000	-3.08337400
H	3.41248500	-5.68374000	-2.21315500
C	3.75071200	-3.37686200	-1.42241000
H	3.66445200	-4.17305100	-0.66705600
N	1.09196800	-4.76763200	-3.12632400
C	-0.86793400	-3.38612700	-2.83646900
C	-1.67937400	-2.39013000	-3.39107900
C	2.23753400	-5.14800600	-3.94681000
H	2.35346100	-4.47324900	-4.80971800
C	0.35036800	-3.81443500	-3.53998400
H	0.57049400	-3.27183000	-4.47226800
H	-3.42458100	1.97494200	3.55967300
H	0.84355100	1.21806000	4.68760300
H	-0.91197000	-2.64281100	4.02225500
H	-1.39598100	-1.91575200	-4.32648900
O	-4.42394200	-2.21874100	-1.00394200
H	-4.54426400	-2.79045200	-0.18118200
H	-0.65782700	-4.76869900	-1.20536900
H	0.12843600	4.87688300	0.42036500
H	4.01918300	-1.05115300	-2.80186000
O	-3.52222400	3.20048500	-1.61744300
H	-3.73491800	2.81592800	-2.52585800
H	0.58616600	3.36200500	-3.57081100
H	4.02499500	-2.68308800	1.16888900

O	4.76539700	1.73759200	0.71845400
H	4.85553300	2.38305600	-0.05180900
C	3.81775100	-1.38930900	7.06774000
C	4.01554100	-2.49497900	7.90359100
C	3.84332100	-0.10510900	7.63148600
C	4.24431500	-2.32533200	9.27145500
H	3.99233800	-3.49645200	7.48104700
C	4.07153900	0.06706200	8.99749700
H	3.66951000	0.75964600	6.99803400
C	4.27446600	-1.04288900	9.82258800
H	4.39528000	-3.19567900	9.90466300
H	4.08777100	1.06884300	9.41894400
H	4.45023400	-0.90846500	10.88652000
C	6.08746000	-1.84802300	5.12541200
C	7.10348700	-1.16157900	5.80137900
C	6.27463400	-3.20590700	4.82737500
C	8.27742200	-1.81625100	6.18258900
H	6.97505800	-0.10707200	6.03274100
C	7.44656100	-3.86208200	5.20667300
H	5.50410300	-3.74431100	4.28369600
C	8.45202200	-3.16969600	5.88750800
H	9.05518800	-1.26670000	6.70637200
H	7.57632900	-4.91441800	4.96750800
H	9.36517700	-3.68045700	6.18108000
C	6.54818200	4.15835300	-2.60858100
C	7.32602200	4.20830500	-3.77142700
C	7.13894400	4.50855000	-1.38560900
C	8.66404400	4.60645200	-3.71911000
H	6.88201400	3.93522900	-4.72543600
C	8.47583400	4.90502300	-1.33073500
H	6.55563500	4.46260500	-0.47028400
C	9.24298900	4.95645400	-2.49794200
H	9.25236400	4.63898000	-4.63221300
H	8.91928800	5.17179700	-0.37511800
H	10.28433100	5.26362200	-2.45418500
C	4.31346400	6.06419500	-3.36263600
C	4.88120700	7.26223600	-2.91303700
C	3.94329900	5.95643600	-4.71128600
C	5.08591600	8.32912500	-3.79159800
H	5.16700500	7.36124000	-1.86880300
C	4.14650600	7.02100600	-5.59051300
H	3.48102400	5.04069800	-5.06777500
C	4.72018800	8.21101800	-5.13381700
H	5.52746400	9.25199900	-3.42490800
H	3.85352700	6.92253900	-6.63251700
H	4.87642400	9.04039900	-5.81833000
C	-3.13573200	6.88539100	2.87615600
C	-4.39623300	7.49428300	2.89525500
C	-1.99323300	7.69565800	2.95129900
C	-4.51687200	8.88243600	2.99762100
H	-5.29017800	6.87897800	2.83084600
C	-2.11143100	9.08243400	3.05327100

H	-1.00936200	7.23754300	2.91547800
C	-3.37436800	9.68088400	3.07835100
H	-5.50356000	9.33784400	3.01068500
H	-1.21649900	9.69660000	3.10979200
H	-3.46612000	10.76089200	3.15579500
C	-3.43166200	5.07326400	5.28640900
C	-2.97552600	5.90652600	6.31468900
C	-4.73263300	4.55476400	5.36439600
C	-3.80189000	6.22535400	7.39500700
H	-1.96710300	6.31020600	6.26992500
C	-5.55926200	4.87063300	6.44345600
H	-5.09964600	3.89402400	4.58401000
C	-5.09695600	5.70849100	7.46217600
H	-3.43081600	6.87417400	8.18384700
H	-6.56448500	4.46026500	6.48956800
H	-5.74063700	5.95289700	8.30277300
C	-5.02346400	-4.55684900	4.44893700
C	-6.33192500	-4.43734700	4.93219900
C	-4.11544500	-5.36369800	5.15031300
C	-6.73152700	-5.11663500	6.08588100
H	-7.04382600	-3.80945100	4.40221600
C	-4.51228700	-6.04272400	6.30310200
H	-3.09120600	-5.44651900	4.79911700
C	-5.82288000	-5.92279700	6.77413800
H	-7.75127500	-5.01192400	6.44680200
H	-3.79672800	-6.66350200	6.83591700
H	-6.13116000	-6.45035600	7.67273500
C	-5.60334300	-5.63019600	1.67371500
C	-5.60954000	-7.00719400	1.92650300
C	-6.75030700	-5.03949400	1.12351600
C	-6.73918600	-7.77953800	1.64556100
H	-4.72558000	-7.47874300	2.34847400
C	-7.87935800	-5.80942100	0.84077600
H	-6.75946100	-3.97509700	0.90640300
C	-7.87813800	-7.18240800	1.10220800
H	-6.72588700	-8.84701400	1.84868600
H	-8.75992200	-5.33681100	0.41383600
H	-8.75710400	-7.78152300	0.88054400
C	2.03425100	-6.56789300	-4.46058300
C	2.23004200	-6.86622100	-5.81446200
C	1.64846500	-7.59982700	-3.59213900
C	2.05459900	-8.16735100	-6.29239100
H	2.52300000	-6.07500100	-6.50019200
C	1.47212500	-8.90020300	-4.06712700
H	1.47163100	-7.37727900	-2.54416900
C	1.67613000	-9.18917100	-5.41944900
H	2.21019000	-8.37965700	-7.34689800
H	1.17190000	-9.68822600	-3.38131200
H	1.53691000	-10.20141400	-5.78946800
C	4.77827000	-5.45171800	-3.85321200
C	5.42903300	-6.64928800	-3.53298500
C	5.29414600	-4.66084600	-4.89055400

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C	6.56436800	-7.05661900	-4.23829400
H	5.04378800	-7.26861500	-2.72664000
C	6.42833200	-5.06508900	-5.59614600
H	4.81238100	-3.71860300	-5.13387300
C	7.06698900	-6.26589000	-5.27343000
H	7.05642700	-7.98931400	-3.97519900
H	6.81606500	-4.44027400	-6.39660500
H	7.95119500	-6.57961000	-5.82176000
C	-4.67199200	2.91384100	-5.94434300
C	-4.47194600	3.36357300	-7.25487900
C	-5.74490700	3.43624400	-5.20732300
C	-5.33006000	4.30754600	-7.82436900
H	-3.64018700	2.97158900	-7.83497500
C	-6.60216200	4.38062900	-5.77355600
H	-5.90716500	3.11094400	-4.18356200
C	-6.39852000	4.81837400	-7.08521300
H	-5.16005200	4.64441500	-8.84346400
H	-7.42844400	4.77636700	-5.18906400
H	-7.06566400	5.55454200	-7.52523100
C	-5.00680200	-0.06767500	-6.38787100
C	-6.39100200	-0.11344000	-6.59208300
C	-4.15937500	-0.56171900	-7.39049800
C	-6.92114500	-0.63162500	-7.77632500
H	-7.05946200	0.25906100	-5.81991000
C	-4.68676400	-1.08017800	-8.57398100
H	-3.08455700	-0.55285800	-7.23528700
C	-6.07005700	-1.11531100	-8.77177900
H	-7.99835100	-0.65960400	-7.91754500
H	-4.01717500	-1.46003100	-9.34121900
H	-6.48038600	-1.52054000	-9.69278800
N	-5.00000000	-2.15077800	-1.82095400
C	-3.03919300	-3.18214400	-0.89176400
C	-2.44531500	-3.74500400	0.23853900
C	-6.37685600	-1.68256800	-1.67797000
H	-6.67959500	-1.71452500	-0.62153100
C	-4.39013100	-2.63487400	-0.79992400
H	-4.87008000	-2.67806400	0.18590800
N	-5.54651000	0.60369300	-1.32242700
C	-3.74278600	2.17917400	-1.13187800
C	-2.81052200	2.96737000	-1.80691300
C	-6.45296500	-0.19463800	-2.14488200
H	-6.13573600	-0.16225300	-3.19696500
C	-4.63803600	1.31024200	-1.89156400
H	-4.50956400	1.30747100	-2.98128100
N	-1.15108200	-5.07153900	2.48059300
C	-1.16927200	-4.32327800	0.18296400
C	-0.49207400	-4.32351800	-1.04188700
C	-0.46302500	-5.78833200	3.55013200
H	0.55368600	-6.08294500	3.24500400
C	-0.55663700	-4.96471200	1.35585600
H	0.45160300	-5.37528500	1.19211900
N	0.78972500	-4.41288600	-3.62683600

C	-1.04692600	-3.77376300	-2.20279600
C	-2.33373900	-3.19224400	-2.13211800
C	1.36981700	-4.46470900	-4.96592900
H	0.76242300	-3.89589100	-5.68753800
C	-0.34072200	-3.83247400	-3.49295300
H	-0.85669000	-3.36646300	-4.34070700
O	-2.87625000	-2.66931700	-3.24019000
N	2.62277100	-2.39382100	-4.54264400
C	3.22989600	-0.57999500	-3.06554800
C	4.02369800	-0.18420700	-1.98312800
C	2.78204400	-3.79419400	-4.92375700
H	3.38018100	-4.34558300	-4.18086900
C	3.25347300	-1.98056100	-3.51245100
H	3.88051800	-2.65436100	-2.90848700
N	-0.92073000	4.75647200	-3.09999300
C	-1.96342700	3.84861000	-1.11970400
C	-2.06902100	3.92206400	0.27376700
C	0.01236900	5.71076300	-3.69000100
H	0.60391800	6.22706900	-2.91715400
C	-1.01409100	4.71989500	-1.82704800
H	-0.39895900	5.36518300	-1.18154800
N	-2.42021500	4.11260100	3.13031300
C	-2.98961700	3.15339200	0.99455200
C	-3.83754300	2.26866300	0.28926400
C	-2.67989200	4.20719000	4.56378800
H	-3.39585700	3.43812100	4.89458400
C	-3.12055100	3.28435300	2.45429500
H	-3.87423600	2.64267400	2.92577200
N	1.75186500	3.97280500	-3.77129800
C	2.49153800	1.73157600	-3.32334800
C	2.46812000	0.39556700	-3.72477800
C	1.01628800	4.92803300	-4.59702700
H	0.42412500	4.39465300	-5.35418400
C	1.72167800	2.72460500	-4.06927400
H	1.13231700	2.35227500	-4.91672600
N	-0.85484400	2.61767400	5.00218400
C	0.88916500	1.16092000	4.22216600
C	2.19665800	1.06284700	3.74582300
C	-1.34122600	3.95670300	5.32910400
H	-0.62171700	4.71335200	4.98571600
C	0.32144400	2.47658000	4.50823400
H	0.96312900	3.34228000	4.30089600
N	0.49428800	-3.68441300	4.38613600
C	0.73305100	-1.29145900	4.22351100
C	0.14175900	-0.03008500	4.46588100
C	-0.31680000	-4.83256200	4.77990500
H	-1.33277500	-4.52390000	5.07291400
C	-0.01689100	-2.52154200	4.52533500
H	-1.03633200	-2.37818500	4.90265700
N	4.95837600	0.71441800	2.90574400
C	2.79550300	-0.18138800	3.50145700
C	2.04630800	-1.33843600	3.74252900

C	6.34292700	0.46910500	2.51399500
H	6.51816400	-0.59923900	2.31015500
C	4.19081500	-0.29513900	3.05170800
H	4.54377800	-1.32212500	2.87118400
N	5.74881900	0.72279200	0.14416700
C	4.08394300	1.14373700	-1.54654600
C	3.30804200	2.11641200	-2.21795100
C	6.62857900	1.24483000	1.18583200
H	6.42726900	2.30951800	1.38407100
C	4.96971400	1.54816300	-0.44273000
H	4.93840800	2.60946500	-0.16925700
H	-3.79725400	-2.34181800	-2.99399700
H	-2.98376100	-3.75005700	1.18193200
H	0.49305900	-4.77497400	-1.11904300
H	4.63445800	-0.91504000	-1.46047700
H	2.77377700	1.96633000	3.57085800
H	-1.43442800	4.60435500	0.83237900
H	2.48684100	-2.31707800	3.57371800
O	-1.11246600	0.02567900	4.93382700
H	-1.33387600	1.00004100	5.07289800
O	3.36321600	3.39179200	-1.81130700
H	2.77486300	3.92642400	-2.43285000
O	-4.72832400	1.53547700	0.96954400
H	-5.25383400	1.00360000	0.29306900
H	-2.74408900	2.91195400	-2.88967000
H	1.85864500	0.10092700	-4.57438600
C	1.43860000	-5.91596600	-5.42410300
C	0.94288300	-6.28400500	-6.68069000
C	1.99282100	-6.90810500	-4.60172200
C	1.00707200	-7.61057600	-7.11452700
H	0.50466600	-5.52682100	-7.32617200
C	2.05734100	-8.23411000	-5.03231200
H	2.36227500	-6.64103300	-3.61614700
C	1.56573300	-8.59017900	-6.29148600
H	0.61707200	-7.87687100	-8.09341100
H	2.48922800	-8.99094600	-4.38261200
H	1.61451200	-9.62309600	-6.62554300
C	3.49033000	-3.86672500	-6.27082000
C	4.59997200	-4.70324800	-6.44130800
C	3.05050700	-3.10049700	-7.36052600
C	5.25231200	-4.78358000	-7.67425900
H	4.95569800	-5.29804600	-5.60364300
C	3.70076300	-3.17829800	-8.59292300
H	2.20440400	-2.43114100	-7.23674400
C	4.80362900	-4.02179300	-8.75478900
H	6.11233800	-5.43840900	-7.78732100
H	3.34783200	-2.57752500	-9.42714800
H	5.31072300	-4.08089200	-9.71409500
C	-0.76796900	6.75229200	-4.48239700
C	-0.51283400	8.11654100	-4.29939100
C	-1.75484000	6.36688900	-5.40158600
C	-1.21917000	9.07872000	-5.02553900

H	0.24425000	8.42890200	-3.58440200
C	-2.46160100	7.32622400	-6.12794800
H	-1.97865900	5.31268500	-5.53510700
C	-2.19502800	8.68596200	-5.94354800
H	-1.00836000	10.13344800	-4.86999900
H	-3.22406100	7.01210500	-6.83595700
H	-2.74721100	9.43257000	-6.50790600
C	2.00328300	5.84835500	-5.30364100
C	1.93476900	6.01675700	-6.69174100
C	2.99325600	6.53785000	-4.58815500
C	2.82771800	6.86333900	-7.35328000
H	1.17611700	5.48409200	-7.25960100
C	3.88728300	7.38282400	-5.24709200
H	3.07280400	6.40832600	-3.51248900
C	3.80642500	7.54983700	-6.63237700
H	2.75902900	6.98215300	-8.43127600
H	4.64901600	7.90928600	-4.67825700
H	4.50344800	8.20705600	-7.14507700
C	-3.26086200	5.58050400	4.87798200
C	-4.42729900	5.69608900	5.64337200
C	-2.64577700	6.74861800	4.40378300
C	-4.96558200	6.95103100	5.93915300
H	-4.91830100	4.79874400	6.01165600
C	-3.18199100	8.00299900	4.69761000
H	-1.75277300	6.67274700	3.79054300
C	-4.34375400	8.10869300	5.46766000
H	-5.87205400	7.02168700	6.53447700
H	-2.69420600	8.89868700	4.32202400
H	-4.76216100	9.08554800	5.69461400
C	-1.50204200	4.08204200	6.83855900
C	-0.90870700	5.15128800	7.52027600
C	-2.23840100	3.13941200	7.57106000
C	-1.05404700	5.28501000	8.90323900
H	-0.33032500	5.88574600	6.96545300
C	-2.38312600	3.26990700	8.95292100
H	-2.69330800	2.29456200	7.06178600
C	-1.79246700	4.34446100	9.62368800
H	-0.58691400	6.12176400	9.41561800
H	-2.95579000	2.53050100	9.50638600
H	-1.90449800	4.44483700	10.69981300
C	-1.25151900	-7.04516100	3.89558800
C	-0.60648800	-8.28531600	3.97407700
C	-2.63208300	-6.98741500	4.13730300
C	-1.31904300	-9.44294500	4.29725400
H	0.46197200	-8.34604300	3.78245000
C	-3.34617400	-8.14216300	4.46022500
H	-3.14951000	-6.03599900	4.05744500
C	-2.69171000	-9.37457700	4.54283400
H	-0.80095600	-10.39673400	4.35294600
H	-4.41566200	-8.08040600	4.64411600
H	-3.24856000	-10.27379600	4.79226600
C	0.34391900	-5.52439700	5.96565300

C	-0.40225100	-5.83481700	7.10895300
C	1.70613200	-5.85817400	5.93872800
C	0.19316700	-6.47377500	8.19953700
H	-1.45747400	-5.57570000	7.14611300
C	2.30339800	-6.49599600	7.02685500
H	2.30144600	-5.60316000	5.06707900
C	1.54834700	-6.80748700	8.16128300
H	-0.40198200	-6.70635600	9.07871600
H	3.36025300	-6.74729200	6.99046900
H	2.01418600	-7.30246600	9.00916400
C	7.26799800	0.90796400	3.64203100
C	8.28280700	0.05649900	4.09549700
C	7.12203000	2.16466100	4.24787900
C	9.14158400	0.45218800	5.12414100
H	8.40341400	-0.92311000	3.63957000
C	7.97854900	2.56233400	5.27549100
H	6.32462300	2.82567100	3.92171900
C	8.99292700	1.70769100	5.71655300
H	9.92303500	-0.22272900	5.46337200
H	7.85162800	3.53919800	5.73491300
H	9.65833900	2.01672000	6.51820000
C	8.07629800	1.09828200	0.73518500
C	8.95089700	2.18960500	0.80205200
C	8.55927400	-0.12255100	0.24103500
C	10.28177800	2.06560600	0.39527500
H	8.58855400	3.14382600	1.17658600
C	9.88799900	-0.24895600	-0.16651900
H	7.88688100	-0.97164600	0.16292500
C	10.75497200	0.84482000	-0.08957800
H	10.94558700	2.92415100	0.45437400
H	10.24618300	-1.20172000	-0.54782500
H	11.78901600	0.74657300	-0.40893200
C	-7.86511500	0.36790600	-2.04261000
C	-8.58403500	0.66954800	-3.20528700
C	-8.46665700	0.59703500	-0.79658000
C	-9.88126800	1.18189900	-3.12870600
H	-8.12747200	0.50182700	-4.17742800
C	-9.76191000	1.11057800	-0.71812300
H	-7.91900200	0.38300100	0.11692800
C	-10.47422800	1.40336300	-1.88440500
H	-10.42481100	1.41043100	-4.04145900
H	-10.21398200	1.28400200	0.25470700
H	-11.48226300	1.80412700	-1.82263400
C	-7.30704500	-2.58251300	-2.48164600
C	-8.43049500	-3.15310000	-1.87177900
C	-7.05841400	-2.85819900	-3.83408000
C	-9.29552500	-3.97549900	-2.59763800
H	-8.63189800	-2.95209300	-0.82263400
C	-7.92060300	-3.68054500	-4.56043400
H	-6.18276100	-2.43774300	-4.32048400
C	-9.04332100	-4.24087700	-3.94480100
H	-10.16292300	-4.40985800	-2.10802000

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H	-7.71394500	-3.88562400	-5.60738600
H	-9.71351200	-4.88206800	-4.51073700
N	-1.47728700	-0.85277800	5.44421000
C	-2.10947300	0.82837600	3.83505200
C	-3.10928000	1.28774200	2.94689100
C	-1.81441500	-2.08276500	6.15571200
H	-2.73660900	-2.53427200	5.75705400
C	-2.30827400	-0.43136200	4.56950300
H	-3.23084500	-0.97703700	4.33837100
N	-0.55613000	-3.41362100	4.51564900
C	0.81596900	-3.53792200	2.53762500
C	2.10980300	-3.37432500	1.99099500
C	-0.66322400	-3.11928900	5.94169000
H	0.26175700	-2.66197900	6.32691900
C	0.57297300	-3.21207800	3.95249900
H	1.43121800	-2.80915000	4.50306400
N	-5.08352000	2.43552400	1.19175100
C	-2.94208700	2.53649700	2.27717300
C	-1.78898500	3.28707200	2.50675600
C	-6.10780100	3.04499200	0.34594000
H	-5.71945500	3.96654100	-0.11053300
C	-3.98019000	3.05996800	1.39226900
H	-3.77798300	4.03040800	0.92154000
N	0.59092200	4.81330400	3.16828200
C	-0.78810600	2.84253100	3.38254200
C	-0.96838800	1.61482300	4.02973700
C	1.78199600	5.55152400	3.57591900
H	2.42929400	4.94150600	4.22592600
C	0.40542900	3.65293700	3.66719100
H	1.12539700	3.20067900	4.36637000
N	3.04051800	4.65347500	1.66881700
C	3.12391500	3.25494800	-0.29757700
C	2.77700600	3.12468100	-1.64711300
C	2.61339700	5.89967000	2.29656200
H	1.95437700	6.48007400	1.63133900
C	2.69830600	4.44324300	0.45718300
H	2.08001200	5.16049500	-0.10407800
N	4.70079100	-3.21969000	0.74057500
C	2.35829500	-3.74551700	0.63578800
C	1.31634900	-4.26166800	-0.13502100
C	6.02528200	-3.20406600	0.12268700
H	5.94718500	-3.46084200	-0.94338400
C	3.69610500	-3.63899400	0.05979100
H	3.80555200	-3.95879400	-0.98422200
N	-0.90761600	-5.43334700	-1.59315700
C	0.02810600	-4.42607300	0.39324000
C	-0.19725800	-4.05757100	1.72456900
C	-2.04839700	-6.06528200	-2.24801900
H	-2.95107200	-6.01633500	-1.61828400
C	-1.06212900	-5.01724900	-0.39571300
H	-2.02700400	-5.10233300	0.12714300
N	5.69952100	-0.83836900	-0.45983400

C	4.36172500	1.15751500	-0.44980700
C	3.91850200	2.25749100	0.28524200
C	6.61013700	-1.75955000	0.21645900
H	6.68675400	-1.50138200	1.28241700
C	5.22771600	0.16701600	0.18454400
H	5.47427400	0.33642800	1.24023000
N	-2.67965300	-3.90248000	-3.24156400
C	-2.29861100	-1.54771300	-3.52802200
C	-1.54452600	-0.55782800	-4.15890200
C	-2.35863200	-5.29015300	-3.56925800
H	-1.45342600	-5.32903800	-4.19170700
C	-1.98639200	-2.95586500	-3.76239100
H	-1.13976300	-3.16616100	-4.42796600
N	-5.24383200	1.80349100	-1.58853400
C	-3.70938000	0.19952300	-2.53033200
C	-3.39671500	-1.16920700	-2.69897800
C	-6.45583800	2.06022900	-0.81636900
H	-6.84298500	1.13603500	-0.35852800
C	-4.87629900	0.58653000	-1.72240600
H	-5.42922500	-0.23891900	-1.25874800
N	-0.14811800	1.59769600	-5.52785000
C	-1.84134200	0.80334200	-3.99736700
C	-2.92103400	1.15585100	-3.18005600
C	0.48113700	2.72393600	-6.21113300
H	0.09013800	3.68527100	-5.84168000
C	-1.08597600	1.85140700	-4.69972000
H	-1.40390600	2.88292200	-4.48321300
N	2.21127500	2.86020100	-4.46732900
C	3.19862600	2.04114700	-2.42577100
C	3.99716600	1.04122000	-1.82444400
C	2.01521900	2.70187900	-5.90577700
H	2.40163400	1.73224800	-6.25759600
C	2.87380200	1.95277400	-3.85858300
H	3.26030900	1.06972100	-4.38108300
H	-1.66370900	4.24455800	2.00941200
H	2.17436900	3.88846700	-2.13054500
H	1.50457500	-4.55781700	-1.16300500
H	-3.18286200	2.20165000	-3.04612700
O	4.41068800	0.00261400	-2.56317700
H	4.98717700	-0.57302800	-1.96959900
H	4.20290800	2.35650500	1.32892900
O	3.08879800	-2.88422600	2.76309100
H	3.93093600	-2.88030600	2.20926900
H	-1.18155900	-4.18686200	2.16567800
O	-4.20884500	0.54561600	2.75867100
H	-4.80719900	1.05683900	2.12762500
H	-0.21601000	1.24943800	4.72313000
H	-0.71517000	-0.84116900	-4.80071700
O	-4.14851600	-2.09213800	-2.08497200
H	-3.78841700	-2.99551700	-2.35528300
C	-1.72392500	-7.52904600	-2.52070000
C	-2.62883100	-8.53347600	-2.15743000

C	-0.51735500	-7.89657400	-3.13411100
C	-2.34195300	-9.87762900	-2.40837900
H	-3.56513100	-8.26261400	-1.67599600
C	-0.22862500	-9.23851900	-3.38564900
H	0.20264200	-7.12859900	-3.40068100
C	-1.14082300	-10.23416100	-3.02439900
H	-3.05587700	-10.64409600	-2.11867700
H	0.71113900	-9.50749200	-3.86081000
H	-0.91461100	-11.27917200	-3.21832800
C	-3.51516900	-5.90561900	-4.34639600
C	-3.28009000	-6.52504200	-5.57964200
C	-4.82660400	-5.86426600	-3.85068000
C	-4.32891200	-7.10076200	-6.30088400
H	-2.26925200	-6.55952300	-5.97822200
C	-5.87605000	-6.43750900	-4.57005700
H	-5.03149400	-5.37479800	-2.90268700
C	-5.63031200	-7.05933600	-5.79747800
H	-4.12756600	-7.57773300	-7.25633200
H	-6.88670200	-6.39634100	-4.17275100
H	-6.44800300	-7.50441900	-6.35776700
C	-7.52672900	2.63413700	-1.73595400
C	-8.81696000	2.09077300	-1.74370900
C	-7.24144500	3.70833400	-2.59167900
C	-9.80665400	2.61286500	-2.58043100
H	-9.04999700	1.25358400	-1.09045700
C	-8.22841700	4.23143700	-3.42815200
H	-6.23886200	4.12497100	-2.61221700
C	-9.51545100	3.68610100	-3.42454100
H	-10.80251800	2.17778100	-2.57364900
H	-7.99145000	5.06350600	-4.08602000
H	-10.28310700	4.09242900	-4.07755200
C	-7.32338600	3.39308000	1.19501600
C	-7.85315500	4.68853200	1.16248000
C	-7.92939500	2.43641300	2.02255800
C	-8.97063600	5.02267200	1.93131000
H	-7.38953100	5.44106600	0.52962700
C	-9.04449800	2.76853100	2.79313400
H	-7.52311400	1.43019800	2.07353700
C	-9.57006100	4.06289400	2.74888800
H	-9.36835500	6.03324100	1.89290300
H	-9.50177500	2.01630900	3.43036200
H	-10.43760000	4.32108500	3.35004600
C	1.35904300	6.79918800	4.34093000
C	1.95696000	7.11203000	5.56760700
C	0.36787400	7.65424400	3.83679300
C	1.58347400	8.25846900	6.27350100
H	2.72235000	6.45485200	5.97297100
C	-0.00712200	8.80000000	4.53996700
H	-0.11959300	7.41101100	2.89745300
C	0.60064500	9.10724300	5.76069000
H	2.05845500	8.48452900	7.22457200
H	-0.77724000	9.45206900	4.13602000

H	0.30683100	9.99841100	6.30879100
C	3.84148500	6.74071000	2.62079200
C	3.88748300	8.09270100	2.25981000
C	4.94632600	6.18131300	3.27962000
C	5.00616900	8.87484400	2.55806100
H	3.04140600	8.53768400	1.74184900
C	6.06511400	6.96028200	3.57840000
H	4.93300800	5.12843100	3.54491900
C	6.09856100	8.31096200	3.21989400
H	5.02379800	9.92245500	2.26918800
H	6.91335000	6.51138400	4.08873400
H	6.97080900	8.91660200	3.45076700
C	2.75936900	3.81511100	-6.63239000
C	3.61971900	3.51371000	-7.69496600
C	2.60380800	5.15601900	-6.25089900
C	4.30323600	4.52747600	-8.37126000
H	3.75503700	2.47812400	-7.99719900
C	3.28537800	6.17048100	-6.92467200
H	1.95708900	5.40191700	-5.41393600
C	4.13687800	5.85986400	-7.98884600
H	4.96701700	4.27405000	-9.19369800
H	3.15425500	7.20447000	-6.61629900
H	4.66881300	6.64991600	-8.51207700
C	0.19814100	2.62454300	-7.70478200
C	-0.27653900	3.73705900	-8.40992100
C	0.40662900	1.42434800	-8.40025400
C	-0.52839900	3.65964200	-9.78202100
H	-0.44808500	4.67192400	-7.88205600
C	0.15558100	1.34432100	-9.77081000
H	0.75333100	0.54783200	-7.86098600
C	-0.31162000	2.46264000	-10.46726000
H	-0.89706700	4.53362600	-10.31256600
H	0.32181800	0.40684900	-10.29517700
H	-0.50879400	2.39940100	-11.53404700
C	7.99465800	-1.66265300	-0.41187400
C	9.11750100	-1.44434600	0.39504800
C	8.17127600	-1.78638500	-1.79763200
C	10.39364000	-1.35905200	-0.16684700
H	8.99394500	-1.34190000	1.47018100
C	9.44510400	-1.70016300	-2.36090400
H	7.31017700	-1.94130100	-2.44167800
C	10.56108800	-1.48733900	-1.54684000
H	11.25416800	-1.18924300	0.47457400
H	9.56554600	-1.79682600	-3.43653900
H	11.55251900	-1.41884400	-1.98606000
C	6.91860800	-4.23037600	0.80777200
C	7.58237300	-5.19987100	0.04689000
C	7.08739100	-4.23063100	2.20013500
C	8.40639000	-6.14673200	0.66010600
H	7.45558000	-5.21425000	-1.03266200
C	7.90903800	-5.17653100	2.81456500
H	6.56812400	-3.49592400	2.80912000

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C	8.57254100	-6.13711100	2.04615200
H	8.91423800	-6.89194900	0.05388700
H	8.02910000	-5.16463400	3.89451000
H	9.21121300	-6.87392500	2.52549000
C	-0.91743900	-4.41731600	6.69802300
C	-0.13568200	-4.75318300	7.80984600
C	-1.93158200	-5.29918900	6.29605600
C	-0.36623200	-5.93769500	8.51420000
H	0.65859800	-4.08246300	8.12826600
C	-2.16332000	-6.48327000	6.99729400
H	-2.53164200	-5.06189600	5.42258400
C	-1.38207400	-6.80623600	8.11054700
H	0.25089800	-6.18159800	9.37496400
H	-2.95269200	-7.15613700	6.67240100
H	-1.56155700	-7.72911400	8.65550200
C	-2.02651800	-1.76344200	7.63008800
C	-3.18042300	-2.20425800	8.28905700
C	-1.07913900	-1.02306900	8.35275100
C	-3.38248800	-1.92334700	9.64273200
H	-3.92587500	-2.77359300	7.73934500
C	-1.27866400	-0.74071800	9.70483300
H	-0.18984800	-0.65602500	7.84906700
C	-2.43089200	-1.19144700	10.35541600
H	-4.28461600	-2.27390000	10.13719000
H	-0.53516900	-0.16547400	10.25047400
H	-2.58663100	-0.96988600	11.40782100
N	-2.95799400	4.94744400	-0.15025900
C	-1.17466700	4.03373000	-1.50008600
C	-0.83685500	3.40163300	-2.70217600
C	-4.38285500	5.21885400	0.00892300
H	-4.97509200	4.73383400	-0.78339500
C	-2.58471800	4.31293100	-1.19387800
H	-3.30726600	3.95620100	-1.94379500
N	-4.62314100	3.17694900	1.36060100
C	-3.67501800	1.20212100	2.34582400
C	-2.91038700	0.67075100	3.38453900
C	-4.85324400	4.62009000	1.37421400
H	-4.24865100	5.09080000	2.16245300
C	-3.88702400	2.64590500	2.26827000
H	-3.40284900	3.25477200	3.04215500
N	-0.06641500	2.23044400	-5.22394900
C	0.49063700	3.15496800	-3.06902200
C	1.52436800	3.55289500	-2.19007800
C	0.38430100	1.68615900	-6.50160300
H	1.47479200	1.53102100	-6.50843400
C	0.82619700	2.53936600	-4.36340200
H	1.89444500	2.38402500	-4.55551800
O	2.79908700	3.32784400	-2.53458100
N	3.49416700	4.53228000	-0.33309400
C	1.19891500	4.19882500	-0.95991200
C	-0.13952600	4.42550300	-0.63891200
C	4.49409500	5.08586300	0.57846300

H	4.00515200	5.47223000	1.48400900
C	2.24792600	4.66814300	-0.05757200
H	1.91561000	5.16667100	0.86172700
N	4.68507000	2.90439300	1.69159700
C	4.07942600	0.57519200	1.84841100
C	4.26078600	-0.72373700	1.31972000
C	5.46251200	3.94365000	1.02278600
H	5.95186700	3.55636700	0.11506000
C	4.76375500	1.71753100	1.22339400
H	5.36879100	1.48397900	0.33940400
O	5.02501300	-0.88624400	0.23183500
N	-1.45536500	-0.56892200	5.57446700
C	-2.72410500	-0.71236100	3.52365800
C	-3.32564500	-1.56165500	2.58830400
C	-0.79063800	-1.25630100	6.67759700
H	-0.74546000	-2.34319500	6.50373600
C	-1.96652500	-1.28256600	4.64756700
H	-1.89124700	-2.38080300	4.65371400
N	-4.70044100	-3.25851100	0.69687800
C	-4.10370000	-1.07632700	1.53116800
C	-4.28091500	0.32052500	1.40116500
C	-5.46449000	-4.05969300	-0.25491200
H	-5.94090400	-3.42670200	-1.02024900
C	-4.77518900	-1.98684800	0.59086900
H	-5.36740600	-1.50608700	-0.19671200
O	-5.02917800	0.79419500	0.39627800
N	1.37510200	-1.08188200	5.53045900
C	2.67082800	-0.34960000	3.62774900
C	3.28484100	0.73378600	2.98944200
C	0.68451900	-0.74402900	6.77119500
H	0.64005900	0.34647600	6.92084600
C	1.89429200	-0.12974900	4.85702300
H	1.81037500	0.91988900	5.17804500
N	-3.47396800	-4.23314200	-1.69179700
C	-1.17093800	-3.73335200	-2.16008200
C	0.16349600	-4.04461700	-1.89873100
C	-4.48465900	-5.02614800	-0.99416600
H	-4.00710100	-5.65599900	-0.23024600
C	-2.23133100	-4.44389900	-1.44896800
H	-1.91092600	-5.18781900	-0.70868100
N	0.15128500	-0.60473200	-5.64148600
C	-0.43493400	-2.11859500	-3.86033600
C	-1.48032400	-2.75598100	-3.15293500
C	-0.28213800	0.28709500	-6.71325900
H	-1.37265200	0.44038300	-6.69068700
C	-0.75329400	-1.15171100	-4.92359500
H	-1.81921000	-0.94785400	-5.08002900
O	-2.75041300	-2.43961900	-3.43760400
N	2.97422400	-4.69169700	-1.54184300
C	1.20993900	-3.41841300	-2.59110100
C	0.88791800	-2.46189000	-3.56058900
C	4.39734600	-4.99872800	-1.44290500

H	5.00188100	-4.30178200	-2.04508100
C	2.61610900	-3.77591200	-2.35676300
H	3.34969000	-3.21284200	-2.95384400
N	4.60715300	-3.44465700	0.45254900
C	3.64213600	-1.84050200	1.95722600
C	2.86129600	-1.63262400	3.09427900
C	4.83890800	-4.82945400	0.04693900
H	4.21884700	-5.50779100	0.65004000
C	3.85655300	-3.19933700	1.46445400
H	3.36120100	-4.00603700	2.01934100
H	-0.39132400	4.92828500	0.29050200
H	-1.61636400	3.09816800	-3.39535500
H	1.67645100	-1.96887200	-4.12220300
H	0.40376500	-4.79720600	-1.15315700
H	3.16703300	1.73794900	3.38705900
H	2.39935900	-2.48099900	3.59110300
H	-3.21105800	-2.63829400	2.67790700
H	-2.45841400	1.33687100	4.11393200
H	-3.33800000	-3.02017700	-2.85827100
H	-5.06181700	1.79788900	0.49883000
H	5.05734100	-1.87643800	0.03804500
H	3.37668700	3.71109800	-1.80144500
C	-4.62124000	6.72253400	-0.05620900
C	-5.62705400	7.24391200	-0.87880200
C	-3.84120400	7.60883800	0.70088400
C	-5.85816000	8.62045400	-0.93895500
H	-6.23477000	6.56876400	-1.47607600
C	-4.06991100	8.98428400	0.64187600
H	-3.04360200	7.21884900	1.32610600
C	-5.08064500	9.49504700	-0.17745200
H	-6.64285500	9.00740800	-1.58364100
H	-3.45619000	9.65821300	1.23387600
H	-5.25724200	10.56622600	-0.22447200
C	-6.32494400	4.89332700	1.65527300
C	-6.69136000	5.76010400	2.69179600
C	-7.33457600	4.28659300	0.89381400
C	-8.03672200	6.02512900	2.95899800
H	-5.91903100	6.23238300	3.29370800
C	-8.67917700	4.54846500	1.16013500
H	-7.07077400	3.59948300	0.09476000
C	-9.03490100	5.42011100	2.19316500
H	-8.30239400	6.70088700	3.76750300
H	-9.44960100	4.06961500	0.56169500
H	-10.08206100	5.62249400	2.40091600
C	6.53706900	4.45792700	1.97288600
C	7.86830300	4.55234400	1.55008800
C	6.21616600	4.83968200	3.28386300
C	8.85935600	5.02778500	2.41256000
H	8.13206900	4.25290300	0.53880800
C	7.20443000	5.31462000	4.14712300
H	5.19147000	4.74933500	3.63188000
C	8.52983600	5.41189100	3.71372100

H	9.88770300	5.09387800	2.06728500
H	6.94010700	5.60585700	5.16033000
H	9.29937000	5.78004000	4.38685400
C	5.22516000	6.23067700	-0.11093200
C	5.31374400	7.48185000	0.51071800
C	5.81515200	6.06000600	-1.37199500
C	5.98504700	8.54006400	-0.10681500
H	4.85609000	7.62968300	1.48566900
C	6.48447600	7.11617500	-1.99154500
H	5.74391900	5.10097400	-1.87745000
C	6.57306900	8.35993200	-1.36006400
H	6.04412700	9.50418100	0.39107500
H	6.93520300	6.96816200	-2.96926200
H	7.09353700	9.18220500	-1.84342200
C	6.30494500	-5.18013900	0.26492000
C	6.65103400	-6.31728700	1.00453300
C	7.32929200	-4.37873000	-0.26018000
C	7.99093400	-6.65518100	1.20975300
H	5.86705000	-6.94418100	1.42188600
C	8.66846100	-4.71332100	-0.05490200
H	7.08097200	-3.48430800	-0.82453900
C	9.00393900	-5.85395400	0.67991400
H	8.24067100	-7.54179400	1.78634500
H	9.45045600	-4.08144400	-0.46745400
H	10.04685400	-6.11322000	0.84045200
C	4.64405500	-6.41637300	-1.94418400
C	5.66509100	-6.67208200	-2.86723700
C	3.85584200	-7.48630000	-1.49551200
C	5.90316100	-7.96961000	-3.32733800
H	6.27930400	-5.85096400	-3.22831700
C	4.09160100	-8.78310400	-1.95403000
H	3.04596100	-7.29782400	-0.79712300
C	5.11758600	-9.02965600	-2.87079800
H	6.69973700	-8.14934100	-4.04446400
H	3.47138600	-9.60148200	-1.59782000
H	5.29969700	-10.03930900	-3.22893800
C	-5.19990400	-5.92478600	-1.99481600
C	-5.29159300	-7.30188500	-1.76030800
C	-5.77284400	-5.39914700	-3.16226700
C	-5.94964700	-8.13811900	-2.66551200
H	-4.84686100	-7.72367200	-0.86247400
C	-6.42891600	-6.23287200	-4.06883000
H	-5.69905400	-4.33527800	-3.36956900
C	-6.52100800	-7.60560200	-3.82259900
H	-6.01139400	-9.20467100	-2.46658900
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H	-7.03109100	-8.25439400	-4.52937900
C	-6.55179500	-4.82535900	0.48904400
C	-7.87507100	-4.79588300	0.03317300
C	-6.25062200	-5.56743200	1.64063700
C	-8.87748100	-5.50030100	0.70476700
H	-8.12366700	-4.21888800	-0.85408400

C	-7.25034200	-6.27137600	2.31332600
H	-5.23239700	-5.58029300	2.01794600
C	-8.56757800	-6.24159900	1.84654100
H	-9.89941700	-5.46563700	0.33662600
H	-7.00129400	-6.84113600	3.20474900
H	-9.34605400	-6.78846900	2.37165300
C	0.02318700	2.66263800	-7.61389200
C	0.98535100	3.05148200	-8.55371800
C	-1.27210500	3.19099000	-7.71768200
C	0.66201800	3.94013300	-9.58228400
H	1.99520700	2.65520900	-8.48160700
C	-1.59751800	4.07922200	-8.74376500
H	-2.02219300	2.91494000	-6.98257000
C	-0.63155000	4.45610900	-9.68118100
H	1.42247700	4.23056400	-10.30241500
H	-2.60567500	4.48011700	-8.80969000
H	-0.88481000	5.14919200	-10.47892500
C	0.09657000	-0.32809900	-8.05451400
C	-0.85336200	-0.43393600	-9.07750300
C	1.39542700	-0.80315900	-8.28921200
C	-0.51439100	-0.99138400	-10.31302900
H	-1.86590300	-0.07646500	-8.90716500
C	1.73638600	-1.36114800	-9.52210000
H	2.13593300	-0.74751900	-7.49686100
C	0.78261400	-1.45581500	-10.53965200
H	-1.26544500	-1.06521000	-11.09515200
H	2.74702800	-1.72534500	-9.68759400
H	1.04791800	-1.89189300	-11.49900400
C	1.43189300	-1.36754700	7.94329400
C	1.75382000	-0.59764400	9.06752000
C	1.81246100	-2.71746600	7.91972100
C	2.43170300	-1.16257500	10.15079800
H	1.47116200	0.45176500	9.09671700
C	2.48978700	-3.28416500	9.00032500
H	1.58878400	-3.31999900	7.04449900
C	2.80069400	-2.50877100	10.12107000
H	2.67361500	-0.54887400	11.01456400
H	2.77819000	-4.33158700	8.96602900
H	3.32988100	-2.94987400	10.96148800
C	-1.56789200	-1.00012600	7.96254900
C	-1.92705900	-2.06588100	8.79641300
C	-1.94218500	0.30027600	8.33213200
C	-2.63489500	-1.84074600	9.97984900
H	-1.64984600	-3.07987500	8.51879900
C	-2.64939000	0.52790000	9.51349100
H	-1.69007200	1.13353000	7.68305400
C	-2.99718300	-0.54221600	10.34292500
H	-2.90524400	-2.68082300	10.61422000
H	-2.93243300	1.54156600	9.78516300
H	-3.54974000	-0.36483400	11.26168000
N	-0.91229700	5.47985900	-1.46787700
C	-1.68035200	3.39144700	-2.39765500

C	-2.76248900	2.49024700	-2.52598200
C	-1.19379300	6.65655700	-0.65057800
H	-2.16226800	6.56238500	-0.13428000
C	-1.82606000	4.59102900	-1.55761700
H	-2.78100800	4.68783900	-1.02764300
N	-0.14585200	5.58707400	1.29990300
C	1.00324900	3.71041300	2.28481100
C	2.23663800	3.03622500	2.43801300
C	-0.09202300	6.77562900	0.45342100
H	0.87739500	6.85610100	-0.06336700
C	0.92032700	4.89141500	1.41044000
H	1.84093700	5.15464000	0.87631000
N	-4.89413400	0.61581000	-2.99535100
C	-2.64187800	1.35534700	-3.38271600
C	-1.45146200	1.14826800	-4.08029200
C	-5.99824100	-0.29902400	-3.27678100
H	-5.65097300	-1.12364800	-3.91541100
C	-3.76236000	0.43696400	-3.57376300
H	-3.59602000	-0.40499500	-4.25750800
N	1.03182600	0.90793800	-5.57689800
C	-0.36930600	2.03214500	-3.96012800
C	-0.50599300	3.13996400	-3.11578500
C	2.28282200	0.87193500	-6.32790500
H	2.97973800	1.65297500	-5.98460500
C	0.87020900	1.84968300	-4.73004200
H	1.65141500	2.60316700	-4.54596900
N	3.28679300	-0.62407600	-4.65527100
C	3.11325900	-1.88511500	-2.60873000
C	2.61461900	-3.05040500	-1.98195900
C	2.97888600	-0.50705300	-6.07739900
H	2.27445700	-1.28986600	-6.40048900
C	2.81134100	-1.62980900	-4.02673300
H	2.17247800	-2.37200100	-4.51991100
O	1.83497500	-3.88603600	-2.68092400
N	4.68428100	1.61770200	2.95879700
C	2.33100300	1.92455900	3.32812800
C	1.19906900	1.51491600	4.03361500
C	5.94207400	0.93828800	3.26121300
H	5.75824500	0.08105000	3.92434000
C	3.60512400	1.24219600	3.54364700
H	3.59942100	0.40345700	4.25109800
N	-1.20382900	0.85002500	5.53792300
C	-0.03104500	2.17262800	3.88889900
C	-0.10447200	3.26079300	3.01177700
C	-2.42862200	0.61003300	6.29532600
H	-3.25575100	1.23836700	5.92842700
C	-1.21639100	1.78324700	4.66655900
H	-2.12264800	2.37530000	4.46613500
N	5.59372900	-0.57142700	1.35839000
C	4.27576300	-1.27532400	-0.53882900
C	3.92990300	-1.02117800	-1.87095400
C	6.54263100	0.37746900	1.93188600

H	6.70919400	1.23483800	1.26040100
C	5.18185100	-0.35927900	0.16848100
H	5.50547200	0.52040900	-0.40859500
N	-3.13854100	-1.10206200	4.67987600
C	-2.71424800	-2.36372100	2.67066700
C	-2.00221300	-3.43344600	2.08069400
C	-2.85989800	-0.88070600	6.09549700
H	-2.02469700	-1.50932700	6.44285300
C	-2.47153000	-2.01142000	4.07920300
H	-1.69883700	-2.59698900	4.59122400
N	-5.37858200	-1.66374000	-1.33336200
C	-3.96040900	-2.04910800	0.58377900
C	-3.67536500	-1.69266500	1.90689600
C	-6.48715200	-0.92763200	-1.93241400
H	-6.81658100	-0.10044200	-1.28365100
C	-5.01918000	-1.34226000	-0.15090600
H	-5.50611900	-0.52282000	0.39966500
N	-0.73107600	-5.64798700	0.74941800
C	-2.27894200	-3.81061200	0.73256400
C	-3.24892800	-3.11322700	0.01192700
C	-0.13196900	-6.80935000	0.09530300
H	-0.44348000	-6.85257500	-0.95807600
C	-1.59596000	-4.94352700	0.11352900
H	-1.87691200	-5.17855300	-0.92079400
N	1.78635400	-5.42411700	-0.57501400
C	2.95666600	-3.32587400	-0.62423200
C	3.77734600	-2.43604000	0.06939000
C	1.42119400	-6.65662100	0.12030500
H	1.73092300	-6.60198200	1.17369500
C	2.50074000	-4.54762200	0.03332700
H	2.81992300	-4.69128300	1.07327500
H	0.31045900	3.84922100	-3.01238000
H	4.31170700	-0.13659100	-2.37288800
H	4.05063500	-2.64825900	1.09906900
H	1.26882000	0.67731600	4.72187300
O	-3.89345200	2.72580500	-1.84774000
H	-4.54679000	1.99873600	-2.09989800
H	-4.21961600	-0.88063600	2.38086000
H	-1.35906400	0.29219000	-4.74255800
H	1.61650600	-4.66379900	-2.07804100
H	-3.47187000	-3.40459100	-1.01047000
O	-1.08427100	-4.08637600	2.80584700
H	-0.71817700	-4.82504100	2.22594800
O	3.30437700	3.46390200	1.75129900
H	4.08383100	2.88280800	2.02283000
H	-1.04065600	3.79810600	2.88837400
C	-7.10473400	0.45355400	-4.00482800
C	-7.62113400	-0.04813100	-5.20539000
C	-7.62316500	1.65346200	-3.49605700
C	-8.64071500	0.62649500	-5.88139500
H	-7.22476100	-0.97432200	-5.61386600
C	-8.64030500	2.33003900	-4.17061200

H	-7.22551000	2.06688900	-2.57349800
C	-9.15371900	1.81795500	-5.36550200
H	-9.02958300	0.22166000	-6.81188500
H	-9.03054000	3.25913500	-3.76381400
H	-9.94460900	2.34608200	-5.89107800
C	-7.66245200	-1.87308800	-2.15032200
C	-8.94488900	-1.51880000	-1.71508300
C	-7.48296200	-3.11014800	-2.78671400
C	-10.02975600	-2.37550400	-1.91810400
H	-9.09680800	-0.56601700	-1.21397100
C	-8.56515100	-3.96730800	-2.99077600
H	-6.48929000	-3.40655400	-3.10912200
C	-9.84325900	-3.60210200	-2.55833800
H	-11.01813100	-2.08444300	-1.57241900
H	-8.40990500	-4.92285900	-3.48485500
H	-10.68537000	-4.27062600	-2.71568200
C	-4.10164000	-1.22944500	6.90626500
C	-4.00812600	-2.08609900	8.00969900
C	-5.35796800	-0.70901400	6.56204500
C	-5.14038400	-2.40975400	8.76166800
H	-3.04192400	-2.50258000	8.28377000
C	-6.49056100	-1.03090600	7.31120100
H	-5.44888300	-0.06134800	5.69520000
C	-6.38568600	-1.88207700	8.41501800
H	-5.04817200	-3.07675500	9.61480500
H	-7.45676300	-0.61952500	7.03073500
H	-7.26809800	-2.13424600	8.99696100
C	-2.17920600	0.93892500	7.76180000
C	-3.06035000	1.77394400	8.45940200
C	-1.06611600	0.41850400	8.43835700
C	-2.84424400	2.07548900	9.80646300
H	-3.92310400	2.19059700	7.94548000
C	-0.84770100	0.71836100	9.78373200
H	-0.36214600	-0.21168300	7.90305600
C	-1.73743000	1.54704300	10.47346000
H	-3.53917400	2.72566300	10.33141200
H	0.01976500	0.30714500	10.29345700
H	-1.56622100	1.78161600	11.52062400
C	-1.23561900	7.88922100	-1.54504400
C	-2.29788000	8.79635000	-1.44894600
C	-0.21815800	8.13925900	-2.47764300
C	-2.34090100	9.93489800	-2.25745800
H	-3.09671400	8.61168200	-0.73501500
C	-0.25933000	9.27538100	-3.28722000
H	0.60000700	7.43235400	-2.57749300
C	-1.32055800	10.17861800	-3.17880700
H	-3.17366400	10.62764800	-2.16884200
H	0.53657300	9.45417900	-4.00555200
H	-1.35315200	11.06231700	-3.81041700
C	-0.28627600	8.01248200	1.32135500
C	0.59546400	9.09507700	1.21819600
C	-1.34492500	8.09068000	2.23837900

C	0.42066800	10.23684700	2.00435700
H	1.42392700	9.04589600	0.51583100
C	-1.52120600	9.22946400	3.02550200
H	-2.02373900	7.24968100	2.34384000
C	-0.63918300	10.30782800	2.91043000
H	1.11535000	11.06739000	1.91022400
H	-2.34627900	9.27389600	3.73169200
H	-0.77555600	11.19378700	3.52474400
C	1.98418200	1.09914700	-7.80434600
C	2.71068000	2.04625000	-8.53600000
C	0.97889700	0.37024000	-8.45672100
C	2.44948500	2.25563300	-9.89250300
H	3.48754100	2.62402600	-8.04132400
C	0.71567100	0.57766100	-9.81148900
H	0.39240500	-0.35080800	-7.89522400
C	1.45151500	1.52051100	-10.53509500
H	3.02371400	2.99552900	-10.44391400
H	-0.06710800	0.00492600	-10.30207000
H	1.24512500	1.68314100	-11.58953800
C	4.26738700	-0.65065400	-6.87747400
C	4.33672200	-1.54793900	-7.94996200
C	5.40596000	0.10208000	-6.55374000
C	5.51238400	-1.68510600	-8.69234400
H	3.46405900	-2.14312800	-8.20728200
C	6.58171500	-0.03351700	-7.29326100
H	5.37293500	0.78509400	-5.71012500
C	6.63870500	-0.92697000	-8.36677600
H	5.54749100	-2.38680000	-9.52158500
H	7.45545500	0.55658600	-7.02909900
H	7.55488200	-1.03376200	-8.94133300
C	7.87530800	-0.32291600	2.16816600
C	9.06988700	0.26580100	1.73656000
C	7.93085900	-1.56509900	2.81714200
C	10.29695800	-0.36545000	1.95532600
H	9.04083800	1.22570600	1.22704600
C	9.15532800	-2.19763400	3.03648500
H	7.00984100	-2.04322100	3.13698000
C	10.34338400	-1.59912000	2.60746000
H	11.21413400	0.10630100	1.61280700
H	9.18158400	-3.16058600	3.53980000
H	11.29643100	-2.09300000	2.77658400
C	6.88417000	1.90862600	3.96207100
C	7.47749600	1.55417400	5.17949900
C	7.17248600	3.16611200	3.41158700
C	8.34913300	2.43017500	5.83106200
H	7.25800700	0.58522200	5.62088600
C	8.04117800	4.04370700	4.06174900
H	6.71026600	3.46586700	2.47526400
C	8.63409600	3.67787800	5.27345500
H	8.80103000	2.13729700	6.77494800
H	8.25351600	5.01475300	3.62246800
H	9.30960600	4.36202700	5.77968800

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C	2.12314300	-7.83961600	-0.53518600
C	2.87663100	-8.72594100	0.24328400
C	2.03341600	-8.06116200	-1.91721800
C	3.52098600	-9.81849700	-0.34204700
H	2.95882900	-8.56247300	1.31481400
C	2.67768800	-9.15113800	-2.50392000
H	1.46701500	-7.37484900	-2.54044000
C	3.42238100	-10.03463600	-1.71767600
H	4.10132400	-10.49681900	0.27751700
H	2.59991900	-9.30888000	-3.57625900
H	3.92465700	-10.88247100	-2.17535200
C	-0.59257400	-8.08188200	0.79539600
C	-1.16695300	-9.12133200	0.05447200
C	-0.45676400	-8.23489500	2.18299100
C	-1.58933200	-10.29574700	0.68215300
H	-1.28391800	-9.01300900	-1.02083700
C	-0.87913000	-9.40677400	2.81185700
H	-0.02891800	-7.43245900	2.77737300
C	-1.44555500	-10.44204900	2.06299600
H	-2.03280800	-11.09264000	0.09135100
H	-0.76816300	-9.51018300	3.88788600
H	-1.77543700	-11.35366800	2.55360500
N	3.59481100	3.76144000	2.42922000
C	3.45958200	1.35454300	2.47544700
C	3.99424100	0.13845900	1.99154400
C	4.23953700	4.96059400	1.90212000
H	4.92881200	4.71592500	1.07837900
C	3.98902400	2.63312400	1.97619100
H	4.76392500	2.55890400	1.20417800
N	2.43124400	5.20440400	0.25146400
C	0.38530700	4.43565900	-0.74659300
C	-1.00452100	4.36778400	-0.64602300
C	3.13833200	5.90535800	1.32148400
H	2.44443900	6.14230100	2.14044300
C	1.15703000	5.06649100	0.32195000
H	0.58718400	5.44028500	1.18199300
N	5.03687800	-2.42563700	1.20456400
C	3.51816500	-1.10168400	2.51262600
C	2.52440500	-1.09580800	3.49216900
C	5.61006200	-3.72165500	0.84847700
H	5.03640300	-4.53146400	1.32150100
C	4.08828500	-2.37101200	2.06826800
H	3.67882500	-3.27962200	2.52737700
N	0.54594400	-0.93909400	5.61817600
C	1.98338000	0.10286000	3.97879400
C	2.46298100	1.30943600	3.45670400
C	-0.40611400	-0.78452500	6.71420200
H	-0.70362000	0.26865200	6.83905000
C	0.97267600	0.11977300	5.04689200
H	0.62147200	1.11976800	5.34438300
N	-2.29046700	-1.04279700	5.15575800
C	-3.10828800	-1.40927200	2.91820300

C	-3.33228800	-2.34845000	1.88524400
C	-1.70143000	-1.59249700	6.37335500
H	-1.40145900	-2.64319400	6.23466600
C	-2.45963500	-1.83643500	4.16856600
H	-2.15309000	-2.88829400	4.21206800
O	-2.91183000	-3.61058900	2.04542500
N	-3.91209100	4.28981100	-0.62456300
C	-1.78626300	3.81496800	-1.67054900
C	-1.13850000	3.32302500	-2.80926600
C	-5.36952700	4.26205700	-0.69930300
H	-5.71456400	3.72369600	-1.59638400
C	-3.25462600	3.78914800	-1.59766800
H	-3.75877800	3.32735300	-2.46045800
N	0.24889300	2.44808400	-5.18433200
C	0.25220600	3.37082900	-2.95732300
C	1.02806600	3.93006100	-1.91601300
C	0.99887300	2.07877200	-6.38132500
H	2.08419200	2.17428800	-6.21948000
C	0.90867400	2.90206900	-4.18855300
H	2.00126800	2.99131500	-4.21011500
O	2.35998800	3.98785400	-2.05086300
N	-5.41879600	2.11452700	0.49484500
C	-4.23009100	0.31605900	1.58642400
C	-3.55958400	-0.09623800	2.74347400
C	-5.91907700	3.48487700	0.54286600
H	-5.55791600	4.01251800	1.43996700
C	-4.73259600	1.69421900	1.48601300
H	-4.49866900	2.34198200	2.34480400
N	1.17570700	-0.24332700	-5.59348000
C	0.68796600	-1.93673300	-3.94072100
C	-0.27530500	-2.81099900	-3.42486700
C	0.71276500	0.57629400	-6.70948400
H	-0.37465900	0.47709400	-6.85469400
C	0.32926200	-1.01341300	-5.02764800
H	-0.72456900	-1.04817800	-5.34400500
N	4.09345100	-3.84406700	-1.08123600
C	2.33636800	-2.91863300	-2.43240600
C	1.99185800	-2.00531300	-3.42946300
C	5.50189900	-3.91033500	-0.69789500
H	6.06229800	-3.09138600	-1.17108700
C	3.71763600	-2.98903800	-1.96237500
H	4.42662200	-2.28594100	-2.41725900
N	-2.17532800	-4.73604000	-2.41042100
C	0.02255800	-3.74540800	-2.42677300
C	1.34059000	-3.80207600	-1.91827800
C	-3.07245600	-5.76333200	-1.88978600
H	-2.61088900	-6.31280600	-1.05398500
C	-0.98961300	-4.69309100	-1.93511800
H	-0.65651300	-5.38065100	-1.14875200
N	-3.97654900	-4.14463000	-0.27114300
C	-4.01270700	-1.94593000	0.69730200
C	-4.44647600	-0.62606600	0.57060500

C	-4.35885800	-5.06975400	-1.33638400
H	-4.81671200	-4.51714600	-2.16903200
C	-4.30456300	-2.90708900	-0.36381500
H	-4.84249100	-2.52143900	-1.23900500
H	2.07170400	2.25459300	3.82269500
H	-1.29101700	-2.79003400	-3.80979500
H	-3.38932600	0.60751100	3.55341100
H	-4.97718000	-0.31906300	-0.32604500
H	-1.71843500	2.90121700	-3.62534900
H	-1.49899200	4.76327400	0.23657400
H	2.72087800	4.44821800	-1.22877500
O	4.95307600	0.17306000	1.05644000
H	5.22244200	-0.78082900	0.87131900
O	1.63568900	-4.69807200	-0.96707200
H	2.61938800	-4.60470500	-0.76579200
H	2.74877400	-1.33863000	-3.83258900
H	2.16636700	-2.03647400	3.90070000
H	-3.19741000	-4.12431500	1.22522000
C	-3.40269300	-6.75284100	-3.00051700
C	-3.28367900	-8.12996900	-2.77861700
C	-3.82749800	-6.30586500	-4.26034300
C	-3.59141600	-9.04492500	-3.78860700
H	-2.94930300	-8.48960300	-1.80871700
C	-4.13518000	-7.21801400	-5.27068800
H	-3.90222200	-5.23968200	-4.45253900
C	-4.01991200	-8.59141500	-5.03763200
H	-3.49294200	-10.11044700	-3.59874300
H	-4.46220300	-6.85604900	-6.24192400
H	-4.25808100	-9.30135900	-5.82506800
C	-5.37100900	-6.07176900	-0.79630900
C	-6.58442300	-6.27286800	-1.46506100
C	-5.11400400	-6.80529600	0.37123500
C	-7.51978200	-7.19325600	-0.98599500
H	-6.79900300	-5.70696000	-2.36809700
C	-6.04769700	-7.72408500	0.85250500
H	-4.18474900	-6.65209400	0.91267800
C	-7.25363200	-7.92229000	0.17446700
H	-8.45626600	-7.33627700	-1.51839200
H	-5.83396600	-8.28377400	1.75917400
H	-7.98080900	-8.63676800	0.55046300
C	6.09302700	-5.23717200	-1.15669200
C	7.26846200	-5.25492400	-1.91677700
C	5.47701200	-6.45532000	-0.83485700
C	7.82518000	-6.46386400	-2.34092400
H	7.75288500	-4.31746900	-2.17782400
C	6.03067500	-7.66387800	-1.25936500
H	4.55588500	-6.46111400	-0.25895500
C	7.20771800	-7.67218000	-2.01288400
H	8.73823400	-6.45898700	-2.93005200
H	5.54096300	-8.59951000	-1.00323700
H	7.63749900	-8.61350700	-2.34414400
C	7.05161000	-3.79311600	1.33577600

C	7.47254200	-4.87227700	2.12192800
C	7.97626900	-2.78869100	1.01465000
C	8.79225000	-4.95432300	2.57239000
H	6.76436700	-5.65462300	2.38276000
C	9.29463800	-2.86819200	1.46517900
H	7.66453100	-1.93559700	0.41862900
C	9.70741500	-3.95233300	2.24459000
H	9.10190100	-5.79925200	3.18146200
H	9.99914800	-2.08148400	1.20906600
H	10.73375100	-4.01293900	2.59604500
C	-2.72795800	-1.52266900	7.49701100
C	-3.00125600	-2.65301900	8.27674800
C	-3.41909600	-0.33286700	7.76983000
C	-3.93556600	-2.59723600	9.31411500
H	-2.47800700	-3.58384800	8.07214700
C	-4.35314100	-0.27459200	8.80507800
H	-3.23331600	0.54529500	7.15867300
C	-4.61378200	-1.40669700	9.58245400
H	-4.13462800	-3.48511000	9.90848000
H	-4.88054800	0.65495800	9.00304200
H	-5.34252400	-1.36150800	10.38729900
C	0.24040000	-1.26549400	8.00713900
C	0.20742200	-0.46478400	9.15520100
C	0.88038100	-2.51200200	8.07308000
C	0.78941600	-0.90114400	10.34811900
H	-0.27888300	0.50684500	9.11651800
C	1.46307800	-2.94990400	9.26316700
H	0.93298500	-3.13328900	7.18398700
C	1.41815000	-2.14638400	10.40611400
H	0.75377400	-0.26576100	11.22916400
H	1.95548600	-3.91829000	9.29751600
H	1.87335500	-2.48695400	11.33222600
C	-5.89422900	5.69115300	-0.75587000
C	-6.83051100	6.06295700	-1.72815000
C	-5.45199300	6.65880800	0.15837200
C	-7.32464700	7.36871800	-1.78270700
H	-7.17713300	5.32500800	-2.44736000
C	-5.94368100	7.96385100	0.10588400
H	-4.70910100	6.38981900	0.90333200
C	-6.88349000	8.32338200	-0.86440500
H	-8.05081900	7.63877800	-2.54492500
H	-5.59023400	8.70192300	0.82125400
H	-7.26473300	9.34014200	-0.90625800
C	-7.44193600	3.45867900	0.57231400
C	-8.14406200	4.20895000	1.52321600
C	-8.16796700	2.68450900	-0.34488400
C	-9.54087600	4.19735100	1.55376200
H	-7.59416700	4.80819400	2.24470700
C	-9.56319200	2.67101300	-0.31651800
H	-7.63565500	2.07961400	-1.07291800
C	-10.25515400	3.42897000	0.63248800
H	-10.06858400	4.78594700	2.29962700

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H	-10.11079500	2.06523600	-1.03386700
H	-11.34152200	3.41667500	0.65572600
C	5.03080600	5.63720800	3.01463600
C	6.36192100	6.01667400	2.80497700
C	4.44597700	5.88759700	4.26473800
C	7.09355900	6.64297100	3.81713100
H	6.82967500	5.82188000	1.84315700
C	5.17500400	6.51278900	5.27724700
H	3.42157400	5.57723800	4.44775600
C	6.50142900	6.89435600	5.05626100
H	8.12603600	6.93031600	3.63682100
H	4.70810800	6.69919100	6.24084300
H	7.06932100	7.37961800	5.84545200
C	3.71781200	7.20506500	0.77806200
C	3.46142800	8.41508600	1.43404600
C	4.50984100	7.21921800	-0.37933800
C	3.99133100	9.61453300	0.95251200
H	2.84438500	8.41929700	2.32903200
C	5.03862700	8.41666300	-0.86329000
H	4.70741000	6.29261200	-0.91081000
C	4.78236800	9.61864000	-0.19787200
H	3.78198100	10.54413400	1.47492900
H	5.64959100	8.41077600	-1.76199400
H	5.19335500	10.55080100	-0.57576000
C	0.59380500	2.99946400	-7.52562500
C	1.57053700	3.64688700	-8.29186100
C	-0.75749800	3.22004400	-7.83065700
C	1.20979100	4.48848500	-9.34719900
H	2.62166000	3.49069100	-8.06209400
C	-1.12053800	4.06037400	-8.88407400
H	-1.52579400	2.74205800	-7.23030300
C	-0.13770800	4.69677900	-9.64757500
H	1.98215400	4.98285200	-9.93053600
H	-2.17212800	4.22130600	-9.10697000
H	-0.42078100	5.35256500	-10.46653700
C	1.41871700	0.12713800	-7.98262300
C	0.68264300	-0.13991400	-9.14328000
C	2.81212400	-0.03092500	-8.01706800
C	1.32186400	-0.54450600	-10.31797100
H	-0.39877100	-0.02872000	-9.12889900
C	3.45294600	-0.43578000	-9.18883900
H	3.39288500	0.15055900	-7.11761400
C	2.70991900	-0.69231500	-10.34470400
H	0.73380500	-0.74716400	-11.20922800
H	4.53337500	-0.55403900	-9.19877100
H	3.20903700	-1.00893800	-11.25657800
N	5.60747800	1.09569300	0.90998300
C	3.61777300	1.62823200	2.14672700
C	2.81370500	1.32132200	3.24476500
C	6.81025000	0.28686200	0.72613000
H	6.80172500	-0.56726700	1.41836100
C	4.80505900	0.82231100	1.87431200

H	4.98988900	-0.02133600	2.55121200
N	5.60747800	-1.09569300	-0.90998300
C	3.61777300	-1.62823200	-2.14672700
C	2.81370500	-1.32132200	-3.24476500
C	6.81025000	-0.28686200	-0.72613000
H	6.80172500	0.56726700	-1.41836100
C	4.80505900	-0.82231100	-1.87431200
H	4.98988900	0.02133600	-2.55121200
N	1.14749700	0.87164500	5.57797500
C	1.69019300	2.09499700	3.56842700
C	1.38264100	3.19290200	2.75678700
C	0.30074300	0.72235000	6.75736100
H	-0.54710100	1.42543300	6.73394600
C	0.87111300	1.80826900	4.75574900
H	0.00970300	2.47693800	4.90601900
N	0.89547800	5.52774300	1.12622200
C	2.15935700	3.54149700	1.64621200
C	3.28996500	2.75277300	1.33194500
C	0.72605500	6.71322500	0.29035300
H	1.41813500	6.70078700	-0.56659100
C	1.85206400	4.73169800	0.83643600
H	2.51290400	4.90834900	-0.02035100
O	4.04547600	3.08453000	0.27628900
N	-0.89547800	5.52774300	-1.12622200
C	-2.15935700	3.54149700	-1.64621200
C	-3.28996500	2.75277300	-1.33194500
C	-0.72605500	6.71322500	-0.29035300
H	-1.41813500	6.70078700	0.56659100
C	-1.85206400	4.73169800	-0.83643600
H	-2.51290400	4.90834900	0.02035100
O	-4.04547600	3.08453000	-0.27628900
N	1.14749700	-0.87164500	-5.57797500
C	1.69019300	-2.09499700	-3.56842700
C	1.38264100	-3.19290200	-2.75678700
C	0.30074300	-0.72235000	-6.75736100
H	-0.54710100	-1.42543300	-6.73394600
C	0.87111300	-1.80826900	-4.75574900
H	0.00970300	-2.47693800	-4.90601900
N	0.89547800	-5.52774300	-1.12622200
C	2.15935700	-3.54149700	-1.64621200
C	3.28996500	-2.75277300	-1.33194500
C	0.72605500	-6.71322500	-0.29035300
H	1.41813500	-6.70078700	0.56659100
C	1.85206400	-4.73169800	-0.83643600
H	2.51290400	-4.90834900	0.02035100
O	4.04547600	-3.08453000	-0.27628900
N	-1.14749700	0.87164500	-5.57797500
C	-1.69019300	2.09499700	-3.56842700
C	-1.38264100	3.19290200	-2.75678700
C	-0.30074300	0.72235000	-6.75736100
H	0.54710100	1.42543300	-6.73394600
C	-0.87111300	1.80826900	-4.75574900

H	-0.00970300	2.47693800	-4.90601900
N	-0.89547800	-5.52774300	1.12622200
C	-2.15935700	-3.54149700	1.64621200
C	-3.28996500	-2.75277300	1.33194500
C	-0.72605500	-6.71322500	0.29035300
H	-1.41813500	-6.70078700	-0.56659100
C	-1.85206400	-4.73169800	0.83643600
H	-2.51290400	-4.90834900	-0.02035100
O	-4.04547600	-3.08453000	0.27628900
N	-1.14749700	-0.87164500	5.57797500
C	-1.69019300	-2.09499700	3.56842700
C	-1.38264100	-3.19290200	2.75678700
C	-0.30074300	-0.72235000	6.75736100
H	0.54710100	-1.42543300	6.73394600
C	-0.87111300	-1.80826900	4.75574900
H	-0.00970300	-2.47693800	4.90601900
N	-5.60747800	-1.09569300	0.90998300
C	-3.61777300	-1.62823200	2.14672700
C	-2.81370500	-1.32132200	3.24476500
C	-6.81025000	-0.28686200	0.72613000
H	-6.80172500	0.56726700	1.41836100
C	-4.80505900	-0.82231100	1.87431200
H	-4.98988900	0.02133600	2.55121200
N	-5.60747800	1.09569300	-0.90998300
C	-3.61777300	1.62823200	-2.14672700
C	-2.81370500	1.32132200	-3.24476500
C	-6.81025000	0.28686200	-0.72613000
H	-6.80172500	-0.56726700	-1.41836100
C	-4.80505900	0.82231100	-1.87431200
H	-4.98988900	-0.02133600	-2.55121200
H	4.81198100	2.43088700	0.24245100
H	4.81198100	-2.43088700	-0.24245100
H	-4.81198100	-2.43088700	0.24245100
H	-4.81198100	2.43088700	-0.24245100
H	3.06522800	0.47332500	3.87517600
H	0.52472600	3.81797300	2.98821900
H	-0.52472600	3.81797300	-2.98821900
H	-3.06522800	0.47332500	-3.87517600
H	3.06522800	-0.47332500	-3.87517600
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H	-0.52472600	-3.81797300	2.98821900
H	-3.06522800	-0.47332500	3.87517600
C	-8.04461300	-1.13332600	1.00893300
C	-9.01409800	-0.67781400	1.91019400
C	-8.23249200	-2.37436500	0.38312700
C	-10.15440300	-1.43947600	2.17636200
H	-8.87761900	0.27949500	2.40667600
C	-9.37022600	-3.13740700	0.64913000
H	-7.48317200	-2.75228400	-0.30674600
C	-10.33592900	-2.67163500	1.54567900
H	-10.89679300	-1.07040300	2.87880300
H	-9.50118300	-4.09760900	0.15747200

H	-11.22084700	-3.26702800	1.75305800
C	-8.04461300	1.13332600	-1.00893300
C	-9.01409800	0.67781400	-1.91019400
C	-8.23249200	2.37436500	-0.38312700
C	-10.15440300	1.43947600	-2.17636200
H	-8.87761900	-0.27949500	-2.40667600
C	-9.37022600	3.13740700	-0.64913000
H	-7.48317200	2.75228400	0.30674600
C	-10.33592900	2.67163500	-1.54567900
H	-10.89679300	1.07040300	-2.87880300
H	-9.50118300	4.09760900	-0.15747200
H	-11.22084700	3.26702800	-1.75305800
C	-1.00744300	7.95604100	-1.12530900
C	-1.87948900	8.94317000	-0.65054000
C	-0.40613600	8.13517300	-2.37999600
C	-2.13956300	10.09044900	-1.40427400
H	-2.35796200	8.81447300	0.31714100
C	-0.66461100	9.28003300	-3.13511700
H	0.25473900	7.36731500	-2.77079200
C	-1.53139500	10.26307800	-2.64913100
H	-2.81979500	10.84559900	-1.01922000
H	-0.19121500	9.40330500	-4.10575300
H	-1.73369900	11.15346500	-3.23835500
C	1.00744300	7.95604100	1.12530900
C	1.87948900	8.94317000	0.65054000
C	0.40613600	8.13517300	2.37999600
C	2.13956300	10.09044900	1.40427400
H	2.35796200	8.81447300	-0.31714100
C	0.66461100	9.28003300	3.13511700
H	-0.25473900	7.36731500	2.77079200
C	1.53139500	10.26307800	2.64913100
H	2.81979500	10.84559900	1.01922000
H	0.19121500	9.40330500	4.10575300
H	1.73369900	11.15346500	3.23835500
C	8.04461300	1.13332600	1.00893300
C	9.01409800	0.67781400	1.91019400
C	8.23249200	2.37436500	0.38312700
C	10.15440300	1.43947600	2.17636200
H	8.87761900	-0.27949500	2.40667600
C	9.37022600	3.13740700	0.64913000
H	7.48317200	2.75228400	-0.30674600
C	10.33592900	2.67163500	1.54567900
H	10.89679300	1.07040300	2.87880300
H	9.50118300	4.09760900	0.15747200
H	11.22084700	3.26702800	1.75305800
C	8.04461300	-1.13332600	-1.00893300
C	9.01409800	-0.67781400	-1.91019400
C	8.23249200	-2.37436500	-0.38312700
C	10.15440300	-1.43947600	-2.17636200
H	8.87761900	0.27949500	-2.40667600
C	9.37022600	-3.13740700	-0.64913000
H	7.48317200	-2.75228400	0.30674600

C	10.33592900	-2.67163500	-1.54567900
H	10.89679300	-1.07040300	-2.87880300
H	9.50118300	-4.09760900	-0.15747200
H	11.22084700	-3.26702800	-1.75305800
C	1.12938200	0.99949300	8.00515800
C	0.65503600	1.87751300	8.98716300
C	2.37760700	0.38800300	8.19437500
C	1.40281800	2.13368900	10.13920300
H	-0.30758100	2.36396500	8.85058800
C	3.12671500	0.64236700	9.34410200
H	2.76811900	-0.27755800	7.43044000
C	2.64121200	1.51535200	10.32190000
H	1.01832700	2.81892000	10.89011100
H	4.09237800	0.16097400	9.47527600
H	3.22586600	1.71459200	11.21598400
C	-1.12938200	-0.99949300	8.00515800
C	-0.65503600	-1.87751300	8.98716300
C	-2.37760700	-0.38800300	8.19437500
C	-1.40281800	-2.13368900	10.13920300
H	0.30758100	-2.36396500	8.85058800
C	-3.12671500	-0.64236700	9.34410200
H	-2.76811900	0.27755800	7.43044000
C	-2.64121200	-1.51535200	10.32190000
H	-1.01832700	-2.81892000	10.89011100
H	-4.09237800	-0.16097400	9.47527600
H	-3.22586600	-1.71459200	11.21598400
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C	0.65503600	-1.87751300	-8.98716300
C	2.37760700	-0.38800300	-8.19437500
C	1.40281800	-2.13368900	-10.13920300
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H	2.76811900	0.27755800	-7.43044000
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H	1.01832700	-2.81892000	-10.89011100
H	4.09237800	-0.16097400	-9.47527600
H	3.22586600	-1.71459200	-11.21598400
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C	-2.37760700	0.38800300	-8.19437500
C	-1.40281800	2.13368900	-10.13920300
H	0.30758100	2.36396500	-8.85058800
C	-3.12671500	0.64236700	-9.34410200
H	-2.76811900	-0.27755800	-7.43044000
C	-2.64121200	1.51535200	-10.32190000
H	-1.01832700	2.81892000	-10.89011100
H	-4.09237800	0.16097400	-9.47527600
H	-3.22586600	1.71459200	-11.21598400
C	-1.00744300	-7.95604100	1.12530900
C	-1.87948900	-8.94317000	0.65054000
C	-0.40613600	-8.13517300	2.37999600
C	-2.13956300	-10.09044900	1.40427400

H	-2.35796200	-8.81447300	-0.31714100
C	-0.66461100	-9.28003300	3.13511700
H	0.25473900	-7.36731500	2.77079200
C	-1.53139500	-10.26307800	2.64913100
H	-2.81979500	-10.84559900	1.01922000
H	-0.19121500	-9.40330500	4.10575300
H	-1.73369900	-11.15346500	3.23835500
C	1.00744300	-7.95604100	-1.12530900
C	1.87948900	-8.94317000	-0.65054000
C	0.40613600	-8.13517300	-2.37999600
C	2.13956300	-10.09044900	-1.40427400
H	2.35796200	-8.81447300	0.31714100
C	0.66461100	-9.28003300	-3.13511700
H	-0.25473900	-7.36731500	-2.77079200
C	1.53139500	-10.26307800	-2.64913100
H	2.81979500	-10.84559900	-1.01922000
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H	1.73369900	-11.15346500	-3.23835500