

## Supporting Information

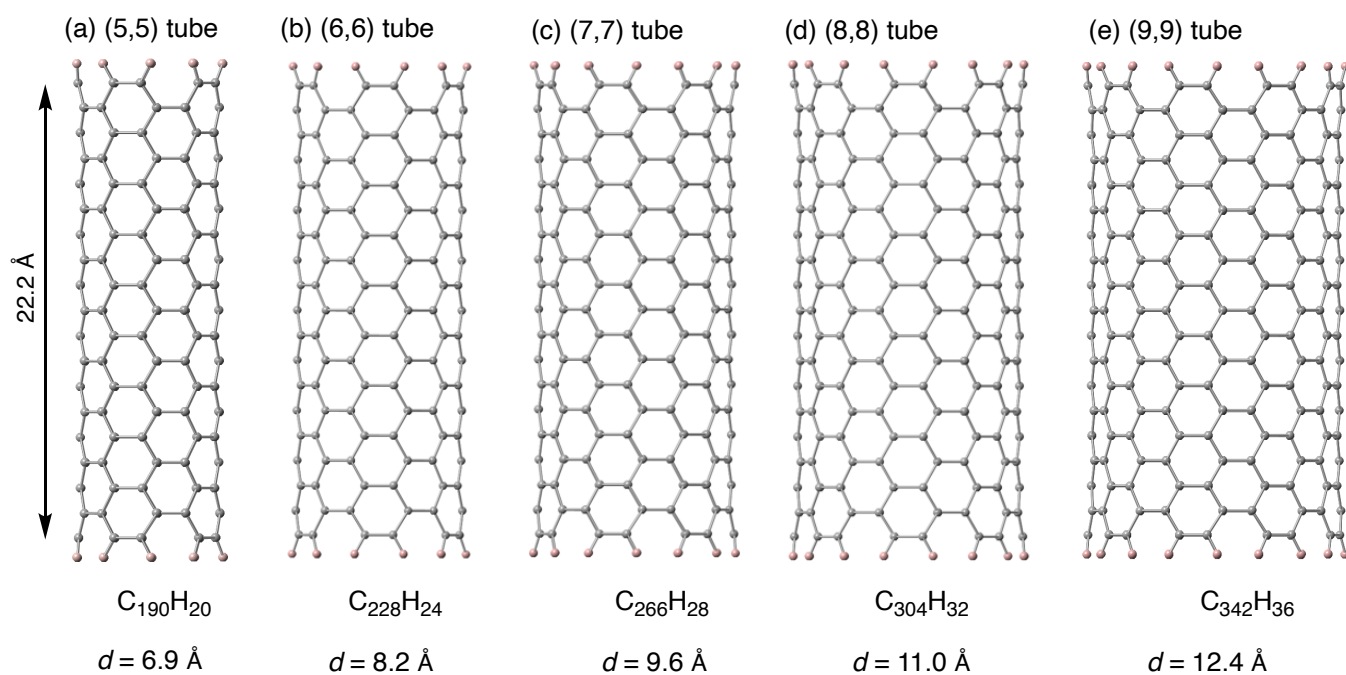
### Theoretical Understandings of Stability of Mechanically Interlocked Carbon Nanotubes and Their Precursors

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## 1. Models of finite-length tubes



**Fig. S1** Optimized structures for finite-length ( $a,a$ ) tubes: (a)  $a = 5$ , (b)  $a = 6$ , (c)  $a = 7$ , (d)  $a = 8$ , and (e)  $a = 9$ . Their tube lengths are 22.2 Å. The optimized tube diameters ( $d$ ) are also given.

## 2 Potential energy surfaces (PESs) of benzene approaching naphthalene

Figure S2 shows PESs of benzene approaching naphthalene in T-shaped and stacking alignments, obtained from our previous study (Ref. 53). According to the energy scanning analyses in Ref. 53, we found attractive interactions originated from CH- $\pi$  and  $\pi$ - $\pi$  interactions between benzene and naphthalene, represented by  $E_{\min}$  values. The local minima of the T-shaped and stacking complexes have the  $E_{\min}$  values of -4.6 and -3.2 kcal/mol at the equilibrium internuclear separations ( $S_e$ ) of 2.87 and 3.65 Å, respectively. Their key parameters are summarized in Table S1. With respect to both equilibrium structures, we newly obtained the height of C<sub>6</sub>H<sub>6</sub> from C<sub>8</sub>H<sub>10</sub> is also given as  $H_e$ . In the equilibrium T-shaped structure, the distance of an H benzene atom neighboring to naphthalene, from the naphthalene plane is defined as the height. In the equilibrium stacking complex, the distance of the center of benzene from that of naphthalene is defined as the height. By using the definition, the  $H_e$  values in the T-shaped and stacking complexes are 2.5 and 3.6 Å, respectively.

In addition, we focus on C<sub>6</sub>H<sub>6</sub>-C<sub>8</sub>H<sub>10</sub> complexes that are energetically identical to the dissociation limit toward C<sub>6</sub>H<sub>6</sub> and C<sub>8</sub>H<sub>10</sub> to represent the internuclear separation denoting the  $S_0$  value. The  $S_0$  values in the T-shaped and stacking complexes are 2.50 and 3.19 Å, respectively, according to Ref. 53. The corresponding  $H_0$  values are newly listed in Table S1: The  $H_0$  values in the T-shaped and stacking structures are 2.1 and 3.1, respectively. When separations between benzene and naphthalene further decrease from the  $S_0$  and  $H_0$  value, benzene and naphthalene begin to interact in repulsive manners. Thus,

the  $S_0$  value is the smallest limit of internuclear separation between  $C_6H_6$  and  $C_8H_{10}$  without any long-range repulsive interactions.

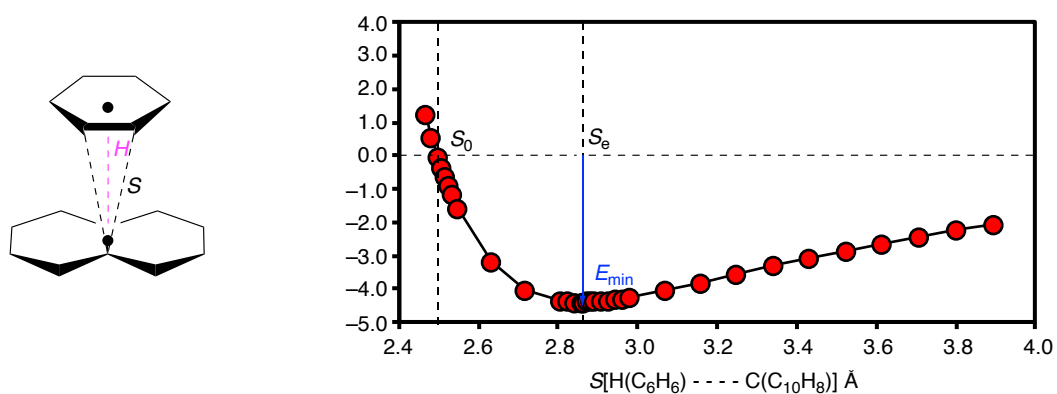
**Table S1.** Key parameters in the potential energy surfaces of benzene approaching naphthalene with two orientation models given in Figure S2.

Models	Stacking model <sup>a</sup>	T-shaped model <sup>a</sup>
Interactions	$\pi$ - $\pi$ interactions	CH- $\pi$ interactions
$S_0$ ( $H_0$ ) <sup>b</sup>	3.15 (3.1)	2.50 (2.1)
$S_c$ ( $H_c$ ) <sup>c</sup>	3.65 (3.6)	2.86 (2.5)
$E_{\min}$ <sup>d</sup>	-3.2	-4.6

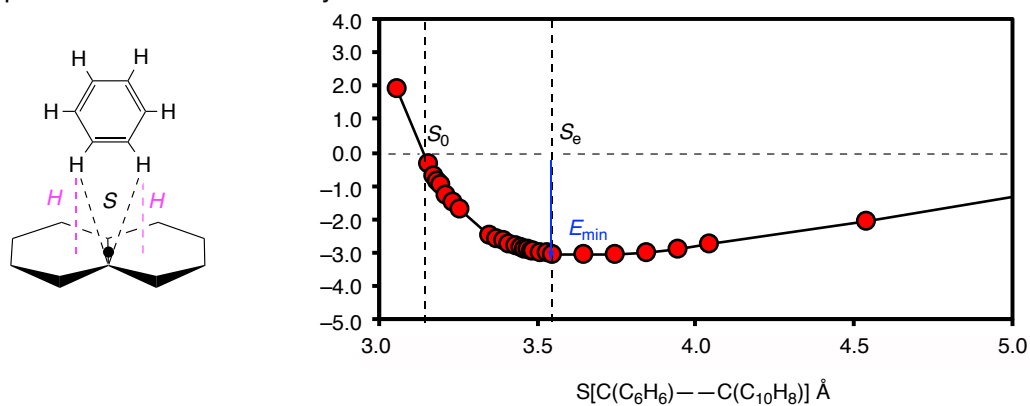
- a) The two models can be seen in Figure S2.
- b) Internuclear separation ( $S_0$  in Å) in a  $C_6H_6$ - $C_8H_{10}$  complex is energetically identical to the dissociation limit toward  $C_6H_6$  and  $C_8H_{10}$ . In T-shaped models, their heights, defined in Figure S2, are given as  $H_0$  in parentheses whose units are in Å.
- c) Internuclear separation ( $S_c$  in Å) in the local minimum of a  $C_6H_6$ - $C_8H_{10}$  complex. In T-shaped models, their heights, defined in Figure S2, are given as  $H_c$  in parentheses whose unit in Å.
- d) Stabilization energy ( $E_{\min}$  in kcal/mol) of the local minimum of a  $C_6H_6$ - $C_8H_{10}$  complex, measured from the dissociation limit toward  $C_6H_6$  and  $C_8H_{10}$ .



(a) stacking orientation stabilized by  $\pi$ - $\pi$  interactions



(b) T-shaped orientation stabilized by CH- $\pi$  interactions



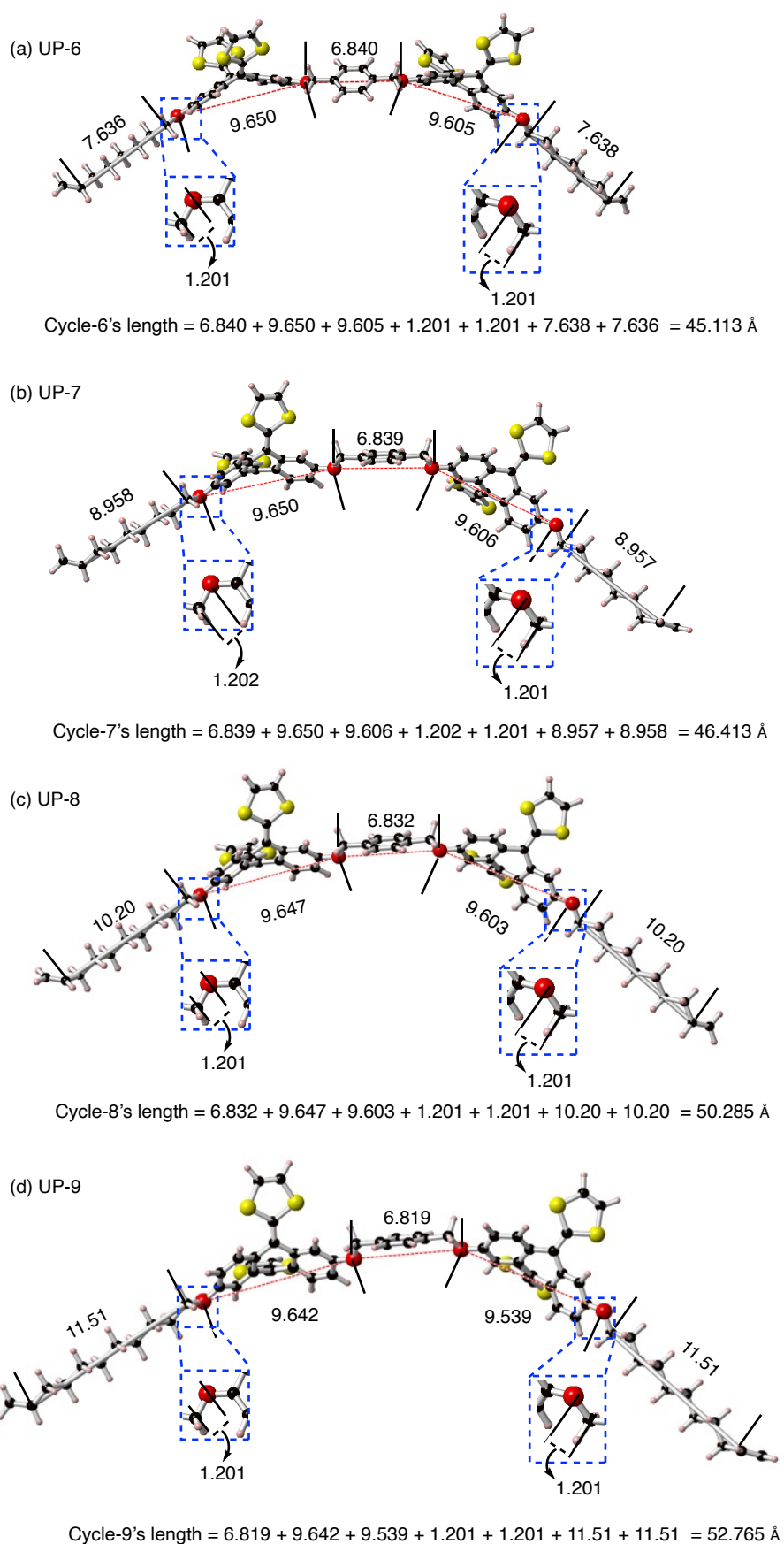
**Fig. S2** Potential energy surfaces (PESs) for benzene approaching naphthalene as a function of atom separations ( $S$ ), obtained from B97D calculations. We also define height of benzene from naphthalene as  $H$  in this figure. There are two types of orientation constructed by benzene and naphthalene: (a) stacking orientation and (b) T-shaped orientation that are stabilized by  $\pi$ - $\pi$  and CH- $\pi$  interactions, respectively. Key parameters in PESs ( $E_{\text{min}}$ , as well as  $S_0$  and  $S_e$  and their corresponding height ( $H_0$  and  $H_e$ )) are defined in this figure and listed in Table S1.

### 3. Lengths of optimized UP- $n$ structures ( $L$ )

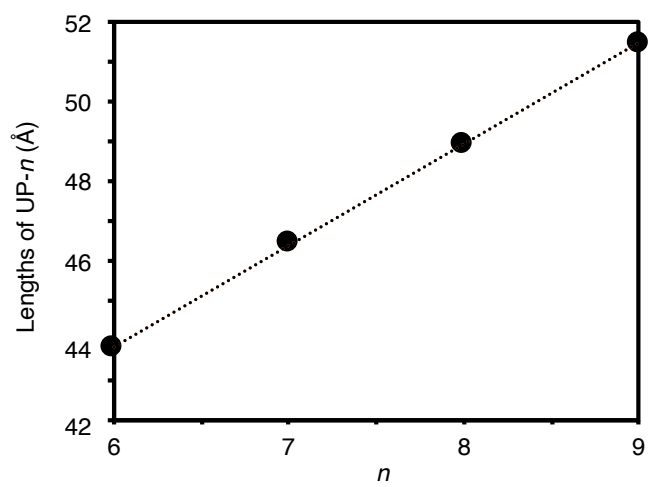
Lengths of optimized UP- $n$  structures in Å are calculated according to Figure S3. Then, we plotted lengths of optimized UP- $n$  structures are a function of  $n$  ( $6 \leq n \leq 9$ ) in Figure S4. Then, we found that the  $L$  values increase in a linear fashion against  $n$ , fitted by the following equation.

$$L = 2.52 \times n + 28.55 \quad (\text{S1})$$

The fitting equation can be used for predicting lengths of optimized UP- $n$  structures, even when  $n$  is large than 9.



**Fig. S3** Three optimized structures for a UP-shaped precursor of *p*-xylene-linked bis-exTTF terminated by an alkyl ( $C_nH_{2n}$ ) linker with terminate ethene (UP-*n*), where *n* is 6~9.

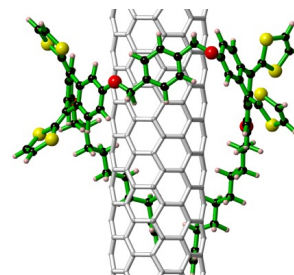
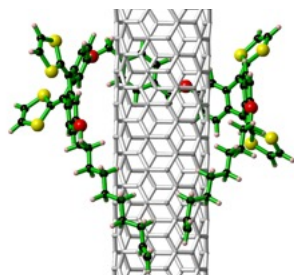
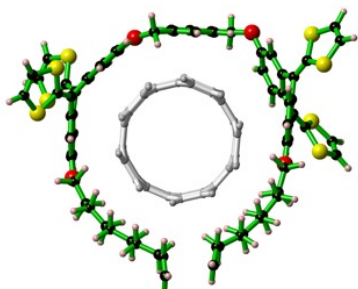


**Fig. S4** Lengths of UP- $n$  in Å are plotted as a function of  $n$ .

#### 4. Optimized structures for UP-8-( $a,a$ ) and UP-9-( $a,a$ )

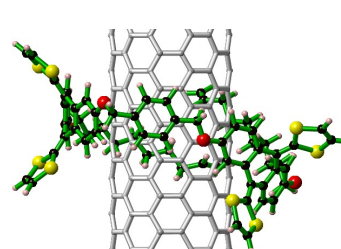
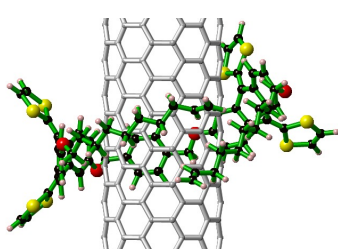
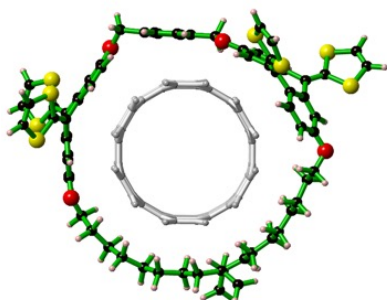
(a) UP-8-(5,5)

$$E_{\text{stabilize}} = -70.2 \text{ kcal/mol}$$



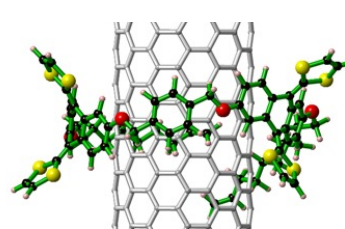
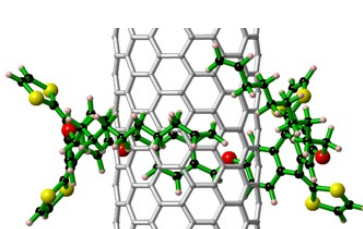
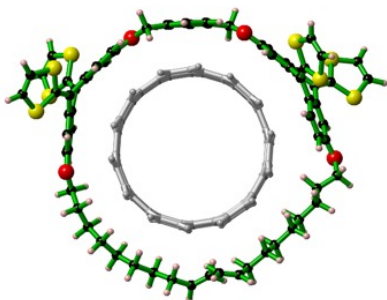
(b) UP-8-(6,6)

$$E_{\text{stabilize}} = -71.2 \text{ kcal/mol}$$



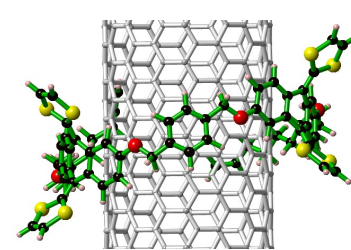
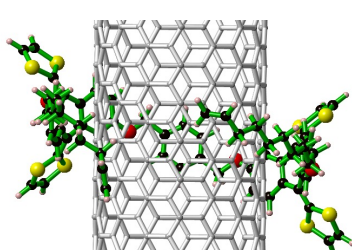
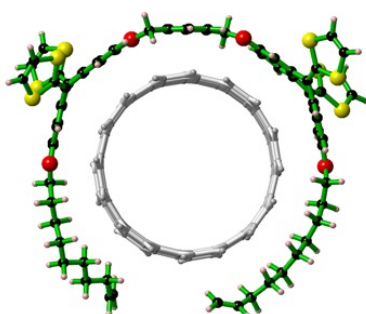
(c) UP-8-(7,7)

$$E_{\text{stabilize}} = -74.2 \text{ kcal/mol}$$



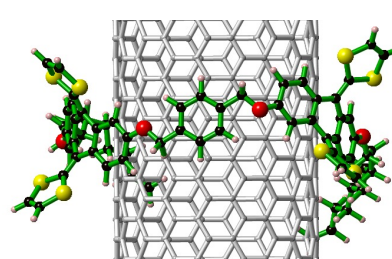
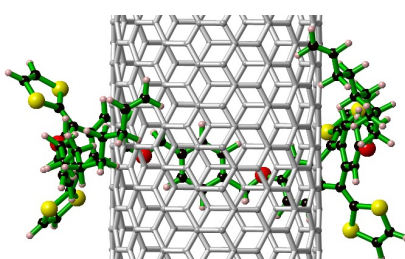
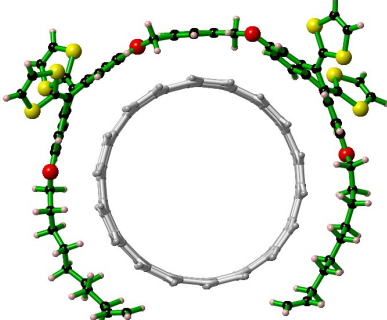
(d) UP-8-(8,8)

$$E_{\text{stabilize}} = -78.5 \text{ kcal/mol}$$



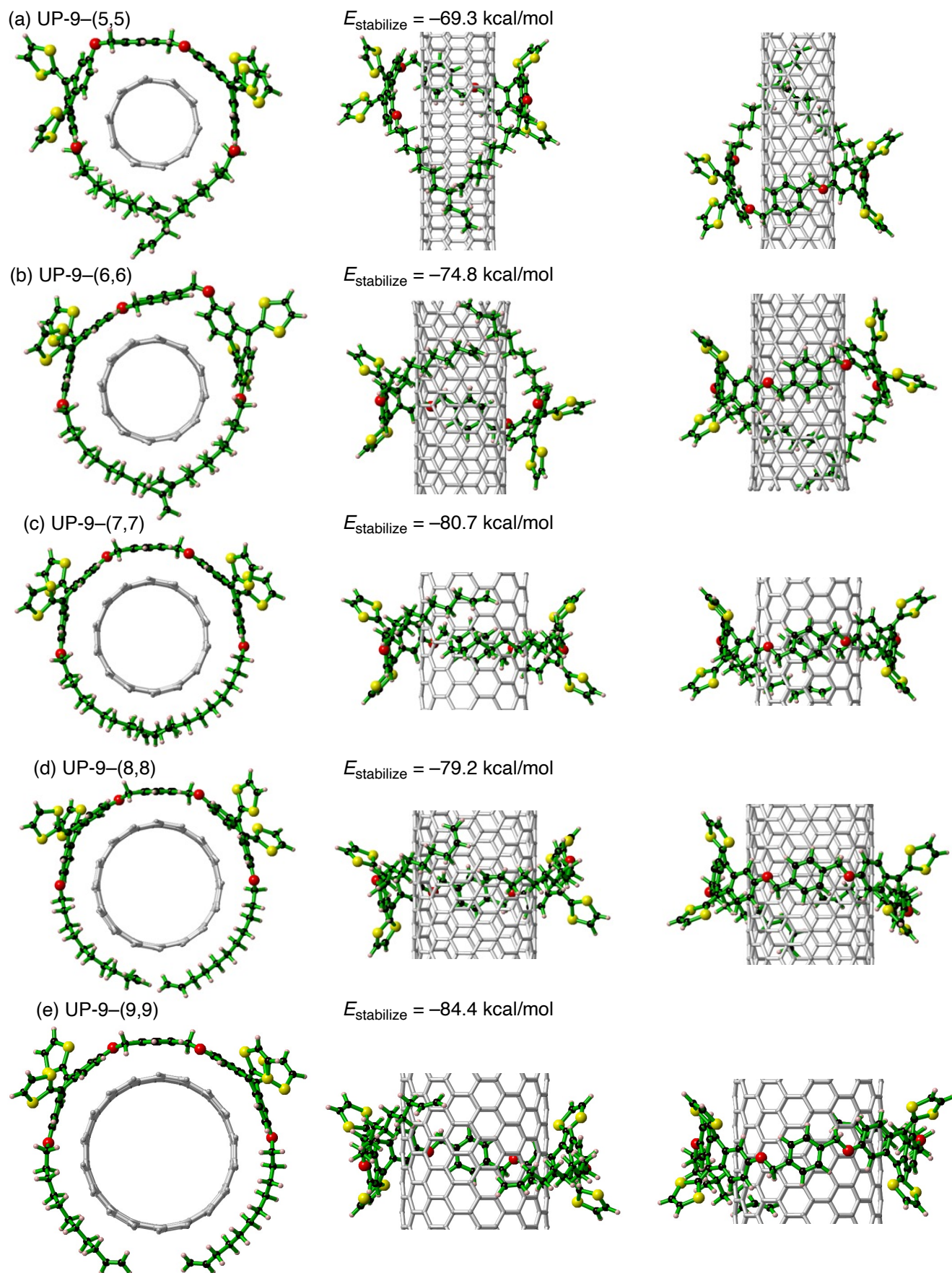
(e) UP-8-(9,9)

$$E_{\text{stabilize}} = -79.4 \text{ kcal/mol}$$



**Fig. S5** Optimized structures for an ( $a,a$ ) tube weakly bound by a UP-shaped bis-exTTF precursor (UP- $n$ ) where  $n$  is 8 (UP-8-( $a,a$ )): (a)  $a = 5$ , (b)  $a = 6$ , (c)  $a = 7$ , (d)  $a = 8$ , and (e)  $a = 9$ . Their stabilization energies ( $E_{\text{stabilize}}$  values) are given.





**Fig. S6** Optimized structures for an  $(a,a)$  tube weakly bound by a UP-shaped bis-exTTF precursor (UP- $n$ ) where  $n$  is 9 (UP-9- $(a,a)$ ): (a)  $a = 5$ , (b)  $a = 6$ , (c)  $a = 7$ , (d)  $a = 8$ , and (e)  $a = 9$ . Their stabilization energies ( $E_{\text{stabilize}}$  values) are given.

## 5. Energy decomposition analyses of $E_{\text{stabilize}}$ values

The stabilization energies of the UP- $n$ -( $a,a$ ) structures ( $E_{\text{stabilize}}$ ), defined in the equation (1), are decomposed to three energy components, host-guest interactions between the UP- $n$  and ( $a,a$ ) tube ( $E_{\text{long-range}}$ ), and both the energy penalties required for the deformation of a UP- $n$  or a tube, when a UP- $n$  wraps around a tube to form a UP- $n$ -( $m,m$ ) structure ( $E_{\text{deform(UP)}}$  and  $E_{\text{deform(tube)}}$ , respectively). The three energy components are defined in the following equations.

$$E_{\text{long-range}}(\text{UP-}n\text{-(}a,a\text{)}) = E(\text{UP-}n\text{-(}a,a\text{)}) - E(\text{UP-}n \text{ from UP-}n\text{-(}a,a\text{)}) - E(\text{tube from UP-}n\text{-(}a,a\text{)}) \quad (\text{S2})$$

$$E_{\text{deform(UP)}} = E(\text{UP-}n \text{ from UP-}n\text{-(}a,a\text{)}) - E(\text{UP-}n) \quad (\text{S3})$$

$$E_{\text{deform(tube)}} = E(\text{tube from UP-}n\text{-(}a,a\text{)}) - E(\text{tube}) \quad (\text{S4})$$

Here,  $E(\text{UP-}n \text{ from UP-}n\text{-(}a,a\text{)})$  and  $E(\text{tube from UP-}n\text{-(}a,a\text{)})$  are the total energies of a UP- $n$  and a tube taken from the optimized UP- $n$ -( $m,m$ ) structure, respectively, as well as  $E(\text{UP-}n)$  and  $E(\text{tube})$  are those of the optimized UP- $n$  and tube structures, respectively.

Similarly, the stabilization energy of an ( $a,b$ )@Cycle- $n$  structure ( $E_{\text{stabilize}}$ ), defined in the equation (2), are decomposed to three energy values, host-guest interactions between the Cycle- $n$  and ( $a,b$ ) tube ( $E_{\text{long-range}}$ ), and both the energy penalties required for the

deformation of a Cycle- $n$  or a tube, when an  $(a,b)@Cycle-n$  structure is formed ( $E_{\text{deform}}(\text{Cycle})$  and  $E_{\text{deform}}(\text{tube})$ , respectively). We defined the three energy components, as follow.

$$E_{\text{long-range}}((a,b)@Cycle-n) = E((a,b)@Cycle-n) - E(\text{Cycle-}n \text{ from } (a,b)@Cycle-n) - E(\text{tube from } (a,b)@Cycle-n) \quad (\text{S5})$$

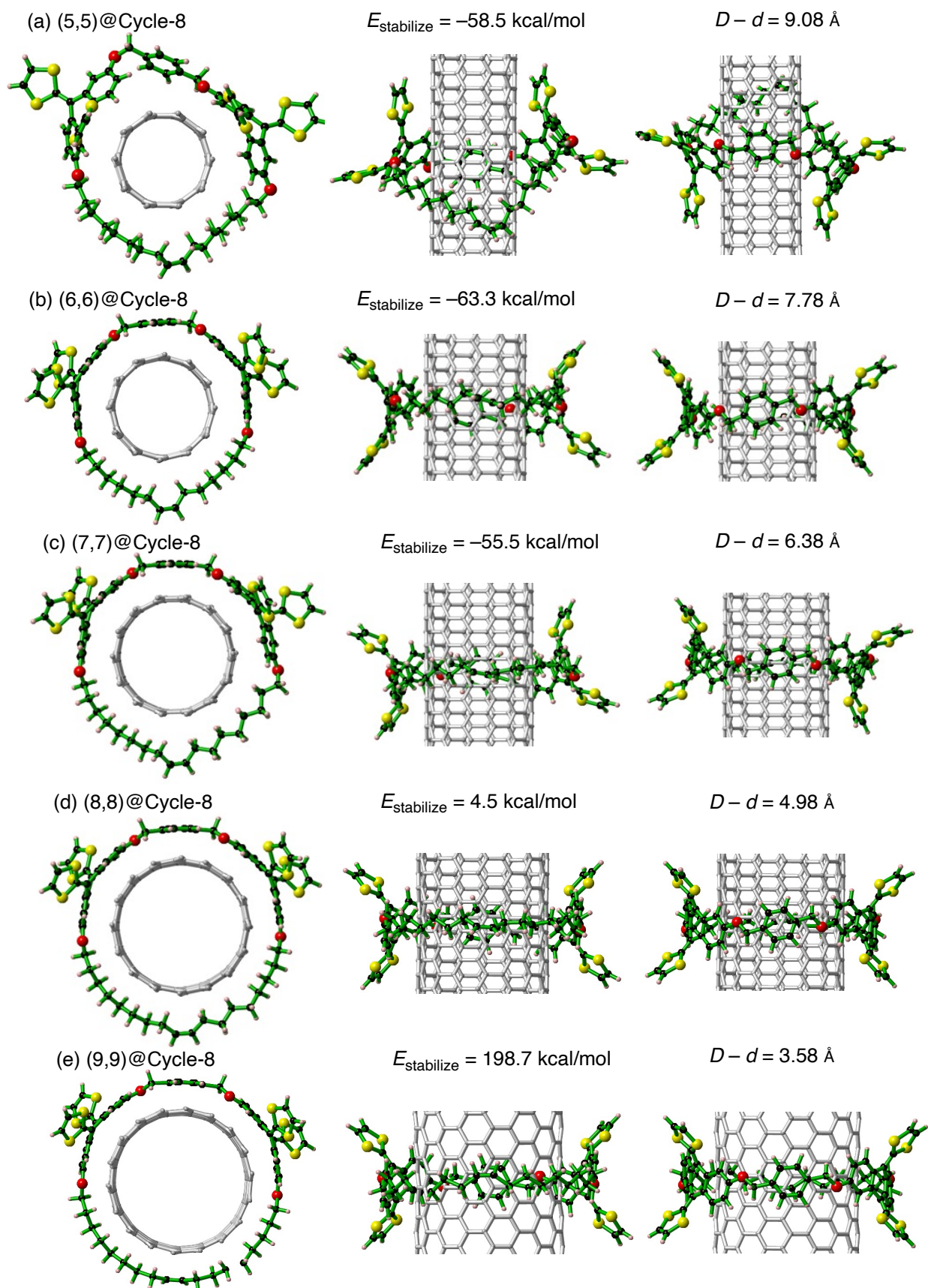
$$E_{\text{deform}}(\text{Cycle}) = E(\text{Cycle-}n \text{ from } (a,b)@Cycle-n) + E(\text{C}_2\text{H}_4) - E(\text{UP-}n) \quad (\text{S6})$$

$$E_{\text{deform}}(\text{tube}) = E(\text{tube from } (a,b)@Cycle-n) - E(\text{tube}) \quad (\text{S7})$$

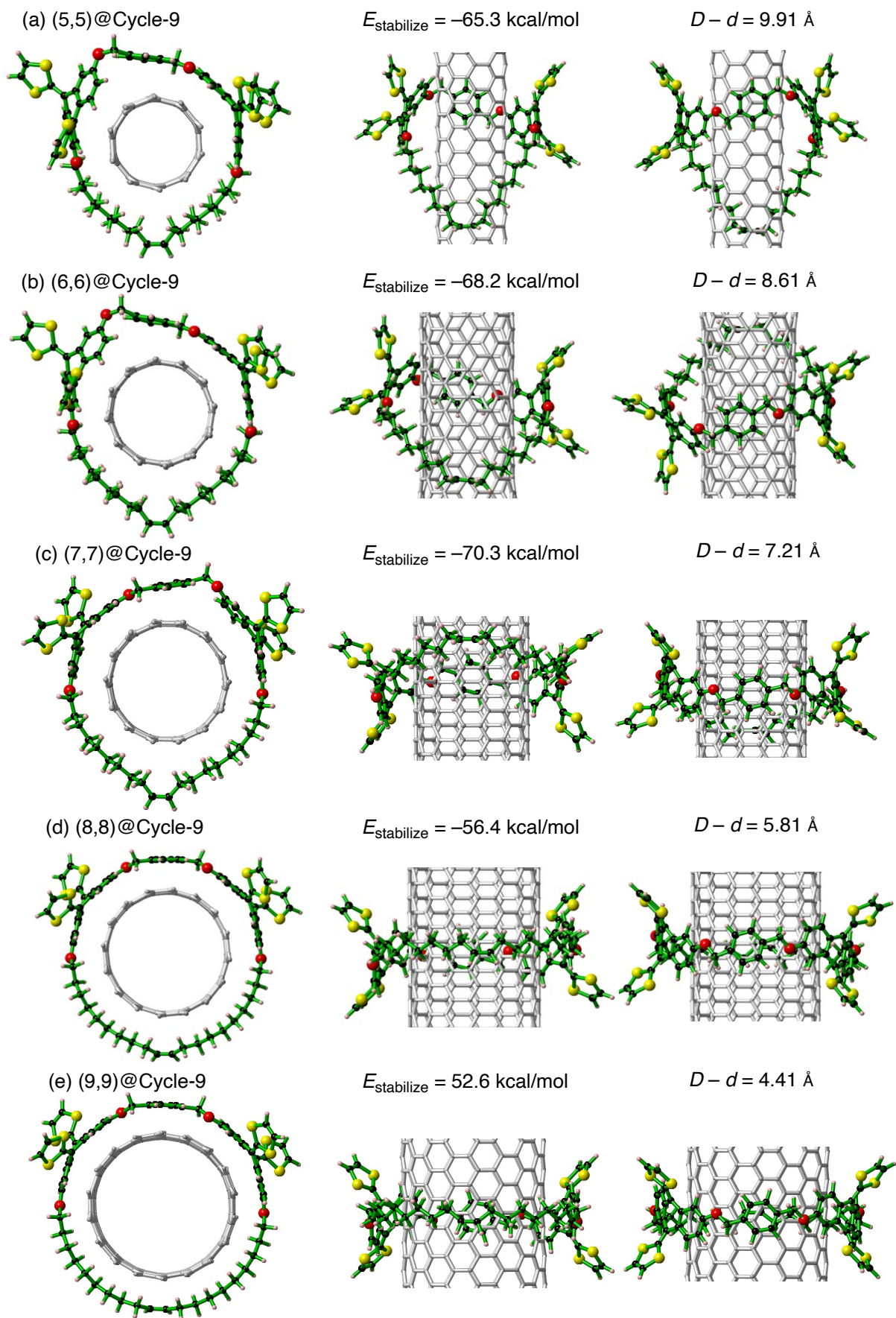
Here,  $E(\text{Cycle-}n \text{ from } (a,b)@Cycle-n)$  and  $E(\text{tube from } (a,b)@Cycle-n)$  are the total energies of a Cycle- $n$  and a tube taken from the optimized  $(a,b)@Cycle-n$  structure, respectively, as well as  $E(\text{C}_2\text{H}_4)$  is that of the optimized  $\text{C}_2\text{H}_4$  structure.



## 6. Optimized structures for $(a,a)$ @Cycle-8, $(a,a)$ @Cycle-9 plus $(10,10)$ @Cycle-9

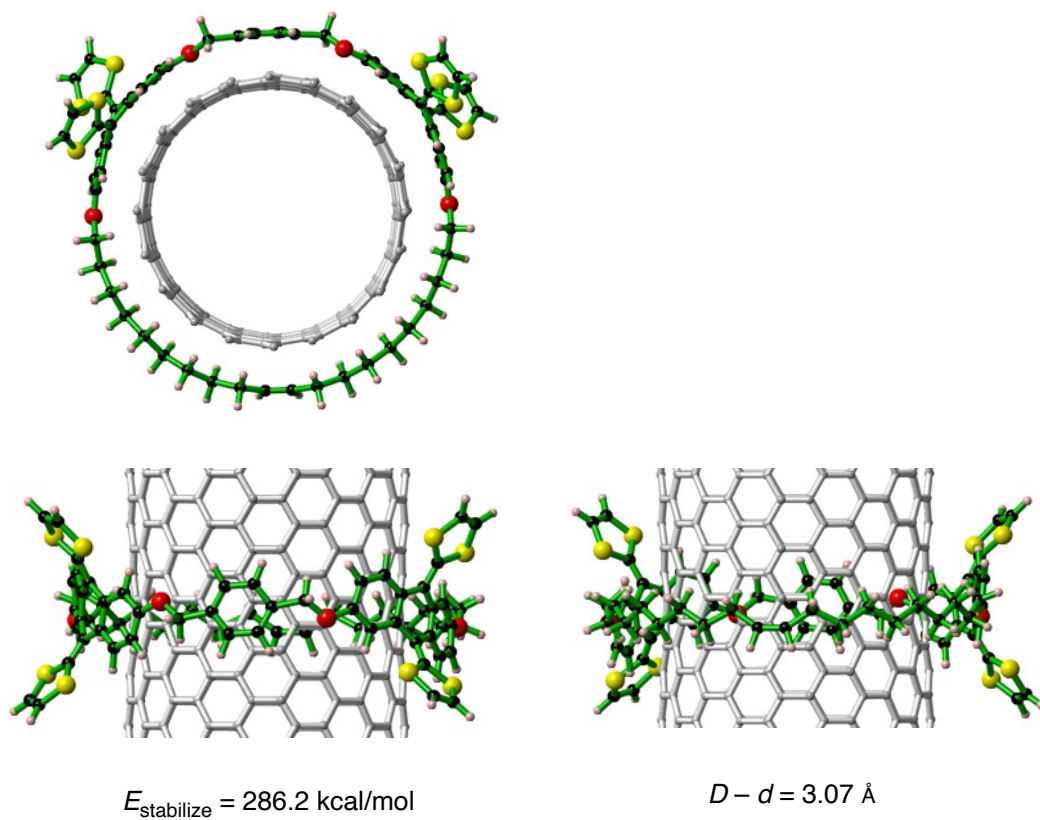


**Fig. S7** Optimized structures for an  $(a,a)$  tube inside the macrocycle formed by ring-closing metathesis of UP-8- $(a,a)$  ( $(a,a)$ @Cycle-8): (a)  $a = 5$ , (b)  $a = 6$ , (c)  $a = 7$ , (d)  $a = 8$ , and (e)  $a = 9$ . Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.



**Fig. S8** Optimized structures for an  $(a,a)$  tube inside the macrocycle formed by ring-closing metathesis of UP-9- $(a,a)$  ( $(a,a)$ @Cycle-9): (a)  $a = 5$ , (b)  $a = 6$ , (c)  $a = 7$ , (d)  $a = 8$ , and (e)  $a = 9$ . Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.

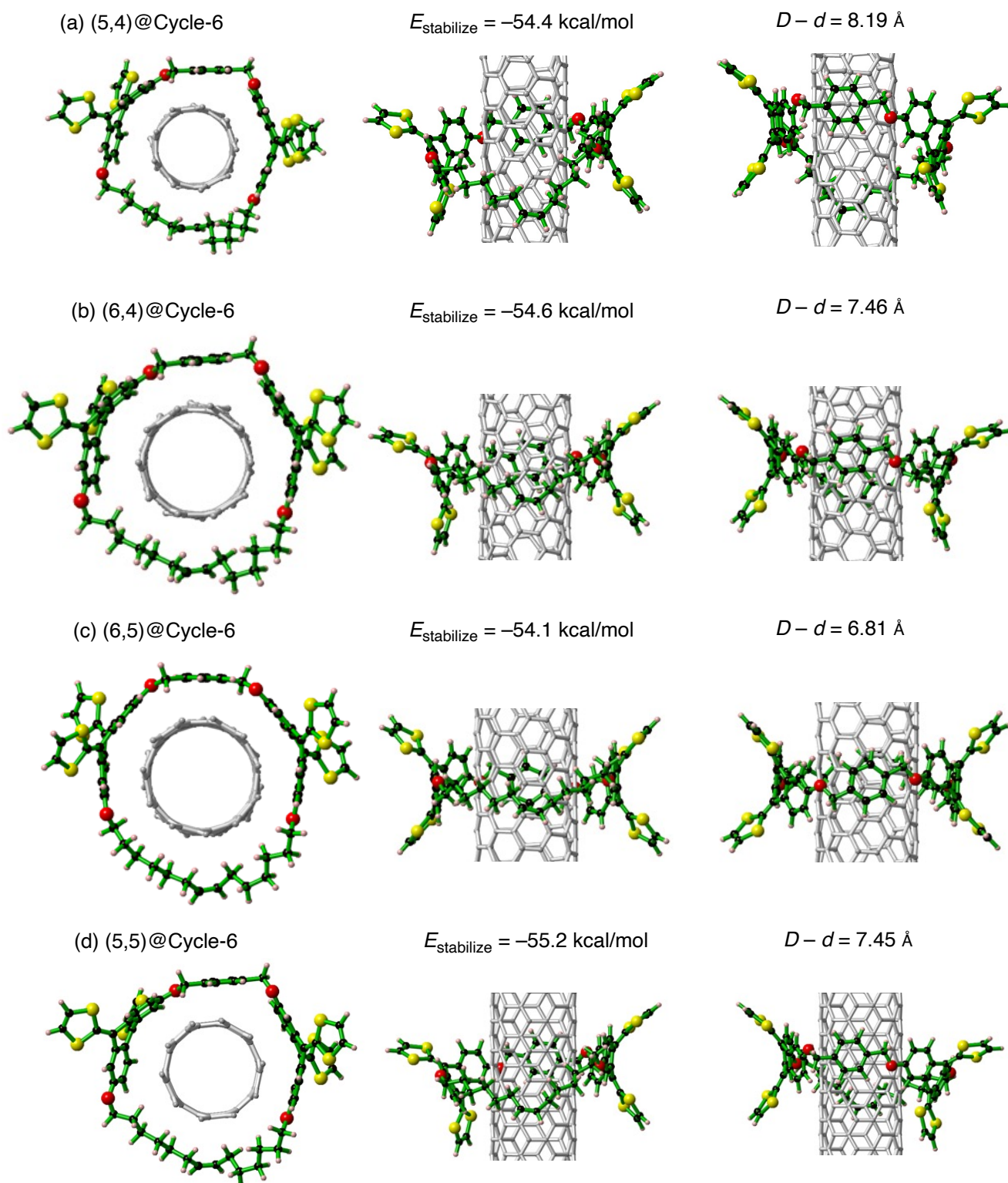
(10,10)@Cycle-9



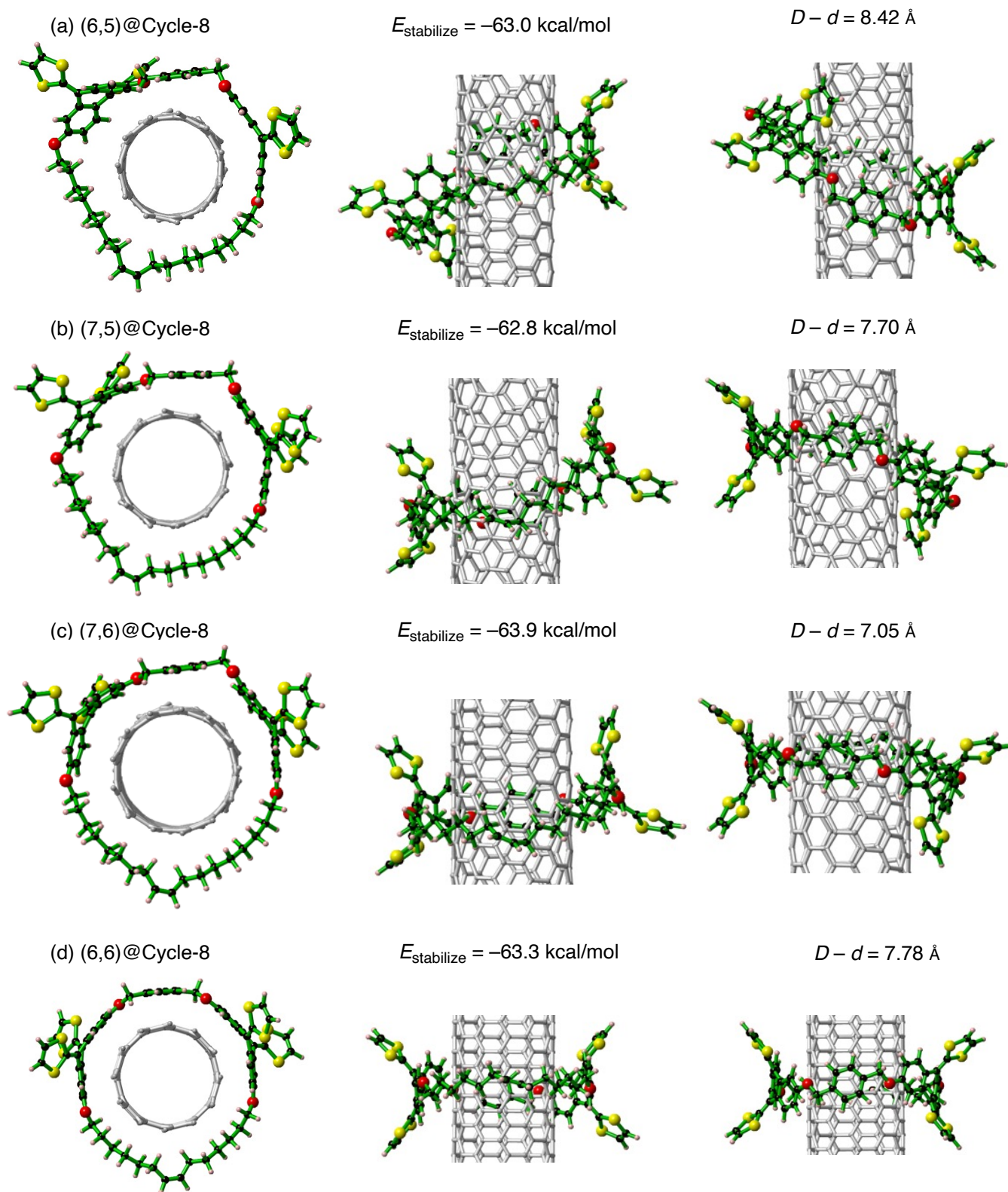
**Fig. S9** Optimized structures for (10,10)@Cycle-9. Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.



## 7. Optimized structures for $(a,b)$ @Cycle- $n$

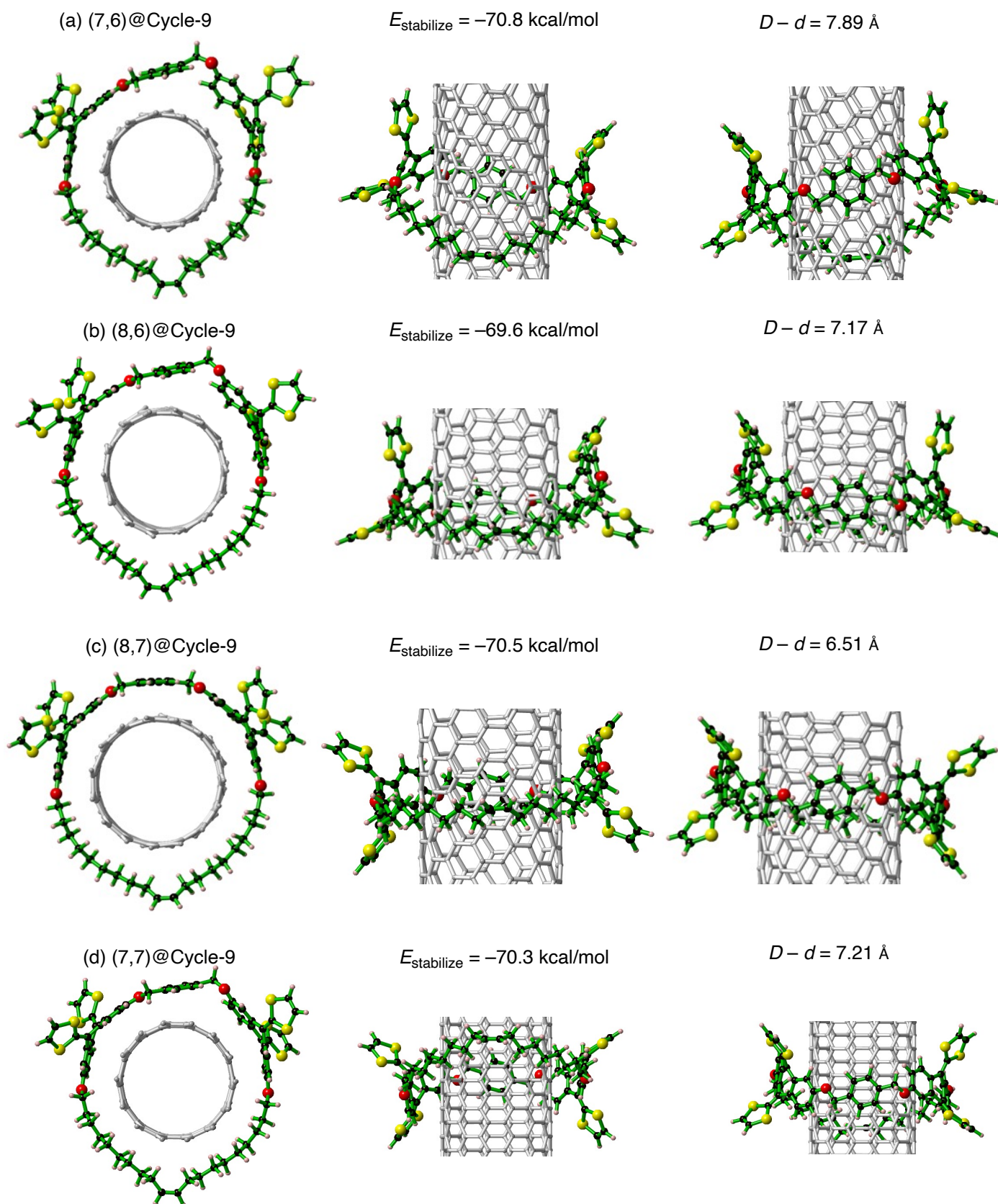


**Fig. S10** Optimized  $(a,b)$ @Cycle-6 structures having tube chirality near that of the armchair tube of the most stable (5,5)@Cycle-6 at  $n = 6$ : (a)  $(a,b) = (5,4)$ , (b)  $(a,b) = (6,4)$ , and (c)  $(a,b) = (6,5)$ . For comparison, the (5,5)@Cycle-6 structure is also given in (d). Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.



**Fig. S11** Optimized  $(a,b)$ @Cycle-8 structures having tube chirality near that of the armchair tube of the most stable (6,6)@Cycle-8 at  $n = 8$ : (a)  $(a,b) = (6,5)$ , (b)  $(a,b) = (7,5)$ , and (c)  $(a,b) = (7,6)$ . For comparison, the (6,6)@Cycle-8 structure is also given in (d). Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.





**Fig. S12** Optimized  $(a,b)$ @Cycle-9 structures having tube chirality near that of the armchair tube of the most stable  $(7,7)$ @Cycle-9 at  $n = 9$ : (a)  $(a,b) = (7,6)$ , (b)  $(a,b) = (8,6)$ , and (c)  $(a,b) = (8,7)$ . For comparison, the  $(7,7)$ @Cycle-9 structure is also given in (d). Their stabilization energies ( $E_{\text{stabilize}}$  values) and  $D - d$  values are given.

## 8. Optimized lengths of $sp^3$ CC bonds in the macrocycle in $(a,a)@Cycle-n$

With respect to the macrocycle deformation in the  $(a,a)@Cycle-n$  structures whose  $D - d$  values are less than 5 Å, we found significant elongation of  $sp^3$  CC bonds in alkyl chains (up to 1.67 Å), relative to those of structures whose  $D - d$  values are larger than 5 Å (around 1.55 Å, being close to the typical  $sp^3$  CC bonds<sup>59</sup>), as shown in Table S2. The  $sp^3$  CC bond elongation in alkyl chains causes high energy penalty, although it partially reduces the number of atom contacts between which repulsive CH- $\pi$  and  $\pi$ - $\pi$  interactions operate in  $(m,m)@Cycle-n$  structures. As a result, the  $(m,m)@Cycle-n$  structures whose  $D - d$  values are less than 5 Å are destabilized.

**Table S2.** Optimized lengths in Å of  $sp^3$  CC bonds in the macrocycle in  $(m,m)@Cycle-n$

<b>(5,5)@Cycle-6</b> <b>(<math>D-d = 7.45</math> Å)</b>	1.538, 1.542, 1.542, 1.536, 1.544, 1.508, 1.510, 1.552, 1.540, 1.543, 1.541, 1.527
<b>(6,6)@Cycle-6</b> <b>(<math>D-d = 6.15</math> Å)</b>	1.536, 1.549, 1.548, 1.547, 1.558, 1.513, 1.510, 1.561, 1.554, 1.544, 1.549, 1.535
<b>(7,7)@Cycle-6</b> <b>(<math>D-d = 4.75</math> Å)</b>	1.581, 1.601, 1.595, 1.596, 1.600, 1.522, 1.541, 1.601, 1.613, 1.587, 1.601, 1.579
<b>(5,5)@Cycle-8</b> <b>(<math>D-d = 9.11</math> Å)</b>	1.530, 1.538, 1.536, 1.535, 1.536, 1.538, 1.546, 1.516, 1.508, 1.544, 1.539, 1.535, 1.538, 1.538, 1.543, 1.527
<b>(6,6)@Cycle-8</b> <b>(<math>D-d = 7.74</math> Å)</b>	1.530, 1.538, 1.537, 1.537, 1.536, 1.538, 1.550, 1.511, 1.507, 1.548, 1.537, 1.537, 1.539, 1.539, 1.544, 1.528
<b>(7,7)@Cycle-8</b> <b>(<math>D-d = 6.37</math> Å)</b>	1.535, 1.550, 1.543, 1.548, 1.548, 1.541, 1.553, 1.512, 1.513, 1.555, 1.545, 1.546, 1.548, 1.549, 1.550, 1.535
<b>(8,8)@Cycle-8</b> <b>(<math>D-d = 4.99</math> Å)</b>	1.569, 1.583, 1.584, 1.581, 1.580, 1.585, 1.584, 1.541, 1.538, 1.590, 1.581, 1.575, 1.603, 1.576, 1.585, 1.566

<b>(9,9)@Cycle-8</b> <b>(D-d = 3.61 Å)</b>	1.632, 1.657, 1.638, 1.684, 1.646, 1.644, 1.665, 1.596, 1.595, 1.664, 1.642, 1.649, 1.651, 1.652, 1.646, 1.628
<b>(5,5)@Cycle-9</b> <b>(D-d = 9.25 Å)</b>	1.525, 1.539, 1.536, 1.538, 1.536, 1.536, 1.536, 1.551, 1.509, 1.510, 1.550, 1.537, 1.536, 1.536, 1.539, 1.537, 1.541, 1.525
<b>(6,6)@Cycle-9</b> <b>(D-d = 8.58 Å)</b>	1.526, 1.544, 1.538, 1.539, 1.538, 1.536, 1.538, 1.549, 1.508, 1.508, 1.550, 1.537, 1.537, 1.537, 1.539, 1.538, 1.540, 1.526
<b>(7,7)@Cycle-9</b> <b>(D-d = 7.21 Å)</b>	1.527, 1.541, 1.539, 1.538, 1.538, 1.537, 1.536, 1.547, 1.507, 1.507, 1.549, 1.535, 1.537, 1.538, 1.540, 1.540, 1.544, 1.528
<b>(8,8)@Cycle-9</b> <b>(D-d = 5.32 Å)</b>	1.545, 1.555, 1.556, 1.553, 1.555, 1.555, 1.550, 1.557, 1.520, 1.520, 1.557, 1.551, 1.553, 1.554, 1.554, 1.555, 1.553, 1.540
<b>(9,9)@Cycle-9</b> <b>(D-d = 4.45 Å)</b>	1.597, 1.600, 1.600, 1.596, 1.601, 1.602, 1.598, 1.609, 1.561, 1.559, 1.610, 1.595, 1.599, 1.600, 1.599, 1.600, 1.596, 1.583
<b>(10,10)@Cycle-9</b> <b>(D-d = 3.07 Å)</b>	1.658, 1.680, 1.676, 1.682, 1.679, 1.683, 1.673, 1.695, 1.627, 1.628, 1.689, 1.679, 1.684, 1.681, 1.674, 1.680, 1.682, 1.669



## 9. Full lists in Refs. 32 and 39

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

## 10. Energies of the optimized geometries, and their Cartesian Coordinates.

10-1. Energies in the optimized geometries for discussion in the main text.

	Total energy in Hartree	BSSE-corrected energy in Hartree
UP-6	-5958.00923548	–
UP-8	-6115.15997155	–
UP-9	-6193.73532113	–
(5,5) tube	-7247.38118947	–
(6,6) tube	-8697.28297945	–
(7,7) tube	-10147.1292194	–
(8,8) tube	-11596.9407313	–
(9,9) tube	-13046.7297408	–
(10,10) tube	-14496.5026810	–
UP-6-(5,5)	-13205.5257409	-13205.491852397500
UP-6-(6,6)	-14655.4310638	-14655.396681160210
UP-6-(7,7)	-16105.2864605	-16105.251385023850
UP-8-(5,5)	-13362.689183	-13362.653067247770
UP-8-(6,6)	-14812.5918457	-14812.556456221300
UP-8-(7,7)	-16262.4447298	-16262.407426582130
UP-8-(8,8)	-17712.2637525	-17712.225754807740
UP-8-(9,9)	-19162.0545704	-19162.016247263110
UP-9-(5,5)	-13441.2633574	-13441.226911963220
UP-9-(6,6)	-14891.1724287	-14891.137453582830
UP-9-(7,7)	-16341.0319202	-16340.993122401110
UP-9-(8,8)	-17790.8417152	-17790.802192140280
UP-9-(9,9)	-19240.6387520	-19240.599589668050
(5,5)@Cycle-6	-13126.9756320	-13126.943786812360
(6,6)@Cycle-6	-14576.8723805	-14576.837236124260
(7,7)@Cycle-6	-16026.5872053	-16026.543418953310
(5,5)@Cycle-8	-13284.1302190	-13284.099701150940
(6,6)@Cycle-8	-14734.0418430	-14734.009219679890
(7,7)@Cycle-8	-16183.8795256	-16183.843035624120
(8,8)@Cycle-8	-17633.6034411	-17633.558970019310
(9,9)@Cycle-8	-19083.1024704	-19083.039120635000
(5,5)@Cycle-9	-13362.7201932	-13362.685955405160
(6,6)@Cycle-9	-14812.6268124	-14812.592379092070
(7,7)@Cycle-9	-16262.4771228	-16262.441978316810
(8,8)@Cycle-9	-17712.2721613	-17712.231320724580
(9,9)@Cycle-9	-19161.8967911	-19161.846638860670
(10,10)@Cycle-9	-20611.3026259	-20611.236189032180

10-2. Cartesian coordinates of the optimized geometries listed in the above table.

**UP-6**

C	0.49688500	-1.15647300	-3.16371900
C	-0.88454600	-1.02737600	-2.95403900
C	-1.45969200	-1.42451000	-1.73695100
C	-0.62931600	-1.94610400	-0.72489500
C	0.74672100	-2.07421900	-0.93368200
C	1.32273100	-1.68416600	-2.15919800
H	0.93747800	-0.83438300	-4.10920900
H	-1.51791800	-0.60536800	-3.73670500
H	-1.07206200	-2.23582100	0.22809000
H	1.39003700	-2.46451700	-0.14484600
C	2.80257400	-1.86653700	-2.40142200
H	3.10874900	-1.37548200	-3.34214800
H	3.05454700	-2.94047400	-2.48711000
C	-2.95405100	-1.33441100	-1.53397200
H	-3.42042100	-0.73670900	-2.33701100
H	-3.41386400	-2.34041900	-1.55759200
O	3.52402900	-1.30557900	-1.29094500
O	-3.21289200	-0.73333800	-0.25254500
C	-4.51360100	-0.70597800	0.18229700
C	-5.61818100	-1.10758400	-0.58943600
C	-4.71490100	-0.19869300	1.48050600
C	-6.92186000	-1.05768500	-0.05625600
H	-5.48278300	-1.41445400	-1.62312300
C	-6.00915800	-0.11241500	1.99510400
H	-3.85418300	0.14462800	2.05308400
C	-8.11774300	-1.46143100	-0.83295900
C	-7.13023500	-0.55434700	1.26071400
H	-6.15549800	0.33686200	2.97696300
C	-9.28333400	-0.57327800	-0.61180800
C	-8.52368800	-0.46744600	1.75712600
C	-10.15480300	-0.16000400	-1.63331400
C	-9.49179500	-0.06297200	0.70973400
C	-11.23543500	0.70005400	-1.38707200
H	-9.97142600	-0.48393600	-2.65756400

C	-10.55211600	0.82257300	0.94712700
C	-11.43704900	1.19259200	-0.08497500
H	-11.88332900	0.99657500	-2.20882300
H	-10.69153800	1.27999800	1.92510600
C	4.88630700	-1.47006000	-1.27495000
C	5.54149300	-0.93687600	-0.14777200
C	5.63577800	-2.08182100	-2.29539800
C	6.93126200	-1.04480600	-0.00082000
H	4.93979800	-0.40375400	0.58633600
C	7.03073100	-2.16095800	-2.16489200
H	5.16009900	-2.46476600	-3.19547200
C	7.66922600	-0.49088600	1.15930300
C	7.70156100	-1.67514700	-1.03044800
H	7.60698800	-2.58020900	-2.98925000
C	8.96097200	0.13148500	0.78507900
C	9.17286800	-1.72308000	-0.86204400
C	9.44218000	1.32669000	1.34529200
C	9.72988900	-0.49411400	-0.24797600
C	10.66194500	1.89580600	0.94959300
H	8.83841000	1.85261500	2.08446400
C	10.93162500	0.09390900	-0.66602100
C	11.41394500	1.27208500	-0.06237200
H	10.99482000	2.82417200	1.40824700
H	11.50025500	-0.32322700	-1.49545700
O	12.60344700	1.73999400	-0.55570600
O	-12.43497000	2.05754600	0.27930900
C	-8.89617100	-0.83495400	3.02825900
S	-10.59511700	-0.85386600	3.61984900
C	-8.98257400	-2.03620700	5.38637400
C	-10.26715100	-1.75054600	5.09934900
H	-8.64327300	-2.56511500	6.27477000
H	-11.11987400	-2.01477500	5.72162200
C	-8.17105500	-2.60420200	-1.59477600
S	-9.66056700	-3.18613400	-2.42051000
C	-7.75619600	-5.05238000	-2.51876200
C	-9.04436200	-4.78918800	-2.81034800

H	-7.24858300	-5.99297000	-2.72315300
H	-9.73177900	-5.48612700	-3.28566300
C	7.25148600	-0.64002800	2.46016800
S	5.74680100	-1.49714300	2.94881700
C	7.24879600	-0.96191000	5.08799400
C	6.13245200	-1.58537800	4.66482700
H	7.58916300	-0.92255200	6.12082500
H	5.43697900	-2.12436000	5.30513400
C	9.92875400	-2.83623500	-1.14170400
S	11.69641300	-2.96279600	-0.83085500
C	10.69181500	-5.34949900	-1.47501100
C	11.80146100	-4.70496100	-1.06600000
H	10.62722700	-6.41706900	-1.67566900
H	12.76655200	-5.17489000	-0.88718000
C	13.12547200	2.95726400	-0.00159500
H	13.27901200	2.83880300	1.08677900
H	12.40098000	3.77892700	-0.15119500
C	14.44457900	3.26377800	-0.70379600
H	15.13221900	2.41590100	-0.55706400
H	14.26140500	3.34789200	-1.78669600
C	15.08516800	4.55827600	-0.17614300
H	15.25409200	4.47125300	0.91125200
H	14.38634100	5.40119700	-0.31696000
C	16.41709500	4.88241300	-0.87139600
H	17.11561300	4.03938100	-0.73103800
H	16.24933200	4.96934100	-1.95899900
C	17.06571300	6.17458500	-0.35066900
H	17.23805900	6.09314700	0.73539900
H	16.36878800	7.01839600	-0.49480600
C	18.40580000	6.49140500	-1.05269800
H	19.11147100	5.65985000	-0.89110900
H	18.21979500	6.54778000	-2.14107300
C	-13.34183100	2.50122000	-0.74164300
H	-13.85365300	1.63138800	-1.19286700
H	-12.78099100	3.01463400	-1.54428800
C	-14.34965600	3.44689500	-0.09586900

H	-14.87294600	2.91314200	0.71314800
H	-13.80605800	4.28497200	0.36823600
C	-15.36635100	3.98072200	-1.11851500
H	-15.89877200	3.13499500	-1.58737600
H	-14.83315800	4.50320200	-1.93182500
C	-16.39089900	4.93741300	-0.48799000
H	-16.92481100	4.41532100	0.32482200
H	-15.85933500	5.78298400	-0.01788300
C	-17.40987500	5.47719600	-1.50375200
H	-17.94678400	4.63715700	-1.97488400
H	-16.87582200	6.00189700	-2.31491700
C	-18.43718900	6.43741100	-0.86214200
H	-18.98824700	5.90890900	-0.06678700
H	-17.88229300	7.26069700	-0.37569900
S	8.21903000	-0.11792300	3.88473400
S	9.23882700	-4.38886900	-1.73528900
S	-7.75140200	-1.48782200	4.25350100
S	-6.80821200	-3.76863400	-1.77318400
C	19.01815100	7.78249000	-0.57305500
H	18.41616700	8.68423600	-0.73343100
C	20.20344100	7.88779600	0.04455600
H	20.82593600	7.00729900	0.22457100
H	20.59166800	8.84933100	0.38498500
C	-19.40730300	7.00179300	-1.86826700
H	-18.96423600	7.59110400	-2.67923300
C	-20.73385700	6.80862200	-1.84848200
H	-21.38834000	7.23008200	-2.61345300
H	-21.20670500	6.22167000	-1.05660000

**UP-8**

C	0.48187600	-1.46878600	-3.19206400
C	-0.89799800	-1.35310100	-2.96475600
C	-1.46734800	-1.84289800	-1.77916200
C	-0.63290500	-2.44516700	-0.81638300
C	0.74148400	-2.55997200	-1.04267100
C	1.31180400	-2.07558800	-2.23685800

H	0.91814600	-1.07435400	-4.11178300
H	-1.53458200	-0.86913700	-3.70794800
H	-1.07101500	-2.80784000	0.11352900
H	1.38805600	-3.01274300	-0.29071900
C	2.79047100	-2.23869900	-2.49900700
H	3.09156200	-1.68114000	-3.40359000
H	3.04355900	-3.30334900	-2.66215700
C	-2.95955800	-1.76140100	-1.55809300
H	-3.43005500	-1.11006600	-2.31568300
H	-3.42434100	-2.76173600	-1.64340900
O	3.51622000	-1.75696700	-1.35454700
O	-3.20403800	-1.24472300	-0.23744400
C	-4.50163200	-1.23277200	0.20720300
C	-5.61508900	-1.57432400	-0.58052100
C	-4.68956500	-0.80630100	1.53615000
C	-6.91486400	-1.54412900	-0.03642900
H	-5.48942500	-1.81784500	-1.63216600
C	-5.97959300	-0.73923900	2.06401100
H	-3.82173500	-0.50816300	2.12312100
C	-8.11990700	-1.88515800	-0.82883600
C	-7.10987300	-1.12212600	1.31081200
H	-6.11493200	-0.35055200	3.07291100
C	-9.27360900	-0.99923800	-0.54512100
C	-8.49940900	-1.05091800	1.82073700
C	-10.14552600	-0.51252500	-1.53328400
C	-9.46869200	-0.57040200	0.80703500
C	-11.21418800	0.34308700	-1.22687100
H	-9.97153100	-0.77312900	-2.57701700
C	-10.51699000	0.31076800	1.10619400
C	-11.40274000	0.75560200	0.10472600
H	-11.86290100	0.69811300	-2.02440500
H	-10.64579500	0.70657900	2.11214900
C	4.87962400	-1.91233200	-1.35977400
C	5.53936700	-1.45545600	-0.20214700
C	5.62568100	-2.44473600	-2.42619500
C	6.93101800	-1.56189200	-0.07337500

H	4.93932800	-0.98063500	0.57223600
C	7.02220600	-2.52134300	-2.31168800
H	5.14577800	-2.76740500	-3.34743200
C	7.67371300	-1.08518200	1.11758400
C	7.69813700	-2.11086300	-1.15083000
H	7.59557700	-2.87748600	-3.16720300
C	8.95687800	-0.42598700	0.77864100
C	9.17122500	-2.15706300	-0.99745800
C	9.43186800	0.73117500	1.41830500
C	9.72258700	-0.96941200	-0.30216800
C	10.64301700	1.33853100	1.05458800
H	8.82955600	1.19749600	2.19759800
C	10.91530400	-0.34154300	-0.68693700
C	11.39228300	0.79536700	-0.00485500
H	10.97088300	2.23531400	1.57537500
H	11.48038200	-0.69264600	-1.54868400
O	12.57349800	1.30861900	-0.47233100
O	-12.38762100	1.60848400	0.52797100
C	-8.86892700	-1.49298400	3.06875400
S	-10.56458400	-1.52892600	3.66886700
C	-8.95643200	-2.83801800	5.34788000
C	-10.23907200	-2.51990300	5.08757100
H	-8.61849100	-3.42523000	6.19940700
H	-11.09136800	-2.81237600	5.69767500
C	-8.19130700	-2.97746100	-1.65991700
S	-9.69280600	-3.49006200	-2.50958800
C	-7.81129000	-5.36826000	-2.73650200
C	-9.09819500	-5.07298600	-3.00173100
H	-7.31620100	-6.30019300	-3.00210100
H	-9.79693800	-5.73149900	-3.51390100
C	7.26772600	-1.32969200	2.40766800
S	5.77395200	-2.23203500	2.84568300
C	7.28879800	-1.83645600	5.00611100
C	6.17409800	-2.43799000	4.54823100
H	7.63710500	-1.86727700	6.03658300
H	5.48814800	-3.02681600	5.15398200



C	9.93452500	-3.24046400	-1.36119100
S	11.70581800	-3.37211200	-1.07381600
C	10.71691000	-5.71662100	-1.87750100
C	11.82414300	-5.09223800	-1.43226400
H	10.66003800	-6.76790100	-2.15266400
H	12.79473900	-5.56463300	-1.29441100
C	13.08934200	2.48674400	0.16615400
H	13.24864300	2.29069300	1.24242400
H	12.35775800	3.31118000	0.07967900
C	14.40307800	2.85560600	-0.51574600
H	15.09877800	2.00551100	-0.43422000
H	14.21575800	3.01861900	-1.58888600
C	15.03270300	4.11299400	0.10618000
H	15.20317900	3.94632600	1.18414100
H	14.32544000	4.95721900	0.02948700
C	16.36101000	4.50284200	-0.56188800
H	17.06855300	3.65906600	-0.48524000
H	16.19174800	4.66926900	-1.63989500
C	16.99681300	5.75894000	0.05450100
H	17.16333200	5.59222700	1.13312400
H	16.28860900	6.60247400	-0.02310000
C	18.32645100	6.14860100	-0.61064400
H	19.03443500	5.30495300	-0.53291100
H	18.16079000	6.31575300	-1.68949300
C	-13.29307200	2.12636500	-0.45894300
H	-13.82090500	1.29278300	-0.95768700
H	-12.72833700	2.67749600	-1.23332900
C	-14.28245800	3.04837100	0.24662600
H	-14.80897700	2.47762000	1.02782600
H	-13.72365500	3.85098400	0.75342200
C	-15.29666500	3.65358700	-0.73797300
H	-15.84732700	2.84312000	-1.24661300
H	-14.75966000	4.20840400	-1.52708400
C	-16.29962100	4.59449500	-0.05143100
H	-16.83696100	4.04121500	0.73823100
H	-15.74903400	5.40495500	0.45693800

C	-17.31657600	5.20414400	-1.02927900
H	-17.86838900	4.39292900	-1.53561200
H	-16.77763300	5.75360900	-1.82098300
C	-18.31680500	6.14965400	-0.34546800
H	-18.85542700	5.60074400	0.44673900
H	-17.76535100	6.96173500	0.16019300
S	8.24254800	-0.90134400	3.85836600
S	9.25344000	-4.75351700	-2.05821800
S	-7.72518900	-2.23458900	4.24341700
S	-6.84320100	-4.14367000	-1.92042500
C	-19.33339400	6.75821500	-1.32434200
H	-19.89185000	5.95256800	-1.82931400
H	-18.79535300	7.30905500	-2.11534800
C	-20.33481900	7.70870400	-0.62939900
H	-20.89002800	7.15562200	0.14617000
H	-19.75837200	8.49691100	-0.11085200
C	18.96168000	7.40452300	0.00664500
H	19.13286600	7.24361700	1.08401700
H	18.25622100	8.24964100	-0.07510100
C	20.29963500	7.78765200	-0.66592300
H	20.11501100	7.92351000	-1.74756000
H	21.01414700	6.95395200	-0.56547000
C	20.89731900	9.04561900	-0.08968200
H	20.28517700	9.95007300	-0.18235300
C	22.08102800	9.11782800	0.53576700
H	22.71352700	8.23344800	0.64993100
H	22.45794200	10.05537800	0.94826200
C	-21.30152200	8.33924400	-1.59875200
H	-20.85302500	8.95591900	-2.38609400
C	-22.63173300	8.17322400	-1.57553400
H	-23.28350000	8.64300800	-2.31426000
H	-23.11035000	7.56029700	-0.80712500

**UP-9**

C	0.48005500	-1.77165900	-3.20399800
C	-0.89907300	-1.66703200	-2.96708200

C	-1.46124200	-2.19207500	-1.79327500
C	-0.62049700	-2.82049800	-0.85295800
C	0.75310200	-2.92504200	-1.08883800
C	1.31639200	-2.40301400	-2.27049200
H	0.91079700	-1.34864400	-4.11357400
H	-1.54060800	-1.16314300	-3.69252200
H	-1.05272600	-3.21124500	0.06842500
H	1.40462300	-3.39740600	-0.35350900
C	2.79494700	-2.54945400	-2.54423400
H	3.09167300	-1.94494500	-3.41964500
H	3.05132800	-3.60336100	-2.76323100
C	-2.95084500	-2.11303500	-1.55607900
H	-3.43156300	-1.46795700	-2.31249000
H	-3.41537000	-3.11450600	-1.62691900
O	3.52195600	-2.12508900	-1.37852200
O	-3.17881200	-1.58555900	-0.23613600
C	-4.47240700	-1.55598300	0.21889400
C	-5.59568600	-1.89829400	-0.55448300
C	-4.64507800	-1.10910100	1.54326800
C	-6.89060800	-1.84615200	-0.00047300
H	-5.48113900	-2.15964900	-1.60312800
C	-5.92989300	-1.02117900	2.08055700
H	-3.76947700	-0.81126000	2.11872400
C	-8.10576900	-2.18478000	-0.77842500
C	-7.07027600	-1.40235300	1.34182900
H	-6.05296300	-0.61679900	3.08485000
C	-9.24646300	-1.28069700	-0.49939200
C	-8.45493300	-1.30716600	1.86111900
C	-10.11937300	-0.79733300	-1.48830300
C	-9.42606400	-0.82971200	0.84769900
C	-11.17449100	0.07666500	-1.18686300
H	-9.95639200	-1.07524600	-2.52933600
C	-10.46070600	0.06925400	1.14140800
C	-11.34777800	0.51119200	0.13980600
H	-11.82438200	0.42848300	-1.98486200
H	-10.57682600	0.48156100	2.14227500

C	4.88773800	-2.25506100	-1.40274800
C	5.54886700	-1.84896900	-0.22720300
C	5.63411500	-2.71472700	-2.50225200
C	6.94355800	-1.93226500	-0.11669900
H	4.94686300	-1.42981400	0.57721900
C	7.03313100	-2.76675300	-2.40446900
H	5.15179500	-2.99886800	-3.43486800
C	7.68733200	-1.50497700	1.09208500
C	7.71183100	-2.40350400	-1.22950200
H	7.60516100	-3.06405800	-3.28304700
C	8.95033000	-0.79659300	0.77826400
C	9.18724700	-2.42119700	-1.09267700
C	9.40333600	0.33499900	1.47671600
C	9.71692600	-1.25957700	-0.33870600
C	10.59390700	0.99320700	1.13448700
H	8.79872900	0.74104300	2.28737300
C	10.88861000	-0.58039300	-0.70048900
C	11.34383800	0.52991300	0.03810800
H	10.90481700	1.86777000	1.70137500
H	11.45218900	-0.86868600	-1.58620100
O	12.50465100	1.10094300	-0.41338000
O	-12.31793700	1.38352200	0.55734700
C	-8.81997100	-1.72594100	3.11840200
S	-10.51108600	-1.73192600	3.73218300
C	-8.90559000	-3.03489200	5.41849900
C	-10.18630000	-2.70498300	5.16339200
H	-8.56804600	-3.61310900	6.27631700
H	-11.03716300	-2.97750500	5.78463400
C	-8.19635300	-3.28832000	-1.59247900
S	-9.70992000	-3.79543800	-2.42380400
C	-7.85226900	-5.69893400	-2.63631600
C	-9.13746800	-5.39228400	-2.89689500
H	-7.37014800	-6.64047600	-2.89169400
H	-9.84754000	-6.04988300	-3.39444800
C	7.30049700	-1.83005400	2.37008800
S	5.83286300	-2.79081100	2.77053100

C	7.36007400	-2.47865800	4.93602500
C	6.25515900	-3.08057200	4.45545800
H	7.71946600	-2.55794400	5.96007900
H	5.58946300	-3.71815400	5.03383500
C	9.97318800	-3.46354100	-1.52194500
S	11.75027500	-3.56499200	-1.25923600
C	10.81150600	-5.88743500	-2.17892700
C	11.90760300	-5.25980400	-1.71128200
H	10.77791000	-6.92350100	-2.50994900
H	12.89115000	-5.71399300	-1.60851200
C	12.98907600	2.26261800	0.27772100
H	13.17441600	2.01699700	1.33957600
H	12.22634000	3.06239300	0.24647600
C	14.27576800	2.71750500	-0.40383800
H	15.00634700	1.89363000	-0.37682800
H	14.06391600	2.92786800	-1.46409500
C	14.86329500	3.96629400	0.27398800
H	15.06189200	3.75003500	1.33825000
H	14.11829400	4.78086800	0.25563300
C	16.15964700	4.45184100	-0.39427200
H	16.90668100	3.63945100	-0.37483900
H	15.96234400	4.66710700	-1.45877900
C	16.74758700	5.70217100	0.27843600
H	16.94416700	5.48561000	1.34317000
H	15.99773100	6.51250600	0.26060800
C	18.04271000	6.19390400	-0.38753800
H	18.79346600	5.38466100	-0.36860500
H	17.84649700	6.40965400	-1.45244400
C	-13.22005400	1.90345900	-0.43158700
H	-13.76516200	1.07246900	-0.91586700
H	-12.65026000	2.43399200	-1.21657600
C	-14.18914700	2.85229300	0.26652800
H	-14.72251400	2.30136900	1.05725900
H	-13.61330100	3.65078200	0.76058900
C	-15.19643100	3.46392200	-0.72123300
H	-15.76404200	2.65758300	-1.21769300

H	-14.65266800	3.99909000	-1.51925200
C	-16.17890300	4.43148800	-0.04215000
H	-16.72397300	3.89745300	0.75542900
H	-15.61111100	5.23676700	0.45541800
C	-17.18732900	5.05011400	-1.02306000
H	-17.75602800	4.24421100	-1.51934400
H	-16.64060600	5.58091600	-1.82218400
C	-18.16740300	6.02157800	-0.34621700
H	-18.71477400	5.49085400	0.45227900
H	-17.59824300	6.82660500	0.15082300
S	8.27997900	-1.45914500	3.83336000
S	9.32245900	-4.95372600	-2.29313600
S	-7.67596600	-2.46379500	4.29521300
S	-6.86398000	-4.47426200	-1.84494200
C	-19.17480900	6.64229000	-1.32709700
H	-19.74423600	5.83733700	-1.82403400
H	-18.62782300	7.17347900	-2.12590800
C	-20.15360100	7.61377100	-0.64882900
H	-20.70690100	7.08867700	0.14744400
H	-19.58502900	8.42063800	-0.15461300
C	18.62730600	7.44578700	0.28555600
H	18.82332200	7.22986300	1.35049300
H	17.87648500	8.25532100	0.26676400
C	19.92202200	7.93817800	-0.38027800
H	19.72602600	8.15758400	-1.44424400
H	20.67861100	7.13622500	-0.36097600
C	-21.16332400	8.23316100	-1.64191900
H	-21.74793900	7.43056000	-2.12127000
H	-20.59275900	8.73722400	-2.44372400
C	20.50234200	9.19712400	0.30348700
H	20.72042100	8.97433100	1.36107600
H	19.72467900	9.98304800	0.29487000
C	21.74650500	9.70470600	-0.37923100
H	21.62743200	10.00189800	-1.42749000
C	22.95782400	9.78435000	0.18994200
H	23.11193700	9.49075200	1.23170700

H	23.82912700	10.14614400	-0.35884300
C	-22.09319100	9.21886600	-0.98208400
H	-21.61394200	10.08621700	-0.51373300
C	-23.42562300	9.08883400	-0.90928500
H	-23.93432700	8.23302000	-1.36098000
H	-24.04947300	9.82816100	-0.40388600

**(5,5) tube**

C	-3.47782000	11.10596500	0.69110000
C	-3.47782000	11.10596500	-0.69110000
C	-3.19013500	9.90428800	-1.41803600
C	-3.36935500	8.67188000	-0.72071600
C	-3.36935500	8.67188000	0.72071600
C	-3.19013500	9.90428800	1.41803600
C	-3.14059500	7.42461800	-1.40024300
C	-2.30221900	7.42467800	-2.55347100
C	-1.72649500	8.67204500	-2.98059700
C	-2.33452500	9.90439700	-2.59476600
C	-0.35556600	8.67209200	-3.42594000
C	0.36302800	9.90451500	-3.47082100
C	-0.41718700	11.10627900	-3.51929300
C	-1.73171400	11.10621200	-3.09229200
C	-3.14059500	7.42461800	1.40024300
C	-3.37912500	6.18576200	0.71987800
C	-3.37912500	6.18576200	-0.71987800
C	-3.15777100	4.95315400	-1.40466800
C	-2.31168100	4.95318800	-2.56842600
C	-1.72863100	6.18583300	-2.99022600
C	-0.35936000	6.18586600	-3.43509800
C	0.36137300	7.42475900	-3.41871200
C	-3.15777100	4.95315400	1.40466800
C	-3.37605900	3.71254900	0.71592100
C	-3.37605900	3.71254900	-0.71592100
C	-3.15878900	2.47329300	-1.40486600
C	-2.31218500	2.47331200	-2.56931900
C	-1.72392700	3.71257200	-2.98855200

C	-0.36217900	3.71258600	-3.43100300
C	0.36027400	4.95322200	-3.43641400
C	-3.15878900	2.47329300	1.40486600
C	-3.15193000	0.00000500	-1.40448800
C	-2.30970700	-0.00000300	-2.56290000
C	-1.72890900	1.23972700	-2.99203200
C	-0.36018500	1.23972000	-3.43675300
C	0.36016900	2.47332700	-3.43742500
C	-3.15193000	0.00000500	1.40448800
C	-3.38095700	-1.23972200	0.71957900
C	-3.38095700	-1.23972200	-0.71957900
C	-3.15877400	-2.47330300	-1.40487300
C	-2.31218000	-2.47331700	-2.56929700
C	-1.72889200	-1.23972200	-2.99202300
C	-0.36018600	-1.23973100	-3.43674300
C	0.36194000	0.00000500	-3.43083200
C	-3.15877400	-2.47330300	1.40487300
C	-3.37606600	-3.71255100	0.71592500
C	-3.37606600	-3.71255100	-0.71592500
C	-3.15776100	-4.95315000	-1.40467000
C	-2.31167700	-4.95319900	-2.56842000
C	-1.72391600	-3.71257300	-2.98855000
C	-0.36217800	-3.71258000	-3.43100300
C	0.36016800	-2.47332700	-3.43745400
C	-3.15776100	-4.95315000	1.40467000
C	-3.37911500	-6.18577400	0.71987300
C	-3.37911500	-6.18577400	-0.71987300
C	-3.14058900	-7.42461400	-1.40024900
C	-2.30222400	-7.42467400	-2.55348000
C	-1.72865000	-6.18584300	-2.99024300
C	-0.35935900	-6.18587500	-3.43511500
C	0.36027900	-4.95323100	-3.43641100
C	-3.14058900	-7.42461400	1.40024900
C	-3.36932800	-8.67188100	0.72070100
C	-3.36932800	-8.67188100	-0.72070100
C	-3.19018100	-9.90430400	-1.41803900



C	-2.33454200	-9.90441000	-2.59480700
C	-1.72648100	-8.67205300	-2.98059200
C	-0.35557300	-8.67210100	-3.42592000
C	0.36137200	-7.42475400	-3.41871200
C	-3.19018100	-9.90430400	1.41803900
C	-3.47788100	-11.10592900	0.69112000
C	-3.47788100	-11.10592900	-0.69112000
C	0.36301600	-9.90453000	-3.47085600
C	-0.41718100	-11.10625600	-3.51932300
C	-1.73174200	-11.10618800	-3.09231200
C	1.71742300	-7.42472200	-2.97813100
C	2.30181700	-8.67201600	-2.56274200
C	1.74681200	-9.90448900	-3.02133200
C	1.72869500	-4.95321200	-2.99178800
C	2.31023200	-6.18584400	-2.56788900
C	3.15685100	-6.18581200	-1.40342100
C	3.36422200	-7.42462900	-0.71292900
C	3.14945100	-8.67193900	-1.39696200
C	3.41478000	-9.90431500	-0.72750500
C	3.21969800	-11.10601500	-1.48439500
C	2.40670500	-11.10614000	-2.60221300
C	3.36422200	-7.42462900	0.71292900
C	3.14945100	-8.67193900	1.39696200
C	3.41478000	-9.90431500	0.72750500
C	3.38067300	-4.95317800	-0.71943600
C	3.38067300	-4.95317800	0.71943600
C	3.15685100	-6.18581200	1.40342100
C	2.31023200	-6.18584400	2.56788900
C	1.71742300	-7.42472200	2.97813100
C	2.30181700	-8.67201600	2.56274200
C	1.74681200	-9.90448900	3.02133200
C	2.40670500	-11.10614000	2.60221300
C	3.21969800	-11.10601500	1.48439500
C	0.36137200	-7.42475400	3.41871200
C	-0.35557300	-8.67210100	3.42592000
C	0.36301600	-9.90453000	3.47085600

C	1.72869500	-4.95321200	2.99178800
C	0.36027900	-4.95323100	3.43641100
C	-0.35935900	-6.18587500	3.43511500
C	-1.72865000	-6.18584300	2.99024300
C	-2.30222400	-7.42467400	2.55348000
C	-1.72648100	-8.67205300	2.98059200
C	-2.33454200	-9.90441000	2.59480700
C	-1.73174200	-11.10618800	3.09231200
C	-0.41718100	-11.10625600	3.51932300
C	-2.31167700	-4.95319900	2.56842000
C	3.15203000	-3.71256300	1.40481600
C	2.31008200	-3.71257600	2.56288000
C	3.15203000	-3.71256300	-1.40481600
C	2.31008200	-3.71257600	-2.56288000
C	-0.36217800	-3.71258000	3.43100300
C	-1.72391600	-3.71257300	2.98855000
C	3.38163900	-2.47331300	0.71987700
C	3.38163900	-2.47331300	-0.71987700
C	1.72942200	-2.47332100	-2.99255300
C	1.72942200	-2.47332100	2.99255300
C	0.36016800	-2.47332700	3.43745400
C	-2.31218000	-2.47331700	2.56929700
C	3.15816100	-1.23972400	1.40471900
C	2.31189600	-1.23973200	2.56872300
C	3.15816100	-1.23972400	-1.40471900
C	2.31189600	-1.23973200	-2.56872300
C	-0.36018600	-1.23973100	3.43674300
C	-1.72889200	-1.23972200	2.99202300
C	3.37587500	0.00000400	0.71615800
C	3.37587500	0.00000400	-0.71615800
C	1.72411800	0.00000300	-2.98823700
C	1.72411800	0.00000300	2.98823700
C	0.36194000	0.00000500	3.43083200
C	-2.30970700	-0.00000300	2.56290000
C	3.15817700	1.23971800	1.40471800
C	2.31189800	1.23972500	2.56873400

C	3.15817700	1.23971800	-1.40471800
C	2.31189800	1.23972500	-2.56873400
C	-0.36018500	1.23972000	3.43675300
C	-1.72890900	1.23972700	2.99203200
C	3.38162900	2.47330600	0.71986900
C	3.38162900	2.47330600	-0.71986900
C	1.72940700	2.47331300	-2.99254000
C	1.72940700	2.47331300	2.99254000
C	0.36016900	2.47332700	3.43742500
C	-2.31218500	2.47331200	2.56931900
C	3.15203500	3.71257100	1.40481500
C	2.31008200	3.71258600	2.56287400
C	3.15203500	3.71257100	-1.40481500
C	2.31008200	3.71258600	-2.56287400
C	-0.36217900	3.71258600	3.43100300
C	-1.72392700	3.71257200	2.98855200
C	3.38069100	4.95317400	0.71944500
C	3.38069100	4.95317400	-0.71944500
C	1.72870500	4.95320200	-2.99178900
C	1.72870500	4.95320200	2.99178900
C	0.36027400	4.95322200	3.43641400
C	-2.31168100	4.95318800	2.56842600
C	3.15683600	6.18580500	1.40342000
C	2.31022900	6.18583800	2.56786700
C	3.15683600	6.18580500	-1.40342000
C	2.31022900	6.18583800	-2.56786700
C	-0.35936000	6.18586600	3.43509800
C	-1.72863100	6.18583300	2.99022600
C	3.36422300	7.42464600	0.71292900
C	3.36422300	7.42464600	-0.71292900
C	1.71742700	7.42472900	-2.97813200
C	1.71742700	7.42472900	2.97813200
C	0.36137300	7.42475900	3.41871200
C	-2.30221900	7.42467800	2.55347100
C	3.14946900	8.67193600	1.39696500
C	2.30182400	8.67201000	2.56276600

C	3.14946900	8.67193600	-1.39696500
C	2.30182400	8.67201000	-2.56276600
C	-0.35556600	8.67209200	3.42594000
C	-1.72649500	8.67204500	2.98059700
C	3.41473000	9.90431300	0.72748100
C	3.41473000	9.90431300	-0.72748100
C	1.74677500	9.90447700	-3.02131500
C	1.74677500	9.90447700	3.02131500
C	0.36302800	9.90451500	3.47082100
C	-2.33452500	9.90439700	2.59476600
C	3.21965300	11.10604500	1.48440100
C	2.40668000	11.10616600	2.60219200
C	3.21965300	11.10604500	-1.48440100
C	2.40668000	11.10616600	-2.60219200
C	-0.41718700	11.10627900	3.51929300
C	-1.73171400	11.10621200	3.09229200
C	-3.38098700	1.23972100	-0.71960900
C	-3.38098700	1.23972100	0.71960900
H	2.14328000	-12.05809000	3.06206800
H	3.57602200	-12.05787800	1.09185400
H	-2.25079600	-12.05802700	2.98417600
H	0.06622000	-12.05815500	3.73681100
H	-3.53534300	-12.05781100	-1.21810400
H	-3.53534300	-12.05781100	1.21810400
H	3.57602200	-12.05787800	-1.09185400
H	2.14328000	-12.05809000	-3.06206800
H	0.06622000	-12.05815500	-3.73681100
H	-2.25079600	-12.05802700	-2.98417600
H	3.57606600	12.05787900	1.09187300
H	2.14327400	12.05808400	3.06213000
H	0.06624700	12.05814000	3.73688000
H	-2.25084900	12.05801500	2.98422400
H	-3.53534700	12.05780700	1.21815000
H	-3.53534700	12.05780700	-1.21815000
H	-2.25084900	12.05801500	-2.98422400
H	0.06624700	12.05814000	-3.73688000

H	2.14327400	12.05808400	-3.06213000
H	3.57606600	12.05787900	-1.09187300

**(6,6) tube**

H	-12.06130100	-0.23560700	-4.41172000
H	-12.06127800	-2.53390500	-3.61918000
H	-12.06128200	-3.93890200	-2.00191400
H	-12.06123800	-4.40161100	0.38483000
H	-12.06125300	-3.70312600	2.41006900
H	-12.06126900	-1.86785400	4.00433200
H	-12.06127000	1.86785300	-4.00433200
H	-12.06125300	3.70312500	-2.41006900
H	-12.06123800	4.40161200	-0.38483000
H	-12.06128200	3.93890300	2.00191300
H	-12.06127900	2.53390400	3.61917900
H	-12.06130100	0.23560700	4.41171900
C	-11.10850100	-0.71040200	-4.18099100
C	-11.10848400	-2.01780000	-3.73016800
C	-11.10851000	-3.97634100	-1.47529000
C	-11.10845900	-4.23958600	-0.11764500
C	-11.10845100	-3.26584800	2.70579700
C	-11.10846400	-2.22177100	3.61264100
C	-11.10846500	2.22177100	-3.61264100
C	-11.10845100	3.26584700	-2.70579700
C	-11.10845900	4.23958700	0.11764500
C	-11.10851000	3.97634200	1.47529000
C	-11.10848500	2.01780000	3.73016800
C	-11.10850100	0.71040200	4.18099000
C	-9.90873400	0.06889200	-4.17331000
C	-9.90872400	-2.62672800	-3.24380600
C	-9.90869700	-3.58001300	-2.14636000
C	-9.90868200	-4.12281100	0.65288700
C	-9.90870100	-3.64888900	2.02706900
C	-9.90869200	-1.49596400	3.89668100
C	-9.90869200	1.49596300	-3.89668000
C	-9.90870100	3.64888900	-2.02706800

C	-9.90868200	4.12281200	-0.65288700
C	-9.90869700	3.58001300	2.14636000
C	-9.90872400	2.62672800	3.24380600
C	-9.90873400	-0.06889200	4.17331000
C	-8.67468400	-0.64288600	-4.07047000
C	-8.67468800	-2.00286700	-3.60156700
C	-8.67467000	-3.84681100	-1.47853900
C	-8.67465100	-4.12074900	-0.06625500
C	-8.67464700	-3.20391900	2.59197500
C	-8.67464900	-2.11773500	3.53522400
C	-8.67464900	2.11773500	-3.53522400
C	-8.67464700	3.20391900	-2.59197500
C	-8.67465100	4.12074900	0.06625500
C	-8.67467000	3.84681100	1.47853900
C	-8.67468800	2.00286600	3.60156700
C	-8.67468400	0.64288600	4.07047000
C	-7.42765500	0.07186200	-4.11230700
C	-7.42764100	-2.59136500	-3.19386900
C	-7.42763600	-3.52555500	-2.11848400
C	-7.42760700	-4.06190700	0.64726900
C	-7.42761000	-3.59751500	1.99390900
C	-7.42763300	-1.47033500	3.84110500
C	-7.42763300	1.47033500	-3.84110500
C	-7.42761000	3.59751500	-1.99390900
C	-7.42760700	4.06190700	-0.64726900
C	-7.42763600	3.52555500	2.11848400
C	-7.42764100	2.59136500	3.19386900
C	-7.42765400	-0.07186200	4.11230700
C	-6.18874300	-0.64592200	-4.07590500
C	-6.18874200	-2.00378000	-3.60776500
C	-6.18872600	-3.85303800	-1.47866700
C	-6.18871500	-4.12655100	-0.06857100
C	-6.18871600	-3.20699100	2.59727000
C	-6.18873100	-2.12261500	3.53916700
C	-6.18873200	2.12261500	-3.53916700
C	-6.18871600	3.20699100	-2.59727000

C	-6.18871500	4.12655100	0.06857100
C	-6.18872600	3.85303800	1.47866700
C	-6.18874200	2.00378000	3.60776500
C	-6.18874300	0.64592200	4.07590500
C	-4.95449700	0.06957400	-4.12940100
C	-4.95448100	-2.60001000	-3.20873100
C	-4.95448300	-3.54144800	-2.12503000
C	-4.95446600	-4.07899800	0.64731600
C	-4.95446800	-3.61103800	2.00438700
C	-4.95448600	-1.47887400	3.85607200
C	-4.95448600	1.47887400	-3.85607200
C	-4.95446800	3.61103800	-2.00438700
C	-4.95446600	4.07899800	-0.64731600
C	-4.95448300	3.54144800	2.12503000
C	-4.95448100	2.60001000	3.20873100
C	-4.95449700	-0.06957400	4.12940200
C	-3.71388800	-0.64917400	-4.07620000
C	-3.71388800	-2.00132600	-3.61001600
C	-3.71387400	-3.85480200	-1.47596500
C	-3.71387100	-4.12714500	-0.07180600
C	-3.71387000	-3.20554300	2.60018900
C	-3.71388200	-2.12573200	3.53812400
C	-3.71388200	2.12573200	-3.53812400
C	-3.71387000	3.20554300	-2.60018900
C	-3.71387100	4.12714500	0.07180600
C	-3.71387400	3.85480200	1.47596500
C	-3.71388800	2.00132600	3.61001600
C	-3.71388800	0.64917400	4.07620000
C	-2.47469300	0.06938000	-4.13158200
C	-2.47468900	-2.60116100	-3.21059300
C	-2.47468700	-3.54338700	-2.12595100
C	-2.47467900	-4.08113400	0.64739500
C	-2.47468000	-3.61280100	2.00563200
C	-2.47468500	-1.47987900	3.85799000
C	-2.47468500	1.47987900	-3.85799000
C	-2.47468000	3.61280100	-2.00563200

C	-2.47467900	4.08113400	-0.64739500
C	-2.47468700	3.54338700	2.12595100
C	-2.47468900	2.60116000	3.21059300
C	-2.47469300	-0.06938000	4.13158200
C	-1.23972800	-0.64746200	-4.08031400
C	-1.23972900	-2.00519100	-3.61221900
C	-1.23972600	-3.85750000	-1.47951100
C	-1.23972400	-4.13098600	-0.06955800
C	-1.23972100	-3.20996400	2.60077100
C	-1.23972600	-2.12570000	3.54258400
C	-1.23972600	2.12570000	-3.54258400
C	-1.23972100	3.20996400	-2.60077100
C	-1.23972400	4.13098600	0.06955800
C	-1.23972600	3.85750000	1.47951100
C	-1.23972900	2.00519100	3.61221900
C	-1.23972800	0.64746200	4.08031400
C	0.00000000	0.07149500	-4.12680600
C	0.00000000	-2.59987800	-3.20555300
C	0.00000000	-3.53819000	-2.12540300
C	0.00000000	-4.07614700	0.64881200
C	0.00000000	-3.60974900	2.00142300
C	0.00000000	-1.47614500	3.85435800
C	0.00000000	1.47614500	-3.85435800
C	0.00000000	3.60974900	-2.00142300
C	0.00000000	4.07614700	-0.64881300
C	0.00000000	3.53819000	2.12540300
C	0.00000000	2.59987800	3.20555300
C	0.00000000	-0.07149500	4.12680600
C	1.23972800	-0.64746200	-4.08031300
C	1.23972900	-2.00519100	-3.61221900
C	1.23972600	-3.85750000	-1.47951100
C	1.23972400	-4.13098600	-0.06955800
C	1.23972100	-3.20996400	2.60077100
C	1.23972600	-2.12570000	3.54258400
C	1.23972600	2.12570000	-3.54258400
C	1.23972100	3.20996400	-2.60077100



C	1.23972400	4.13098600	0.06955800
C	1.23972600	3.85750000	1.47951100
C	1.23972900	2.00519100	3.61221800
C	1.23972800	0.64746200	4.08031300
C	2.47469200	0.06938000	-4.13158200
C	2.47468900	-2.60116000	-3.21059300
C	2.47468600	-3.54338700	-2.12595100
C	2.47467900	-4.08113400	0.64739500
C	2.47468000	-3.61280100	2.00563200
C	2.47468500	-1.47987900	3.85799100
C	2.47468500	1.47987900	-3.85799100
C	2.47468000	3.61280100	-2.00563200
C	2.47467900	4.08113400	-0.64739500
C	2.47468600	3.54338700	2.12595100
C	2.47468900	2.60116000	3.21059300
C	2.47469200	-0.06938000	4.13158200
C	3.71388800	-0.64917400	-4.07620000
C	3.71388800	-2.00132600	-3.61001600
C	3.71387400	-3.85480200	-1.47596500
C	3.71387000	-4.12714400	-0.07180600
C	3.71387000	-3.20554200	2.60018900
C	3.71388200	-2.12573200	3.53812400
C	3.71388200	2.12573200	-3.53812400
C	3.71387000	3.20554200	-2.60018900
C	3.71387100	4.12714400	0.07180600
C	3.71387400	3.85480200	1.47596500
C	3.71388800	2.00132600	3.61001600
C	3.71388800	0.64917400	4.07620000
C	4.95449700	0.06957400	-4.12940100
C	4.95448100	-2.60001000	-3.20873100
C	4.95448300	-3.54144800	-2.12503000
C	4.95446600	-4.07899800	0.64731600
C	4.95446800	-3.61103800	2.00438700
C	4.95448600	-1.47887400	3.85607200
C	4.95448600	1.47887400	-3.85607200
C	4.95446800	3.61103800	-2.00438700

C	4.95446600	4.07899800	-0.64731600
C	4.95448300	3.54144800	2.12503000
C	4.95448100	2.60001000	3.20873100
C	4.95449700	-0.06957400	4.12940100
C	6.18874300	-0.64592200	-4.07590600
C	6.18874200	-2.00378000	-3.60776500
C	6.18872500	-3.85303800	-1.47866700
C	6.18871500	-4.12655100	-0.06857100
C	6.18871600	-3.20699100	2.59727000
C	6.18873100	-2.12261500	3.53916800
C	6.18873100	2.12261500	-3.53916800
C	6.18871600	3.20699100	-2.59727100
C	6.18871500	4.12655100	0.06857100
C	6.18872500	3.85303800	1.47866700
C	6.18874200	2.00378000	3.60776500
C	6.18874300	0.64592200	4.07590600
C	7.42765400	0.07186200	-4.11230800
C	7.42764100	-2.59136600	-3.19386900
C	7.42763600	-3.52555500	-2.11848400
C	7.42760800	-4.06190800	0.64726900
C	7.42760900	-3.59751600	1.99391000
C	7.42763300	-1.47033500	3.84110600
C	7.42763300	1.47033500	-3.84110600
C	7.42760900	3.59751600	-1.99391000
C	7.42760800	4.06190700	-0.64726900
C	7.42763600	3.52555500	2.11848500
C	7.42764100	2.59136600	3.19387000
C	7.42765400	-0.07186200	4.11230800
C	8.67468400	-0.64288600	-4.07047000
C	8.67468800	-2.00286700	-3.60156800
C	8.67467000	-3.84681100	-1.47853900
C	8.67465100	-4.12074900	-0.06625500
C	8.67464700	-3.20391900	2.59197500
C	8.67464900	-2.11773500	3.53522500
C	8.67464900	2.11773500	-3.53522500
C	8.67464700	3.20391900	-2.59197500

C	8.67465100	4.12074900	0.06625500
C	8.67467000	3.84681100	1.47853900
C	8.67468800	2.00286700	3.60156800
C	8.67468400	0.64288600	4.07047100
C	9.90873400	0.06889200	-4.17331200
C	9.90872500	-2.62672900	-3.24380700
C	9.90869800	-3.58001400	-2.14636000
C	9.90868200	-4.12281200	0.65288800
C	9.90870200	-3.64889000	2.02706900
C	9.90869200	-1.49596400	3.89668200
C	9.90869200	1.49596400	-3.89668200
C	9.90870200	3.64889000	-2.02706900
C	9.90868200	4.12281200	-0.65288800
C	9.90869800	3.58001400	2.14636000
C	9.90872500	2.62672800	3.24380700
C	9.90873400	-0.06889200	4.17331100
C	11.10850200	-0.71040200	-4.18099200
C	11.10848500	-2.01780000	-3.73016900
C	11.10851000	-3.97634200	-1.47529000
C	11.10846000	-4.23958700	-0.11764500
C	11.10845200	-3.26584800	2.70579800
C	11.10846500	-2.22177200	3.61264300
C	11.10846500	2.22177100	-3.61264200
C	11.10845200	3.26584800	-2.70579800
C	11.10846000	4.23958800	0.11764500
C	11.10851000	3.97634200	1.47529000
C	11.10848500	2.01780000	3.73016900
C	11.10850200	0.71040200	4.18099200
H	12.06130200	-0.23560700	-4.41172100
H	12.06127900	-2.53390500	-3.61918100
H	12.06128200	-3.93890300	-2.00191300
H	12.06123900	-4.40161300	0.38483100
H	12.06125300	-3.70312700	2.41007100
H	12.06127000	-1.86785500	4.00433500
H	12.06127000	1.86785400	-4.00433400
H	12.06125300	3.70312600	-2.41007000

H	12.06123900	4.40161300	-0.38483000
H	12.06128200	3.93890300	2.00191400
H	12.06127900	2.53390500	3.61918000
H	12.06130200	0.23560700	4.41172100

**(7,7) tube**

H	-12.06287700	5.10292600	-0.03658200
H	-12.06290800	4.50870600	-2.38972100
H	-12.06272900	3.15290300	-4.01253000
H	-12.06267900	0.94272100	-5.01533000
H	-12.06269400	-1.17164700	-4.96701300
H	-12.06266200	-3.33362500	-3.86407900
H	-12.06289100	-4.61337400	-2.18076100
H	-12.06290000	-5.09924400	0.19709700
H	-12.06280300	4.68012800	2.03502700
H	-12.06272200	3.21016600	3.96640800
H	-12.06270200	1.32670800	4.92742900
H	-12.06265300	-1.09970600	4.98301500
H	-12.06271600	-3.02490400	4.10918100
H	-12.06283800	-4.58177700	2.24727300
C	-11.10946200	4.90876000	-0.52583100
C	-11.10945300	4.57002300	-1.86702500
C	-11.10933800	2.64913300	-4.16521300
C	-11.10930400	1.38944200	-4.73682700
C	-11.10929600	-1.60510200	-4.66834300
C	-11.10929900	-2.83732000	-4.03968400
C	-11.10945600	-4.65064200	-1.65576900
C	-11.10947400	-4.92763800	-0.30047900
C	-11.10939400	4.30936800	2.40866300
C	-11.10936100	3.47155900	3.50941300
C	-11.10928700	0.80343500	4.87050500
C	-11.10926600	-0.57952800	4.90219600
C	-11.10934400	-3.30701000	3.66469600
C	-11.10938500	-4.19440100	2.60351000
C	-9.91082700	4.85451400	0.24990500
C	-9.91082300	4.15373500	-2.52390100

C	-9.91078300	3.22160600	-3.63868600
C	-9.91072500	0.61624900	-4.82090700
C	-9.91071700	-0.83652500	-4.78768500
C	-9.91075000	-3.38501300	-3.48744100
C	-9.91079500	-4.26498600	-2.33102500
C	-9.91084000	-4.83797400	0.47200200
C	-9.91079200	4.56361200	1.67363800
C	-9.91074400	2.83097100	3.95030900
C	-9.91071800	1.53653600	4.61062700
C	-9.91068100	-1.32367500	4.67618400
C	-9.91069400	-2.64696800	4.07579600
C	-9.91079600	-4.48219900	1.88095700
C	-8.67610500	4.77926200	-0.46521900
C	-8.67609900	4.42716600	-1.85883100
C	-8.67604100	2.61545200	-4.02540500
C	-8.67601300	1.30654900	-4.61941100
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C	-8.67609900	-4.50756800	-1.65406400
C	-8.67611900	-4.79550400	-0.24577600
C	-8.67605700	4.21368800	2.30178000
C	-8.67603900	3.34311700	3.44556600
C	-8.67598500	0.82728200	4.72885200
C	-8.67597500	-0.60974300	4.76177100
C	-8.67602000	-3.18171800	3.59501900
C	-8.67605600	-4.10385600	2.49239800
C	-7.42935300	4.78418400	0.25035500
C	-7.42934900	4.09156200	-2.49085100
C	-7.42932300	3.17804200	-3.58312000
C	-7.42926500	0.60323800	-4.75133000
C	-7.42926600	-0.82032600	-4.71877200
C	-7.42930800	-3.33892000	-3.43387400
C	-7.42933700	-4.20133900	-2.30081100
C	-7.42936500	-4.76775400	0.46930400
C	-7.42933300	4.49898900	1.64545300
C	-7.42928400	2.78664000	3.89535100

C	-7.42927100	1.51823400	4.54238100
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C	-7.42926400	-2.60516300	4.01881300
C	-7.42933500	-4.41903300	1.84987600
C	-6.19040300	4.77995500	-0.46693800
C	-6.19040100	4.42860800	-1.85765200
C	-6.19035400	2.61451800	-4.02681100
C	-6.19033200	1.30832800	-4.61953900
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C	-6.19040600	-4.79627000	-0.24742200
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C	-6.19031200	-0.60821400	4.76255200
C	-6.19033500	-3.18341500	3.59439700
C	-6.19036500	-4.10367800	2.49410400
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C	-4.95518600	4.10687700	-2.49730100
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C	-4.95518200	-4.21691300	-2.30652200
C	-4.95519000	-4.78432200	0.46848200
C	-4.95517600	4.51354000	1.65331500
C	-4.95513900	2.79810800	3.90716900
C	-4.95513100	1.52111600	4.55860400
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C	-4.95517300	-4.43321100	1.85840600
C	-3.71458500	4.78391500	-0.47051400
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C	-3.71454300	1.31252600	-4.62269100

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C	-3.71458100	-4.51403900	-1.65126400
C	-3.71458300	-4.80037800	-0.25080200
C	-3.71456400	4.21576900	2.30825300
C	-3.71455000	3.34999300	3.44565500
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C	-2.47543500	4.80440500	0.24871700
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C	-2.47540900	-0.82636700	-4.73790100
C	-2.47542100	-3.35104600	-3.45002600
C	-2.47543100	-4.22028000	-2.30809500
C	-2.47543600	-4.78804400	0.46861900
C	-2.47542900	4.51693400	1.65476500
C	-2.47541200	2.80042300	3.90999900
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C	-2.47540600	-1.31137500	4.62703800
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C	-1.23970200	4.43604900	-1.85963600
C	-1.23969400	2.61777400	-4.03364600
C	-1.23968800	1.31138100	-4.62642000
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C	-1.23970200	-4.51642900	-1.65439600
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C	-1.23969200	3.35076500	3.44948000
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C	-1.23968600	-0.60813500	4.77010900

C	-1.23969100	-3.18915900	3.59927600
C	-1.23969600	-4.10958600	2.49886500
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C	1.23969100	3.35076500	3.44948100
C	1.23968600	0.82610800	4.73732200
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C	1.23969500	-4.10958600	2.49886500
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C	2.47542300	3.18943000	-3.59984700
C	2.47540700	0.60838700	-4.77070400
C	2.47540800	-0.82636700	-4.73790200
C	2.47542100	-3.35104600	-3.45002700



C	2.47543100	-4.22028100	-2.30809500
C	2.47543500	-4.78804500	0.46861900
C	2.47542800	4.51693400	1.65476500
C	2.47541100	2.80042300	3.91000000
C	2.47540800	1.52207000	4.56213300
C	2.47540600	-1.31137500	4.62703800
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C	2.47542600	-4.43654100	1.86002200
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C	3.71458300	4.43380400	-1.85639400
C	3.71455600	2.61419700	-4.03205300
C	3.71454300	1.31252600	-4.62269100
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C	3.71455200	-2.79627800	-3.90816900
C	3.71458100	-4.51404000	-1.65126500
C	3.71458300	-4.80037900	-0.25080200
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C	3.71455000	3.34999300	3.44565600
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C	3.71454500	-3.18856500	3.59541300
C	3.71456100	-4.10565600	2.49897200
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C	4.95516600	3.18713500	-3.59695900
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C	4.95515900	-3.34862000	-3.44725000
C	4.95518200	-4.21691400	-2.30652300
C	4.95519000	-4.78432300	0.46848200
C	4.95517600	4.51354100	1.65331500
C	4.95513800	2.79810900	3.90717000
C	4.95513000	1.52111600	4.55860500
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C	6.19035400	2.61451900	-4.02681200
C	6.19033200	1.30832800	-4.61953900
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C	6.19040600	-4.79627100	-0.24742200
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C	6.19032200	0.82583100	4.72977400
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C	7.42932400	3.17804200	-3.58312100
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C	7.42930800	-3.33892100	-3.43387500
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C	7.42936500	-4.76775500	0.46930400
C	7.42933300	4.49899000	1.64545300
C	7.42928400	2.78664100	3.89535200
C	7.42927100	1.51823400	4.54238200
C	7.42925300	-1.30846300	4.60712600
C	7.42926400	-2.60516300	4.01881300
C	7.42933500	-4.41903400	1.84987600
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C	8.67604200	2.61545300	-4.02540600
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C	8.67602200	-2.79724200	-3.90151800
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C	8.67603900	3.34311800	3.44556600
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C	8.67605700	-4.10385600	2.49239800
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C	9.91082400	4.15373600	-2.52390200
C	9.91078400	3.22160700	-3.63868700
C	9.91072500	0.61624900	-4.82090800
C	9.91071800	-0.83652500	-4.78768600
C	9.91075000	-3.38501300	-3.48744200
C	9.91079600	-4.26498600	-2.33102600
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C	9.91079300	4.56361300	1.67363800
C	9.91074500	2.83097200	3.95031000
C	9.91071900	1.53653600	4.61062800
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C	11.10946300	4.90876000	-0.52583100
C	11.10945400	4.57002300	-1.86702500
C	11.10933900	2.64913300	-4.16521400
C	11.10930400	1.38944200	-4.73682800
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C	11.10945700	-4.65064300	-1.65576900
C	11.10947500	-4.92763800	-0.30047900
C	11.10939400	4.30936900	2.40866300
C	11.10936200	3.47156000	3.50941300
C	11.10928800	0.80343600	4.87050600
C	11.10926700	-0.57952800	4.90219600
C	11.10934400	-3.30701100	3.66469600
C	11.10938600	-4.19440100	2.60351000
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H	12.06290900	4.50870400	-2.38972100

H	12.06273000	3.15290400	-4.01253100
H	12.06268000	0.94272200	-5.01533100
H	12.06269500	-1.17164600	-4.96701200
H	12.06266400	-3.33362500	-3.86407800
H	12.06289200	-4.61337500	-2.18076200
H	12.06290100	-5.09924500	0.19709700
H	12.06280400	4.68012900	2.03502600
H	12.06272300	3.21016700	3.96640700
H	12.06270300	1.32670800	4.92742900
H	12.06265400	-1.09970600	4.98301500
H	12.06271700	-3.02490500	4.10918100
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**(8,8) tube**

H	12.06373400	-2.07426800	5.40759300
H	12.06389600	-4.10525300	4.08486800
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H	12.06369900	-5.40781000	-2.07437100
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H	12.06389500	-2.35640700	-5.28960500
H	12.06382600	0.01473100	-5.79120100
H	12.06381600	-0.01472600	5.79127200
H	12.06388900	2.35641700	5.28968000
H	12.06387500	4.08497600	4.10532500
H	12.06371200	5.40773400	2.07432300
H	12.06380800	5.79132900	0.01477200
H	12.06388800	5.28973700	-2.35637400
H	12.06389300	4.10526200	-4.08486700
H	12.06373500	2.07427700	-5.40759200
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C	11.10997500	-5.32530600	1.83243300
C	11.10993800	-5.61164700	0.47878100
C	11.10990300	-5.06208100	-2.47001400
C	11.10995600	-4.30697400	-3.62938800

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C	11.10997000	1.83249100	5.32530000
C	11.10996500	4.30693400	3.62936000
C	11.10991100	5.06204100	2.46998500
C	11.10993300	5.61167800	-0.47879400
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C	11.10997200	3.62933000	-4.30684600
C	11.10992100	2.46994400	-5.06194600
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C	9.91204300	-5.54082100	-0.29454800
C	9.91204900	-5.27460800	-1.72302500
C	9.91212800	-3.70971700	-4.12598600
C	9.91214300	-2.51106500	-4.94746400
C	9.91205500	0.29450500	-5.54075300
C	9.91205300	-0.29450600	5.54076900
C	9.91214500	2.51106200	4.94747200
C	9.91213300	3.70970400	4.12597700
C	9.91205200	5.27459600	1.72301500
C	9.91204300	5.54082700	0.29454100
C	9.91214800	4.94749000	-2.51101700
C	9.91214200	4.12596100	-3.70964200
C	9.91206600	1.72298300	-5.27451200
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C	8.67708600	-5.46750600	0.42110200
C	8.67707600	-4.94825100	-2.36414700
C	8.67710800	-4.16402900	-3.56828400
C	8.67710300	-1.82703900	-5.17004600
C	8.67709300	-0.42113600	-5.46745200
C	8.67709100	0.42113600	5.46745500
C	8.67710300	1.82703800	5.17005100

C	8.67711200	4.16402300	3.56827900
C	8.67708000	4.94824500	2.36414200
C	8.67708600	5.46750800	-0.42110600
C	8.67710300	5.17007100	-1.82700300
C	8.67712000	3.56825800	-4.16396300
C	8.67709100	2.36411500	-4.94817000
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C	7.43060400	-5.19983200	-1.69420000
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C	7.43061600	-0.29448700	5.46067300
C	7.43063500	2.47866900	4.87434100
C	7.43063600	3.65321000	4.06949500
C	7.43060600	5.19983100	1.69419800
C	7.43060800	5.46071800	0.29451100
C	7.43063900	4.87435900	-2.47863800
C	7.43064300	4.06948100	-3.65315900
C	7.43061700	1.69417200	-5.19976600
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C	6.19161500	-5.16540000	1.82412000
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C	6.19159700	-4.94293400	-2.36293500
C	6.19160800	-4.16072800	-3.56394100
C	6.19161200	-1.82414600	-5.16538400
C	6.19160400	-0.42187600	-5.46194600
C	6.19160300	0.42187600	5.46193300
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C	6.19161100	4.16072700	3.56394000
C	6.19159900	4.94293400	2.36293500
C	6.19159900	5.46199100	-0.42185700
C	6.19161300	5.16539700	-1.82412000

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C	6.19161000	2.36291300	-4.94287700
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C	4.95574600	-4.07917900	3.66500200
C	4.95574100	-4.88885500	2.48339000
C	4.95573100	-5.47587800	-0.29299300
C	4.95572800	-5.21343300	-1.70110200
C	4.95573600	-3.66504000	-4.07918700
C	4.95573400	-2.48341000	-4.88883700
C	4.95573800	0.29297900	-5.47583900
C	4.95573800	-0.29297800	5.47584600
C	4.95573500	2.48340800	4.88882800
C	4.95573900	3.66504600	4.07919300
C	4.95572900	5.21343400	1.70110400
C	4.95573000	5.47587200	0.29299400
C	4.95573900	4.88885100	-2.48338900
C	4.95574500	4.07917900	-3.66500400
C	4.95573900	1.70108400	-5.21338300
C	3.71508500	-2.36872400	4.94776400
C	3.71508700	-3.56605500	4.16796500
C	3.71508200	-5.17294800	1.82346500
C	3.71507600	-5.46862000	0.42549400
C	3.71507300	-4.94780200	-2.36873500
C	3.71507600	-4.16799300	-3.56605700
C	3.71508000	-1.82348200	-5.17293400
C	3.71507800	-0.42550300	-5.46857500
C	3.71507900	0.42550400	5.46856100
C	3.71508100	1.82348800	5.17294700
C	3.71507700	4.16799400	3.56605900
C	3.71507300	4.94780200	2.36873600
C	3.71507400	5.46861600	-0.42549300
C	3.71508000	5.17294400	-1.82346400
C	3.71508600	3.56605400	-4.16796800
C	3.71508500	2.36872400	-4.94776500
C	2.47594100	-1.70295100	5.21849100
C	2.47594300	-4.08311000	3.66877500

C	2.47594000	-4.89378800	2.48569000
C	2.47593300	-5.48130200	-0.29310600
C	2.47593000	-5.21853500	-1.70296200
C	2.47593300	-3.66880200	-4.08311200
C	2.47593400	-2.48569700	-4.89376000
C	2.47593900	0.29310100	-5.48127500
C	2.47594000	-0.29310000	5.48128200
C	2.47593400	2.48569700	4.89375700
C	2.47593400	3.66880900	4.08312100
C	2.47593000	5.21853700	1.70296500
C	2.47593200	5.48129300	0.29310700
C	2.47593900	4.89378100	-2.48568800
C	2.47594200	4.08311300	-3.66878100
C	2.47594000	1.70295400	-5.21850100
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C	1.23969200	-5.17569000	1.82651000
C	1.23969000	-5.47235000	0.42382100
C	1.23968700	-4.95189700	-2.36852600
C	1.23968800	-4.16945800	-3.56989300
C	1.23969000	-1.82651600	-5.17567400
C	1.23969200	-0.42382200	-5.47230900
C	1.23969300	0.42382300	5.47230100
C	1.23969100	1.82652400	5.17568600
C	1.23968800	4.16946400	3.56989900
C	1.23968800	4.95189400	2.36852700
C	1.23968900	5.47234500	-0.42382000
C	1.23969100	5.17568400	-1.82650900
C	1.23969800	3.56990100	-4.16944800
C	1.23969800	2.36852600	-4.95187800
C	0.00000600	-1.70036200	5.21656600
C	0.00000500	-4.08240600	3.66563000
C	0.00000400	-4.89059000	2.48616600
C	-0.00000400	-5.47855000	-0.29483200
C	-0.00000600	-5.21658700	-1.70036100
C	-0.00000500	-3.66564200	-4.08240100



C	-0.0000300	-2.48616100	-4.89055500
C	0.0000400	0.29483700	-5.47853600
C	0.0000500	-0.29483400	5.47853500
C	-0.0000200	2.48616500	4.89055900
C	-0.0000500	3.66564700	4.08240700
C	-0.0000500	5.21659300	1.70036600
C	-0.0000400	5.47853700	0.29483300
C	0.0000200	4.89058100	-2.48616300
C	0.0000400	4.08241000	-3.66563700
C	0.0000500	1.70036400	-5.21657200
C	-1.23968600	-2.36852600	4.95187700
C	-1.23968700	-3.56990700	4.16945500
C	-1.23969100	-5.17569300	1.82651600
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C	-1.23969900	-4.95189100	-2.36852100
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C	-1.23969100	-1.82651100	-5.17567500
C	-1.23968900	-0.42381700	-5.47231200
C	-1.23968900	0.42381900	5.47230700
C	-1.23969100	1.82651600	5.17567900
C	-1.23969900	4.16945700	3.56989700
C	-1.23969800	4.95188400	2.36852200
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C	-1.23969100	5.17568600	-1.82651500
C	-1.23968800	3.56990400	-4.16945300
C	-1.23968800	2.36853100	-4.95188900
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C	-2.47593900	2.48569000	4.89376000

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C	-2.47593500	4.89377900	-2.48569700
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C	-3.71508100	-5.17295500	1.82348200
C	-3.71508000	-5.46859900	0.42550600
C	-3.71508500	-4.94778100	-2.36872100
C	-3.71508700	-4.16796400	-3.56603800
C	-3.71508100	-1.82346700	-5.17293600
C	-3.71507500	-0.42549100	-5.46858700
C	-3.71507400	0.42549300	5.46858400
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C	-3.71508800	4.16797700	3.56605100
C	-3.71508500	4.94777600	2.36872100
C	-3.71507900	5.46860000	-0.42550300
C	-3.71508000	5.17294800	-1.82347900
C	-3.71507700	3.56606300	-4.16798700
C	-3.71507400	2.36874100	-4.94779500
C	-4.95572600	-1.70110200	5.21341100
C	-4.95573700	-4.07919600	3.66503400
C	-4.95573600	-4.88885600	2.48341000
C	-4.95574000	-5.47586200	-0.29297700
C	-4.95573900	-5.21339200	-1.70107900
C	-4.95574500	-3.66501200	-4.07917400
C	-4.95573900	-2.48338700	-4.88883000
C	-4.95573200	0.29299500	-5.47586400
C	-4.95572900	-0.29299400	5.47585600
C	-4.95574000	2.48339100	4.88883400
C	-4.95574700	3.66501300	4.07917400
C	-4.95573900	5.21340500	1.70108700
C	-4.95573800	5.47585300	0.29297900
C	-4.95573400	4.88885000	-2.48340700

C	-4.95573700	4.07919700	-3.66503600
C	-4.95572900	1.70110300	-5.21341200
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C	-6.19161400	-5.16540500	1.82414700
C	-6.19160600	-5.46196400	0.42187700
C	-6.19161100	-4.94289400	-2.36291200
C	-6.19161900	-4.16068500	-3.56391600
C	-6.19161400	-1.82412200	-5.16538700
C	-6.19159900	-0.42185600	-5.46196800
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C	-6.19161400	1.82412100	5.16538300
C	-6.19162200	4.16069200	3.56392300
C	-6.19161100	4.94289300	2.36291200
C	-6.19160300	5.46196800	-0.42187500
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C	-6.19160000	2.36293800	-4.94292100
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C	-7.43063600	-4.87436200	2.47867100
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C	-7.43063900	-2.47863900	-4.87434300
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C	-7.43060600	-0.29451200	5.46070500
C	-7.43064200	2.47863600	4.87434000
C	-7.43064600	3.65316200	4.06947000
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C	-7.43060800	1.69419700	-5.19980900
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C	-8.67710600	-5.17005900	1.82703700
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C	-8.67709000	-4.94818900	-2.36411600
C	-8.67711900	-4.16397300	-3.56825500
C	-8.67710400	-1.82700500	-5.17005500
C	-8.67708700	-0.42110600	-5.46748500
C	-8.67708500	0.42110100	5.46749000
C	-8.67710600	1.82699800	5.17005000
C	-8.67712400	4.16396600	3.56824600
C	-8.67709200	4.94818600	2.36411000
C	-8.67708900	5.46748200	-0.42113500
C	-8.67710000	5.17007100	-1.82703800
C	-8.67711000	3.56828500	-4.16401200
C	-8.67708100	2.36414400	-4.94822500
C	-9.91204700	-1.72302600	5.27460000
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C	-9.91214700	-2.51102300	-4.94747200
C	-9.91204500	0.29454000	-5.54079900
C	-9.91204100	-0.29454900	5.54081000
C	-9.91215200	2.51100800	4.94745900
C	-9.91214600	3.70963600	4.12593900
C	-9.91206300	5.27453200	1.72297600
C	-9.91205100	5.54079300	0.29450500
C	-9.91214100	4.94749600	-2.51106100
C	-9.91213200	4.12598900	-3.70969500
C	-9.91205500	1.72301500	-5.27457200
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C	-11.10997900	-5.32525200	1.83248000
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C	-11.10991700	-5.06199100	-2.46996700
C	-11.10996700	-4.30688800	-3.62934800

C	-11.10997200	-1.83244900	-5.32530700
C	-11.10993700	-0.47879700	-5.61164300
C	-11.10993600	0.47878000	5.61163600
C	-11.10997500	1.83243100	5.32529100
C	-11.10997800	4.30683900	3.62930300
C	-11.10992400	5.06194800	2.46992700
C	-11.10993600	5.61166300	-0.47883700
C	-11.10996600	5.32534000	-1.83249200
C	-11.10996300	3.62936900	-4.30692000
C	-11.10991100	2.46998800	-5.06202000
H	-12.06369800	-2.07437300	5.40780700
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H	-12.06390300	-5.28958000	2.35639300
H	-12.06383300	-5.79117000	-0.01474300
H	-12.06372500	-5.40767900	-2.07432000
H	-12.06388400	-4.08493500	-4.10530400
H	-12.06389000	-2.35637600	-5.28968900
H	-12.06381200	0.01477100	-5.79128500
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H	-12.06389800	2.35635000	5.28966700
H	-12.06390000	4.08485100	4.10523100
H	-12.06373600	5.40759100	2.07424900
H	-12.06381100	5.79132900	0.01472400
H	-12.06388200	5.28974100	-2.35642600
H	-12.06387700	4.10532600	-4.08496000
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**(9,9) tube**

C	11.10936100	-5.40947600	3.28401800
C	9.91213700	-5.68956200	2.56050300
C	8.67715900	-5.29644000	3.16333500
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C	11.10935400	-4.56584900	4.38064200
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C	6.19206200	-5.28596900	3.15791600

C	6.19203600	-4.41240000	4.29323900
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C	4.95584200	-5.62160400	2.52748400
C	3.71517400	-5.29197800	3.16502600
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C	4.95576500	-3.88900200	4.77904300
C	2.47610600	-5.62818600	2.53051200
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C	4.95587600	-6.05311400	1.16263400
C	3.71524600	-6.15016100	0.45147900
C	2.47616300	-6.06033200	1.16381500
C	6.19214300	-6.14102600	0.45394000
C	6.19216500	-6.07949500	-0.97719100
C	4.95590900	-5.93095600	-1.67573100
C	3.71528200	-6.08877800	-0.97555500
C	7.43109500	-6.03955000	1.16243900
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C	8.67727900	-6.09098100	-0.97984400
C	7.43113700	-5.91754200	-1.67434900
C	9.91220400	-6.12762600	1.17500300
C	11.10946500	-6.31438800	0.42209700
C	11.10946900	-6.25495300	-0.96020100
C	9.91224100	-6.00424600	-1.69434700
C	7.43114100	-5.37321000	-2.98994200
C	8.67728200	-5.00531000	-3.60397300
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C	2.47620800	-5.93801500	-1.67759600
C	1.23968000	-6.09298800	-0.97813500
C	1.23967100	-6.15450600	0.45356400
C	1.23968700	-5.00545500	-3.60652200

C	0.00009000	-5.38963600	-2.99983700
C	0.00010800	-5.93610900	-1.67893800
C	-1.23950600	-6.09314900	-0.97820500
C	-1.23952900	-6.15459500	0.45349200
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C	-1.23963100	-5.29674400	3.16557100
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C	1.23958700	2.19826800	5.76134700
C	2.47606800	1.51499900	5.97686600
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C	-4.95569700	6.08674100	0.97738200
C	-6.19194100	5.92707400	1.67348400
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C	-3.71516800	5.62478400	-2.52632500
C	-2.47611100	5.29611300	-3.16474500
C	-1.23955400	5.62795900	-2.52988400
C	-0.00003600	5.29371100	-3.16557900
C	1.23961700	5.62781400	-2.52995200



C	1.23966600	6.06023200	-1.16375600
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C	2.47622300	6.09301400	0.97853100
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C	1.23946500	3.89323300	-4.78439700
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C	11.10944800	-4.17309200	-4.75417400
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**(10,10) tube**

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C	3.71533100	6.83511500	-0.35151400
C	4.95601400	6.83018800	0.36559200
C	4.95602900	6.60456700	1.77846200
C	6.19258100	6.37768200	2.45497100
C	6.19260300	5.72601300	3.73011800
C	3.71531100	6.61343600	-1.76222600
C	2.47624600	6.39713500	-2.44633900
C	1.23954100	6.61835400	-1.76530100
C	-0.00001500	6.39593800	-2.44771100
C	-1.23957400	6.61837000	-1.76526800
C	-1.23956500	6.84079100	-0.35004100
C	-2.47626500	6.83921500	0.36602600
C	-2.47625200	6.61323700	1.78097400
C	-0.00003600	5.74848500	-3.72195700
C	1.23952000	5.32838700	-4.30391700
C	2.47623000	5.74808800	-3.72377300
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C	6.19254900	6.82523800	-0.34796900
C	3.71528300	4.31445900	-5.31274200

C	2.47622000	3.73734800	-5.73908300
C	1.23951500	4.31659800	-5.31811200
C	-0.00003600	3.73554300	-5.73948600
C	-1.23960100	4.31654300	-5.31805500
C	-1.23959000	5.32835000	-4.30387500
C	-2.47629500	5.74801000	-3.72369100
C	-2.47629400	6.39710400	-2.44629000
C	-0.00002600	2.46283200	-6.38996700
C	1.23953300	1.78090500	-6.61387600
C	2.47623300	2.46145700	-6.39115100
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C	6.19249200	5.31718800	-4.29315800
C	3.71532400	0.36768000	-6.83415100
C	2.47628200	-0.34980500	-6.83986600
C	1.23955000	0.36623200	-6.83983800
C	0.00000400	-0.35153100	-6.83916500
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C	-2.47630100	2.46138600	-6.39109300
C	-2.47630200	3.73728500	-5.73898700
C	0.00001600	-1.76353200	-6.61739300
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C	4.95603500	-1.76286300	-6.60883400
C	4.95602200	-0.34943400	-6.83093300
C	6.19255800	0.36411700	-6.82427900
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C	-1.23954100	-2.44682000	-6.39761300
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C	1.23959100	-5.73991100	-3.73757000
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C	0.00001900	-6.61314600	-1.77913800
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H	-12.06351900	-7.16955700	-0.09704800
H	-12.06344700	-4.27915200	-5.75328900
H	-12.06358000	-0.08016100	-7.16917500
H	-12.06352300	2.30766700	-6.78795600
H	-12.06349500	-2.12334200	-6.84855600
H	-12.06349500	4.14930400	-5.84715400

**UP-6-(5,5)**

C	1.23412300	-0.30139000	-6.46897200
C	3.55726900	-0.98474100	-6.42456000
C	1.61300600	1.02427000	-6.19974900
H	0.17586500	-0.54903900	-6.57299700
C	3.93408600	0.33001700	-6.14869300
H	4.30784600	-1.77262600	-6.48689700
H	0.85869700	1.79898400	-6.07379700
H	4.98709200	0.56829400	-5.98771900
C	2.31516700	6.88050200	0.11181500
C	4.23809500	8.17777800	-0.83838200
C	3.30564500	7.17322100	-0.94708500
C	3.12545700	6.34040700	-2.15247000
C	4.20335600	5.80435800	-2.87654900
C	1.61395700	5.06832700	-3.58857500
C	4.01556400	4.93233500	-3.95350400
H	5.22246100	6.01823500	-2.55878300
H	0.62714600	4.67964500	-3.82639700
H	4.88551200	4.54261200	-4.47565200
C	2.96783400	1.34887700	-6.03993500
C	2.71049500	4.52649900	-4.28261500
C	3.46351200	2.74366900	-5.71910700
H	3.89628000	3.22808100	-6.61436500
H	4.26437800	2.64570600	-4.97103600
O	2.40055100	3.56311600	-5.21241400
C	1.79472800	5.98320300	-2.53863500
C	0.66769300	6.53020800	-1.74120700
C	-0.51622000	6.94174200	-2.31569700
S	-0.85981100	6.87433700	-4.08058100
S	-1.85734100	7.72479800	-1.41029400
C	-2.33280700	7.83363800	-4.02868000
H	-2.81860700	8.05233400	-4.97748600
C	-2.78548900	8.21826100	-2.82002400
H	-3.69185500	8.79395500	-2.64387900
S	5.33838300	8.67374300	-2.17242400

C	5.45960800	10.42564500	-0.16572100
H	5.73540200	11.30095500	0.41909600
S	4.40769700	9.24104500	0.60257800
C	5.88169400	10.16989900	-1.41899100
H	6.54861100	10.80646600	-1.99699700
C	1.70758000	6.49592600	2.44915500
C	0.96359600	6.62815600	-0.29181600
C	0.01297200	6.40127600	0.72045100
H	-1.01451200	6.16543100	0.45543600
C	0.35976000	6.36064600	2.07584200
H	-0.40488800	6.14397500	2.81894300
C	2.67102600	6.77959000	1.46441200
H	3.71400900	6.83991700	1.76995200
O	2.17880100	6.32693000	3.72346400
C	2.42766500	4.69260100	5.47750600
H	2.95765300	5.38144500	6.15352400
H	3.17960700	4.25856500	4.80187500
C	1.74463200	3.55377700	6.26185600
H	1.02984900	3.04825000	5.59237200
H	1.15386500	3.95721600	7.10111700
C	2.75255400	2.50191300	6.76240500
H	3.34412500	2.90329400	7.60266000
H	3.46718100	2.29858800	5.94914700
C	2.09409100	1.16838100	7.15592200
H	1.40477500	0.87213700	6.34905800
H	1.48049200	1.28240100	8.06460700
C	1.43156300	5.45678900	4.60553000
H	0.72506100	6.05486200	5.20731300
H	0.85137200	4.73517500	4.00937900
C	3.12853100	0.03602500	7.36043800
O	1.71537700	-6.12404400	3.11133700
C	2.19032000	-6.29350500	1.83970300
C	2.93884000	-6.50715900	-0.88338100
C	1.20991800	-6.32482000	0.83179900
H	0.17801500	-6.16567200	1.13448900
C	3.55028100	-6.36879000	1.49136800

H	4.33145700	-6.28362500	2.24178700
C	3.90171300	-6.45672300	0.13964200
H	4.95742900	-6.41190100	-0.12188400
C	1.55522300	-6.44283700	-0.52217800
C	0.54836400	-6.42280900	-1.60953800
C	3.28785700	-6.54414300	-2.31963900
C	2.38465100	-5.73659500	-3.16919300
C	0.99542200	-5.69848500	-2.82074400
C	2.83653000	-5.00279500	-4.27612700
H	3.89733300	-4.94824100	-4.51210200
C	0.13956900	-4.92491900	-3.62365600
H	-0.90117200	-4.80184400	-3.33530800
C	0.58713000	-4.22888400	-4.75299900
H	-0.12812900	-3.62897400	-5.30993500
C	1.94699400	-4.28181100	-5.09596300
O	2.52331600	-3.71628500	-6.20755100
C	2.19854500	-1.31349000	-6.59352000
C	1.81963400	-2.72750600	-6.98692000
C	4.28553800	-7.34444000	-2.83056100
C	-0.66211300	-7.07863500	-1.52095700
S	4.66134000	-7.50735200	-4.58248000
S	5.27307700	-8.46803300	-1.83003400
S	-1.18542200	-8.05037100	-0.10025800
S	-1.85437400	-7.17693800	-2.86353600
C	5.96462500	-9.36325400	-3.17874300
H	6.60060600	-10.21331100	-2.93978700
C	5.68725400	-8.92916500	-4.42312900
H	6.06544000	-9.37615300	-5.34040300
C	-2.87389500	-8.40871000	-2.13087900
H	-3.71407400	-8.77456800	-2.71759800
C	-2.57013100	-8.80394400	-0.87986100
H	-3.12813500	-9.53823400	-0.30231700
H	2.14637800	-2.92520300	-8.01955100
H	0.73016500	-2.86919300	-6.95728800
H	3.85667800	0.09353000	6.53258900
H	3.69133800	0.19202800	8.29519600

C	-1.85538100	-3.28123100	6.16407100
H	-2.55091100	-4.13644400	6.19615100
C	-0.72459200	-3.48170000	7.19548600
H	-0.07520800	-2.59116600	7.20371700
H	-1.16546700	-3.55475100	8.20273900
C	0.13211400	-4.72979500	6.91370800
H	-0.51979500	-5.61949800	6.86033800
H	0.81169300	-4.90017200	7.76650900
C	0.96870300	-4.64547400	5.62354300
H	0.31350600	-4.59486800	4.74211400
H	1.56758800	-3.71980400	5.62836800
C	1.90654100	-5.85633100	5.48610500
H	1.32837200	-6.78885800	5.59235200
H	-1.40681700	-3.27574300	5.15846200
C	2.67351300	-5.92003400	4.16843600
H	3.23392300	-4.98798200	3.97775200
H	3.39023600	-6.75961000	4.18360700
H	2.64618800	-5.84303200	6.30400800
C	10.26214000	3.16463400	-0.85913800
C	10.29598500	2.32912600	-1.96014500
C	9.10472300	1.67254800	-2.41188600
C	7.86173900	2.24767700	-2.00945400
C	7.82608400	3.12039900	-0.86213400
C	9.03527600	3.38676100	-0.15210800
C	6.62496500	1.66666900	-2.45965700
C	6.62776200	0.30211800	-2.87999800
C	7.86773000	-0.42623700	-2.83198300
C	9.10789500	0.28083900	-2.83964300
C	7.83716100	-1.79313100	-2.37345300
C	9.04813600	-2.40785100	-1.93411100
C	10.27346200	-1.82083500	-2.39048000
C	10.30258800	-0.51084600	-2.83166600
C	6.55646200	3.36311300	-0.22928000
C	5.34326400	3.15296000	-0.96096700
C	5.37990700	2.27752900	-2.10306100
C	4.15932500	1.69416900	-2.55457000

C	4.16170500	0.32234900	-2.97771500
C	5.38512500	-0.40839300	-2.93084800
C	5.35410200	-1.77615500	-2.48059700
C	6.56914200	-2.35523300	-1.98985900
C	4.08834800	3.39964700	-0.32845700
C	2.87510900	3.16560500	-1.05538600
C	2.91149400	2.29851200	-2.18961200
C	1.68862900	1.72423600	-2.66283700
C	1.69107200	0.35103700	-3.07977900
C	2.91581600	-0.38577500	-3.01555700
C	2.88413100	-1.74115300	-2.56616700
C	4.10087500	-2.34042100	-2.09647600
C	1.61375100	3.41302500	-0.42542500
C	-0.78148000	1.75297200	-2.77260600
C	-0.77886200	0.38189000	-3.18741100
C	0.45088500	-0.35294900	-3.12069500
C	0.41864300	-1.70732300	-2.65041600
C	1.62591200	-2.30245400	-2.17948500
C	-0.85313200	3.42116400	-0.52077400
C	-2.06685600	3.21760300	-1.25557600
C	-2.03075200	2.35969200	-2.41093300
C	-3.25366400	1.78021100	-2.86930000
C	-3.25054000	0.40204700	-3.28788300
C	-2.02454900	-0.32865000	-3.22735900
C	-2.05538100	-1.68798600	-2.75240000
C	-0.84107100	-2.26515100	-2.25829800
C	-3.32188300	3.46189500	-0.61853500
C	-4.53729800	3.23592500	-1.34625300
C	-4.50239900	2.37737900	-2.49196100
C	-5.73182900	1.79855600	-2.95570600
C	-5.72838200	0.42229200	-3.37626000
C	-4.49563600	-0.31066200	-3.31227700
C	-4.52524400	-1.66502400	-2.84665700
C	-3.30878700	-2.25709300	-2.37026500
C	-5.80029300	3.48379800	-0.70984200
C	-7.00901100	3.26150600	-1.43599700



C	-6.97391400	2.39726200	-2.58692400
C	-8.20218700	1.80853200	-3.03344400
C	-8.19867800	0.44532600	-3.45139700
C	-6.96697600	-0.28650300	-3.40916600
C	-6.99664100	-1.64829800	-2.94273600
C	-5.78640000	-2.23564200	-2.46540100
C	-8.27078300	3.48939800	-0.79503800
C	-9.49388400	3.27594300	-1.52212400
C	-9.45857700	2.41037900	-2.67426800
C	-10.67830000	1.85911600	-3.17009300
C	-10.67469600	0.46835600	-3.59742800
C	-9.45168200	-0.26044500	-3.49426900
C	-9.48144500	-1.62415100	-3.02811500
C	-8.25660700	-2.20426600	-2.54512300
C	-10.74784600	3.56224300	-0.90313200
C	-11.92229200	3.36650000	-1.70175000
C	-11.88839100	2.53630300	-2.80631900
C	-10.73337000	-2.21532400	-2.68057700
C	-11.90961500	-1.60951100	-3.23247700
C	-11.88106700	-0.30181400	-3.67927700
C	-8.30836000	-3.02545300	-1.38060000
C	-9.58273100	-3.23293600	-0.74587500
C	-10.78609600	-3.05307000	-1.49220100
C	-5.83873800	-3.06574700	-1.29087700
C	-7.09862400	-3.26571200	-0.65033000
C	-7.15333900	-3.24556300	0.78832600
C	-8.41456100	-2.98546900	1.41770300
C	-9.63743000	-3.21230500	0.69444500
C	-10.89363400	-3.01162100	1.34179700
C	-12.06955800	-3.29896900	0.57372600
C	-12.01712300	-3.31914500	-0.80736800
C	-8.44990500	-2.13029200	2.55814600
C	-9.70688700	-1.53592800	2.92814500
C	-10.92983400	-2.13811800	2.50482200
C	-5.94538200	-3.02654300	1.51649300
C	-5.98076300	-2.16343300	2.66771800

C	-7.22274400	-1.56223500	3.03351000
C	-7.22621000	-0.18555900	3.45573100
C	-8.45610300	0.54673600	3.37983200
C	-9.71009800	-0.15793400	3.35129300
C	-10.93603800	0.57306500	3.33797600
C	-12.14657000	-0.19474700	3.35255300
C	-12.14353200	-1.51594600	2.94648600
C	-8.42593400	1.89526300	2.91724900
C	-9.65076200	2.48520700	2.44657100
C	-10.90512500	1.94946600	2.86727000
C	-5.98746300	0.52243400	3.49179400
C	-5.95715900	1.88307700	3.02375500
C	-7.16681600	2.46959800	2.54442500
C	-7.11410800	3.29893500	1.36867100
C	-8.32425200	3.50877900	0.62969900
C	-9.59839800	3.31551700	1.26941900
C	-10.80226900	3.58329400	0.55068000
C	-12.03326500	3.41083100	1.26485000
C	-12.08339700	2.61463600	2.39364700
C	-5.85445900	3.50191900	0.72824800
C	-4.75138000	-1.58061200	3.12548200
C	-4.75522600	-0.21203300	3.54596200
C	-4.68241100	-3.26859900	0.87828100
C	-4.62765900	-3.28755100	-0.55269000
C	-4.69602300	2.44667700	2.63329100
C	-4.64282700	3.27031400	1.46259300
C	-3.50423600	-2.18440300	2.75857200
C	-3.46851700	-3.05250700	1.61131400
C	-3.36105300	-3.09031300	-1.19654400
C	-3.51190700	0.49966100	3.58786900
C	-3.48115500	1.86104100	3.12136500
C	-3.37644300	3.47645400	0.82083500
C	-2.28351400	-1.60165300	3.21202600
C	-2.28719100	-0.23173200	3.64316200
C	-2.21248000	-3.29827800	0.97774500
C	-2.15792300	-3.31358600	-0.46004500

C	-2.22649300	2.42359500	2.73616000
C	-2.17293600	3.24410500	1.55446600
C	-1.03453000	-2.20179900	2.84498800
C	-0.99783900	-3.06598700	1.70488700
C	-0.89237200	-3.09435700	-1.09482300
C	-1.04141100	0.47755200	3.68097400
C	-1.01123100	1.83051500	3.21432900
C	-0.90830300	3.42521300	0.90736700
C	0.19248900	-1.63069800	3.32017400
C	0.18973700	-0.25698200	3.74561300
C	0.26420600	-3.30710100	1.07013300
C	0.31669100	-3.32609200	-0.36433400
C	0.24911700	2.39100800	2.82167900
C	0.30069000	3.20759200	1.64347100
C	1.43511300	-2.23011900	2.95072100
C	1.47128300	-3.08524700	1.79715500
C	1.57365700	-3.12954500	-1.00794400
C	1.43057800	0.45107800	3.77347100
C	1.46098600	1.80837600	3.30160800
C	1.55853400	3.42082800	1.00806800
C	2.66341100	-1.64973700	3.41007000
C	2.66150100	-0.28079800	3.82357600
C	2.72958600	-3.32116100	1.15516800
C	2.78199500	-3.35195200	-0.27239000
C	2.71684000	2.37376600	2.90832000
C	2.76638200	3.20388100	1.74500700
C	3.91266400	-2.25230000	3.03997400
C	3.94578500	-3.10705200	1.88487200
C	4.04783800	-3.16352100	-0.91973500
C	3.90706300	0.43108400	3.85608000
C	3.93582400	1.79059300	3.39069000
C	4.03366100	3.42247300	1.10783400
C	5.13481500	-1.67528400	3.49887300
C	5.13195500	-0.29789000	3.91741500
C	5.19851400	-3.35712500	1.25152800
C	5.25089900	-3.38853100	-0.18710900

C	5.18702300	2.36222600	3.01270000
C	5.23725100	3.20066700	1.84216200
C	6.38154100	-2.26635400	3.11426900
C	6.41333300	-3.12362000	1.97427000
C	6.51634100	-3.17723400	-0.82508100
C	6.37577600	0.41324800	3.93592400
C	6.40365300	1.76394500	3.47787100
C	6.50283600	3.38758800	1.19621000
C	7.61806200	-1.69318300	3.57500300
C	7.61510800	-0.31502900	3.99849000
C	7.68218000	-3.37884300	1.34568400
C	7.73503900	-3.40599700	-0.09498500
C	7.67076400	2.33308800	3.10325600
C	7.72161300	3.16786600	1.92878300
C	8.85719400	-2.31934700	3.24407000
C	8.89006600	-3.19918900	2.08507800
C	8.99450800	-3.24980600	-0.74814900
C	8.85159800	0.39341400	4.07824200
C	8.88017000	1.77238400	3.61387900
C	8.98059300	3.41164400	1.30201800
C	10.04615400	-1.71777100	3.77221400
C	10.04343100	-0.39656500	4.17912300
C	10.11402200	-3.51443700	1.40882000
C	10.16476900	-3.53876800	0.02763300
C	10.10232000	2.41726900	3.23288100
C	10.15117700	3.21612400	2.10593000
C	0.44660300	2.32965800	-2.30635200
C	0.40870600	3.18740500	-1.15538800
H	-13.10115500	0.30139900	3.52514200
H	-13.09582800	-2.02733900	2.80936300
H	-12.96626300	3.77040300	0.83195400
H	-13.05451100	2.36717600	2.82130600
H	-12.82512200	2.27396500	-3.29714200
H	-12.88482000	3.73691100	-1.35027600
H	-13.04132400	-3.33979900	1.06485400
H	-12.94891600	-3.37531300	-1.36935200

H	-12.86990300	-2.11801400	-3.15200000
H	-12.81958500	0.18674700	-3.93945600
H	10.99688500	-2.24563600	3.70398800
H	10.99198600	0.08182200	4.42098700
H	11.03409400	2.15167500	3.73125800
H	11.12027900	3.55891200	1.74462900
H	11.20246400	3.51862100	-0.43763600
H	11.26218500	2.04728900	-2.37756700
H	11.26719700	-0.03873800	-3.01569500
H	11.21583300	-2.34614100	-2.23817900
H	11.13480200	-3.61583300	-0.46261600
H	11.04518100	-3.57288900	1.97163600
C	2.49717200	-1.33092400	7.35226600
H	1.92257500	-1.57465600	6.45175500
C	2.58236000	-2.23521800	8.33836500
H	2.09610300	-3.20809900	8.26346300
H	3.14448400	-2.02377500	9.25176700
C	-2.60954000	-1.99436900	6.36919200
H	-1.99490600	-1.08889000	6.41085800
C	-3.94079700	-1.88690800	6.49272600
H	-4.58533100	-2.76842300	6.44852800
H	-4.42940700	-0.92058300	6.62429900

**UP-6-(6,6)**

C	-2.00858500	-0.24880200	-6.75106000
C	0.23493300	-1.15402400	-6.78507700
C	-1.49610700	1.05391400	-6.75659600
H	-3.08828200	-0.39794800	-6.69149000
C	0.74773000	0.14866500	-6.78830900
H	0.90947700	-2.00707700	-6.74848200
H	-2.16812800	1.90808300	-6.70013300
H	1.82894200	0.29742900	-6.76108300
C	-0.27124400	7.26569300	-0.97296000
C	1.81542400	8.24346100	-1.95965400
C	0.77199500	7.34617400	-2.02193000
C	0.52444200	6.45036200	-3.17223800

C	1.54770300	5.77838000	-3.86297500
C	-1.09322600	5.20980000	-4.52527700
C	1.28466100	4.85926800	-4.88491600
H	2.58303400	5.91522600	-3.55732300
H	-2.11350200	4.89764800	-4.73755100
H	2.11893100	4.37125000	-5.38226100
C	-0.10675400	1.26306700	-6.73705200
C	-0.04951900	4.53702100	-5.18777500
C	0.51760100	2.63776900	-6.58749000
H	0.90397400	3.02080200	-7.54982600
H	1.36761300	2.53941400	-5.89608300
O	-0.44915800	3.56849500	-6.07447700
C	-0.83019400	6.18395900	-3.54930100
C	-1.90347300	6.91786200	-2.83690000
C	-2.99904800	7.43903900	-3.49023900
S	-3.29452000	7.27058700	-5.25732300
S	-4.23376800	8.48632600	-2.70706300
C	-4.58596700	8.46250000	-5.34852100
H	-4.99254400	8.68229000	-6.33368500
C	-5.01176100	9.01238900	-4.19525300
H	-5.81386900	9.74246300	-4.10765300
S	2.99563200	8.50679900	-3.29127400
C	3.28514900	10.37801400	-1.41613600
H	3.65298500	11.25465700	-0.88662200
S	2.07920000	9.39045400	-0.59918800
C	3.70120600	9.97869600	-2.63324200
H	4.45508800	10.48278800	-3.23456200
C	-0.98700800	7.22331600	1.37163800
C	-1.63195400	7.11398900	-1.39511300
C	-2.62906800	7.09113500	-0.40416600
H	-3.66596400	6.92030500	-0.68619100
C	-2.33156600	7.18054100	0.96116000
H	-3.14204900	7.14087300	1.68504100
C	0.02894000	7.28074000	0.39737700
H	1.06166500	7.25947100	0.73990300
O	-0.55935700	7.16305900	2.67049100

C	-0.74739700	6.04188000	4.80886200
H	-0.15506300	6.76341700	5.39268300
H	-0.04032700	5.33754500	4.34727600
C	-1.72241500	5.25643200	5.70758900
H	-2.40859400	4.68899700	5.05778100
H	-2.35187100	5.94815100	6.29305500
C	-1.02425900	4.25254000	6.64129700
H	-0.43712000	4.78168500	7.41088600
H	-0.30382400	3.67014900	6.04681600
C	-2.01968200	3.28177400	7.30405800
H	-2.75140000	2.94637300	6.55250400
H	-2.59490100	3.80543000	8.08695600
C	-1.50390200	6.74369200	3.67973200
H	-2.07177100	7.61885900	4.04139600
H	-2.21645000	6.02939100	3.24209600
C	-1.33427900	2.03053100	7.90013100
O	-0.20497400	-7.24259000	2.71688300
C	0.17347300	-7.26990900	1.40102000
C	0.71717900	-7.10145700	-1.38478000
C	-0.87403200	-7.34695600	0.46291500
H	-1.89421900	-7.36520700	0.84122700
C	1.49912800	-7.17110800	0.94467800
H	2.33174200	-7.10879300	1.64125700
C	1.74596800	-7.04974700	-0.42806900
H	2.76571800	-6.83889600	-0.74272300
C	-0.62251200	-7.30411800	-0.91656500
C	-1.69641100	-7.41958300	-1.92977000
C	0.93432800	-6.89948600	-2.83485300
C	-0.18832500	-6.21117600	-3.51582400
C	-1.51917200	-6.51706600	-3.08681300
C	0.00432700	-5.24407100	-4.51479700
H	1.00359900	-4.89718800	-4.76853800
C	-2.58972000	-5.87992000	-3.73700100
H	-3.60648400	-6.04310000	-3.38482000
C	-2.39595500	-4.97071000	-4.78298500
H	-3.26265500	-4.50984600	-5.25014100

C	-1.08625000	-4.61982700	-5.14878000
O	-0.75423600	-3.65679900	-6.06838200
C	-1.15159000	-1.36373900	-6.72603900
C	-1.75909900	-2.74199800	-6.53665900
C	2.02917100	-7.38043300	-3.52077700
C	-2.70214900	-8.35667400	-1.83965500
S	2.25884600	-7.21624400	-5.29837800
S	3.33273300	-8.36871900	-2.77295700
S	-2.87824400	-9.52103100	-0.47960400
S	-3.91172200	-8.65964500	-3.13661900
C	4.07819800	-8.87977100	-4.28272200
H	4.91113400	-9.57686100	-4.21681800
C	3.59140100	-8.35827900	-5.42494900
H	3.97205000	-8.57121200	-6.42191700
C	-4.52913100	-10.16825600	-2.47237800
H	-5.27603600	-10.70202700	-3.05658300
C	-4.06025900	-10.55742900	-1.27132200
H	-4.37192400	-11.45427600	-0.73958000
H	-2.19180800	-3.13651200	-7.47427600
H	-2.57257200	-2.64806500	-5.80147700
H	-0.78689400	1.50228900	7.10508200
H	-0.58147100	2.34947800	8.64278000
C	0.49156000	-1.90162900	7.64951400
H	-0.25476200	-2.08405600	8.43851400
C	1.19334400	-3.21379000	7.23730100
H	1.97773800	-2.96469300	6.50441100
H	1.70739600	-3.65712300	8.10574900
C	0.22615200	-4.23176900	6.59893400
H	-0.49068400	-3.68690700	5.96453100
H	-0.37001900	-4.73713300	7.37711500
C	0.95229100	-5.26231300	5.71598500
H	1.63555800	-4.70701400	5.05237900
H	1.58705200	-5.92021000	6.33328800
C	-0.00427600	-6.09662000	4.83972400
H	-0.75913300	-5.42918000	4.39944700
H	-0.06731700	-1.53969000	6.77003800



C	0.75116900	-6.75465100	3.68418600
H	1.39576400	-5.99765300	3.21313300
H	1.39170300	-7.58672400	4.02587600
H	-0.54228800	-6.84968100	5.43600900
C	-2.32861200	1.09752100	8.54214000
C	-2.61833700	-0.13662700	8.10349900
H	-2.10526200	-0.56178200	7.24024200
H	-3.37178400	-0.75802400	8.59139600
C	1.45496700	-0.82779400	8.08228800
C	1.35418900	-0.10835100	9.20930600
H	0.52775900	-0.26731700	9.90593600
H	2.07947300	0.66776900	9.46095900
H	2.28697200	-0.63679400	7.39523500
H	-2.87109200	1.49777600	9.40672400
H	-11.86411000	-2.47521500	-3.16020400
H	-11.83397900	-4.08132300	-1.33564800
H	-11.81045800	-4.51143600	0.76204000
H	-11.79606000	-3.73889700	3.06756600
H	-11.79857100	-2.12786100	4.47846500
H	-11.81612000	0.25730200	4.94961100
H	-11.88712600	-0.44863400	-3.85004800
H	-11.90224400	1.93644200	-3.37967900
H	-11.90144300	3.54845700	-1.96895400
H	-11.88711800	4.32075700	0.33656400
H	-11.86699700	3.88969500	2.43245900
H	-11.83937700	2.28392600	4.25754400
C	-10.90473400	-2.76633400	-2.73423100
C	-10.88760000	-3.68016900	-1.69627900
C	-10.85542800	-4.27623600	1.23026000
C	-10.84726800	-3.83686700	2.54146000
C	-10.85018500	-1.59299100	4.51070900
C	-10.86022500	-0.23629400	4.77860700
C	-10.93685100	0.06122000	-3.69634400
C	-10.94544300	1.41806600	-3.42909900
C	-10.94499900	3.66254100	-1.46017700
C	-10.93688600	4.10163900	-0.14887700

C	-10.90810500	3.50439500	2.77691600
C	-10.89245100	2.59096100	3.81522600
C	-9.71417900	-2.07573700	-3.12477800
C	-9.67885700	-3.96064500	-0.98419300
C	-9.66306000	-4.25065900	0.44004800
C	-9.64622800	-3.34411600	3.14296900
C	-9.64774900	-2.25190800	4.10206400
C	-9.66824600	0.54517300	4.65522200
C	-9.72971400	-0.69980700	-3.59362900
C	-9.74734900	2.09791500	-3.04269800
C	-9.74700600	3.19029400	-2.08370200
C	-9.73026000	4.09504900	0.61987000
C	-9.71650300	3.80439600	2.04411000
C	-9.68399800	1.92094300	4.18600200
C	-8.47141200	-2.63270300	-2.69381300
C	-8.45357300	-3.58387100	-1.61420100
C	-8.42329900	-4.14396600	1.14148400
C	-8.41474100	-3.68614200	2.50535900
C	-8.41743900	-1.57447900	4.36165100
C	-8.42797700	-0.16332000	4.64129900
C	-8.50149000	0.02970900	-3.60142500
C	-8.51043100	1.44156800	-3.32418600
C	-8.51010900	3.55337700	-1.46858500
C	-8.50165500	4.00885900	-0.10371900
C	-8.47463200	3.44768100	2.65274100
C	-8.45834000	2.49848500	3.73402500
C	-7.23309800	-2.02203000	-3.09579000
C	-7.19841700	-3.88592400	-0.98081700
C	-7.18263500	-4.16978400	0.41529300
C	-7.16583700	-3.27135600	3.08550900
C	-7.16739200	-2.20166200	4.02647800
C	-7.18781000	0.56133800	4.57705600
C	-7.24795900	-0.67341300	-3.55651900
C	-7.26574600	2.09185800	-3.01396400
C	-7.26545800	3.16188700	-2.07321300
C	-7.24852700	4.05192400	0.60042000

C	-7.23546800	3.76780500	1.99692000
C	-7.20355700	1.90977200	4.11711200
C	-5.98645100	-2.61759700	-2.71875200
C	-5.96844500	-3.56858500	-1.64186400
C	-5.93741600	-4.13040000	1.12272900
C	-5.92861600	-3.67083500	2.48404600
C	-5.93153300	-1.55300200	4.34814100
C	-5.94228100	-0.14435400	4.63059500
C	-6.01591000	0.05407800	-3.63221100
C	-6.02472300	1.46468800	-3.35782200
C	-6.02429900	3.58178200	-1.49453000
C	-6.01589200	4.03208900	-0.12962100
C	-5.98966400	3.47108700	2.63808700
C	-5.97325200	2.52600300	3.72059500
C	-4.76098100	-2.01029200	-3.12831300
C	-4.72624900	-3.88169100	-1.01118700
C	-4.70977300	-4.16943300	0.39559000
C	-4.69222000	-3.26427700	3.07179100
C	-4.69416700	-2.18649000	4.02132500
C	-4.71544700	0.58318900	4.57964900
C	-4.77515000	-0.65119800	-3.59473000
C	-4.79306500	2.12265400	-3.05820100
C	-4.79310100	3.19990400	-2.10827500
C	-4.77611400	4.08059000	0.57599800
C	-4.76395700	3.79912300	1.98446700
C	-4.73198100	1.94196300	4.11595800
C	-3.51499600	-2.59581900	-2.73188900
C	-3.49653200	-3.54445200	-1.66444900
C	-3.46237500	-4.10906400	1.10208800
C	-3.45370700	-3.64951300	2.45741200
C	-3.45750300	-1.52692600	4.32894100
C	-3.46865500	-0.12502300	4.61140900
C	-3.54133000	0.07856100	-3.64642400
C	-3.54952900	1.48433600	-3.38335300
C	-3.54993900	3.59965700	-1.51361200
C	-3.54268500	4.03309400	-0.15263700

C	-3.51765100	3.48173400	2.61794900
C	-3.50087600	2.54639600	3.69792900
C	-2.28537900	-1.98878600	-3.14288400
C	-2.24916500	-3.86228000	-1.03759400
C	-2.23145700	-4.14253200	0.36856400
C	-2.21312300	-3.23602900	3.04410400
C	-2.21489600	-2.15984100	3.99601000
C	-2.23771800	0.60626000	4.55697600
C	-2.29795400	-0.63053100	-3.59738600
C	-2.31282100	2.14086700	-3.07615800
C	-2.31319800	3.21429700	-2.12416900
C	-2.30042600	4.08048300	0.55568000
C	-2.28713300	3.80380500	1.95938700
C	-2.25345500	1.96171000	4.09099200
C	-1.04523000	-2.58659200	-2.76906500
C	-1.02694100	-3.53811100	-1.69838000
C	-0.98933400	-4.07299500	1.06841800
C	-0.98093800	-3.60922800	2.42442900
C	-0.98487500	-1.49941700	4.29803800
C	-0.99549200	-0.09554700	4.59088400
C	-1.06964600	0.09162000	-3.65220700
C	-1.07717600	1.49854600	-3.39012800
C	-1.07881900	3.60872800	-1.52580000
C	-1.07274000	4.05496500	-0.16697000
C	-1.04564900	3.50611600	2.59652200
C	-1.02887700	2.56713300	3.67757300
C	0.18296800	-1.97883500	-3.18206400
C	0.22198400	-3.84277000	-1.06899500
C	0.23931700	-4.09568300	0.33460100
C	0.25836100	-3.18718500	3.00480200
C	0.25815500	-2.12228100	3.95435900
C	0.23657300	0.63524100	4.53543800
C	0.16952400	-0.62029900	-3.61785100
C	0.15797500	2.14673900	-3.07162800
C	0.15775900	3.21362400	-2.12591800
C	0.16838700	4.11875900	0.54347800

C	0.18339100	3.84102700	1.94355500
C	0.22014500	1.98680300	4.07162200
C	1.43097600	-2.58072100	-2.81523500
C	1.45008400	-3.52522800	-1.73574200
C	1.48379600	-4.02766500	1.03584100
C	1.49409000	-3.56894600	2.39155000
C	1.49320900	-1.47191100	4.27492300
C	1.48352500	-0.06922200	4.57346600
C	1.40304800	0.10390700	-3.68321100
C	1.39651900	1.50863600	-3.40126800
C	1.39518400	3.62349000	-1.53660000
C	1.40225800	4.09168600	-0.18288000
C	1.43078900	3.55038600	2.58707400
C	1.44968100	2.60478900	3.66813800
C	2.65719000	-1.97277700	-3.22792600
C	2.69414000	-3.82451100	-1.10219400
C	2.71062400	-4.07456200	0.30992100
C	2.73056900	-3.17336500	2.98579100
C	2.73023900	-2.10336900	3.94257900
C	2.71116800	0.66044100	4.52031800
C	2.64216800	-0.60484700	-3.66959500
C	2.62810000	2.16281000	-3.09603700
C	2.62702500	3.23706700	-2.14462900
C	2.64169800	4.16123200	0.52322600
C	2.65693400	3.88456100	1.93377700
C	2.69433300	2.02219400	4.06096700
C	3.90611200	-2.55993300	-2.83922400
C	3.92438800	-3.50046000	-1.76107300
C	3.95375800	-4.02286400	1.01793600
C	3.96459100	-3.56408900	2.37369700
C	3.96633000	-1.45037000	4.25515800
C	3.95680800	-0.04922700	4.54632700
C	3.87461300	0.12566500	-3.72255400
C	3.86709400	1.52726500	-3.43050000
C	3.86577900	3.65127200	-1.55975500
C	3.87392500	4.11915900	-0.20723800

C	3.90489200	3.57310200	2.56698300
C	3.92395300	2.63007900	3.64342800
C	5.13801600	-1.94650600	-3.24704700
C	5.17273700	-3.80543500	-1.12232500
C	5.18787600	-4.07335500	0.28857500
C	5.20695700	-3.16052000	2.96552800
C	5.20781100	-2.08663500	3.91922600
C	5.19084400	0.68052800	4.48953100
C	5.12225100	-0.58268500	-3.69709600
C	5.10414000	2.18546900	-3.12279000
C	5.10322700	3.26378500	-2.17408000
C	5.12075800	4.17999400	0.49903300
C	5.13663500	3.90299500	1.90800600
C	5.17408600	2.04149000	4.03194000
C	6.38127300	-2.53010800	-2.85608100
C	6.39903000	-3.47664600	-1.77534400
C	6.42785000	-4.01231900	0.99432600
C	6.43760100	-3.54734000	2.35411600
C	6.43988300	-1.43388200	4.22462300
C	6.43112900	-0.02676900	4.51438400
C	6.34954100	0.14615400	-3.74474700
C	6.34047000	1.55331600	-3.45349800
C	6.33943200	3.67219300	-1.58896200
C	6.34816100	4.13744400	-0.22952700
C	6.38014000	3.59350000	2.53763300
C	6.39925200	2.64651600	3.61776500
C	7.61117600	-1.91063100	-3.24993800
C	7.64565600	-3.76754200	-1.13290900
C	7.66041500	-4.03942600	0.26571700
C	7.67869600	-3.12826100	2.93313400
C	7.67984800	-2.06068700	3.87677700
C	7.66332600	0.69935600	4.44281100
C	7.59533700	-0.55878600	-3.69957600
C	7.57629100	2.20176000	-3.13220200
C	7.57565800	3.27159900	-2.19099600
C	7.59362200	4.18203700	0.47572700

C	7.60979100	3.90771300	1.87363500
C	7.64713600	2.05011000	3.99041000
C	8.86701500	-2.49968400	-2.87070600
C	8.88463800	-3.44866700	-1.78962800
C	8.91361400	-3.98926400	0.96954600
C	8.92302600	-3.52420700	2.33103200
C	8.92507700	-1.41428400	4.19160100
C	8.91658900	-0.00493600	4.48026500
C	8.83550100	0.16692900	-3.76052800
C	8.82585100	1.57630300	-3.47164700
C	8.82483100	3.68806100	-1.61322100
C	8.83391700	4.15282300	-0.25169700
C	8.86606200	3.60988500	2.50686300
C	8.88518600	2.66084000	3.58782000
C	10.09214000	-1.91984200	-3.32128600
C	10.12709500	-3.80143000	-1.17975900
C	10.14197500	-4.08188800	0.24656900
C	10.16030200	-3.16129500	2.94583400
C	10.16150200	-2.07016300	3.90648700
C	10.14475500	0.72412800	4.47680500
C	10.07586700	-0.54108700	-3.78194100
C	10.05647000	2.25327600	-3.21159200
C	10.05585400	3.34487600	-2.25133100
C	10.07405100	4.26515900	0.44794500
C	10.09066800	3.98423100	1.87416000
C	10.12842200	2.10271200	4.01576100
C	11.30108200	-2.59029000	-2.95302300
C	11.31802800	-3.50321300	-1.91422300
C	11.34870800	-4.08301700	1.01487000
C	11.35763700	-3.63672300	2.32391400
C	11.35989700	-1.39289200	4.29597100
C	11.35181200	-0.03778700	4.57244400
C	11.26760100	0.24121200	-3.90132300
C	11.25815800	1.59637100	-3.62493400
C	11.25697300	3.83952300	-1.65210400
C	11.26583600	4.28587500	-0.34304800

C	11.30002600	3.70686100	2.58636900
C	11.31843600	2.79414100	3.62527200
H	12.24755000	-2.28249500	-3.39584700
H	12.27734300	-3.88744100	-1.56968700
H	12.29874900	-4.30488900	0.53027600
H	12.31436300	-3.52097100	2.83171700
H	12.31656800	-1.91107700	4.24279300
H	12.30230900	0.47094400	4.72843300
H	12.22333800	-0.25142900	-4.07603600
H	12.20678700	2.13071600	-3.59068400
H	12.20570900	3.73873700	-2.17781200
H	12.22124500	4.52288900	0.12346400
H	12.24586600	4.10818100	2.22451000
H	12.27812600	2.50354400	4.05088100

**UP-6-(7,7)**

C	-3.49737600	1.13539700	-7.00420100
C	-1.82491400	-0.60284700	-7.19906400
C	-2.49872200	2.11386700	-7.02341600
H	-4.53927200	1.43490300	-6.87894800
C	-0.82344000	0.37744100	-7.21254400
H	-1.55839000	-1.65778500	-7.22303200
H	-2.76009500	3.16444700	-6.91426000
H	0.22390300	0.07249900	-7.25171000
C	2.07458100	7.45719700	-1.77568700
C	3.97836000	7.77316100	-3.38140400
C	2.76231600	7.21158700	-3.06346300
C	1.97183800	6.38796900	-4.00311200
C	2.54077900	5.40580600	-4.83170400
C	-0.22561100	5.70062700	-4.82094500
C	1.76685800	4.59327700	-5.66991700
H	3.61196600	5.21801700	-4.78217800
H	-1.31142600	5.70928200	-4.75803000
H	2.25556100	3.84146000	-6.28482400
C	-1.14493500	1.73966200	-7.09522100
C	0.36912600	4.72701400	-5.64451700



C	-0.02166300	2.75238100	-6.98684400
H	0.38124000	3.03263800	-7.97825800
H	0.79722400	2.30203700	-6.40375600
O	-0.51210000	3.93099700	-6.32921300
C	0.54842800	6.54531400	-4.01205500
C	-0.04657900	7.54921900	-3.09738100
C	-1.10728600	8.35150200	-3.45780600
S	-1.92860100	8.28797000	-5.05742700
S	-1.75030200	9.68346900	-2.43366100
C	-2.84011200	9.78065700	-4.86388100
H	-3.44160900	10.11039400	-5.70862700
C	-2.76018400	10.41174700	-3.67683700
H	-3.28751900	11.32766600	-3.41781600
S	4.76085900	7.62340900	-4.99427800
C	6.05014300	9.41683600	-3.50188100
H	6.76993400	10.17403500	-3.19737000
S	4.90771900	8.85580400	-2.28611000
C	5.98506300	8.85965800	-4.72630200
H	6.64371500	9.09853100	-5.55887100
C	2.06817100	7.64291700	0.66587000
C	0.65815000	7.65988000	-1.79889800
C	0.00117600	7.87309600	-0.57261200
H	-1.08365200	7.95490200	-0.55169400
C	0.68367300	7.89240200	0.64958600
H	0.12835400	8.03749300	1.57309100
C	2.74844500	7.42771400	-0.54634800
H	3.80224300	7.16188500	-0.49507200
O	2.83389600	7.53724200	1.79318200
C	3.16057900	6.76894300	4.03734900
H	3.98420900	7.46682200	4.25473300
H	3.60075400	5.89765300	3.53161500
C	2.47521100	6.29499800	5.33050300
H	1.57348100	5.72669200	5.05274200
H	2.12980800	7.15518600	5.92833400
C	3.38068800	5.38171000	6.18004300
H	4.12791900	5.98125200	6.72717000

H	3.94625000	4.71885300	5.50623200
C	2.58010100	4.50546800	7.15582900
H	1.80082900	3.96973300	6.59213800
H	2.05571100	5.13672400	7.89393300
C	2.16851800	7.40403300	3.06583100
H	1.81822000	8.39317700	3.41100100
H	1.29095100	6.74773600	2.95540700
C	3.45931900	3.46666200	7.88681100
O	-6.73047200	-6.96231000	1.46968400
C	-5.99599300	-6.91872500	0.31781200
C	-4.65719600	-6.62952500	-2.17395800
C	-6.71573200	-6.58826600	-0.84550800
H	-7.77284700	-6.35379300	-0.73725400
C	-4.60895600	-7.12955800	0.23588300
H	-4.02335100	-7.36208700	1.12249800
C	-3.96307300	-6.96102100	-0.99590300
H	-2.87667500	-7.01609300	-1.01003100
C	-6.07791500	-6.46472800	-2.08741400
C	-6.81037100	-6.10936900	-3.32271800
C	-3.99511200	-6.37136800	-3.47544000
C	-4.64607300	-5.30577400	-4.27620800
C	-6.06976600	-5.17696500	-4.19784900
C	-3.92259100	-4.37897300	-5.04313400
H	-2.83579000	-4.37531000	-5.03750300
C	-6.69085800	-4.13086300	-4.90221100
H	-7.76149600	-3.97020600	-4.78684700
C	-5.96729800	-3.23460400	-5.69756800
H	-6.48989500	-2.43201900	-6.21211900
C	-4.56840300	-3.35242000	-5.75401700
O	-3.73455900	-2.48304200	-6.41001400
C	-3.17159900	-0.23186400	-7.05988100
C	-4.28428600	-1.24632700	-6.89010700
C	-2.91665300	-7.09841600	-3.93519200
C	-8.01758200	-6.67412900	-3.66607400
S	-2.13926500	-6.85868200	-5.53990600
S	-2.19601500	-8.49107200	-3.05380500

S	-8.88316600	-7.89446800	-2.66682800
S	-8.84660200	-6.38765100	-5.23732000
C	-1.18381800	-9.05731700	-4.37603800
H	-0.61052300	-9.96728900	-4.21078600
C	-1.15900300	-8.31854500	-5.50167900
H	-0.56269900	-8.54145600	-6.38417900
C	-10.01134400	-7.69836700	-5.07655900
H	-10.67621100	-7.88146600	-5.91833000
C	-10.02672800	-8.37930600	-3.91464700
H	-10.70651400	-9.19539000	-3.67766900
H	-4.82426400	-1.43062100	-7.83817600
H	-5.01128200	-0.84945400	-6.16215800
H	4.01497000	2.87623400	7.14117000
H	4.20710700	4.00382700	8.49861200
C	-7.60035100	-3.21233000	7.68976300
H	-8.30933100	-3.80542900	8.29092300
C	-6.60823000	-4.14948700	6.96376400
H	-5.85365200	-3.53537100	6.44777700
H	-6.06412200	-4.75898100	7.70396300
C	-7.30688000	-5.04610600	5.92920900
H	-7.92713000	-4.40430100	5.28381600
H	-8.00116500	-5.73891500	6.43471800
C	-6.32965100	-5.83195500	5.03488800
H	-5.51737700	-5.15543900	4.72448400
H	-5.85672300	-6.64907700	5.60537900
C	-7.02368900	-6.37179100	3.77143200
H	-7.57662600	-5.54584700	3.30088900
H	-8.19131800	-2.68657000	6.91919000
C	-6.03245200	-6.89527900	2.73194400
H	-5.18457800	-6.19815600	2.64384100
H	-5.63387400	-7.89140700	2.99392300
H	-7.76082400	-7.14937000	4.02633400
H	13.49080100	2.09739400	-1.37087600
H	13.63529000	2.13234100	1.05174000
H	13.55618600	1.26030700	2.97638300
H	13.24831700	-0.57439400	4.53518700

H	12.84322700	-2.58385100	5.05560300
H	12.31306400	-4.90372300	4.57854000
H	11.88516300	-6.54050200	3.31039100
H	11.53253700	-7.60271300	1.15655100
H	13.18497500	1.17089000	-3.24644200
H	12.69696700	-0.70644800	-4.70551700
H	12.23637800	-2.72790900	-5.11974900
H	11.77091200	-5.03329300	-4.52078600
H	11.50013000	-6.63276400	-3.16385100
H	11.40747700	-7.63214900	-0.95398200
C	12.57691100	2.23874900	-0.79557400
C	12.65929900	2.25860900	0.58525300
C	12.54731100	1.02455700	3.31210300
C	12.37187400	-0.02125100	4.20055100
C	11.79803000	-2.86704200	4.93953900
C	11.49582100	-4.18937900	4.66756900
C	10.89044400	-6.50648700	2.86823100
C	10.68940800	-7.11194800	1.64071500
C	12.14375300	0.92772500	-3.45352900
C	11.86560200	-0.14235400	-4.28506800
C	11.21284400	-3.00633300	-4.87277700
C	10.94752600	-4.32051000	-4.53141900
C	10.56451200	-6.58519100	-2.60842300
C	10.51172000	-7.15483000	-1.34883900
C	11.31234300	2.24311900	-1.46045000
C	11.48259700	2.28396500	1.39515100
C	11.42836400	1.68549600	2.71841200
C	11.06538200	-0.47725000	4.55604300
C	10.78702400	-1.85778800	4.91478600
C	10.16201500	-4.59283600	4.35208600
C	9.86833500	-5.71655100	3.47858200
C	9.45268100	-6.96858000	0.93978800
C	11.10220300	1.60724600	-2.75021300
C	10.52687500	-0.60585700	-4.46992900
C	10.21023100	-1.99531100	-4.75513500
C	9.66135600	-4.71334700	-4.04899800

C	9.47551800	-5.81200400	-3.11593300
C	9.36640500	-6.98972400	-0.51074900
C	10.17092300	2.61327300	-0.68468600
C	10.25643100	2.63340700	0.75009200
C	10.15113000	1.47117900	3.32198100
C	9.96891100	0.38475800	4.24550100
C	9.42797700	-2.29804600	4.94333400
C	9.11397400	-3.67193500	4.66030600
C	8.54348100	-5.85501700	2.96144500
C	8.33459900	-6.48396400	1.68591000
C	9.76257200	1.37810900	-3.19123700
C	9.47359500	0.26611600	-4.05509400
C	8.85815800	-2.43406200	-4.61002300
C	8.58242100	-3.79957400	-4.25539700
C	8.22150400	-5.93431400	-2.44194400
C	8.16673000	-6.52564800	-1.13289400
C	8.87714800	2.70026300	-1.30538300
C	9.04512700	2.73944000	1.51702000
C	8.99222500	2.15364000	2.81413500
C	8.63391100	0.01734100	4.63181300
C	8.36123100	-1.33533000	4.98388100
C	7.74354300	-4.03773300	4.42625000
C	7.45585800	-5.13787800	3.56909400
C	7.04515700	-6.37442300	1.05966700
C	8.67121400	2.07751100	-2.56944400
C	8.10260700	-0.10984400	-4.26880300
C	7.79235700	-1.47128500	-4.54871800
C	7.24999100	-4.15730200	-3.85121600
C	7.06794200	-5.23367000	-2.93678000
C	6.96044800	-6.39569500	-0.36164200
C	7.74568600	3.14023000	-0.54681900
C	7.83093100	3.15916600	0.88552200
C	7.72553200	1.99542400	3.46193400
C	7.54385900	0.91192700	4.38493600
C	7.00245300	-1.77445900	5.08458000
C	6.68895000	-3.14532600	4.80093600

C	6.11778100	-5.32927400	3.09740500
C	5.90933400	-5.95619500	1.82410600
C	7.33663700	1.90347200	-3.05716000
C	7.04824600	0.79310100	-3.91917500
C	6.43201000	-1.91089900	-4.47539700
C	6.15670800	-3.27374400	-4.12157000
C	5.79546400	-5.41056400	-2.30518400
C	5.74095700	-5.99952000	-0.99824500
C	6.46668200	3.24127300	-1.17341400
C	6.63458800	3.27782300	1.65561000
C	6.58113900	2.68721300	2.96152100
C	6.22285300	0.54837900	4.78658400
C	5.94823400	-0.81358300	5.14120400
C	5.32917600	-3.52054900	4.58001300
C	5.03949300	-4.62685500	3.71553900
C	4.62811800	-5.86388400	1.20057300
C	6.25910500	2.61359900	-2.44622500
C	5.68921600	0.42048700	-4.14893300
C	5.37656200	-0.95046500	-4.43101600
C	4.83314700	-3.64193600	-3.73257400
C	4.64987100	-4.72515100	-2.81127100
C	4.54254100	-5.88648200	-0.23033600
C	5.33164400	3.67066100	-0.40886800
C	5.41651400	3.68672500	1.01890700
C	5.31022700	2.51667200	3.60381000
C	5.12939300	1.43856900	4.52577000
C	4.58665000	-1.25555600	5.22909300
C	4.27384800	-2.62118700	4.94558200
C	3.70086500	-4.80899700	3.23373800
C	3.49318800	-5.43267600	1.96423500
C	4.92055800	2.42769800	-2.92726500
C	4.63328700	1.32072500	-3.78680800
C	4.01459500	-1.39291700	-4.34672100
C	3.73990700	-2.75146100	-3.99420500
C	3.37765900	-4.89384900	-2.17054600
C	3.32365900	-5.47894800	-0.86712100

C	4.04810300	3.76747800	-1.03727800
C	4.21576300	3.79822800	1.79121000
C	4.16106000	3.20392200	3.09604400
C	3.80378900	1.07097700	4.92641100
C	3.52894700	-0.29122800	5.28403000
C	2.90930600	-2.99779100	4.72261100
C	2.61945300	-4.10418500	3.85572500
C	2.20777700	-5.34048000	1.33757900
C	3.83988400	3.13649800	-2.31004600
C	3.27009900	0.94367200	-4.01554200
C	2.95622100	-0.42846300	-4.30093200
C	2.41188700	-3.12315700	-3.60435800
C	2.22814300	-4.20759000	-2.68109100
C	2.12152500	-5.36522100	-0.09540300
C	2.91675800	4.18383300	-0.27286800
C	3.00146800	4.19862400	1.15639800
C	2.89496600	3.03091900	3.73471800
C	2.71414900	1.95539500	4.66382700
C	2.17201800	-0.73095100	5.37196400
C	1.85825100	-2.10106700	5.08800200
C	1.28586700	-4.28530400	3.37478600
C	1.07792500	-4.91064500	2.10011100
C	2.50733600	2.94282800	-2.78235200
C	2.21947000	1.83749200	-3.64558800
C	1.59946200	-0.86986900	-4.21328100
C	1.32344300	-2.23451700	-3.86401100
C	0.96099300	-4.37636600	-2.04174200
C	0.90748800	-4.95995200	-0.73134100
C	1.63068000	4.26711200	-0.89606500
C	1.79968900	4.30056600	1.92628000
C	1.74593500	3.71525800	3.22684200
C	1.38853400	1.58942800	5.06348000
C	1.11435000	0.23430900	5.42304600
C	0.49310200	-2.47351500	4.85888100
C	0.20469700	-3.57541300	3.99373800
C	-0.20663500	-4.81105400	1.47202900

C	1.42538900	3.64601000	-2.16301300
C	0.85533400	1.46037800	-3.86752900
C	0.54241900	0.09540800	-4.14945300
C	-0.00360300	-2.60108800	-3.46564000
C	-0.18708900	-3.68298100	-2.54767900
C	-0.29249700	-4.83528800	0.04370400
C	0.49824500	4.68724800	-0.13346300
C	0.58370500	4.70999700	1.29308900
C	0.47911200	3.55716900	3.87602700
C	0.29793600	2.48196400	4.80646200
C	-0.24659400	-0.20467200	5.51582800
C	-0.56102200	-1.57489400	5.22911500
C	-1.13328300	-3.75870600	3.51361800
C	-1.33983100	-4.38191300	2.23770100
C	0.09203300	3.46355000	-2.64382800
C	-0.19677300	2.36000900	-3.50573900
C	-0.81708100	-0.34195600	-4.05763500
C	-1.09303500	-1.70489600	-3.71820800
C	-1.45653600	-3.84737900	-1.90414500
C	-1.50887200	-4.42521800	-0.59230200
C	-0.77961100	4.78676400	-0.75780500
C	-0.61054600	4.83594200	2.06589300
C	-0.66389000	4.25217400	3.37472600
C	-1.02435400	2.12194700	5.20979000
C	-1.30019600	0.76010800	5.56829900
C	-1.92204600	-1.94665000	5.00085400
C	-2.21119400	-3.05113300	4.13123700
C	-2.61899700	-4.27891500	1.60928400
C	-0.98515600	4.17026000	-2.03010300
C	-1.55504400	1.99028600	-3.73453700
C	-1.86767600	0.62080400	-4.00095400
C	-2.41364800	-2.06615300	-3.31895900
C	-2.59677600	-3.14830200	-2.40087300
C	-2.70165500	-4.29195100	0.17995000
C	-1.91106500	5.22260800	0.00343800
C	-1.82594800	5.24681000	1.42942600



C	-1.93350200	4.08821500	4.01843800
C	-2.11518900	3.01291900	4.94309300
C	-2.66180300	0.32117000	5.65014800
C	-2.97497600	-1.04361100	5.36253300
C	-3.54662800	-3.22349500	3.64077100
C	-3.75165700	-3.84179200	2.36951100
C	-2.31902700	3.99753600	-2.51931100
C	-2.60680800	2.89466200	-3.38002600
C	-3.22525900	0.18390300	-3.91153400
C	-3.50031200	-1.17020600	-3.56654300
C	-3.86351700	-3.30634100	-1.75683000
C	-3.91534500	-3.87908000	-0.45537500
C	-3.19323500	5.33051800	-0.62776000
C	-3.02742400	5.36807200	2.20248300
C	-3.08196200	4.78154100	3.51047800
C	-3.44393100	2.64966200	5.34209300
C	-3.72002100	1.28885900	5.69999200
C	-4.34073500	-1.41255600	5.12761000
C	-4.62843900	-2.50872700	4.25160400
C	-5.03384400	-3.73976600	1.73701900
C	-3.40009100	4.71033200	-1.90449700
C	-3.97125900	2.51973000	-3.60520700
C	-4.28337300	1.14818900	-3.87320300
C	-4.82830000	-1.54109700	-3.18292100
C	-5.01212900	-2.62400200	-2.26798800
C	-5.11767000	-3.76842600	0.31009500
C	-4.32437000	5.75437400	0.13393600
C	-4.24066600	5.77165900	1.56656700
C	-4.34897100	4.61435900	4.14713000
C	-4.53215900	3.53500800	5.07441800
C	-5.07714100	0.85254500	5.77961400
C	-5.39136200	-0.51561100	5.48653800
C	-5.95716600	-2.67710800	3.75918400
C	-6.16355600	-3.30667500	2.49074000
C	-4.73331600	4.52493500	-2.38151000
C	-5.02290000	3.41513600	-3.24371000

C	-5.63856400	0.70889400	-3.79200500
C	-5.91458400	-0.65354000	-3.43976300
C	-6.27705700	-2.79306400	-1.63450500
C	-6.32985100	-3.37144300	-0.32657700
C	-5.61060300	5.84043100	-0.48955500
C	-5.44464500	5.87739400	2.33451500
C	-5.49917500	5.29493200	3.63312200
C	-5.86114100	3.16691700	5.46002500
C	-6.13567100	1.81573200	5.81515700
C	-6.75331500	-0.87780500	5.23641500
C	-7.03739100	-1.96502900	4.36616000
C	-7.44435200	-3.21097000	1.86156300
C	-5.81689000	5.22034900	-1.75528300
C	-6.38666500	3.03321300	-3.45649200
C	-6.69715700	1.67126800	-3.73627300
C	-7.23980000	-1.02021200	-3.04706700
C	-7.42286600	-2.10063400	-2.13729100
C	-7.52945700	-3.24908100	0.44178200
C	-6.75039100	6.27904900	0.26894500
C	-6.66596800	6.29877800	1.70406700
C	-6.77434000	5.14273900	4.27948200
C	-6.95861200	4.06056300	5.20772700
C	-7.50278400	1.38069400	5.90920600
C	-7.81696900	0.00953200	5.61617500
C	-8.38099300	-2.15778600	3.89555900
C	-8.58818400	-2.79262700	2.62278700
C	-7.15974000	5.04586800	-2.23899200
C	-7.44968000	3.93411600	-3.10363000
C	-8.06452500	1.23255100	-3.66401300
C	-8.34038700	-0.13577800	-3.31554400
C	-8.70287800	-2.27790000	-1.50925000
C	-8.75737900	-2.86259300	-0.19618300
C	-8.01915500	6.43057600	-0.37083500
C	-7.85004300	6.47278900	2.48497100
C	-7.90599800	5.87765300	3.80941200
C	-8.27303300	3.72233900	5.65526700

C	-8.55334300	2.34269600	6.01573000
C	-9.17712000	-0.38914200	5.43821000
C	-9.46780000	-1.50657500	4.55473900
C	-9.88001100	-2.76398200	2.01323500
C	-8.23032900	5.79464300	-1.66024200
C	-8.80667000	3.58157100	-3.38105400
C	-9.12300100	2.19266400	-3.67074800
C	-9.67181800	-0.53090000	-2.97813500
C	-9.85837700	-1.63342100	-2.04871600
C	-9.96683100	-2.79901400	0.56243400
C	-9.09343100	6.93347800	0.42583600
C	-9.01166900	6.95436000	1.80650000
C	-9.12714100	5.72646200	4.53598600
C	-9.30477200	4.68434100	5.42817600
C	-9.88204700	1.83920600	6.16924200
C	-10.18364300	0.51803500	5.89130400
C	-10.78294100	-1.79327100	4.07516700
C	-10.98173600	-2.39922300	2.84698900
C	-9.52914600	5.61936600	-2.22952700
C	-9.80779200	4.54952900	-3.06110700
C	-10.45938500	1.68669400	-3.66050700
C	-10.72452900	0.37049800	-3.32628500
C	-11.10838400	-1.89973000	-1.40926400
C	-11.16102700	-2.46339700	-0.14678100
H	-10.03990900	7.19573400	-0.04485900
H	-9.89624500	7.23274000	2.37758200
H	-9.97832100	6.36472100	4.30315400
H	-10.28984200	4.53574400	5.86829200
H	-10.69817600	2.52483500	6.39272500
H	-11.22691200	0.20593100	5.90555900
H	-11.65000700	-1.42807900	4.62371900
H	-11.99911100	-2.49051400	2.46910500
H	-10.34939000	6.26340500	-1.91560100
H	-10.83808700	4.38689400	-3.37449800
H	-11.29741800	2.36804800	-3.80065700
H	-11.76233600	0.05975500	-3.21389200

H	-12.03413000	-1.54740000	-1.86210400
H	-12.12615800	-2.53650400	0.35259700
C	2.64130400	2.54493600	8.75481500
H	2.07212700	3.02372800	9.56000800
C	2.53695000	1.22016200	8.57526400
H	3.08399100	0.71430500	7.77730500
H	1.90609600	0.60088700	9.21556800
C	-6.90571300	-2.19758400	8.55933000
H	-6.20789300	-1.53268800	8.03962000
C	-7.06865100	-2.07424900	9.88434200
H	-7.75480600	-2.72564000	10.43246800
H	-6.52900400	-1.32175300	10.46233400

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C	7.57207000	0.35011200	-4.88692400
C	5.68877700	1.84973700	-5.12333600
C	6.72883800	-0.75256100	-5.06879200
H	8.63576700	0.18672100	-4.70154400
C	4.84479900	0.74725100	-5.30627200
H	5.28260000	2.85881200	-5.13060400
H	7.12922600	-1.76293600	-5.01741200
H	3.77304100	0.90722800	-5.43800300
C	2.67813000	-6.75272900	-0.53086900
C	1.03401200	-7.49842200	-2.27958600
C	2.08963800	-6.70734800	-1.89001000
C	2.80255300	-5.78158000	-2.79660300
C	2.15204800	-4.94661800	-3.72234900
C	4.91238300	-4.71313900	-3.41334700
C	2.85084300	-4.01456000	-4.50007200
H	1.06610300	-4.96677100	-3.79386000
H	5.96930100	-4.52207900	-3.24310400
H	2.30847200	-3.36381200	-5.18270200
C	5.35120400	-0.56332600	-5.26919600
C	4.23641100	-3.87829200	-4.31862800
C	4.38340800	-1.72425400	-5.39957300
H	4.06625400	-1.86912800	-6.44912200

H	3.48107500	-1.50677100	-4.80450600
O	5.01274600	-2.92515900	-4.92435600
C	4.22394700	-5.67206200	-2.65817100
C	4.89499300	-6.51837600	-1.64382300
C	6.11157300	-7.12536500	-1.86082300
S	7.06093500	-6.97713200	-3.38149100
S	6.87618000	-8.27213400	-0.70587000
C	8.20252100	-8.26602600	-3.01809700
H	8.93348800	-8.51541500	-3.78467400
C	8.11983900	-8.85134000	-1.80778100
H	8.77387200	-9.64400800	-1.44997700
S	0.38140700	-7.54706400	-3.95495100
C	-0.69178900	-9.49730000	-2.48713000
H	-1.28866500	-10.36275800	-2.20633600
S	0.23042900	-8.70629600	-1.21346000
C	-0.62324800	-8.97424000	-3.72628000
H	-1.15633000	-9.35370200	-4.59569400
C	2.45340500	-6.74590500	1.90543600
C	4.09732800	-6.69381500	-0.41058900
C	4.65464300	-6.70670000	0.88605200
H	5.72941300	-6.59100500	1.01162700
C	3.85707300	-6.74939400	2.02790600
H	4.29843000	-6.69604100	3.02178900
C	1.87507600	-6.77017600	0.62478900
H	0.79684500	-6.72777700	0.50684700
O	1.75613100	-6.64064300	3.07705600
C	1.39609400	6.33884600	0.84731800
C	2.94073400	6.57022900	-1.52052900
C	2.80418300	6.34812100	0.90980600
H	3.26514000	6.18716600	1.88211300
C	0.75867600	6.41945400	-0.40356400
H	-0.32281000	6.37831600	-0.49540200
C	1.53841200	6.49130700	-1.56333700
H	1.03298300	6.45665700	-2.52756500
C	3.58889600	6.50614300	-0.24470000
C	5.06904000	6.60712600	-0.21654800

C	3.77939800	6.70368000	-2.72951200
C	5.06770500	5.98376100	-2.64063100
C	5.74130900	5.97705000	-1.37770300
C	5.63578100	5.30467400	-3.73189100
H	5.09846700	5.22362000	-4.67517000
C	6.99909100	5.34859700	-1.30771600
H	7.51927200	5.28354500	-0.35567000
C	7.59161500	4.73329600	-2.41596000
H	8.56704000	4.26417300	-2.30819500
C	6.89074300	4.68387600	-3.62941700
O	7.38924800	4.10228100	-4.77850300
C	7.06264400	1.65959000	-4.90195900
C	8.02254000	2.81818200	-4.67369900
C	3.46330200	7.53276500	-3.78351400
C	5.74313600	7.33592700	0.74255300
S	4.53350900	7.81499300	-5.20304300
S	2.00149500	8.58161400	-3.83320000
S	4.94318200	8.21887000	2.09117900
S	7.51571700	7.64343600	0.71379500
C	2.52087300	9.56506400	-5.19801100
H	1.87858300	10.39406700	-5.48850700
C	3.66537300	9.21800400	-5.81706800
H	4.08684300	9.72486900	-6.68289500
C	7.51821900	8.89290600	1.95175100
H	8.46729700	9.37957200	2.16735100
C	6.35296300	9.15310900	2.57461200
H	6.21769200	9.88270100	3.37059600
H	8.80696000	2.81160100	-5.44645600
H	8.52056500	2.69079900	-3.69864400
O	0.74693300	6.19673000	2.04511700
C	-0.69167300	6.24915500	2.02480900
H	-1.08100300	5.54642700	1.27196100
H	-1.01771500	7.26620300	1.74123600
C	-1.23546400	5.84173300	3.38925500
H	-0.84726900	6.51026900	4.17265600
H	-0.87087700	4.82861700	3.61418200

C	-2.77913000	5.85012700	3.36116200
H	-3.15190700	6.88253800	3.46930300
H	-3.12138700	5.50021300	2.37306600
C	-3.42577100	4.94209000	4.41985100
H	-3.15575500	5.28178800	5.43448700
H	-3.01197800	3.92690300	4.30860000
C	-4.95498700	4.87795600	4.27109400
H	-5.39464200	5.86488700	4.49815200
H	-5.19759200	4.66744400	3.21567900
C	-5.61660500	3.79740900	5.14016500
H	-5.39349200	3.97525000	6.20622500
H	-5.16869100	2.82246700	4.88765000
C	-7.13946500	3.72114700	4.93036200
H	-7.62958200	4.58998900	5.40009300
H	-7.35814100	3.78571600	3.85188500
C	0.32199700	-6.49707100	3.02442800
H	0.03284900	-5.86507900	2.17323200
H	-0.14204700	-7.49056200	2.89116200
C	-0.14872100	-5.80871100	4.30159100
H	0.11774000	-6.40907200	5.18529000
H	0.38468400	-4.84953300	4.38247800
C	-1.66558000	-5.55094000	4.24810700
H	-2.21523200	-6.50220900	4.35099600
H	-1.92755900	-5.14807000	3.25483300
C	-2.14857900	-4.54496300	5.30394600
H	-1.89467800	-4.90129200	6.31675400
H	-1.59609500	-3.60279000	5.15770900
C	-3.65985800	-4.26547900	5.20227700
H	-4.22799100	-5.10338700	5.64148200
H	-3.94576500	-4.22209700	4.13913200
C	-4.07472300	-2.94431500	5.86723500
H	-3.80217400	-2.95937800	6.93713000
H	-3.49654900	-2.12354700	5.41118400
C	-5.57419100	-2.64482900	5.72172500
H	-6.16373700	-3.43170600	6.22105500
H	-5.85038800	-2.67586200	4.65557900

C	-5.96470500	-1.26950900	6.30712800
H	-5.37604700	-0.49595000	5.78224200
H	-5.67823900	-1.22755300	7.37129400
C	-7.75187300	2.41504600	5.47952300
H	-7.24511700	1.56902900	4.98283900
H	-7.54144200	2.31132400	6.55552900
C	-9.23350900	2.32066200	5.22962400
H	-9.54584000	2.42977500	4.18681900
C	-7.43474100	-0.97506400	6.16151000
H	-7.80882500	-0.89737500	5.13621700
C	-12.55102500	-2.44740800	0.48854500
C	-12.35268800	-3.15287500	-0.68336100
C	-11.03392700	-3.30990800	-1.22364400
C	-9.94341400	-3.14185700	-0.31822700
C	-10.15056400	-2.40734200	0.90486000
C	-11.44076400	-1.86257300	1.18174700
C	-8.59340400	-3.32540700	-0.78124000
C	-8.33073000	-3.19291700	-2.17651100
C	-9.42893800	-2.88377900	-3.05285600
C	-10.76598000	-3.17648100	-2.64741900
C	-9.20654200	-1.93470400	-4.11474000
C	-10.32845100	-1.30895800	-4.73697200
C	-11.59261900	-1.97256900	-4.60776000
C	-11.80586000	-2.88247100	-3.58943800
C	-8.99575800	-1.89846100	1.59505300
C	-7.70801800	-2.48379100	1.36158500
C	-7.50073100	-3.21697100	0.13993100
C	-6.16510300	-3.40795400	-0.32727200
C	-5.89986800	-3.27424500	-1.73525700
C	-6.98403200	-2.95575900	-2.60724600
C	-6.76189700	-2.00733400	-3.66734200
C	-7.89878200	-1.34796500	-4.23938500
C	-6.56913000	-1.97562400	2.05500300
C	-5.27527700	-2.54385200	1.80307800
C	-5.06923200	-3.27652600	0.59055900
C	-3.72729100	-3.47298300	0.12347300



C	-3.46160700	-3.34119700	-1.28541700
C	-4.55204900	-3.01643500	-2.15878700
C	-4.33103200	-2.07218300	-3.21236600
C	-5.46677100	-1.42216900	-3.80315500
C	-4.13249400	-2.03292100	2.50102000
C	-1.29614400	-3.52635000	0.57158500
C	-1.03134400	-3.40106300	-0.83068800
C	-2.12074200	-3.08828800	-1.70997300
C	-1.89810900	-2.13799000	-2.76867300
C	-3.02816800	-1.48731700	-3.35281800
C	-1.70412500	-2.08816100	2.95148100
C	-0.41342600	-2.66260900	2.71174200
C	-0.20428100	-3.39322000	1.49184100
C	1.13159200	-3.58461400	1.02832100
C	1.39651000	-3.46584500	-0.37927900
C	0.31553100	-3.15265000	-1.25601000
C	0.53816800	-2.20016000	-2.31192000
C	-0.59657100	-1.54583400	-2.89648900
C	0.72271900	-2.15832400	3.41459300
C	2.01462800	-2.72733400	3.16394100
C	2.22135200	-3.45134300	1.94817100
C	3.56169300	-3.65042000	1.48350000
C	3.82685400	-3.53350300	0.07842800
C	2.74081600	-3.21054800	-0.79947800
C	2.96136500	-2.25797700	-1.84004700
C	1.83164700	-1.60935800	-2.43495000
C	3.15906700	-2.22322400	3.86847600
C	4.44354100	-2.79261500	3.61745100
C	4.64848400	-3.52580400	2.39787000
C	5.98845100	-3.71418100	1.92978200
C	6.25102700	-3.59322500	0.53329400
C	5.16449800	-3.28501100	-0.34460600
C	5.38704500	-2.33035600	-1.39562800
C	4.26172100	-1.67214100	-1.97037700
C	5.59210100	-2.27336900	4.29987400
C	6.88801900	-2.85139100	4.06303300

C	7.09145100	-3.59614200	2.84527700
C	8.42232600	-3.83867900	2.38937200
C	8.68994900	-3.71339900	0.96347300
C	7.60487500	-3.35427300	0.10897000
C	7.82842700	-2.39997200	-0.94842800
C	6.68385200	-1.74064500	-1.51874700
C	8.02173500	-2.37207400	4.78596400
C	9.27230400	-3.02504000	4.53294100
C	9.46705700	-3.74006800	3.36568500
C	9.12943100	-1.83814800	-1.11927400
C	10.22607700	-2.56769200	-0.55489500
C	10.01187800	-3.48274900	0.45958900
C	6.77662100	-0.34991300	-1.80943400
C	8.01022000	0.32731100	-1.52064300
C	9.22426100	-0.41522900	-1.41805300
C	4.35827100	-0.27531100	-2.27340400
C	5.57472200	0.40446100	-1.98100400
C	5.50671000	1.72690100	-1.42706600
C	6.64226000	2.21227500	-0.70806400
C	7.94008900	1.64768700	-0.95325600
C	9.08627800	2.19430200	-0.30225300
C	10.35229200	1.60936400	-0.63141300
C	10.41897100	0.33741700	-1.17395500
C	6.43464800	2.94164900	0.49387700
C	7.53761400	3.08770500	1.40329700
C	8.87560600	2.94802100	0.92627200
C	4.22637900	2.31204200	-1.19589000
C	4.01493800	3.04030400	0.02491800
C	5.09624500	3.16527300	0.94653300
C	4.82925400	3.04062000	2.35538100
C	5.91865300	2.71212700	3.22800700
C	7.27227200	2.96894200	2.81340600
C	8.35447500	2.69794800	3.70289700
C	9.67061000	3.02260500	3.23594600
C	9.92459200	3.14635400	1.88254200
C	5.70127100	1.76915900	4.27501300

C	6.84548000	1.12365900	4.86317600
C	8.13233300	1.73460300	4.77075500
C	3.49015400	2.78516900	2.77596000
C	3.26997900	1.83757100	3.83666400
C	4.39934500	1.18766200	4.42041400
C	4.30761700	-0.21676500	4.72403200
C	5.52325900	-0.96441300	4.86091600
C	6.75429200	-0.28356000	5.16183900
C	7.95222000	-1.03528800	5.35710900
C	9.13124000	-0.29491200	5.69779100
C	9.21875100	1.05497300	5.41293900
C	3.08949600	-0.90275100	4.43500200
C	2.67004200	3.21957300	0.48903100
C	2.40287100	3.08604500	1.88877800
C	3.08384100	1.79903800	-1.89686400
C	3.15058900	0.47837200	-2.44354300
C	1.96963100	1.24423700	3.96792000
C	1.87674900	-0.15137100	4.27504200
C	1.58314400	3.09880500	-0.43568600
C	1.79285800	2.37601700	-1.66034400
C	1.92898700	-0.20822900	-2.74944500
C	1.05864200	2.83347700	2.31267200
C	0.83462400	1.89577600	3.38104500
C	0.65122100	-0.84006700	3.98779200
C	0.24576900	3.27926400	0.02860400
C	-0.02160900	3.13359900	1.43081200
C	0.65467400	1.86522300	-2.35904900
C	0.72333400	0.54070700	-2.91745100
C	-0.46039200	1.30924100	3.51897000
C	-0.55503200	-0.09204700	3.83045000
C	-0.84567300	3.15744200	-0.89280100
C	-0.63848300	2.43461600	-2.11136700
C	-0.50242900	-0.14906700	-3.20474500
C	-1.36717800	2.87840100	1.85113000
C	-1.59209100	1.95112000	2.91661000
C	-1.77709500	-0.77874300	3.52542700

C	-2.18769900	3.35306700	-0.42786400
C	-2.45431900	3.20765800	0.97862900
C	-1.78354000	1.92599000	-2.81076900
C	-1.71420500	0.60169600	-3.37088800
C	-2.89487900	1.36976400	3.05615700
C	-2.99000700	-0.03014000	3.37046800
C	-3.27636900	3.23376300	-1.34547800
C	-3.06924600	2.49999500	-2.56649900
C	-2.93393200	-0.08399500	-3.66142500
C	-3.79536300	2.96134600	1.40250800
C	-4.01970600	2.01667100	2.46214000
C	-4.20563500	-0.71588500	3.07153600
C	-4.61877500	3.41921500	-0.87551000
C	-4.88264100	3.28202000	0.52527200
C	-4.21609600	1.98366900	-3.25623100
C	-4.14703400	0.66671700	-3.81415900
C	-5.31970200	1.42793000	2.59153300
C	-5.41507000	0.03505300	2.90522500
C	-5.71402400	3.29896000	-1.79586400
C	-5.50764800	2.56296200	-3.01502600
C	-5.37254700	-0.01983100	-4.11128300
C	-6.23037400	3.03496300	0.95210700
C	-6.45239700	2.08132700	2.00537200
C	-6.63907900	-0.65284600	2.61591000
C	-7.04961900	3.48881100	-1.32842200
C	-7.31405900	3.35400300	0.08028800
C	-6.64756500	2.05212600	-3.70580200
C	-6.57808900	0.72858200	-4.26797500
C	-7.74557800	1.49564300	2.13875600
C	-7.84220800	0.09648700	2.45406800
C	-8.14494200	3.34551400	-2.24169100
C	-7.94051200	2.61573100	-3.44951900
C	-7.80541300	0.04169600	-4.54449400
C	-8.65836000	3.08499700	0.49822200
C	-8.87677000	2.14055100	1.54307400
C	-9.06402800	-0.58732400	2.15164500

C	-9.49394600	3.54195600	-1.78107900
C	-9.75842100	3.40810100	-0.37043400
C	-9.09341100	2.11315400	-4.14813100
C	-9.02368900	0.78846300	-4.71211700
C	-10.18686500	1.56371700	1.68502900
C	-10.28288000	0.16004700	1.99802700
C	-10.57929000	3.45849600	-2.70424400
C	-10.37049200	2.71519300	-3.93746700
C	-10.23328200	0.10907600	-5.04780200
C	-11.09899100	3.19664700	0.07224100
C	-11.32203800	2.23866400	1.14444000
C	-11.50973200	-0.52597600	1.75232500
C	-11.89151500	3.70728400	-2.18305600
C	-12.14485500	3.57982800	-0.83020500
C	-11.46546900	2.19150500	-4.70034700
C	-11.39853100	0.92144300	-5.24147200
C	-12.60036500	1.62708200	1.36202200
C	-12.69175400	0.27982700	1.65721900
C	-2.63904600	-3.34203800	1.03947600
C	-2.84652000	-2.60180500	2.25565700
H	10.51007100	3.01090800	3.93047400
H	10.95731000	3.23005000	1.54524100
H	10.02443500	-0.82176100	6.03210600
H	10.17882000	1.55689500	5.52921600
H	10.47093200	-4.08638000	3.12177400
H	10.12756300	-2.82758100	5.17844600
H	11.27349200	2.09015200	-0.30340500
H	11.39131400	-0.14732200	-1.25788700
H	11.24933600	-2.28755900	-0.80375700
H	10.87197600	-3.89975700	0.98250500
H	-12.73048200	3.83669900	-2.86604300
H	-13.17669100	3.61209800	-0.48186500
H	-13.51147700	2.18024200	1.13634200
H	-13.67256300	-0.19463200	1.65591900
H	-13.56875200	-2.20150400	0.78997700
H	-13.21940500	-3.44527200	-1.27531500

H	-12.81686600	-3.24815500	-3.41264400
H	-12.44110100	-1.64429700	-5.20728800
H	-12.29847200	0.48434700	-5.67296400
H	-12.41644600	2.72292500	-4.71925700
C	-8.29317500	-0.82832200	7.18098100
H	-7.95494400	-0.90007700	8.21861500
C	-10.16871700	2.13419600	6.17251700
H	-9.89554400	2.02372600	7.22471200
H	-9.34833500	-0.61340000	7.00994200
H	-11.23030500	2.07950100	5.92285300

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C	0.70917200	-0.77688800	-7.01151500
C	3.04451400	-0.15066800	-6.89319500
C	0.33358200	0.54984300	-6.74208100
H	-0.06186300	-1.53622600	-7.15766900
C	2.67574100	1.16612200	-6.61899200
H	4.09845000	-0.42841700	-6.92900800
H	-0.71684500	0.82052300	-6.65540100
H	3.44571200	1.91835500	-6.43904900
C	-3.17680700	7.15376800	-1.82743400
C	-1.78369900	8.88592500	-2.98501900
C	-2.14258400	7.57060800	-2.79680700
C	-1.63606600	6.45933800	-3.62617700
C	-0.28737600	6.34664700	-4.00220600
C	-2.05731200	4.34829000	-4.77443200
C	0.18366000	5.29375000	-4.79483900
H	0.43033800	7.08206500	-3.64124700
H	-2.68584800	3.49111800	-5.00004400
H	1.23518500	5.26869800	-5.06772200
C	1.31696700	1.53116500	-6.54591100
C	-0.71006300	4.27847000	-5.17419400
C	1.01093000	2.98012600	-6.23404900
H	1.24932800	3.63090200	-7.09652000
H	1.66208100	3.28241500	-5.39920300
O	-0.36459000	3.15025300	-5.88032600

C	-2.55078900	5.43174700	-4.02705800
C	-3.96597000	5.54885000	-3.58938700
C	-5.02836100	5.16012500	-4.38429400
S	-4.86224200	4.42838200	-6.01884600
S	-6.75439700	5.43682100	-3.96364400
C	-6.56445200	4.50412200	-6.44864400
H	-6.84302600	4.15911100	-7.44228800
C	-7.42227800	4.95983100	-5.51580900
H	-8.50055800	5.03794600	-5.63895600
S	-0.67233400	9.44862800	-4.28378600
C	-1.86616200	11.52789100	-3.11717700
H	-2.16053600	12.55126100	-2.89290100
S	-2.48341400	10.26188200	-2.06075500
C	-1.04731400	11.16164300	-4.12177600
H	-0.58116300	11.84377400	-4.82994500
C	-4.24188200	7.26223500	0.37412800
C	-4.13445000	6.18003300	-2.25570300
C	-5.15400100	5.82787900	-1.34870300
H	-5.87935300	5.06621300	-1.62018000
C	-5.22958500	6.36506200	-0.06039000
H	-6.02433200	6.05199300	0.61504500
C	-3.22348300	7.64926300	-0.51197600
H	-2.44593500	8.31429300	-0.14044600
O	-4.25690100	7.82388100	1.62990000
C	2.75047200	-6.95373700	1.09506700
C	3.83002400	-6.54113700	-1.49407200
C	1.92163500	-7.00427800	-0.03924400
H	0.85130900	-7.09961700	0.12835800
C	4.12328600	-6.69929100	0.94272700
H	4.77313700	-6.61135400	1.81105600
C	4.63608300	-6.47670600	-0.34212600
H	5.67858300	-6.17771800	-0.43441300
C	2.43549600	-6.82420000	-1.33079300
C	1.57459700	-6.83910900	-2.53472800
C	4.33243000	-6.26998300	-2.86013800
C	3.36304300	-5.55841600	-3.72550500

C	1.96951000	-5.85501100	-3.56463900
C	3.75059200	-4.60612600	-4.67929400
H	4.78933500	-4.29662100	-4.76975400
C	1.04672200	-5.15735000	-4.36298500
H	-0.01863100	-5.27582000	-4.17679400
C	1.44339500	-4.23658600	-5.34145800
H	0.68391000	-3.69169000	-5.89659800
C	2.81147800	-3.97870800	-5.52041000
O	3.35411400	-3.13551600	-6.45674400
C	2.06273700	-1.13875200	-7.09925300
C	2.50326100	-2.54101500	-7.46326700
C	5.54573600	-6.73823800	-3.31877500
C	0.55631900	-7.75209600	-2.71424700
S	6.14377700	-6.54276300	-5.00454600
S	6.65987600	-7.75223200	-2.33461000
S	0.13034800	-9.03939200	-1.53220100
S	-0.41453700	-7.88979200	-4.22211700
C	7.69616200	-8.24817100	-3.66729000
H	8.49043300	-8.95774600	-3.44417400
C	7.46203600	-7.70148700	-4.87554900
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C	-1.15823300	-9.43624700	-3.83204200
H	-1.80059800	-9.88563100	-4.58667900
C	-0.91078300	-9.95582600	-2.61448300
H	-1.32338500	-10.88916100	-2.23656300
H	3.14279900	-2.50608800	-8.35785900
H	1.64264700	-3.18852900	-7.68890300
O	2.10962600	-7.10715500	2.29279200
C	2.68977800	-6.50890200	3.47441400
H	3.18603800	-5.56375800	3.20223600
H	3.44730700	-7.18573700	3.90750900
C	1.52875000	-6.24036800	4.43377900
H	1.13288000	-7.19234600	4.82108000
H	0.72771500	-5.78308200	3.83505500
C	1.87845600	-5.28040400	5.58614100
H	2.56699900	-5.75704700	6.30387700



H	2.41103800	-4.41078900	5.17028000
C	0.60724200	-4.77713200	6.29924300
H	0.17178100	-5.57966200	6.91860700
H	-0.14337300	-4.54502700	5.52577200
C	0.81839800	-3.50215000	7.13671400
H	1.44137500	-3.71349600	8.02198800
H	1.38506900	-2.78369200	6.52387900
C	-0.51722600	-2.84956100	7.55251000
H	-0.94025200	-3.36247800	8.43295700
H	-1.24320700	-2.99376800	6.73533400
C	-0.41589000	-1.33761000	7.81776100
H	0.21260600	-1.12762500	8.69848800
H	0.08655000	-0.86493900	6.95915500
C	-1.80745900	-0.68717500	7.99922800
H	-2.27862100	-1.05256500	8.92654200
H	-2.44416900	-1.02429200	7.16137300
C	-4.22595200	6.91654200	2.76092700
H	-4.80469800	7.40925000	3.55679600
H	-4.72058800	5.96347200	2.51094000
C	-2.78177200	6.68207400	3.20989200
H	-2.23511700	6.16928000	2.40273200
H	-2.30364400	7.66503500	3.34964800
C	-2.67131100	5.86284200	4.50832900
H	-3.08522900	4.85455400	4.34659900
H	-3.28172900	6.33051900	5.30062000
C	-1.20918300	5.74861100	4.97491700
H	-0.59489000	5.41674300	4.12351600
H	-0.83547400	6.75014600	5.25025000
C	-0.98526700	4.76773600	6.13743400
H	-1.39870100	3.78862000	5.84974800
H	-1.55144000	5.09190700	7.02738700
C	0.50889900	4.60042700	6.49108900
H	1.10413200	4.64084000	5.56425000
H	0.84795900	5.44685000	7.11259700
C	0.80663600	3.26900100	7.19682300
H	0.45720200	2.45109600	6.54866900

H	0.22844200	3.18418700	8.13016400
C	2.30479900	3.04577000	7.49847000
H	2.66302600	3.79244000	8.22633300
H	2.87054900	3.20876100	6.56398500
H	-12.36038100	0.38642100	4.04439500
H	-12.60686600	1.87053800	2.13493600
H	-12.64677400	2.19208600	0.01889200
H	-12.48370700	1.32203800	-2.24504600
H	-12.19424500	-0.32674400	-3.58101500
H	-11.78411200	-2.69523200	-3.94352500
H	-12.02130900	-1.57264300	4.84375400
H	-11.60701600	-3.94067100	4.47826600
H	-11.31647300	-5.58363800	3.13623600
H	-11.15609000	-6.45571500	0.87272900
H	-11.20105500	-6.14434500	-1.24580000
H	-11.44894400	-4.65820300	-3.15373500
C	-11.46622600	0.82332300	3.60150100
C	-11.60634400	1.66720200	2.51463100
C	-11.66253700	2.10696600	-0.44006100
C	-11.56966900	1.61260100	-1.72849700
C	-11.16532500	-0.68430300	-3.59406100
C	-10.93204700	-2.03188500	-3.80010200
C	-10.99485200	-1.91024400	4.70594300
C	-10.75920400	-3.25699300	4.49784900
C	-10.35301000	-5.55073500	2.62908300
C	-10.26173900	-6.04681200	1.34126800
C	-10.32395200	-5.61364300	-1.61412200
C	-10.46490900	-4.76831000	-2.69966200
C	-10.17359500	0.38118700	4.02628400
C	-10.46264300	2.12130800	1.78508600
C	-10.48917700	2.33252400	0.34653700
C	-10.29779800	1.31322100	-2.31112200
C	-10.10124500	0.19629900	-3.22111600
C	-9.62036100	-2.58191800	-3.64549900
C	-9.94370200	-0.95054200	4.56213200
C	-9.45820900	-3.72658400	4.13246800

C	-9.26063300	-4.84295400	3.22261200
C	-9.07224000	-5.86698000	0.56724300
C	-9.10230700	-5.65696900	-0.87096800
C	-9.39300800	-3.91392900	-3.10925200
C	-9.04875900	1.13018600	3.56441400
C	-9.19487800	2.00654300	2.43272500
C	-9.24593300	2.40969100	-0.35264100
C	-9.14923100	1.89668200	-1.69413600
C	-8.76899700	-0.26220000	-3.45617900
C	-8.52612100	-1.66419300	-3.67038700
C	-8.60463400	-1.44654700	4.59619800
C	-8.35972200	-2.84712000	4.37757500
C	-7.97714700	-5.00736400	2.61792500
C	-7.88202400	-5.52460100	1.27883300
C	-7.94000200	-5.11927500	-1.50363400
C	-8.08648800	-4.24022300	-2.63302700
C	-7.72329300	0.77490800	3.99600700
C	-8.00879600	2.49001400	1.77969000
C	-8.03369400	2.68839300	0.36867200
C	-7.84496400	1.68414100	-2.26123900
C	-7.65212600	0.59228600	-3.15612800
C	-7.17660900	-2.15278000	-3.57552200
C	-7.49759300	-0.53203100	4.51606200
C	-7.01815600	-3.27450700	4.08566400
C	-6.82461000	-4.36871700	3.19400400
C	-6.63787700	-5.38418300	0.57176700
C	-6.66688500	-5.17959300	-0.83778300
C	-6.95382200	-3.45783700	-3.04925800
C	-6.60144600	1.56654400	3.58913700
C	-6.74839700	2.43935500	2.45770100
C	-6.79578100	2.82191900	-0.33773300
C	-6.70037100	2.31712000	-1.67958700
C	-6.31935500	0.15943000	-3.45427200
C	-6.07617000	-1.24054400	-3.66754300
C	-6.15476800	-1.02111600	4.61468400
C	-5.91063500	-2.41972700	4.39317500

C	-5.52727300	-4.58792300	2.62855600
C	-5.43179600	-5.10667700	1.29230200
C	-5.48912700	-4.70272500	-1.49870000
C	-5.63526600	-3.82474000	-2.62650700
C	-5.28834100	1.21353300	4.02606800
C	-5.57663400	2.92579000	1.80477400
C	-5.59876500	3.10151200	0.38361000
C	-5.41042000	2.10820600	-2.25105900
C	-5.21628100	1.01585000	-3.16026900
C	-4.73858700	-1.73420000	-3.58228400
C	-5.06101800	-0.10535400	4.54608100
C	-4.58116700	-2.85645700	4.11057700
C	-4.38590500	-3.96031300	3.21280600
C	-4.19797700	-4.98271100	0.58482200
C	-4.22670900	-4.77805200	-0.83621700
C	-4.51391500	-3.05020700	-3.05254000
C	-4.16307000	1.99687100	3.59957900
C	-4.30952400	2.86718900	2.47459000
C	-4.35869500	3.22238100	-0.32124600
C	-4.26347400	2.72223900	-1.65189900
C	-3.87934100	0.57628100	-3.43873500
C	-3.63705500	-0.81684300	-3.65439900
C	-3.71600700	-0.59943000	4.62361100
C	-3.47349100	-1.99266600	4.40306700
C	-3.08904400	-4.17034600	2.63636200
C	-2.99299000	-4.68960900	1.30629000
C	-3.04936500	-4.28677800	-1.49308700
C	-3.19499100	-3.41018300	-2.61521000
C	-2.84426800	1.63837500	4.02905600
C	-3.13766800	3.36076800	1.81306200
C	-3.16593300	3.55343600	0.39259600
C	-2.97021500	2.53067900	-2.22881400
C	-2.77343200	1.43712600	-3.13622100
C	-2.29421600	-1.31192400	-3.56853700
C	-2.61827700	0.31884100	4.54863100
C	-2.13979900	-2.43205500	4.11760500

C	-1.94386500	-3.53938100	3.22317100
C	-1.75399600	-4.56821400	0.59562600
C	-1.78233500	-4.36505300	-0.82714800
C	-2.06948800	-2.63064600	-3.04121000
C	-1.72522700	2.41144900	3.59142800
C	-1.87415100	3.29384600	2.47217500
C	-1.93798200	3.70164800	-0.31893300
C	-1.83741400	3.17361900	-1.64816200
C	-1.44285000	1.00110200	-3.41057200
C	-1.19983000	-0.39567100	-3.63204200
C	-1.28142100	-0.17463700	4.62208800
C	-1.03840700	-1.57001000	4.40464800
C	-0.65353100	-3.74421000	2.64685400
C	-0.55566700	-4.27022200	1.31439000
C	-0.61142300	-3.87082000	-1.47934100
C	-0.75817800	-2.98650100	-2.60079100
C	-0.40599300	2.04858300	4.01232600
C	-0.70272500	3.79020100	1.81232500
C	-0.73582000	4.00690700	0.39955500
C	-0.53966500	2.96467500	-2.21546500
C	-0.33970500	1.85733800	-3.09390700
C	0.14152500	-0.88750700	-3.53040100
C	-0.18236700	0.74050400	4.53881300
C	0.29466700	-2.00280300	4.11492900
C	0.48875900	-3.10022700	3.22406100
C	0.67936700	-4.12923600	0.60425600
C	0.65223400	-3.93212400	-0.80941800
C	0.36471500	-2.19600800	-3.00845100
C	0.71541100	2.83212900	3.59128900
C	0.56548300	3.72154600	2.47640200
C	0.50203200	4.14631100	-0.31133400
C	0.60026000	3.61573700	-1.64106500
C	0.99405800	1.42130300	-3.37160200
C	1.23886400	0.02894400	-3.59528100
C	1.15951500	0.25043400	4.63165400
C	1.40190500	-1.14561000	4.41659000

C	1.78426400	-3.30776000	2.65184100
C	1.88049100	-3.82989200	1.32298800
C	1.82731400	-3.44171500	-1.46351600
C	1.68062200	-2.55573500	-2.57639100
C	2.02732000	2.47746600	4.02655900
C	1.73392100	4.22496600	1.82777200
C	1.70204900	4.44115300	0.40768200
C	1.89348000	3.40296200	-2.20808300
C	2.09312900	2.28530100	-3.08711700
C	2.57374400	-0.46339000	-3.51544000
C	2.25360400	1.16423000	4.55539100
C	2.73185400	-1.58296700	4.13922300
C	2.92581600	-2.68358000	3.23963900
C	3.11354600	-3.70501800	0.61837800
C	3.08815100	-3.51582300	-0.80065300
C	2.79910800	-1.78109000	-3.00022400
C	3.14955700	3.26373000	3.60872600
C	3.00145700	4.14710900	2.49346100
C	2.94228500	4.56448200	-0.30101200
C	3.03889800	4.03945100	-1.62826300
C	3.42740000	1.84528500	-3.36888000
C	3.67041200	0.45381100	-3.58244600
C	3.59576700	0.67157700	4.64499700
C	3.83836000	-0.72152400	4.43334500
C	4.22151900	-2.89522700	2.66717100
C	4.31543700	-3.41094800	1.33819300
C	4.26204300	-3.02381000	-1.45546200
C	4.11544800	-2.14378400	-2.57038000
C	4.46781200	2.90752500	4.04977500
C	4.17782900	4.64597200	1.84088500
C	4.14801000	4.85598200	0.42071200
C	4.33754600	3.82481100	-2.20146700
C	4.53445000	2.71258200	-3.08855500
C	5.01303900	-0.04184400	-3.51166300
C	4.69437900	1.59014800	4.57471700
C	5.17411800	-1.16246200	4.15211400

C	5.36911500	-2.26800000	3.25693000
C	5.55671500	-3.29687900	0.63060900
C	5.52928400	-3.09987000	-0.79118900
C	5.23941000	-1.36389200	-2.99748700
C	5.58759800	3.68627500	3.62791800
C	5.44014300	4.56900000	2.50392400
C	5.38273400	4.97830900	-0.28592100
C	5.47931000	4.45430800	-1.62021000
C	5.86365700	2.27235200	-3.36886300
C	6.10678600	0.87205300	-3.58424100
C	6.03189800	1.09717500	4.65658400
C	6.27582700	-0.30203600	4.44037400
C	6.65910800	-2.47827900	2.68362100
C	6.75482500	-3.00382800	1.34925400
C	6.69953200	-2.60796300	-1.44380200
C	6.55180100	-1.72333300	-2.56688900
C	6.90661900	3.31851900	4.04871900
C	6.61770900	5.04903600	1.84473700
C	6.58887400	5.25452300	0.43532500
C	6.77773100	4.22821300	-2.18182000
C	6.97188400	3.12722000	-3.06527900
C	7.44865300	0.38016400	-3.48761300
C	7.13108000	2.01066500	4.56727300
C	7.60861600	-0.73422500	4.14300300
C	7.80225800	-1.83307900	3.25680200
C	7.99106700	-2.86440600	0.63949600
C	7.96269900	-2.66345400	-0.77121100
C	7.67302400	-0.92988700	-2.97321200
C	8.03828700	4.10400000	3.63617700
C	7.89076500	4.98756100	2.51053600
C	7.83393400	5.39202500	-0.27110400
C	7.93046000	4.86782500	-1.60743000
C	8.31321000	2.69541500	-3.35316300
C	8.55639400	1.29358600	-3.56881000
C	8.48082900	1.52263000	4.65891700
C	8.72467100	0.12151900	4.44168500

C	9.10723800	-2.04909800	2.69291100
C	9.20352100	-2.57580300	1.35727300
C	9.14702700	-2.17568100	-1.42510400
C	8.99911500	-1.29016600	-2.54962200
C	9.34534100	3.77597000	4.10968200
C	9.05284500	5.52684600	1.87904400
C	9.02370800	5.73515800	0.44070800
C	9.21490000	4.69690600	-2.20845500
C	9.41263900	3.57457300	-3.11109900
C	9.89490900	0.79574500	-3.53745200
C	9.57427700	2.44121200	4.63777800
C	10.05723100	-0.33668300	4.20810000
C	10.25494400	-1.45856900	3.30496600
C	10.44604900	-2.50022100	0.65693800
C	10.41670800	-2.29284700	-0.78165100
C	10.12367800	-0.53963600	-3.01030000
C	10.41630800	4.63376800	3.70458200
C	10.27444900	5.48307000	2.62243700
C	10.21458200	5.91041300	-0.33249800
C	10.30723400	5.40679100	-1.61719900
C	10.71345000	3.10182900	-3.47311900
C	10.94721200	1.75444900	-3.67972400
C	10.88647600	1.89167800	4.78933800
C	11.12065900	0.54470700	4.58072500
C	11.52721800	-1.76119400	2.72503300
C	11.61973000	-2.26620600	1.44084700
C	11.55921100	-1.83835200	-1.51307000
C	11.41708100	-0.98777700	-2.59422800
H	11.40011000	4.52342000	4.15901800
H	11.15071200	6.01664100	2.25629700
H	11.10868700	6.32045100	0.13547100
H	11.27163600	5.43544900	-2.12285100
H	11.56245300	3.78403200	-3.45315800
H	11.97347100	1.41565300	-3.81623600
H	11.73799800	2.55526800	4.93455200
H	12.14965000	0.18752600	4.56821500



H	12.44095000	-1.46561300	3.23913100
H	12.60364300	-2.35275200	0.98143100
H	12.56046100	-2.04602900	-1.13759800
H	12.31060500	-0.55079000	-3.03840700
C	-1.75674700	0.81726000	7.99742200
H	-1.32897600	1.27068300	7.09963100
C	-2.17384600	1.61384100	8.99164700
H	-2.60128500	1.20124200	9.90942200
H	-2.10297700	2.70052500	8.91779200
C	2.57054800	1.65318600	8.01013400
H	2.26190600	0.84117300	7.34449000
C	3.11446600	1.35346900	9.19813900
H	3.26663300	0.31974100	9.51432300
H	3.42668000	2.13823700	9.89238700

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C	1.75471300	-0.40201000	-7.24947800
C	3.88940600	-1.49575000	-6.93348300
C	2.37885700	0.84868500	-7.22834800
H	0.66801300	-0.45605900	-7.34204800
C	4.51444700	-0.24149000	-6.90283300
H	4.47110700	-2.40216700	-6.77563300
H	1.78209700	1.75562000	-7.29602100
H	5.58842300	-0.18397200	-6.71727300
C	3.19610500	7.72165200	-1.91191400
C	5.24820200	8.58811000	-3.07274100
C	4.27443800	7.62462200	-2.92026300
C	4.12274600	6.48524500	-3.84977200
C	5.21126500	5.73630800	-4.33070700
C	2.64542900	5.00639500	-5.10747000
C	5.05169500	4.67283900	-5.22840700
H	6.21306500	5.95646900	-3.96513500
H	1.65933800	4.61411700	-5.34116700
H	5.92497000	4.12477900	-5.57412600
C	3.76312600	0.94222900	-7.00937400
C	3.75368400	4.30314400	-5.61309000

C	4.44174500	2.28040700	-6.77580100
H	4.98911000	2.63547200	-7.66880700
H	5.16802600	2.16414000	-5.95585800
O	3.43790200	3.24526300	-6.42371900
C	2.80124400	6.10609700	-4.25070700
C	1.65386100	6.86125900	-3.69450700
C	0.52087300	7.14642600	-4.43151000
S	0.27248500	6.65696300	-6.14575000
S	-0.83549200	8.16879800	-3.83879200
C	-1.13625600	7.66859100	-6.43708100
H	-1.54658600	7.67230500	-7.44492200
C	-1.63854300	8.35360600	-5.39230800
H	-2.51681300	8.99511100	-5.42633700
S	6.44797200	8.59172900	-4.41489200
C	6.51225000	10.91538200	-3.11026500
H	6.78318500	11.93248900	-2.83395600
S	5.38153500	10.06898500	-2.05931200
C	6.99542600	10.24755200	-4.17523700
H	7.71533400	10.64335500	-4.88885500
C	2.36543100	8.32904900	0.31720000
C	1.86898000	7.35701700	-2.31519700
C	0.84501600	7.46649000	-1.35896600
H	-0.15255800	7.10786700	-1.59774700
C	1.06580700	7.95034400	-0.06343700
H	0.23303500	7.98503800	0.63456900
C	3.42346800	8.15997500	-0.59894000
H	4.43240200	8.36798400	-0.24819500
O	2.71730000	8.86997600	1.52537900
C	0.93267900	-8.01497500	0.78677000
C	2.26179400	-7.76370800	-1.71207900
C	0.19557900	-7.94844000	-0.40963600
H	-0.88867300	-7.89738800	-0.33539200
C	2.33876200	-7.99437400	0.73437500
H	2.93493600	-8.02231700	1.64280500
C	2.97582400	-7.84303200	-0.50211200
H	4.05507200	-7.70634300	-0.50417900

C	0.83496700	-7.85505100	-1.65499500
C	0.08500200	-7.77686000	-2.92929100
C	2.90022800	-7.49830200	-3.02207400
C	2.08374700	-6.64881400	-3.92248800
C	0.66103700	-6.81583400	-3.89381200
C	2.63819100	-5.65805700	-4.74755100
H	3.69798900	-5.41926600	-4.69405900
C	-0.11988500	-6.01228000	-4.74134800
H	-1.20540300	-6.07303300	-4.68896000
C	0.44312000	-5.06421000	-5.60475300
H	-0.21373300	-4.46993800	-6.23467300
C	1.83243000	-4.85717400	-5.57886000
O	2.49855400	-3.87114900	-6.26501400
C	2.49350500	-1.58370400	-7.06819000
C	1.72326200	-2.88450800	-6.96275200
C	4.10310100	-8.04942500	-3.40878100
C	-0.98578200	-8.59523300	-3.21280000
S	4.85948900	-7.80050900	-5.02225400
S	5.03874900	-9.21755900	-2.41079300
S	-1.63397800	-9.83409000	-2.08098900
S	-1.81341100	-8.65221800	-4.80888700
C	6.15339300	-9.70695600	-3.68107700
H	6.86908600	-10.49094300	-3.44185600
C	6.07152200	-9.06612900	-4.86274100
H	6.71109400	-9.25486800	-5.72265700
C	-2.73042200	-10.12170700	-4.49543500
H	-3.33640200	-10.51487800	-5.30922000
C	-2.64788600	-10.65566900	-3.26177700
H	-3.17773300	-11.54625500	-2.92965500
H	1.44430900	-3.28155100	-7.95679300
H	0.79389000	-2.67229800	-6.41129100
O	0.19416700	-8.03894400	1.93818000
C	0.87742900	-7.75829300	3.17810300
H	1.58019900	-6.92481000	3.02396300
H	1.45887700	-8.64297600	3.49392400
C	-0.16195000	-7.35209000	4.22131300

H	-0.80347200	-8.20775700	4.48263200
H	-0.80811700	-6.59120800	3.76034700
C	0.51220800	-6.74961500	5.47218600
H	0.96438400	-7.54326700	6.09012100
H	1.34221000	-6.10492400	5.13979200
C	-0.44393000	-5.88237900	6.31485200
H	-1.15656400	-6.51545100	6.86989400
H	-1.04511600	-5.26947700	5.62522300
C	0.29893200	-4.92893100	7.27079000
H	0.76344700	-5.49118600	8.09866600
H	1.12667000	-4.46544600	6.71019000
C	-0.59619500	-3.80284600	7.82297000
H	-1.27684500	-4.19414700	8.59847400
H	-1.23732900	-3.43190400	7.00736000
C	0.21013800	-2.61620700	8.37696800
H	0.79859900	-2.93207300	9.25568600
H	0.93582200	-2.29099800	7.61516700
C	-0.68554100	-1.41378100	8.75302700
H	-1.38809300	-1.73290200	9.54463600
H	-1.29375300	-1.12934400	7.88000100
C	1.68415400	9.05766500	2.51608700
H	2.07475600	9.84052200	3.18096400
H	0.76845800	9.44881000	2.04045100
C	1.40411400	7.76634100	3.29113400
H	1.37374300	6.93301700	2.57868400
H	2.24717700	7.56704100	3.97167600
C	0.07610900	7.79620600	4.07195800
H	-0.75720500	7.70719100	3.35330600
H	-0.05514300	8.76645400	4.58228000
C	-0.00554900	6.65192800	5.10078500
H	0.43983800	5.74912300	4.66163200
H	0.61887400	6.90431100	5.97506900
C	-1.43374500	6.31286100	5.55638100
H	-2.02620200	6.02405100	4.67215100
H	-1.92177900	7.20745500	5.98151700
C	-1.46905800	5.16534200	6.58095500

H	-0.88782100	4.31629900	6.18844600
H	-0.96099700	5.48238400	7.50857300
C	-2.89053500	4.68347300	6.91098600
H	-3.40794000	4.40546700	5.98055700
H	-3.47090900	5.50999400	7.35691600
C	-2.89463000	3.47384300	7.87209900
H	-2.37948100	3.76964500	8.80488900
H	-2.30545800	2.65393000	7.43340100
C	-4.28511700	2.98719400	8.19061600
C	0.11388700	-0.22525700	9.22276200
H	0.73642100	-0.38763200	10.11028700
H	-4.97622300	3.74305800	8.58178900
H	11.77231200	-2.38414600	-3.01008300
H	11.89594600	0.01540300	-3.34694800
H	11.90983800	2.03326100	-2.72163900
H	11.81309600	3.81456800	-1.07662100
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H	11.59028300	-4.14103700	-1.85018000
H	11.33731100	-5.36858800	0.22799400
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H	10.93292800	-4.65213700	4.57782700
H	10.84937100	-3.10278200	6.01332900
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C	10.91465500	-0.45505800	-3.30338100
C	10.93399000	2.40594600	-2.41343000
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C	9.59238200	-2.47615100	-2.89155900
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C	9.74789000	1.74407000	-2.85670300
C	9.63405400	3.84640400	-0.91773700
C	9.51870600	4.37565400	0.43113700
C	9.22569600	4.13990900	3.26677800
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C	8.79776600	-4.20316900	4.45589800
C	8.73977000	-3.13973900	5.44470500
C	8.75689300	-0.40828900	6.29686800
C	8.41010900	-1.74054900	-3.21292500
C	8.48361400	-0.31762200	-3.41102500
C	8.50216200	2.38278500	-2.57016000
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C	7.73092700	-5.03358200	2.37553300
C	7.61829800	-4.51107300	3.71043600
C	7.50539100	-2.44524900	5.63375600
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C	7.11971400	-2.36009800	-3.07553000
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C	7.16128700	3.88653800	-1.12734900

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C	-3.86558800	3.90460100	-2.85200700
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C	-4.65770900	2.17942200	4.42608700
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C	-5.03536700	0.90543200	-4.72483800
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C	-5.14413300	4.35017500	-2.37832900
C	-5.25846800	4.86554800	-1.04494500
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C	-7.64103600	-1.80020800	-4.55175800
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C	-9.07428100	-3.43185200	-3.38042900
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C	-9.74516700	-1.80017900	3.91059300
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C	-3.19652200	-7.16717200	-3.52940600
C	-2.43264000	-7.61902100	-2.43858600
H	-1.35136900	-7.69558600	-2.53518600
C	-3.00208000	-7.89537200	-1.19137900
H	-2.36310000	-8.21814500	-0.37403500
C	-5.16102000	-7.20461900	-2.06957800

H	-6.20082300	-6.95814600	-1.86644200
O	-5.02682600	-7.80550300	0.20018500
C	1.99045800	8.28851000	-0.12072700
C	1.14674700	8.02001400	-2.81493900
C	2.90679200	7.91230000	-1.12315100
H	3.90946400	7.63376800	-0.80613800
C	0.65286800	8.55082000	-0.46872700
H	-0.08578200	8.82254500	0.28060700
C	0.24843200	8.38183100	-1.79700300
H	-0.81160200	8.47668800	-2.02618000
C	2.51916700	7.80032400	-2.46866300
C	3.45588700	7.41057200	-3.55329700
C	0.72804000	7.79217500	-4.21262400
C	1.45698100	6.68820200	-4.87301500
C	2.85088000	6.53566400	-4.58613200
C	0.81791000	5.77000600	-5.71770400
H	-0.26223700	5.79351200	-5.84704500
C	3.54678800	5.50899600	-5.25235600
H	4.59089300	5.32163800	-5.01272600
C	2.92172700	4.63703400	-6.15359600
H	3.50289300	3.84847000	-6.62544100
C	1.53550000	4.74425700	-6.35630400
O	0.77488800	3.89305600	-7.11397600
C	0.22842000	1.63780600	-7.76193700
C	1.33895200	2.65229300	-7.55832200
C	-0.17747700	8.58681400	-4.87949500
C	4.74433000	7.89820800	-3.62994600
S	-0.62409000	8.37536800	-6.61002700
S	-0.94756200	10.04797800	-4.16607500
S	5.47258300	9.02689900	-2.43336500
S	5.85529300	7.59302400	-5.01154100
C	-1.58791200	10.68155800	-5.67873500
H	-2.09106100	11.64574400	-5.64256400
C	-1.44095000	9.92517700	-6.78327300
H	-1.80748400	10.18737500	-7.77378100
C	7.06404100	8.78787200	-4.55846800

H	7.90487500	8.92798300	-5.23477200
C	6.88943700	9.43717700	-3.39161800
H	7.56857900	10.18246100	-2.98239600
H	1.91207200	2.82164200	-8.48923500
H	2.03743000	2.25887800	-6.80264300
O	2.48077900	8.31080000	1.15828900
C	1.52429800	8.46932900	2.22615200
H	0.65023300	7.83174500	2.02410700
H	1.17981100	9.51838900	2.26300800
C	2.15209600	8.02728000	3.54657400
H	2.93958900	8.72891700	3.86173700
H	2.63088200	7.05217000	3.38086600
C	1.05714600	7.88381400	4.62621500
H	0.73835800	8.87719100	4.98425800
H	0.16961900	7.42532200	4.15978500
C	1.45863100	6.99314000	5.81502900
H	2.23153000	7.48643800	6.42850200
H	1.91359200	6.07059500	5.42159500
C	0.24679600	6.60505600	6.68156500
H	-0.16314000	7.49611900	7.18772700
H	-0.54883100	6.23597900	6.01318700
C	0.55979500	5.50567200	7.70996000
H	1.25091700	5.88682600	8.48147100
H	1.09067400	4.68926800	7.19514100
C	-0.70292800	4.92741100	8.37202100
H	-1.16768800	5.68248600	9.02918600
H	-1.44331100	4.69379200	7.59194600
C	-0.41150200	3.64050400	9.17704100
H	0.29402700	3.88846000	9.99157200
H	0.09608200	2.91359500	8.52310300
C	-4.20976700	-8.02154400	1.36726900
H	-3.76600500	-9.03282500	1.32951300
H	-3.38611400	-7.29071200	1.37339600
C	-5.06095200	-7.83753200	2.61925900
H	-5.58855300	-6.87650400	2.54438200
H	-5.82521800	-8.62791300	2.68336400



C	-4.16188000	-7.84214800	3.86858100
H	-3.33715600	-7.13212900	3.70449600
H	-3.69857500	-8.83693900	3.99068700
C	-4.90215400	-7.46654200	5.16331200
H	-5.33412800	-6.45738900	5.05087000
H	-5.74837700	-8.15889600	5.30862100
C	-3.98759000	-7.50177200	6.40663800
H	-3.49446700	-8.48868800	6.46131100
H	-4.60076300	-7.40819000	7.31859400
C	-2.91683900	-6.39738300	6.41062800
H	-2.35574200	-6.41506900	5.46369500
H	-3.41322500	-5.41364400	6.44862400
C	-1.91013000	-6.51003300	7.56683200
H	-1.38025400	-7.47508200	7.50003100
H	-2.44232100	-6.50843500	8.53410300
C	-0.88032200	-5.35795700	7.53391300
H	-1.42793200	-4.40668900	7.65709600
H	-0.41325600	-5.32225700	6.53941600
C	0.19622900	-5.46543800	8.58119700
C	-1.66104300	3.01951300	9.74698800
H	-2.25745300	3.66021100	10.40682600
H	-0.14230600	-5.52127000	9.62233900
H	12.48630600	0.26185300	-4.87794200
H	12.89544900	2.09921600	-3.35159500
H	13.14958600	3.06464300	-1.50987100
H	13.28286000	3.28825000	0.89958700
H	13.24160700	2.68054100	2.90359200
H	13.02162900	1.16280200	4.78005900
H	12.71058200	-0.65578400	5.77236100
H	12.26420300	-3.02470000	6.02292000
H	12.08717600	-1.70647200	-5.47177800
H	11.64093000	-4.07582100	-5.22508000
H	11.32682400	-5.89397800	-4.23332800
H	11.10285900	-7.40965900	-2.35542900
H	11.05811300	-8.01786400	-0.35173400
H	11.19110200	-7.79344500	2.05796100

H	11.44796300	-6.82811200	3.89915300
H	11.86101200	-4.99355600	5.42819800
C	11.63117600	0.78977800	-4.45866700
C	11.86473300	1.83886800	-3.58740000
C	12.22848800	3.22081100	-0.95044800
C	12.30459600	3.34829300	0.42512700
C	12.24575400	2.47868600	3.29507500
C	12.12019800	1.61213100	4.36627400
C	11.67461900	-0.99073100	5.78972300
C	11.41983000	-2.34305200	5.93293200
C	11.05906100	-2.02818300	-5.31296800
C	10.80432100	-3.38080500	-5.17221900
C	10.35497100	-5.98362900	-3.75040500
C	10.22711700	-6.84886200	-2.67839100
C	10.16483900	-7.71524800	0.19254600
C	10.24079300	-7.58713700	1.56799500
C	10.60744400	-6.20753600	4.20592600
C	10.84326600	-5.16034700	5.07875900
C	10.30955400	0.30945900	-4.70421200
C	10.79374700	2.48391700	-2.89840500
C	10.97004000	3.15367800	-1.62087600
C	11.12761500	3.41739100	1.22992900
C	11.09905200	2.99573600	2.62021600
C	10.83860200	1.19960400	4.84060700
C	10.62294400	-0.06069600	5.53094700
C	10.09473700	-2.86362900	5.82814400
C	10.03241600	-1.05550700	-5.11886600
C	9.50432800	-3.85918500	-4.82742300
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C	9.02189100	-6.91263300	-1.91604100
C	8.99201200	-7.33103500	-0.52488700
C	9.14943600	-7.06531100	2.32593800
C	9.32686700	-6.39800900	3.60438000
C	9.81543200	-4.22810900	5.41397000
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C	9.89042500	3.65970200	0.55663200
C	9.83467100	2.83723100	3.26740000
C	9.70425600	1.93723600	4.38012200
C	9.28381700	-0.51939200	5.72794400
C	9.01919600	-1.92384600	5.87742300
C	8.68459600	-1.52924100	-5.07811000
C	8.41986500	-2.93424400	-4.93253900
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C	7.86317600	-6.28958300	-2.47449000
C	7.80563600	-7.10304000	0.23875700
C	7.88459500	-6.96972400	1.66738900
C	8.23009500	-5.67030600	4.16114800
C	8.47487000	-4.58359600	5.06885900
C	7.86992800	0.74033200	-4.54303100
C	8.34870900	2.89102500	-2.75761800
C	8.52157600	3.54815000	-1.50581700
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C	8.39156900	1.61813600	4.87083500
C	8.18054300	0.38416200	5.54911900
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C	7.59816400	-0.59686000	-4.95118100
C	7.07600300	-3.36858700	-4.66521000
C	6.86273300	-4.60364300	-3.98957200
C	6.60180600	-6.37217800	-1.79042300
C	6.57328900	-6.77959800	-0.42647100
C	6.72911500	-6.51600800	2.39182900
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C	5.36870800	-6.62306300	0.33019300
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C	6.03619000	-4.11183900	5.15925200
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C	5.75360100	0.85462800	5.66074500
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C	2.21051600	-2.44211900	-4.51524200
C	1.99506600	-3.68754800	-3.83657800
C	1.73567700	-5.45358000	-1.62561400
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C	-5.57110200	0.89064800	6.43375800
C	-5.89557800	1.28805100	-4.54422600
C	-6.16036300	-0.11284800	-4.39035800
C	-6.58230300	-2.56879900	-3.04065700
C	-6.71459100	-3.46931700	-1.93284900
C	-6.77096500	-4.28056200	0.78119900
C	-6.69282500	-4.14358200	2.20638500
C	-6.35396900	-2.84849300	4.70606100
C	-6.11309000	-1.76795500	5.61717100
C	-6.70186800	3.55831400	-4.01927500
C	-6.22205700	5.70231500	-2.22838800
C	-6.04981600	6.35177700	-0.97280600
C	-5.89646600	6.60199300	1.84760100
C	-5.92568700	6.19069800	3.21085400
C	-6.18608000	4.42681100	5.41633900
C	-6.39935800	3.19582300	6.09994700
C	-6.92451400	0.42639900	6.39659400
C	-6.97463100	2.22030600	-4.42418000
C	-7.49663200	-0.55206800	-4.12659600



C	-7.70863600	-1.78745200	-3.44901800
C	-7.96905600	-3.56387400	-1.25225600
C	-7.99758100	-3.97191800	0.11269500
C	-7.84377000	-3.70280800	2.93337400
C	-7.67306200	-3.05060800	4.18828300
C	-7.19712600	-0.90983800	5.98641600
C	-7.79311600	4.41789300	-3.65044300
C	-7.54972200	5.50505400	-2.74262300
C	-7.20648900	6.79942500	-0.24621200
C	-7.12865600	6.92750000	1.18310700
C	-7.18635400	6.10971400	3.89625600
C	-7.31844500	5.21530400	5.01344400
C	-7.74367400	2.76452000	6.36990900
C	-8.01003200	1.36030200	6.51930500
C	-8.33500800	1.75615600	-4.45716400
C	-8.59970700	0.35107100	-4.30756800
C	-9.02195900	-2.10824400	-2.96068600
C	-9.15369000	-3.00789100	-1.84690100
C	-9.21067100	-3.82111600	0.86842300
C	-9.13287900	-3.68506800	2.29757200
C	-8.79339700	-2.38415400	4.79364900
C	-8.55196900	-1.29843400	5.70404400
C	-9.13335500	4.06017600	-3.99499500
C	-8.64778000	6.22981900	-2.18442900
C	-8.47148500	6.89456400	-0.90446300
C	-8.31526300	7.15287800	1.94728400
C	-8.34475900	6.73387400	3.33835800
C	-8.60885500	4.94760900	5.56635300
C	-8.82720400	3.68999100	6.26076200
C	-9.35844100	0.88810200	6.55728200
C	-9.41140200	2.69519300	-4.40903100
C	-9.93891400	-0.10864900	-4.11196000
C	-10.15533200	-1.36971300	-3.42191100
C	-10.41796600	-3.16319300	-1.19894900
C	-10.44723800	-3.58040900	0.19328600
C	-10.29243700	-3.31099300	3.04483100

C	-10.11819100	-2.64310000	4.32387900
C	-9.63643200	-0.47562600	6.13928600
C	-10.16244700	4.99082700	-3.65930500
C	-9.92814400	6.03781800	-2.78577400
C	-9.56382200	7.41230700	-0.14517600
C	-9.48841900	7.53736400	1.23059000
C	-9.54902300	6.67337000	4.10240900
C	-9.67653200	5.81148300	5.17711300
C	-10.12783600	3.21401000	6.60671100
C	-10.38427900	1.86198600	6.74954300
C	-10.73608600	2.17372900	-4.51454200
C	-10.99048900	0.82120100	-4.37141700
C	-11.43728800	-1.78119900	-2.94758800
C	-11.56390100	-2.64619500	-1.87507400
C	-11.62445400	-3.50826500	0.99728600
C	-11.54997900	-3.37852800	2.37287200
C	-11.19028800	-1.99873700	5.01183800
C	-10.95795900	-0.95297400	5.88742500
H	-11.18014100	4.82247300	-4.00816400
H	-10.76973600	6.65646100	-2.47797900
H	-10.51450100	7.61797800	-0.63472600
H	-10.38232400	7.83734100	1.77525700
H	-10.42423900	7.23514200	3.77975400
H	-10.64760700	5.72511700	5.66215300
H	-10.96363300	3.91009900	6.65784900
H	-11.41282200	1.54151200	6.90805200
H	-11.58084700	2.85486400	-4.60495200
H	-12.02644600	0.48611700	-4.35458800
H	-12.33843100	-1.33162000	-3.36180000
H	-12.56012800	-2.84628000	-1.48358300
H	-12.60235200	-3.44887000	0.52195700
H	-12.47181500	-3.22183400	2.93086500
H	-12.22064100	-2.25681600	4.77216900
H	-11.81364300	-0.42498700	6.30546700
C	-2.09152600	1.77918200	9.47327800
H	-1.52545900	1.11855800	8.81338500

H	-3.01784400	1.38470800	9.89473000
C	1.51040000	-5.50039300	8.31419600
H	1.87771900	-5.44431300	7.28659200
H	2.25769200	-5.57784300	9.10608700

**UP-8-(9,9)**

C	3.42135700	0.36006700	-8.13364200
C	1.31520800	1.54418000	-8.26533500
C	2.74670400	-0.86549800	-8.21078300
H	4.50747700	0.36676000	-8.02142800
C	0.64292000	0.32053700	-8.34984100
H	0.75664500	2.47721500	-8.25508300
H	3.30131400	-1.79981800	-8.15234200
H	-0.44737200	0.31116500	-8.39968600
C	0.15723500	-8.17126300	-4.00557900
C	-1.76680900	-8.62315300	-5.55068800
C	-0.69477300	-7.84321200	-5.17325400
C	-0.21891100	-6.67679900	-5.94928000
C	-1.07747100	-5.75026000	-6.56704700
C	1.66199200	-5.27720700	-6.64573000
C	-0.60057000	-4.62166600	-7.24688500
H	-2.15485600	-5.86287300	-6.46334800
H	2.71661700	-5.01227100	-6.60716700
H	-1.30974900	-3.93029700	-7.69508900
C	1.34502300	-0.89587000	-8.29521900
C	0.78061500	-4.36617500	-7.25591700
C	0.54756800	-2.18461400	-8.26445400
H	0.16172700	-2.45512200	-9.26554600
H	-0.31904800	-2.04102200	-7.59895300
O	1.37635400	-3.24675800	-7.77474200
C	1.19237200	-6.44402000	-6.02699200
C	2.09744300	-7.43285400	-5.39818000
C	3.27027100	-7.84753900	-5.99159600
S	3.88118600	-7.23043000	-7.56780900
S	4.30355400	-9.17472500	-5.35288600
C	5.11033400	-8.46971000	-7.79342200

H	5.67158300	-8.45113200	-8.72553000
C	5.30219000	-9.34888600	-6.79145600
H	6.04175100	-10.14711600	-6.79160700
S	-2.71786700	-8.36556000	-7.05597000
C	-3.37907500	-10.69009600	-5.93355300
H	-3.85923200	-11.65257200	-5.76836800
S	-2.29617800	-10.10403700	-4.67652300
C	-3.57113200	-9.90408800	-7.01009000
H	-4.22926100	-10.13465800	-7.84541300
C	0.46468900	-8.92276500	-1.69331600
C	1.57249900	-8.00223100	-4.13845300
C	2.38599300	-8.32323600	-3.03705700
H	3.45582400	-8.12951400	-3.08472500
C	1.85993600	-8.80830100	-1.83473800
H	2.53056700	-9.02464200	-1.00756900
C	-0.37159700	-8.59351100	-2.77642400
H	-1.44656800	-8.61798700	-2.61031600
O	-0.17595000	-9.28797300	-0.54085500
C	0.12823700	8.88885900	-1.41643300
C	0.38671500	8.15230700	-4.14118300
C	1.39998000	8.65394700	-1.97671900
H	2.25370400	8.67916300	-1.30391400
C	-1.01924800	8.73775300	-2.21472100
H	-2.01759000	8.87433200	-1.80921700
C	-0.87237700	8.33808200	-3.54679100
H	-1.77215900	8.12289100	-4.12104900
C	1.55691700	8.32425300	-3.33305800
C	2.88178200	8.12227900	-3.97300500
C	0.55465600	7.74606900	-5.54972800
C	1.70140800	6.84270900	-5.77505800
C	2.89783000	7.07210800	-5.01939500
C	1.64637700	5.77409800	-6.68003900
H	0.71132600	5.51048000	-7.17052900
C	4.00910300	6.25652600	-5.30149300
H	4.91527800	6.35406000	-4.70847500
C	3.97897200	5.24442500	-6.27102700

H	4.86992200	4.64395400	-6.44076200
C	2.77477900	4.97567400	-6.93914600
O	2.57643200	3.97257500	-7.85239200
C	2.71396600	1.57398700	-8.13281500
C	3.48344500	2.86440100	-7.90857500
C	-0.19969100	8.25822900	-6.58317000
C	3.97081600	8.92191400	-3.68444600
S	0.06311600	7.86588900	-8.31993200
S	-1.46749800	9.51767700	-6.37060100
S	3.94865200	10.27747500	-2.50066100
S	5.54703900	8.82999800	-4.54654200
C	-1.62793800	9.91429600	-8.07841200
H	-2.29809400	10.73075700	-8.34005500
C	-0.93534200	9.16750600	-8.95940300
H	-0.96141800	9.29040300	-10.04034800
C	6.21060900	10.32841500	-3.90866700
H	7.18536400	10.63949800	-4.27891900
C	5.48530900	10.98360900	-2.98243800
H	5.78519600	11.90631300	-2.48961200
H	4.21635400	3.03640300	-8.71748800
H	4.04145100	2.77283400	-6.96460500
O	0.11373800	9.19859200	-0.08250600
C	-1.17333500	9.38150800	0.54048200
H	-1.83402000	8.54415700	0.26894100
H	-1.63460500	10.31428600	0.16888800
C	-0.99980200	9.39027700	2.05656100
H	-0.43782000	10.28008400	2.37895400
H	-0.40021700	8.51040200	2.32757300
C	-2.37457200	9.30758600	2.75329900
H	-2.86909200	10.29343400	2.74796700
H	-3.02380500	8.63368000	2.16973500
C	-2.31168800	8.75193300	4.18658500
H	-1.78190100	9.45412000	4.85263700
H	-1.71857500	7.82428000	4.17431000
C	-3.71162900	8.43838300	4.74158200
H	-4.27811300	9.37504500	4.88484500

H	-4.26398700	7.85834400	3.98442400
C	-3.69972100	7.63456300	6.05164100
H	-3.20923500	8.21792000	6.85039900
H	-3.09151400	6.72674200	5.91073800
C	-5.11464500	7.23109100	6.49644800
H	-5.71171000	8.13950100	6.68952000
H	-5.61713300	6.69884700	5.67477400
C	-5.12757100	6.33456200	7.75393200
H	-4.59012600	6.86351200	8.56301900
H	-4.57025200	5.40647300	7.55097300
C	0.62609300	-9.42380400	0.64842500
H	1.26612400	-10.32102800	0.56698700
H	1.28302800	-8.54596700	0.74691000
C	-0.29871900	-9.49520900	1.85885900
H	-0.97728300	-8.63240800	1.81099600
H	-0.92300200	-10.40043200	1.81190500
C	0.51270700	-9.44759200	3.17301100
H	1.41329600	-8.82699800	3.02404000
H	0.87214600	-10.45610100	3.43791700
C	-0.27682100	-8.83474700	4.34048200
H	-0.56745200	-7.81721100	4.04999900
H	-1.21793100	-9.38714200	4.49615400
C	0.53466000	-8.78791900	5.65270000
H	1.59879900	-8.62446100	5.41034700
H	0.47715500	-9.77171700	6.14887500
C	0.09493800	-7.68076800	6.63400600
H	0.61770100	-7.82518000	7.59511100
H	0.42784100	-6.70700200	6.24593200
C	-1.41901900	-7.60425100	6.89040600
H	-1.80528100	-8.59739700	7.18035300
H	-1.93864600	-7.32256400	5.96157100
C	-1.75983800	-6.58127600	7.99696600
H	-1.32821300	-5.60092100	7.74088900
H	-1.26390200	-6.91319500	8.92853000
C	-3.24161100	-6.43962100	8.23433200
C	-6.52914700	6.00795800	8.20363800

H	-7.17125700	6.87185400	8.41207900
H	-3.79184000	-7.37528900	8.38827300
C	10.88447900	6.16174500	2.77318500
C	9.61452700	5.94465900	3.38586400
C	8.46164600	6.01631900	2.54386500
C	8.61211700	6.02991400	1.11481000
C	9.91509200	5.96861700	0.53010600
C	11.02928000	6.17273800	1.39728500
C	7.14796000	5.87389400	3.10950700
C	5.99003700	6.02201400	2.28172100
C	6.14039500	6.03988200	0.85678600
C	7.44547200	5.90378200	0.28529000
C	4.68602300	5.90103500	2.85118900
C	3.52670000	6.04050300	2.01954000
C	3.67626400	6.05985300	0.59896300
C	4.98433000	5.93711400	0.02556900
C	2.22028500	5.91093500	2.59163100
C	1.06676800	6.03498400	1.75864500
C	1.21628600	6.05355200	0.33566100
C	2.51848300	5.94752300	-0.23715000
C	4.54310100	5.39715100	4.18401400
C	3.24270000	5.04339500	4.67311100
C	2.07693000	5.41303300	3.92853300
C	5.70651100	5.02359700	4.92256100
C	5.58701500	4.09634600	6.00827200
C	4.30601300	3.56078800	6.34115400
C	3.12314600	4.12239200	5.75890900
C	7.00564200	5.37267200	4.43474600
C	8.17742800	5.01865700	5.18791800
C	8.05769900	4.08670200	6.27511800
C	6.76861000	3.53248700	6.58542400
C	9.46902800	5.43467000	4.73868800
C	10.58381800	5.11031700	5.56766000
C	10.46858100	4.21236400	6.61391800
C	9.22948200	3.57096300	6.91097800
C	6.68650800	2.29697100	7.28822800

C	7.89415200	1.62025800	7.67391400
C	9.14615800	2.30812000	7.62502200
C	5.42325000	1.63634300	7.41085000
C	4.22307600	2.32001000	7.05034900
C	2.95816700	1.65651600	7.17203500
C	1.75524900	2.34358900	6.80932400
C	1.83906400	3.58438100	6.09617300
C	0.66053700	4.14091900	5.51118200
C	0.78171200	5.05709700	4.41620900
C	0.49420000	1.68102400	6.92967700
C	-0.70865100	2.36572900	6.55897500
C	-0.62409500	3.60005000	5.84344100
C	-1.80493400	4.15490300	5.25191600
C	-1.68241400	5.05931900	4.14925100
C	-0.38294000	5.41129100	3.66304400
C	-0.23857600	5.89417200	2.32777300
C	0.06187600	5.93247300	-0.50025400
C	-1.24225700	6.04506500	0.07270000
C	-1.39368800	6.02575000	1.49426300
C	-2.69622100	5.91114900	2.06325700
C	-2.84187500	5.41860400	3.39829200
C	-3.85102100	6.06109400	1.23219800
C	-3.70042000	6.08540200	-0.18785500
C	-2.39621500	5.95621500	-0.76250100
C	-2.25657600	5.50361300	-2.11350800
C	-0.96407000	5.15072100	-2.60680700
C	0.20152100	5.48066100	-1.84513900
C	1.49714300	5.12917500	-2.33593500
C	2.65836200	5.46997300	-1.57960300
C	-4.86118200	5.98879500	-1.02264000
C	-4.72272900	5.52564200	-2.37043000
C	-3.42565800	5.17092300	-2.86895500
C	-3.31653500	4.27307200	-3.97527500
C	-2.03831500	3.72332500	-4.31590200
C	-0.85303100	4.25617200	-3.71949500
C	0.42386700	3.69483300	-4.04424800



C	1.60826100	4.22118900	-3.43548100
C	0.48794400	2.45870200	-4.75668600
C	-0.72364500	1.79734400	-5.13880100
C	-1.97316700	2.48298100	-5.03273300
C	-3.18534200	1.81470900	-5.40306500
C	-4.44093300	2.49602600	-5.28303300
C	-4.50694200	3.73235800	-4.56344900
C	-5.78193300	4.27721400	-4.22118200
C	-5.89093000	5.18269000	-3.11597300
C	-3.17125000	0.40634800	-5.64673400
C	-1.94538500	-0.32123000	-5.51171500
C	-0.71174400	0.38444600	-5.36965200
C	0.51093600	-0.34501200	-5.22408500
C	1.74848500	0.35630800	-5.09526500
C	1.73635400	1.76573800	-4.85789100
C	2.94246100	2.41863100	-4.46654000
C	2.87661100	3.64783600	-3.74188100
C	0.47181600	-1.74895300	-4.98278200
C	-0.79031900	-2.41277100	-4.87781100
C	-1.98505000	-1.73278900	-5.26238100
C	-3.24644800	-2.40134800	-5.15993500
C	-4.44807500	-1.71505200	-5.53293900
C	-4.41025800	-0.30379100	-5.77691500
C	-5.63480100	0.41980200	-5.90040400
C	-5.65027600	1.83068700	-5.64938300
C	-3.33175300	-3.64306500	-4.45676800
C	-2.15524400	-4.20372800	-3.86673600
C	-0.87640400	-3.65462500	-4.17752000
C	0.30138900	-4.22250900	-3.60265700
C	1.58519700	-3.68723500	-3.93447400
C	1.67065800	-2.44135400	-4.62840400
C	2.93101900	-1.78534200	-4.74876300
C	2.96759100	-0.37358700	-4.97280900
C	0.18050700	-5.14870300	-2.52685800
C	-1.11769800	-5.50646200	-2.04446300
C	-2.27741100	-5.14171000	-2.79172400

C	-3.57724300	-5.49410800	-2.30660900
C	-4.74163500	-5.11587700	-3.05166200
C	-4.61809800	-4.18682300	-4.13501400
C	-5.79429000	-3.62139100	-4.71423800
C	-5.70860800	-2.37636300	-5.41947300
C	-3.72258400	-5.98794800	-0.97349400
C	-2.56600100	-6.12303900	-0.14025500
C	-1.26303600	-5.99763300	-0.70959800
C	-0.10698000	-6.11862800	0.12338500
C	1.19824900	-6.00330600	-0.44851100
C	1.34318400	-5.51507400	-1.78266400
C	2.63873400	-5.17584400	-2.27334700
C	2.76206600	-4.25821100	-3.36376000
C	-0.25561800	-6.11632700	1.54125000
C	-1.56101200	-5.99282500	2.11461000
C	-2.71667000	-6.12000200	1.28505900
C	-4.02134400	-5.98800500	1.85964800
C	-5.18154700	-6.09916500	1.02516800
C	-5.03122000	-6.09707900	-0.39911100
C	-6.18547700	-5.95116200	-1.22672800
C	-6.03943500	-5.45652000	-2.56386600
C	-4.15848600	-5.50722000	3.19812200
C	-2.99027100	-5.16141100	3.95059700
C	-1.69824500	-5.51168700	3.45493700
C	-0.52865800	-5.16634100	4.20416200
C	0.76513500	-5.53446800	3.71553500
C	0.90159500	-6.01321600	2.37488000
C	2.20308900	-6.15180700	1.80357900
C	2.35244600	-6.14338800	0.37988700
C	-5.45434300	-5.14428000	3.68998700
C	-6.62077500	-5.48091800	2.93854500
C	-6.48323800	-5.96083000	1.59526200
C	1.93126100	-5.21122300	4.47250600
C	-0.63737200	-4.27501000	5.31205500
C	-1.91514700	-3.72676500	5.65283600
C	-3.09869200	-4.25631900	5.05469400

C	-4.37478900	-3.70361400	5.38965800
C	-5.56272000	-4.23755300	4.79255600
C	-4.44180900	-2.48118700	6.12364300
C	-3.23196700	-1.82347500	6.51782600
C	-1.98111800	-2.50313100	6.39393200
C	-0.76800100	-1.84323900	6.77808300
C	0.48543500	-2.52670000	6.65472300
C	0.55069600	-3.75419800	5.91868400
C	1.82359600	-4.30985000	5.58146600
C	-3.24709000	-0.41530000	6.78537000
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C	-0.78270900	-0.43825800	7.04073000
C	0.45690200	0.26897800	7.17270400
C	1.68183500	-0.45819400	7.29201400
C	1.69621600	-1.86804200	7.03265000
C	2.94941700	-2.54989400	6.90131600
C	3.01335600	-3.77854700	6.17516500
C	4.29065200	-4.33310800	5.83318300
C	-6.83646500	-3.68562000	5.12518300
C	-6.90392400	-2.45612600	5.85764200
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C	-4.47361200	0.31243800	6.65509400
C	-4.43589100	1.71924600	6.41228100
C	-3.17272200	2.38494400	6.30490300
C	-1.97358800	1.70242500	6.67844500
C	2.92132400	0.24922000	7.41439800
C	4.15041100	-0.47903400	7.53121000
C	4.16458600	-1.88720800	7.27385300
C	5.41475800	-2.56458500	7.14313100
C	5.47831900	-3.79845900	6.41788100
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C	-8.15625700	-1.77347700	5.97213100
C	-8.17205600	-0.37408300	6.23426600

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C	-3.08715400	3.61956600	5.58257000
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C	-5.55034100	3.63388800	5.30854400
C	-9.40690900	0.35308400	6.12594800
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C	-8.00864700	3.65359700	5.04558500
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C	-5.30365400	5.44470500	3.13676700
C	-4.14033100	5.07162400	3.88350100
C	5.38664700	0.22486200	7.65263800
C	-7.91488300	-5.11318300	3.42587900
C	4.39690700	-5.24050300	4.73045000
C	3.22464200	-5.57886300	3.97921900
C	3.36128600	-6.05207100	2.63813200
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C	-8.95471100	-5.95033200	1.33644700
C	-7.64209400	-6.06225300	0.76213200
C	-7.49255800	-6.05586200	-0.65405300
C	5.68769700	-5.59806400	4.23478600
C	5.82378100	-6.07541800	2.89040400
C	4.66672000	-6.18578500	2.06175600
C	4.81581300	-6.17935600	0.63718500
C	3.65797500	-6.03897900	-0.19528600
C	3.80209700	-5.55098300	-1.52989400
C	-8.65644900	-5.93507400	-1.48839200
C	-8.50990100	-5.43911100	-2.82912500
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C	6.26460600	-5.57215300	-1.27228400
C	5.10400800	-5.20750700	-2.02022600

C	5.22776700	-4.28637800	-3.11023600
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C	-6.90990700	-1.69008400	-5.78446200
C	-6.87286900	-0.28692900	-6.02540300
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C	6.59542200	-2.49644200	-4.12984900
C	5.39768700	-1.81411900	-4.50193600
C	5.43461700	-0.40032600	-4.72773700
C	4.20652500	0.32871400	-4.84282300
C	4.19233600	1.73021000	-4.57892100
C	-8.10474300	0.43827800	-6.17367400
C	-8.12090100	1.85214000	-5.91777500
C	-6.90444200	2.50774100	-5.52296100
C	-6.97060500	3.73543000	-4.80475700
C	6.66898900	0.30346800	-4.58614700
C	6.65402700	1.71182300	-4.32011200
C	5.40501700	2.39150400	-4.20033300
C	5.33717500	3.62073200	-3.47187000
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C	3.95246600	5.09802900	-2.05941000
C	-8.25323100	4.29852900	-4.48317700
C	-8.36241600	5.20766900	-3.37581900
C	-7.18606400	5.53160400	-2.61650600
C	-7.32289700	5.99786800	-1.27783200
C	-6.16299400	6.10826600	-0.44776900
C	-6.31317900	6.08818000	0.97719500
C	-5.15884100	5.94525500	1.80423900
C	6.52193000	4.16076300	-2.88977300
C	6.41363200	5.08439500	-1.79924100
C	5.12294700	5.45220700	-1.31378300
C	-8.63423600	6.14156100	-0.70683200
C	-8.78420200	6.12693800	0.72255700
C	-7.61928400	5.96492100	1.54825900

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C	-10.63208800	-1.78107300	5.79003700
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C	-10.48164700	3.73668700	4.85599800
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C	-10.49815200	-4.25008400	4.32891400
C	-9.66637100	-5.12715900	-3.60907300
C	-9.54058200	-4.19055500	-4.71300700
C	-9.95913300	-6.11882400	-0.92941400
C	-10.11159400	-6.12757400	0.51574000
C	-10.08741400	6.07840900	1.30820700
C	-10.23399000	5.57863500	2.66520800
C	-9.78822700	6.10452800	-1.54946700
C	-9.64921500	5.62583100	-2.91459200
C	-9.36323900	2.55692500	-5.86290400
C	-9.43121200	3.80820900	-5.12730100
C	-9.33073600	-0.26799000	-6.37685600
C	-9.36831700	-1.69983000	-6.13219000
C	6.61441800	-0.50098000	7.76553300
C	6.62849500	-1.90153300	7.51003500
C	7.58281900	5.42404100	-1.04848400
C	7.89473100	-0.42274300	-4.45505600
C	7.85748700	-1.82800300	-4.22546400
C	7.86359700	2.37119100	-3.93362900
C	7.79742000	3.60103800	-3.21775800
C	6.75431500	-4.34789600	6.07448500
C	6.85941600	-5.25196700	4.97940100
C	7.27628000	-6.19431700	0.89861400
C	7.12799500	-6.20088000	2.31515800
C	7.56460000	-5.21753800	-1.75356800
C	7.68746800	-4.29848300	-2.83464800
C	-11.62073300	4.39457800	4.30395200
C	-11.50144400	5.28179300	3.24882000

C	-11.80359300	1.79304100	5.79049500
C	-11.84089500	0.42913900	6.02076200
C	-11.19886400	6.31214200	0.44511600
C	-11.05480600	6.32425000	-0.93099500
C	-11.74413600	-3.71162400	4.76808100
C	-11.80878000	-2.52199800	5.47164200
C	-11.38299300	-6.07487700	1.16041100
C	-11.51601700	-5.61406200	2.45821300
C	-11.06802200	-6.05450900	-1.82451300
C	-10.92693100	-5.57680600	-3.11537600
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C	-10.66301500	4.45669200	-4.81553400
C	-10.52227600	1.87372700	-6.33718500
C	-10.50647700	0.51265400	-6.58522200
C	-10.58398300	-2.44456300	-6.08097500
C	-10.66699900	-3.64435500	-5.39697000
C	8.98116700	-3.76929100	-3.16953500
C	9.06724900	-2.51887300	-3.87264300
C	8.73618500	-5.60457800	-1.01647700
C	8.59049500	-6.10008200	0.32464400
C	9.14075800	0.28346600	-4.33227100
C	9.12530200	1.69678100	-4.06974500
C	8.15867400	-5.63318100	4.49735400
C	8.29452600	-6.11400900	3.14994300
C	7.88600400	-2.58919300	7.40522700
C	7.94952000	-3.82771900	6.67962400
C	7.85775700	0.20414500	7.91461000
C	8.99401000	4.15147600	-2.64309900
C	8.88512800	5.07298200	-1.54511100
C	9.07363800	-0.52281400	8.10468500
C	9.08799800	-1.95232300	7.84434500
C	10.05485900	5.47824300	-0.83071900
C	10.37073800	-0.44267900	-4.27698300
C	10.33301300	-1.87631000	-4.04174500
C	10.33937400	2.38257400	-3.75498200
C	10.27216600	3.63826500	-3.02597100

C	9.21491900	-4.42862900	6.39544500
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C	9.74435700	-6.30880400	1.14221200
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C	10.03583400	-5.31570900	-1.53667800
C	10.16123800	-4.37538700	-2.63735900
C	11.41557000	-3.84590700	-3.06341700
C	11.49834900	-2.64180500	-3.73982700
C	11.15671100	-5.79057700	-0.79285100
C	11.01635900	-6.26943400	0.49755400
C	11.57605000	0.31895100	-4.22669100
C	11.56100900	1.67956200	-3.97568800
C	10.57289100	-5.82146800	4.77926400
C	10.70349800	-6.28527000	3.48234300
C	10.29164500	-2.71528000	7.77885200
C	10.35269700	-3.90841700	7.08105500
C	10.26194200	0.23766500	8.31622400
C	10.29679300	1.60144500	8.08538500
C	11.42250800	4.27308000	-2.47002500
C	11.31780400	5.15926200	-1.41261900
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H	-12.06780500	-6.29618000	-1.46755600
H	-11.64003500	-4.12487000	-5.30914500
H	-12.28541600	-6.31291900	0.59975500
H	-11.46886700	2.40519600	-6.42050200
H	-11.44125600	0.02372400	-6.85453400
H	-11.56743500	4.19393100	-5.36177100
H	-11.49479500	-2.02571400	-6.50568800
H	-12.20140900	6.39281900	0.86192600
H	-11.94948100	6.41384500	-1.54492500
H	-12.41043600	5.68454400	2.80507600
H	-11.75120800	5.72627600	-3.49708000
H	-12.51807500	-5.50670700	2.87017800
H	-12.67626600	-4.18850200	4.46966400
H	-12.81165600	-0.06013700	6.08104700
H	-12.74644200	2.32579900	5.67815200



H	-12.78911200	-2.10705900	5.70009800
H	-12.61904900	4.13210400	4.65019200
H	11.25160700	2.11748200	8.17139000
H	11.19056900	-0.26839600	8.57497600
H	11.36940200	3.92918000	7.15585700
H	11.21080400	-2.31547500	8.20391000
H	12.03308400	6.24673300	0.98213400
H	11.77968100	6.22796200	3.38928500
H	12.23331100	5.54213200	-0.96461600
H	11.57111700	5.50006800	5.32537200
H	12.53888300	-0.18478900	-4.29438900
H	12.51256500	2.19485500	-3.85568500
H	12.48501100	-2.23648800	-3.95803300
H	12.41648700	3.99256700	-2.81456500
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H	11.91472500	-6.53147000	1.05399700
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H	11.69793900	-6.54261100	3.12145700
H	12.34025300	-4.34278900	-2.77452500
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H	-6.43025700	3.88923400	8.12372200
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**UP-9-(5,5)**

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C	5.54425800	1.78814900	-5.39862800
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H	8.51732700	0.25235500	-4.74066300
C	4.73652000	0.65058000	-5.51402500
H	5.11446400	2.78249800	-5.50356900
H	7.07616400	-1.76098300	-4.95072800
H	3.66556400	0.76718000	-5.69129900

C	2.73233700	-6.73461600	-0.42125500
C	1.03928800	-7.50075000	-2.11354200
C	2.11395300	-6.71298300	-1.76864200
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C	2.15634700	-5.01194700	-3.65819800
C	4.91938200	-4.76679500	-3.38827400
C	2.84368700	-4.09791200	-4.46530200
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H	2.29001100	-3.46579600	-5.15585600
C	5.27823600	-0.63813200	-5.36104800
C	4.23097800	-3.94886300	-4.29930400
C	4.34375200	-1.82999900	-5.44854200
H	4.03594300	-2.01894300	-6.49386900
H	3.43390400	-1.61083600	-4.86718500
O	4.99465600	-2.99952000	-4.92802400
C	4.24076600	-5.71432100	-2.60847000
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S	7.04118000	-7.05541800	-3.37570000
S	6.91548200	-8.30389400	-0.67435300
C	8.17694800	-8.35231800	-3.02227000
H	8.88352400	-8.62312300	-3.80430300
C	8.12087600	-8.91677800	-1.80062300
H	8.77516100	-9.71142000	-1.44767400
S	0.35533200	-7.59261900	-3.77455800
C	-0.71675800	-9.48153900	-2.22892600
H	-1.32007500	-10.32934800	-1.91056400
S	0.23975400	-8.66520500	-0.99749300
C	-0.66446300	-8.99732800	-3.48450500
H	-1.21910800	-9.39475800	-4.33212400
C	2.57388800	-6.71420600	2.02234000
C	4.15608400	-6.68989300	-0.33735900
C	4.74635900	-6.70094700	0.94442800
H	5.82497200	-6.59350300	1.04125400
C	3.97942900	-6.73359700	2.10749900

H	4.44777100	-6.68236500	3.08919100
C	1.96074100	-6.73483000	0.75704900
H	0.87966400	-6.67561900	0.67348200
O	1.91052800	-6.60890300	3.21369500
C	1.46136700	6.31970300	0.92025100
C	2.90645000	6.58199600	-1.50633000
C	2.87067800	6.30445900	0.92110900
H	3.36918400	6.10322400	1.86693800
C	0.77204500	6.45186300	-0.29838400
H	-0.31300200	6.43625800	-0.34455000
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H	0.95461100	6.54059200	-2.43042100
C	3.60876800	6.47335500	-0.26283200
C	5.09152100	6.53081000	-0.29851200
C	3.69245100	6.71860100	-2.74953300
C	4.96275100	5.96294300	-2.73480900
C	5.69425500	5.91342300	-1.50462000
C	5.46308400	5.29794200	-3.86666400
H	4.87846800	5.24823200	-4.78354600
C	6.94083000	5.25972100	-1.51257600
H	7.50683600	5.16201600	-0.58990100
C	7.46827700	4.66054000	-2.66233800
H	8.43875700	4.17296000	-2.60655600
C	6.71215800	4.65615700	-3.84261000
O	7.14374200	4.11393600	-5.03679800
C	6.91542400	1.65659900	-5.12313600
C	7.84111800	2.85974000	-5.01717400
C	3.35231400	7.57936500	-3.77018500
C	5.82821600	7.20787200	0.65312000
S	4.36232700	7.86223400	-5.23313300
S	1.92173200	8.67091700	-3.72823100
S	5.11327700	8.07066200	2.06123300
S	7.60694200	7.46113900	0.56073500
C	2.40695400	9.67078000	-5.09373000
H	1.77742400	10.52498100	-5.33500200
C	3.51027100	9.30489900	-5.77369100

H	3.90630700	9.81953700	-6.64691700
C	7.70191400	8.66427200	1.83992500
H	8.67500200	9.11139000	2.03292000
C	6.57193900	8.94003400	2.51859800
H	6.49333900	9.64452500	3.34424900
H	8.51016200	2.89400400	-5.89132100
H	8.47744600	2.75779900	-4.12359800
O	0.86182600	6.14036100	2.13916400
C	-0.57713800	6.16801400	2.17515600
H	-0.98263700	5.50070100	1.39897400
H	-0.93046100	7.19280500	1.96031700
C	-1.06996800	5.67533700	3.53128700
H	-0.67313400	6.30796900	4.33971900
H	-0.68026300	4.65915000	3.68957800
C	-2.61395600	5.65493100	3.54014600
H	-3.00272300	6.67149700	3.71910900
H	-2.97164500	5.36056900	2.53919100
C	-3.22774800	4.67067100	4.54937600
H	-2.95537100	4.95318400	5.58064900
H	-2.79499500	3.67327600	4.37230900
C	-4.75626500	4.58669400	4.40427600
H	-5.21568500	5.53923900	4.72165300
H	-4.99983900	4.46918600	3.33449100
C	-5.39846200	3.41817400	5.16683300
H	-5.18356100	3.49525300	6.24635300
H	-4.93596600	2.47873200	4.82478500
C	-6.91980100	3.34748400	4.94582200
H	-7.41122900	4.15124900	5.52167800
H	-7.14408200	3.54648400	3.88449700
C	0.49356200	-6.33460500	3.20754400
H	0.23784500	-5.67672700	2.36513600
H	-0.06524200	-7.28020200	3.09024800
C	0.13952400	-5.61130900	4.50469700
H	0.39981900	-6.23504200	5.37375200
H	0.76157600	-4.70563400	4.55600800
C	-1.35111800	-5.21552200	4.54109500

H	-1.97016500	-6.08938400	4.80547000
H	-1.67299300	-4.90195800	3.53440500
C	-1.63021000	-4.05828000	5.51404300
H	-1.29807100	-4.33402400	6.53000300
H	-1.01661000	-3.19387100	5.21239200
C	-3.10938500	-3.64111000	5.55105600
H	-3.71032700	-4.45905600	5.98605800
H	-3.47548900	-3.50030300	4.52216300
C	-3.34427600	-2.35061200	6.35217800
H	-2.89287000	-2.45799400	7.35465700
H	-2.81522100	-1.51792400	5.85998600
C	-4.83199000	-1.99875500	6.51764000
H	-5.34460200	-2.85457000	6.99222500
H	-5.29905200	-1.86530700	5.52724600
C	-5.05651600	-0.74203700	7.37881000
H	-4.77477100	0.16162000	6.81336500
H	-4.38362300	-0.78529500	8.25363200
C	-7.52659200	1.99242000	5.33437300
H	-7.15556000	1.21613700	4.64717400
H	-7.18420000	1.71573000	6.34238900
C	-9.06894200	2.01926100	5.31030700
H	-9.42540400	2.37743700	4.33064200
H	-9.39911800	2.76669600	6.05685400
C	-6.50781300	-0.61036900	7.89107500
H	-6.77706000	-1.56831000	8.37512000
H	-7.20271300	-0.47778600	7.04738900
C	-12.44337200	-2.63927700	0.04707700
C	-12.21612100	-3.28754500	-1.15243800
C	-10.88690100	-3.39959400	-1.67792700
C	-9.81306500	-3.25724600	-0.74842900
C	-10.05042600	-2.58382000	0.50351600
C	-11.35293300	-2.07172500	0.78421000
C	-8.45296200	-3.39609400	-1.19748200
C	-8.17204200	-3.19130600	-2.58038200
C	-9.26225900	-2.85780700	-3.45818900
C	-10.59984200	-3.19269400	-3.08932600

C	-9.04071100	-1.85289000	-4.46754400
C	-10.16386700	-1.21491000	-5.07498200
C	-11.41792700	-1.90512600	-4.99947600
C	-11.63031900	-2.86914200	-4.03193200
C	-8.91452300	-2.09028300	1.23552800
C	-7.61436700	-2.64526200	0.99849500
C	-7.37648600	-3.31412400	-0.25440900
C	-6.03101100	-3.45884600	-0.70852600
C	-5.74757400	-3.25262000	-2.10419700
C	-6.82367000	-2.91077900	-2.97737500
C	-6.60222800	-1.90818800	-3.98672200
C	-7.74150800	-1.23956700	-4.54276400
C	-6.49617900	-2.15556300	1.73781500
C	-5.18910900	-2.69079300	1.47966900
C	-4.95176000	-3.35445900	0.23261200
C	-3.60025600	-3.50552200	-0.22303200
C	-3.31616300	-3.30197000	-1.62018300
C	-4.39852000	-2.95305400	-2.49392400
C	-4.17794600	-1.95653000	-3.49835400
C	-5.31550800	-1.29654800	-4.07430700
C	-4.06569400	-2.20005100	2.22319700
C	-1.17517800	-3.54166300	0.25858800
C	-0.89228900	-3.34460800	-1.13185200
C	-1.97398300	-3.00814300	-2.01200900
C	-1.75165500	-2.00601500	-3.02171500
C	-2.88325600	-1.34570200	-3.59159000
C	-1.64090700	-2.22978600	2.69954800
C	-0.33772800	-2.76730200	2.45024600
C	-0.09948300	-3.43485400	1.19984400
C	1.24584700	-3.57797200	0.74894300
C	1.52862100	-3.38788600	-0.64506100
C	0.45529400	-3.05343900	-1.52344600
C	0.67821400	-2.05258000	-2.53293200
C	-0.45815600	-1.38893200	-3.10320300
C	0.77812300	-2.28451400	3.19747800
C	2.08333700	-2.81876400	2.93906600

C	2.32006500	-3.47313600	1.69091600
C	3.66941800	-3.62523500	1.23835500
C	3.95222300	-3.44039400	-0.15432300
C	2.87424300	-3.09432500	-1.03207800
C	3.09658100	-2.09995400	-2.03190800
C	1.96422400	-1.43924400	-2.61159900
C	3.20779000	-2.33698500	3.68921200
C	4.50506100	-2.87149500	3.42773600
C	4.73994200	-3.53313400	2.17412200
C	6.08885800	-3.68030100	1.71757600
C	6.36974800	-3.49233600	0.33225200
C	5.29210400	-3.15810200	-0.54758700
C	5.51654400	-2.15946700	-1.55658000
C	4.39078400	-1.49221800	-2.12026900
C	5.63537500	-2.37143700	4.15380600
C	6.94345300	-2.91624500	3.90608600
C	7.17603800	-3.59439000	2.65484700
C	8.51690000	-3.79610600	2.20837000
C	8.80357600	-3.59993200	0.79445400
C	7.72639100	-3.21736800	-0.05988200
C	7.95198100	-2.21393100	-1.07044700
C	6.80685500	-1.54606500	-1.62992100
C	8.05913100	-2.45732500	4.66917100
C	9.32336900	-3.07790300	4.40239100
C	9.54575800	-3.73106600	3.20431800
C	9.24693200	-1.62631200	-1.19409100
C	10.34584300	-2.36539900	-0.64606200
C	10.12969100	-3.32831900	0.32234300
C	6.88243700	-0.14249900	-1.85344700
C	8.09998600	0.53840800	-1.50923800
C	9.32418400	-0.18962700	-1.42246900
C	4.46989900	-0.08015400	-2.35658500
C	5.67054700	0.60189200	-2.00958800
C	5.57106800	1.88842600	-1.38007300
C	6.68620900	2.34931000	-0.61428400
C	7.99799100	1.82407800	-0.87032600

C	9.12431000	2.35635800	-0.17549100
C	10.40525600	1.80909300	-0.51317800
C	10.50222800	0.56819300	-1.11836900
C	6.45016700	3.02092800	0.61510700
C	7.53727700	3.14499900	1.54653900
C	8.88378400	3.04783000	1.08387800
C	4.27914800	2.44187300	-1.14035900
C	4.03714400	3.10115900	0.11304000
C	5.10145500	3.20122900	1.05621200
C	4.81605100	3.00946100	2.45399500
C	5.89816500	2.65857500	3.32722800
C	7.25325600	2.95621200	2.94577500
C	8.32675600	2.66012300	3.83787300
C	9.64428200	3.02630700	3.40635500
C	9.91561300	3.21697700	2.06422500
C	5.68043400	1.66560800	4.32686600
C	6.82630600	1.01070600	4.90119700
C	8.10465800	1.64439300	4.85591500
C	3.47555000	2.71410300	2.84196800
C	3.25439000	1.71765600	3.85669000
C	4.38553000	1.05859700	4.42661300
C	4.31136300	-0.35971100	4.66275100
C	5.53725900	-1.09445600	4.77995200
C	6.75310200	-0.41048300	5.13128500
C	7.96016800	-1.15262400	5.30601800
C	9.12258400	-0.41188800	5.69960200
C	9.19264300	0.95121900	5.48118300
C	3.10822700	-1.04914900	4.32297000
C	2.68304000	3.23667500	0.56410800
C	2.39744100	3.03609600	1.95154900
C	3.15569200	1.95083600	-1.88681500
C	3.25230200	0.66368600	-2.50279100
C	1.96146800	1.09990900	3.94150400
C	1.88594000	-0.30956400	4.18176700
C	1.61234400	3.14722900	-0.38247100
C	1.85207400	2.49563200	-1.64045300



C	2.04475300	-0.02391500	-2.85923800
C	1.05120100	2.74528600	2.34257600
C	0.82499700	1.76003800	3.36640700
C	0.67572800	-1.00156900	3.84037200
C	0.26613000	3.28661900	0.06915000
C	-0.01972700	3.06966700	1.45845000
C	0.73202900	2.00733700	-2.38258600
C	0.82989700	0.71437200	-3.00712200
C	-0.46285400	1.14939600	3.45724500
C	-0.54030400	-0.26623600	3.70189600
C	-0.81003400	3.19833700	-0.87336300
C	-0.57365500	2.54338800	-2.12453600
C	-0.38130200	0.02177900	-3.34463200
C	-1.36736500	2.77839100	1.84649300
C	-1.59433500	1.79958600	2.86431800
C	-1.74495300	-0.95597000	3.34045200
C	-2.16157700	3.35228200	-0.41913800
C	-2.44630500	3.13475200	0.97462000
C	-1.70114900	2.05447000	-2.86560000
C	-1.60269400	0.76148600	-3.49077600
C	-2.88995300	1.19236000	2.95572300
C	-2.96892600	-0.22138800	3.20551400
C	-3.23549800	3.26341300	-1.35744500
C	-2.99939900	2.59521700	-2.61077100
C	-2.80715200	0.07224900	-3.83145300
C	-3.78950200	2.84818600	1.36596200
C	-4.01487300	1.84827000	2.37352200
C	-4.16889800	-0.91215700	2.85873700
C	-4.58738400	3.40482400	-0.89869100
C	-4.86917300	3.19521700	0.48967700
C	-4.12834200	2.09662500	-3.34188600
C	-4.03010400	0.81063100	-3.96405900
C	-5.30725200	1.23490400	2.45590700
C	-5.38722000	-0.17180200	2.70653800
C	-5.66793400	3.31375500	-1.83964000
C	-5.43269300	2.64249000	-3.09049100

C	-5.24004600	0.12049600	-4.31215100
C	-6.21878100	2.90726300	0.88452200
C	-6.44160600	1.90063200	1.88730300
C	-6.59705800	-0.86376900	2.36501300
C	-7.01281100	3.46003300	-1.38282000
C	-7.29501400	3.25392700	0.01408400
C	-6.55454100	2.14911700	-3.82229100
C	-6.45546900	0.85662900	-4.44898500
C	-7.72806600	1.29105800	1.97464900
C	-7.80792400	-0.12471200	2.21696900
C	-8.09295700	3.34485300	-2.31771400
C	-7.86001700	2.67842700	-3.55673200
C	-7.66714100	0.16500000	-4.77693300
C	-8.64055300	2.94649900	0.39973000
C	-8.85963300	1.94988200	1.39581400
C	-9.01130900	-0.80949900	1.85214000
C	-9.45125600	3.49837900	-1.86778800
C	-9.73328600	3.29468000	-0.46887800
C	-8.99491600	2.19290200	-4.29583500
C	-8.89536300	0.89963600	-4.92456000
C	-10.16148000	1.34502000	1.48344300
C	-10.23789600	-0.07484700	1.71212700
C	-10.52228700	3.44313500	-2.80973400
C	-10.28452800	2.76346400	-4.07429200
C	-10.08849500	0.21869800	-5.31189800
C	-11.07685500	3.04363500	-0.05640900
C	-11.29990600	2.03022300	0.96394200
C	-11.45032400	-0.76567400	1.41680500
C	-11.84527400	3.64740100	-2.29689700
C	-12.11565400	3.45295900	-0.95518800
C	-11.36009200	2.26081100	-4.87761300
C	-11.26450400	1.02076900	-5.48084800
C	-12.57079100	1.38880800	1.13418400
C	-12.64369000	0.02532300	1.35393300
C	-2.52758000	-3.40276200	0.71467500
C	-2.76527700	-2.73004100	1.96378500

H	10.47381000	2.99513300	4.11213500
H	10.95159400	3.33258000	1.74691900
H	10.01924200	-0.94084500	6.02113000
H	10.14289400	1.46145000	5.63568900
H	10.55807600	-4.05084300	2.95906800
H	10.16604100	-2.90028300	5.06987000
H	11.31297800	2.28801600	-0.14712400
H	11.48373900	0.10373000	-1.20997300
H	11.36844200	-2.05975300	-0.86594700
H	10.98766900	-3.75712500	0.83916300
H	-12.67658100	3.79562700	-2.98541100
H	-13.15278500	3.45207000	-0.62123700
H	-13.48811100	1.93962000	0.92854100
H	-13.61689800	-0.46321400	1.31718300
H	-13.46919100	-2.42069000	0.34232600
H	-13.06891800	-3.56375900	-1.77177000
H	-12.63735200	-3.26005900	-3.88981100
H	-12.26304000	-1.56100400	-5.59488600
H	-12.15130400	0.59135800	-5.94598200
H	-12.31971300	2.77678400	-4.88319800
C	-6.67575900	0.50489900	8.89399800
H	-5.89607100	0.56079800	9.66296500
C	-7.67804600	1.39623200	8.92398800
H	-8.47946800	1.37966200	8.18325100
H	-7.73285900	2.16606200	9.69584200
C	-9.70213400	0.68597900	5.62232100
H	-9.26542500	0.13099800	6.45980000
C	-10.74247800	0.15507200	4.96378900
H	-11.20733100	0.67572400	4.12484500
H	-11.16147500	-0.81491800	5.23797200

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C	1.47494000	1.05194600	-7.21926300
C	-0.49956700	2.45222500	-7.25304600
C	0.67401500	-0.08385200	-7.02244400
H	2.56033100	0.94221200	-7.27636200

C	-1.29767800	1.32374200	-7.04339500
H	-0.94976400	3.44117600	-7.33456600
H	1.12944000	-1.06614300	-6.91468800
H	-2.37981100	1.43570900	-6.95040900
C	-2.42477400	-6.85951400	-2.44914300
C	-4.41578600	-7.30862800	-3.91620100
C	-3.27618500	-6.58709800	-3.63449200
C	-2.73039700	-5.54069500	-4.53054200
C	-3.52372200	-4.59287800	-5.20372800
C	-0.75348600	-4.34243100	-5.33344400
C	-2.96595400	-3.53957500	-5.93995000
H	-4.60516900	-4.61425200	-5.08636400
H	0.31960800	-4.16457100	-5.31908800
H	-3.61882500	-2.80604000	-6.40645400
C	-0.72286000	0.04108000	-6.95992100
C	-1.56885000	-3.38905300	-5.96326900
C	-1.65146000	-1.14874200	-6.83182500
H	-2.19626500	-1.31371800	-7.78090600
H	-2.40324500	-0.94980200	-6.05227100
O	-0.89981900	-2.32267900	-6.50421800
C	-1.30848700	-5.42827200	-4.64401700
C	-0.47094400	-6.42481300	-3.94267600
C	0.65284300	-6.98202900	-4.51213400
S	1.26105700	-6.56665900	-6.15384400
S	1.60599000	-8.31117300	-3.76492900
C	2.40403400	-7.89938100	-6.27466800
H	2.94547200	-8.00826300	-7.21227800
C	2.56049100	-8.68843000	-5.19447900
H	3.24732600	-9.52977900	-5.12776500
S	-5.37878900	-7.11349500	-5.42340000
C	-6.20644400	-9.25662300	-4.07270100
H	-6.76116100	-10.15497700	-3.80922900
S	-5.04065600	-8.65619100	-2.89909900
C	-6.35961000	-8.55925100	-5.21456700
H	-7.05658000	-8.80876000	-6.01210800
C	-2.11218900	-7.39653300	-0.08039400

C	-1.00723500	-6.81409300	-2.62329000
C	-0.18446100	-7.07907600	-1.50908400
H	0.89428000	-6.96663900	-1.59864800
C	-0.71694500	-7.39168100	-0.26163400
H	-0.07356200	-7.55467500	0.60152400
C	-2.95828400	-7.12870000	-1.17151300
H	-4.03166600	-7.06257900	-1.01520700
O	-2.52952900	-7.62773900	1.19882500
C	-1.12989400	7.37424700	0.19406800
C	-0.28915300	7.82135400	-2.47017300
C	0.16032700	6.98661900	-0.21881900
H	0.77978900	6.46384500	0.50408500
C	-2.01090900	7.96631300	-0.72994300
H	-3.02231000	8.24760100	-0.44860300
C	-1.58004100	8.17341900	-2.04520200
H	-2.28466100	8.58514500	-2.76728600
C	0.59856400	7.19296400	-1.53718100
C	1.90895000	6.72339700	-2.05713400
C	0.16631000	8.00343200	-3.86651800
C	0.93439800	6.84463700	-4.36749600
C	1.82854700	6.21256000	-3.45013400
C	0.76421400	6.30991600	-5.65286400
H	0.04497000	6.74277200	-6.34600000
C	2.50284500	5.05868500	-3.88090100
H	3.15384900	4.53611200	-3.18951400
C	2.33349000	4.51934100	-5.16109200
H	2.84061700	3.59136100	-5.41368900
C	1.46928300	5.16338400	-6.06224200
O	1.23898300	4.77367000	-7.36090800
C	0.89718500	2.32244600	-7.37139400
C	1.74799300	3.50591300	-7.79994100
C	-0.02881700	9.15677100	-4.58470300
C	3.09323000	6.78954900	-1.35712900
S	0.60450600	9.42933700	-6.24674300
S	-0.83390400	10.62309500	-3.92060200
S	3.24969700	7.34107400	0.34411900

S	4.69508600	6.42237700	-2.08879800
C	-0.35947400	11.70113300	-5.23052000
H	-0.63071700	12.75078600	-5.13643600
C	0.28991700	11.16217500	-6.28033700
H	0.62065900	11.71223800	-7.15911100
C	5.65306700	6.78446800	-0.66432600
H	6.72728400	6.62645900	-0.73132300
C	4.99960200	7.20107500	0.43778700
H	5.46896800	7.44223900	1.38917600
H	1.73111300	3.58772900	-8.89753100
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H	-3.46952200	6.74885300	1.14505700
H	-3.08965100	8.35363500	1.83014900
C	-3.06364000	6.70839800	3.26321900
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C	-4.57243200	6.66480000	3.56233900
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H	-5.08343600	6.18315300	2.71161700
C	-4.93754900	5.87977200	4.83112100
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C	-8.40454200	4.42305800	6.01896400
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H	-8.81716600	4.39320300	4.99678100
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C	2.60202600	0.62921700	-3.24885900
C	2.39062300	-2.16784500	-2.93881700
C	2.23219200	-3.31017000	-2.08154600
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H	13.30183400	3.09146900	0.17264900
H	13.07819300	3.38203800	2.57615500
H	12.83109500	2.53302400	4.52707600
H	12.56740200	0.58441600	5.95696400
H	12.41245600	-1.53834300	6.18769600
H	12.36958400	-3.76763200	5.21837100
C	-7.29793500	0.60584400	8.53342700
H	-6.60870100	1.25294700	7.98054800
C	-7.62789100	0.92741600	9.79337700
H	-8.31014200	0.30110700	10.37453100
H	-7.23266900	1.81963400	10.28247700
C	-10.67972400	1.59673100	7.44565800

H	-10.19577500	1.33951200	8.39294300
C	-11.48819900	0.70457100	6.85503700
H	-11.97432200	0.93008300	5.90253600
H	-11.69470900	-0.27154200	7.29722300

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C	3.14856600	0.08472900	-7.22360200
C	0.97271500	1.13193500	-7.38102200
C	2.55418400	-1.18241400	-7.26434400
H	4.23069000	0.16377900	-7.10364000
C	0.37860200	-0.13472200	-7.41959400
H	0.35433400	2.02736100	-7.38048200
H	3.16645000	-2.07743900	-7.17518700
H	-0.70966700	-0.21410000	-7.45361000
C	0.79746300	-7.77031900	-1.96742400
C	-1.26469000	-8.56496100	-3.15672300
C	-0.19526200	-7.70180800	-3.06586800
C	0.13603900	-6.69588000	-4.09927300
C	-0.82829500	-5.91615300	-4.75985300
C	1.85928000	-5.40820700	-5.26429500
C	-0.48481000	-4.92221800	-5.68485200
H	-1.88017600	-6.03220700	-4.50599100
H	2.89879700	-5.11917300	-5.40455200
H	-1.27486500	-4.35088400	-6.16549200
C	1.15660800	-1.30238200	-7.32574300
C	0.87235300	-4.64118200	-5.91185800
C	0.44431600	-2.63710600	-7.20939500
H	0.04464900	-2.97746300	-8.18263100
H	-0.40566000	-2.50417300	-6.52284100
O	1.35077100	-3.62815200	-6.70314000
C	1.51627700	-6.45162700	-4.39170300
C	2.52677900	-7.29063500	-3.70627600
C	3.63637600	-7.78984300	-4.35306000
S	4.03264500	-7.46497700	-6.07821000
S	4.78824700	-8.95824800	-3.61537600
C	5.28292400	-8.69535900	-6.22107900

H	5.73364400	-8.83632600	-7.20145800
C	5.62562600	-9.37026900	-5.10719900
H	6.39480000	-10.13797100	-5.05153500
S	-2.39415100	-8.62328100	-4.55623400
C	-2.81673700	-10.70271900	-2.94302100
H	-3.23094700	-11.62604000	-2.54293100
S	-1.61820000	-9.86573200	-1.96270600
C	-3.16755000	-10.14169600	-4.11590500
H	-3.90768000	-10.54282800	-4.80538500
C	1.39328900	-8.01845400	0.39452400
C	2.17552800	-7.61673000	-2.30627700
C	3.12806200	-7.71660500	-1.27059900
H	4.17862600	-7.53200700	-1.48559200
C	2.75727100	-7.93829700	0.05356300
H	3.50124100	-7.96638900	0.84788000
C	0.42181500	-7.94112900	-0.61964000
H	-0.63373500	-7.95321500	-0.36143300
O	1.12868200	-8.12582700	1.72999300
C	1.41125800	7.95451600	0.46882200
C	0.87799500	7.56213300	-2.29567300
C	2.46815300	7.86135800	-0.45790900
H	3.48389500	7.84295900	-0.06757600
C	0.08403800	7.90266500	0.00798300
H	-0.75474300	7.96501100	0.69728200
C	-0.15916800	7.67735700	-1.35288800
H	-1.18901800	7.51166700	-1.66217900
C	2.22481700	7.70475500	-1.82949300
C	3.31504100	7.62367200	-2.82813000
C	0.65873500	7.23094700	-3.72236700
C	1.72704500	6.38693600	-4.31009800
C	3.07421000	6.61896800	-3.88486900
C	1.46568000	5.34843100	-5.21736700
H	0.44400300	5.06808200	-5.46370400
C	4.09357900	5.82913700	-4.44379200
H	5.11529200	5.93829900	-4.08508300
C	3.83652700	4.83974300	-5.39964600



H	4.66626100	4.26092800	-5.79693100
C	2.50577900	4.57394300	-5.76452300
O	2.10068100	3.56506600	-6.60097800
C	2.36583700	1.25150400	-7.24435200
C	3.05645000	2.58489300	-7.03358700
C	-0.38686000	7.72885400	-4.47043400
C	4.39540100	8.47782200	-2.81753700
S	-0.62380300	7.40101400	-6.22375600
S	-1.60294700	8.89684000	-3.84424300
S	4.65139600	9.76480100	-1.58679700
S	5.64450800	8.53475400	-4.11111000
C	-2.30189600	9.30468200	-5.40652100
H	-3.07485000	10.07041300	-5.42248900
C	-1.85781300	8.62819300	-6.48300700
H	-2.21783700	8.76558800	-7.50067100
C	6.38002600	10.04959700	-3.59833300
H	7.17810000	10.45207300	-4.21895100
C	5.92960800	10.60540700	-2.45725200
H	6.30976400	11.52555600	-2.01790800
H	3.55038700	2.94683900	-7.95440800
H	3.83337000	2.43887000	-6.26787000
O	1.78755900	8.04676700	1.77980100
C	0.79453000	7.82566600	2.80437000
H	0.07887300	7.05941100	2.46995100
H	0.23803400	8.76139000	2.98994100
C	1.51741000	7.32205100	4.05200300
H	2.16716900	8.11011000	4.46357500
H	2.17137300	6.49552400	3.73697700
C	0.53496300	6.79688400	5.11574700
H	-0.04456400	7.62561800	5.55616600
H	-0.19392000	6.13751900	4.61699700
C	1.24514900	5.98341400	6.21642600
H	1.78106900	6.65569000	6.90743000
H	2.01441800	5.35901700	5.73432200
C	0.29803300	5.04711700	6.99131000
H	-0.36428700	5.62508400	7.65814800

H	-0.35757800	4.54567000	6.26158300
C	1.05073700	3.95910300	7.78022400
H	1.56904700	4.39858700	8.64950900
H	1.83928400	3.55246700	7.12656700
C	0.15287300	2.79047800	8.22947100
H	-0.48214700	3.09370000	9.07976700
H	-0.53492100	2.53220700	7.40845000
C	-0.21704000	-7.92767500	2.21384100
H	-0.72418700	-7.15573500	1.61634400
H	-0.78750700	-8.86876500	2.12171400
C	-0.09579500	-7.45373500	3.66068500
H	0.38974500	-8.23360900	4.26813000
H	0.57938400	-6.58488600	3.65805700
C	-1.43810200	-7.03473900	4.28779500
H	-2.08435700	-7.91343800	4.45265300
H	-1.97510900	-6.37559600	3.58667500
C	-1.21300700	-6.26787200	5.60443800
H	-0.76351400	-6.93689900	6.35775700
H	-0.46295300	-5.48556300	5.40475200
C	-2.47291800	-5.58776100	6.17499700
H	-3.12052600	-6.32462400	6.67979600
H	-3.06216800	-5.17495800	5.34079300
C	-2.11580700	-4.43189600	7.12723700
H	-1.60654100	-4.81728700	8.02686100
H	-1.37912000	-3.79523000	6.61231500
C	-3.31218200	-3.55107400	7.53288600
H	-3.93275600	-4.06531500	8.28683900
H	-3.95713000	-3.39410800	6.65374700
C	-2.86127200	-2.18124700	8.06610800
H	-2.20712500	-1.70758100	7.31887000
H	-2.24204300	-2.31439200	8.96857400
C	0.96402800	1.53612800	8.59368400
H	1.62535200	1.28619200	7.74968200
H	1.62321400	1.74644100	9.45385300
C	0.07264400	0.31359200	8.90495200
H	-0.62962200	0.15189400	8.07416400

H	-0.54224700	0.54565800	9.79330500
C	0.87929200	-0.93606400	9.14625100
H	1.59268300	-0.89481800	9.97773600
C	-3.53539100	0.09327100	8.92530300
H	-2.94364700	0.02095800	9.84454700
C	-4.02991900	-1.21879700	8.37141200
H	-4.70404300	-1.70417100	9.10122900
H	-4.61660200	-1.04624700	7.45547700
H	11.74299400	4.55082000	2.41985000
H	11.53954500	3.49492200	4.59582500
H	11.37787300	1.83868200	5.89961200
H	11.24644800	-0.52772600	6.42313800
H	11.20202500	-2.58434200	5.93615700
H	11.23832500	-4.47505900	4.41490100
H	11.33928000	-5.39548500	2.51489500
H	11.51635900	-5.39863700	0.09421400
H	11.90019900	4.54685200	0.31147700
H	12.02022500	3.49367900	-1.87158100
H	12.05205300	1.84540500	-3.19373600
H	11.99840300	-0.51601900	-3.74983300
H	11.88224700	-2.57816300	-3.29793000
H	11.69439100	-4.47898400	-1.80076300
C	10.74896900	4.29929300	2.78701500
C	10.63304500	3.69741000	4.02719500
C	10.40385200	1.35207900	5.87530200
C	10.32895000	0.00336900	6.17364300
C	10.26501400	-2.91131300	5.48762300
C	10.28566100	-3.98892600	4.62035800
C	10.43013900	-5.28815900	1.92491200
C	10.53096300	-5.29017000	0.54520400
C	10.97116900	4.29811100	-0.19955000
C	11.03958800	3.69761700	-1.44391900
C	11.08472500	1.36050600	-3.31738100
C	11.05414600	0.01429000	-3.63463600
C	10.88941300	-2.90679900	-2.99389900
C	10.78231300	-3.99028500	-2.14049500

C	9.61593900	4.44935500	1.92971000
C	9.37610700	3.20391900	4.49406400
C	9.26487300	2.06598500	5.39109900
C	9.10985000	-0.72319300	6.00878000
C	9.07879200	-2.13766700	5.67669900
C	9.12164700	-4.36677900	3.88309900
C	9.19181300	-4.99565700	2.57472600
C	9.40060600	-4.99980200	-0.27902800
C	9.72372400	4.44971900	0.48035000
C	9.86518800	3.20754300	-2.09345300
C	9.88718700	2.07308800	-3.00192400
C	9.82391700	-0.71203400	-3.65840100
C	9.74399600	-2.12977100	-3.34840500
C	9.52263200	-4.37009700	-1.58325000
C	8.32616100	4.28078800	2.52101700
C	8.20565200	3.65402400	3.80919100
C	7.98940900	1.44268800	5.55321700
C	7.91145600	0.04142100	5.86437900
C	7.85068600	-2.70784200	5.22046900
C	7.87236200	-3.82738800	4.31899400
C	8.00922200	-5.04748400	1.77427300
C	8.11391000	-5.04969900	0.34019600
C	8.53561000	4.28342200	-0.29556800
C	8.60680700	3.65853200	-1.58854600
C	8.64938100	1.45221000	-3.35425100
C	8.61735700	0.05303400	-3.68491200
C	8.46216600	-2.70270400	-3.08301600
C	8.35089000	-3.82846400	-2.19565500
C	7.14179200	4.48154800	1.73145600
C	6.90452900	3.24636100	4.26511500
C	6.79543700	2.13138800	5.14482500
C	6.64198900	-0.62495300	5.75907200
C	6.61132700	-2.01140900	5.43517800
C	6.65398300	-4.21371900	3.66144800
C	6.72322800	-4.82710300	2.37781100
C	6.92958200	-4.82950600	-0.44464000

C	7.24743400	4.48404100	0.31085200
C	7.38720400	3.25347700	-2.23259700
C	7.40899200	2.14076200	-3.12208400
C	7.34615900	-0.61321700	-3.77363100
C	7.26779100	-2.00332600	-3.47186500
C	7.04896400	-4.21633800	-1.72500000
C	5.84944500	4.38198800	2.33935900
C	5.72910600	3.75353200	3.62425200
C	5.51237100	1.53836900	5.37276200
C	5.43409200	0.14003600	5.68587800
C	5.37299400	-2.61378500	5.04371300
C	5.39518600	-3.73046000	4.14296400
C	5.53293200	-4.94647100	1.59191100
C	5.63739800	-4.94378800	0.16042500
C	6.05954300	4.38820100	-0.48165500
C	6.13046100	3.76050700	-1.77056400
C	6.17322300	1.54951400	-3.53753500
C	6.14055000	0.15292000	-3.86925100
C	5.98558900	-2.60890200	-3.27238400
C	5.87478900	-3.73173600	-2.38506700
C	4.67760900	4.59733800	1.55276900
C	4.43986800	3.35560900	4.09133500
C	4.32970000	2.23342700	4.97781400
C	4.17522500	-0.52818300	5.59871500
C	4.14388800	-1.92423900	5.27384900
C	4.18759700	-4.12836800	3.49419500
C	4.25831200	-4.74043000	2.19994100
C	4.46545500	-4.73139900	-0.62501100
C	4.78385200	4.60119500	0.12250600
C	4.92440900	3.36139900	-2.41872900
C	4.94675400	2.24391900	-3.31437300
C	4.88171800	-0.51393600	-3.96704500
C	4.80315100	-1.91526700	-3.67134000
C	4.58493400	-4.12810500	-1.91911000
C	3.38331500	4.47599000	2.15755600
C	3.26379100	3.84871800	3.43638300

C	3.04622100	1.63051000	5.19227100
C	2.96736000	0.23910200	5.50857200
C	2.90507000	-2.52122500	4.86583700
C	2.92760600	-3.63289400	3.96763000
C	3.06905100	-4.83994200	1.40678600
C	3.17392500	-4.82861100	-0.01461700
C	3.59405500	4.48266800	-0.66835200
C	3.66520200	3.85819300	-1.94907100
C	3.70829400	1.64461000	-3.71569800
C	3.67436100	0.25489800	-4.03744100
C	3.51804100	-2.51398800	-3.45290900
C	3.40824800	-3.63162300	-2.56971500
C	2.20820100	4.68005600	1.36601300
C	1.97124300	3.44400400	3.90186100
C	1.86047700	2.32481700	4.79021600
C	1.70463300	-0.43010700	5.41669800
C	1.67312500	-1.82555700	5.09065500
C	1.71767200	-4.02858800	3.31031500
C	1.78980000	-4.64272800	2.01639600
C	1.99905800	-4.63672100	-0.80713700
C	2.31411100	4.68796000	-0.06209700
C	2.45837000	3.46187200	-2.60556400
C	2.47988400	2.34657400	-3.50096800
C	2.41119500	-0.41090800	-4.12985600
C	2.33240800	-1.80955200	-3.83775400
C	2.11654300	-4.02508000	-2.09486100
C	0.92125900	4.55529300	1.96773300
C	0.80063600	3.93421300	3.25085400
C	0.58215300	1.72899600	5.00816800
C	0.50297100	0.33568600	5.32765800
C	0.44023000	-2.41636100	4.67732100
C	0.46319300	-3.52962400	3.77546300
C	0.60790600	-4.75009600	1.22491400
C	0.71324900	-4.75728600	-0.20257400
C	1.13141700	4.56613500	-0.85068200
C	1.20496000	3.95754800	-2.14169400

C	1.24881600	1.75403300	-3.91013500
C	1.21429400	0.35721200	-4.21569200
C	1.05454700	-2.40201400	-3.61477500
C	0.94482800	-3.52542100	-2.73657300
C	-0.25501900	4.75511600	1.17700900
C	-0.49307600	3.53562600	3.71722000
C	-0.60361400	2.42364700	4.60510600
C	-0.76153400	-0.33028500	5.22964200
C	-0.79182300	-1.71794900	4.89286700
C	-0.74488400	-3.91814800	3.11171800
C	-0.67247200	-4.53892700	1.82936900
C	-0.46348200	-4.55140500	-0.99132000
C	-0.14885600	4.75516300	-0.24321600
C	-0.00315300	3.56774200	-2.80369100
C	0.01900900	2.45607400	-3.69969900
C	-0.04866900	-0.30749700	-4.30767700
C	-0.12909300	-1.69718000	-3.99910000
C	-0.34582800	-3.92229600	-2.26581000
C	-1.54728500	4.66216400	1.78692200
C	-1.66828600	4.04402600	3.07509200
C	-1.88876700	1.83485800	4.83488800
C	-1.96813600	0.43767500	5.14568800
C	-2.02746900	-2.31127900	4.47783100
C	-2.00383100	-3.42609100	3.58044700
C	-1.86246500	-4.67011400	1.04158200
C	-1.75647900	-4.67772000	-0.38861300
C	-1.33531800	4.66481900	-1.03738800
C	-1.26177100	4.06753800	-2.33773100
C	-1.21848800	1.86120600	-4.11072700
C	-1.25230700	0.46065300	-4.41681900
C	-1.41216200	-2.29726800	-3.79019900
C	-1.52182900	-3.41994100	-2.90949100
C	-2.71839100	4.88112800	0.99943100
C	-2.95892700	3.65382300	3.54614500
C	-3.06993900	2.53312200	4.43599700
C	-3.22564100	-0.22919200	5.03856500

C	-3.25545300	-1.62077000	4.70112200
C	-3.21004700	-3.83269200	2.93332000
C	-3.13957200	-4.46649200	1.64853200
C	-2.93042100	-4.46999300	-1.17614400
C	-2.61041200	4.88309100	-0.43265800
C	-2.46901800	3.67807600	-2.99557800
C	-2.44728300	2.55827700	-3.89406500
C	-2.51111400	-0.20721600	-4.51758900
C	-2.59199800	-1.60569600	-4.19966400
C	-2.81025000	-3.83193500	-2.45637100
C	-4.01135900	4.76872700	1.60632000
C	-4.13265600	4.14948100	2.88989900
C	-4.35329800	1.93142600	4.64265400
C	-4.43114200	0.53698700	4.94407500
C	-4.49064600	-2.21986700	4.29422200
C	-4.46846100	-3.33743900	3.40427600
C	-4.32917800	-4.57870500	0.85747600
C	-4.22322000	-4.57834500	-0.56851200
C	-3.79886700	4.77912800	-1.22570900
C	-3.72753800	4.16841200	-2.51720100
C	-3.68507000	1.95494100	-4.29132300
C	-3.71733400	0.56051200	-4.60788500
C	-3.87465600	-2.20610900	-3.98456700
C	-3.98457300	-3.32876000	-3.10507300
C	-5.18833100	4.98056800	0.81441500
C	-5.42891800	3.75046400	3.35605600
C	-5.54036300	2.62894100	4.24235900
C	-5.69461600	-0.13313400	4.85058100
C	-5.72499500	-1.52866300	4.52396400
C	-5.68111200	-3.74181700	2.75488900
C	-5.61046400	-4.36702100	1.46633900
C	-5.40094800	-4.36230200	-1.35870600
C	-5.08083500	4.98644700	-0.61590600
C	-4.94050200	3.76991100	-3.17087100
C	-4.91909200	2.65074800	-4.06718600
C	-4.98195300	-0.11076800	-4.69982400



C	-5.06146200	-1.50812600	-4.38581400
C	-5.28031400	-3.73211200	-2.64140700
C	-6.47783900	4.86558700	1.41703700
C	-6.59968200	4.24171800	2.70333100
C	-6.81890000	2.02918900	4.45160900
C	-6.89718700	0.63062400	4.76157300
C	-6.95738700	-2.12398800	4.11863100
C	-6.93508800	-3.24421200	3.22237000
C	-6.79596800	-4.47117200	0.67751200
C	-6.68969300	-4.46786700	-0.75334500
C	-6.26659000	4.87600500	-1.40357500
C	-6.19547800	4.25868800	-2.69684000
C	-6.15294800	2.05150900	-4.46383100
C	-6.18488700	0.65343500	-4.78475800
C	-6.34084800	-2.10317500	-4.16789400
C	-6.45157000	-3.22855700	-3.28441800
C	-7.65400700	5.06514600	0.62589100
C	-7.89347800	3.83260800	3.15986100
C	-8.00391300	2.71851200	4.04007600
C	-8.15820300	-0.03799400	4.65357200
C	-8.18857100	-1.42488800	4.33073100
C	-8.14505800	-3.63266300	2.56339300
C	-8.07480800	-4.24925700	1.28155900
C	-7.86559400	-4.24208900	-1.53801600
C	-7.54754500	5.07040000	-0.79420400
C	-7.40725300	3.85208600	-3.34147400
C	-7.38592600	2.74036300	-4.23112500
C	-7.44867100	-0.01434800	-4.86595500
C	-7.52719200	-1.40205300	-4.55565800
C	-7.74570200	-3.61848900	-2.81270600
C	-8.95459400	4.96512600	1.23050400
C	-9.07642600	4.33760700	2.51809300
C	-9.29495700	2.12703200	4.26295300
C	-9.37343500	0.72604700	4.57565400
C	-9.43413000	-2.02483600	3.93683800
C	-9.41196800	-3.14690900	3.03845600

C	-9.27266900	-4.36781100	0.49556100
C	-9.16625900	-4.36374500	-0.93796100
C	-8.74390300	4.97509600	-1.58576300
C	-8.67260300	4.35510000	-2.88062900
C	-8.63000800	2.15042900	-4.64460100
C	-8.66193100	0.75007200	-4.96759300
C	-8.81760200	-2.00250100	-4.35302500
C	-8.92868600	-3.12883900	-3.46668600
C	-10.12510000	5.23426300	0.45660700
C	-10.36721600	3.98433600	3.01911500
C	-10.47969600	2.84670800	3.91651000
C	-10.63607200	0.05826400	4.53946900
C	-10.66724200	-1.35723500	4.21177300
C	-10.62320900	-3.59030700	2.42368600
C	-10.55157100	-4.21787600	1.11488400
C	-10.33981000	-4.20948300	-1.73832800
C	-10.01663800	5.23973200	-0.99255200
C	-9.87461200	4.00510400	-3.56931900
C	-9.85279600	2.87033300	-4.47697000
C	-9.91632100	0.08319600	-5.12087900
C	-9.99637000	-1.33304700	-4.80479500
C	-10.21749300	-3.57441000	-3.03979000
C	-11.38103400	5.17725500	1.13541300
C	-11.49820700	4.57275900	2.37422800
C	-11.72996300	2.22699000	4.22337600
C	-11.80555500	0.87892300	4.52474400
C	-11.87006500	-2.03876200	3.85110800
C	-11.84875100	-3.11842100	2.98646800
C	-11.70092600	-4.41012400	0.28820000
C	-11.59849100	-4.40600800	-1.09141000
C	-11.15758200	5.18857500	-1.85107400
C	-11.08891200	4.59136600	-3.09701300
C	-11.04386700	2.25228800	-4.96753200
C	-11.07453300	0.90471400	-5.27890600
C	-11.23951700	-2.01465600	-4.62798900
C	-11.34647400	-3.09821700	-3.77459700

H	-12.28674600	5.50480500	0.62698200
H	-12.49220300	4.44445000	2.80038800
H	-12.65594600	2.78791800	4.10498000
H	-12.78852500	0.42283100	4.63352000
H	-12.83377800	-1.63717900	4.16109100
H	-12.79644500	-3.53154600	2.64394100
H	-12.69238300	-4.44119600	0.73782700
H	-12.51273200	-4.43415200	-1.68259900
H	-12.12882900	5.51395400	-1.48099700
H	-12.00836800	4.46619900	-3.66718000
H	-11.97691900	2.81370500	-4.98681300
H	-12.03068300	0.44959000	-5.53340300
H	-12.14698800	-1.61052500	-5.07442300
H	-12.33462600	-3.51142800	-3.57723600
C	0.80662900	-2.04829300	8.39977100
H	0.11157900	-2.11903100	7.56264400
C	-3.71974100	1.29787500	8.36518800
H	-4.29251800	1.41436500	7.44384100
H	1.43305600	-2.91963700	8.59960300
H	-3.30144500	2.20286300	8.80941900

**UP-9-(8,8)**

C	0.31117500	0.31070500	-7.86246000
C	2.61653300	-0.41349700	-7.77710300
C	0.71284900	1.64610400	-7.75890100
H	-0.75404900	0.07478100	-7.89463400
C	3.02129200	0.92530700	-7.67977500
H	3.35448300	-1.21326000	-7.74206000
H	-0.02956300	2.43953200	-7.71637400
H	4.08343300	1.15578800	-7.57652600
C	-0.55208500	8.16575700	-2.62680100
C	1.69822700	9.24180200	-2.89850400
C	0.80354700	8.24320200	-3.22501400
C	1.05326400	7.24494200	-4.29126300
C	2.30584100	6.65639700	-4.53912400
C	0.13116500	5.80112700	-6.04039600

C	2.50531400	5.70024000	-5.54518500
H	3.14969800	6.89187600	-3.89383300
H	-0.71736400	5.38505600	-6.58018400
H	3.50043200	5.28741000	-5.69460900
C	2.07504500	1.96480800	-7.63306300
C	1.40100000	5.24211000	-6.28006400
C	2.55251300	3.38205800	-7.35747200
H	3.21422500	3.74547500	-8.16412800
H	3.13564300	3.36877800	-6.42503400
O	1.42833600	4.26558900	-7.24341700
C	-0.05173400	6.82724900	-5.10226500
C	-1.35345500	7.49911700	-4.89720900
C	-2.15229500	7.89739400	-5.94812100
S	-1.76390900	7.60737900	-7.68158300
S	-3.63196600	8.90406000	-5.75929900
C	-2.96575900	8.71608500	-8.33332900
H	-2.98050900	8.85676000	-9.41230600
C	-3.81109800	9.30223200	-7.46424800
H	-4.61217900	9.98729300	-7.73464600
S	3.28119400	9.48471300	-3.71889400
C	2.73526700	11.56484400	-2.14616600
H	2.82507300	12.52580000	-1.64348000
S	1.36549700	10.55145400	-1.70724700
C	3.60215700	11.08290500	-3.05682600
H	4.49854800	11.59454000	-3.40151300
C	-2.10523100	8.39107300	-0.74514200
C	-1.64162100	7.82739600	-3.48565800
C	-2.94033800	7.78766400	-2.93641100
H	-3.77272300	7.44512500	-3.54853100
C	-3.18338400	8.09611700	-1.60097200
H	-4.18587300	8.03317000	-1.18133500
C	-0.79543500	8.40346100	-1.25671500
H	0.04392000	8.55327400	-0.58282700
O	-2.44337400	8.60107700	0.56100600
C	0.87819900	-8.56455800	-1.00022900
C	2.21125300	-7.61999800	-3.33616700

C	0.18014700	-8.41533000	-2.21250800
H	-0.89542200	-8.58196600	-2.20584700
C	2.25920300	-8.30278200	-0.96669000
H	2.82644400	-8.40322900	-0.04438000
C	2.89172400	-7.81665100	-2.11792600
H	3.92806400	-7.50452200	-2.02183500
C	0.82894200	-7.98915200	-3.37979100
C	0.11619600	-7.85102100	-4.66691800
C	2.81183900	-6.97258800	-4.53132300
C	1.84781500	-6.17837300	-5.33930700
C	0.49200600	-6.63509400	-5.41339300
C	2.18345300	-4.97094800	-5.97636900
H	3.16366500	-4.52062600	-5.84047600
C	-0.44086900	-5.87121800	-6.13415600
H	-1.48849300	-6.16839300	-6.13319600
C	-0.08713500	-4.69508900	-6.80489700
H	-0.85055000	-4.14461000	-7.34849800
C	1.23496500	-4.22976900	-6.70735300
O	1.68780400	-3.03850400	-7.22118000
C	1.25043100	-0.73476700	-7.83742300
C	0.72522400	-2.15599200	-7.82013300
C	4.13448800	-7.13056000	-4.89880600
C	-0.73275600	-8.81710200	-5.15521500
S	4.88219300	-6.38613700	-6.35617800
S	5.29498800	-8.20864300	-4.04537600
S	-1.12019500	-10.34695500	-4.29080300
S	-1.47426700	-8.76771900	-6.79408800
C	6.57998600	-8.10805800	-5.23976800
H	7.47310400	-8.70368400	-5.06209600
C	6.39194900	-7.28350200	-6.28770200
H	7.11017100	-7.11143000	-7.08681400
C	-2.03188800	-10.43814700	-6.79706700
H	-2.49952400	-10.80652900	-7.70796200
C	-1.87080600	-11.15102500	-5.66580800
H	-2.18911600	-12.18238000	-5.52712300
H	0.48513300	-2.52190300	-8.83629800

H	-0.20680000	-2.16094400	-7.23235300
O	0.11538000	-8.92930400	0.07237600
C	0.65447100	-8.79166800	1.40514600
H	1.25431400	-7.87078000	1.47228000
H	1.31050300	-9.65049900	1.63351400
C	-0.54364400	-8.70739600	2.34955500
H	-1.10739100	-9.65312000	2.31871500
H	-1.20982900	-7.92611900	1.95482700
C	-0.16575100	-8.34491200	3.79718100
H	0.40972100	-9.15973500	4.26791600
H	0.49425300	-7.46344700	3.77945000
C	-1.41619000	-8.00759200	4.63486400
H	-1.96734300	-8.93044200	4.88362100
H	-2.09345300	-7.40510000	4.00810200
C	-1.12063000	-7.19626800	5.90924800
H	-0.55589400	-7.80284100	6.63752400
H	-0.46667200	-6.35375900	5.63296600
C	-2.40387700	-6.63107300	6.55136600
H	-2.95122500	-7.42879200	7.08199200
H	-3.06990700	-6.28701900	5.74338100
C	-2.15639900	-5.43915500	7.49296100
H	-1.60142800	-5.76329200	8.39018900
H	-1.50941100	-4.71411800	6.97337100
C	-1.41501400	8.65130800	1.57158800
H	-0.66294400	7.87107800	1.37788100
H	-0.91008100	9.63319500	1.54410400
C	-2.11256900	8.37884800	2.90431800
H	-2.77900300	9.21786100	3.15861900
H	-2.75448100	7.49915000	2.74867200
C	-1.14320200	8.07600100	4.06272400
H	-0.61516000	8.98919100	4.38470700
H	-0.37153600	7.37478800	3.70743300
C	-1.88410300	7.42509400	5.24696900
H	-2.54426000	8.16323200	5.73358200
H	-2.54632500	6.64565900	4.83706600
C	-0.96821000	6.75679700	6.28908400

H	-0.41931100	7.51450600	6.87370100
H	-0.20810800	6.16400300	5.75551600
C	-1.75596800	5.81681300	7.22378400
H	-2.37525900	6.40524900	7.92245900
H	-2.45906200	5.23277200	6.60792600
C	-0.87519400	4.82512000	8.00252900
H	-0.26129500	5.35711200	8.74990400
H	-0.16976100	4.35407100	7.30008800
C	-1.69713500	3.71909400	8.68568500
H	-2.35161400	3.24709500	7.93631800
H	-2.36100500	4.15835300	9.45043100
C	-3.46035700	-4.73048700	7.89878500
H	-4.04452500	-4.52512100	6.98889700
H	-4.08045200	-5.39856300	8.51948400
C	-3.21774000	-3.40538100	8.63876200
H	-2.49595500	-2.80089700	8.06266300
H	-2.71397900	-3.60420200	9.60342900
C	-4.44360000	-2.55705700	8.88769600
C	-1.62613000	1.49892600	9.91539400
H	-2.37986000	1.78748500	10.65733600
C	-0.81433300	2.62741300	9.33116600
H	-0.20152900	3.09757800	10.12258900
H	-0.11461900	2.23063600	8.57885100
H	12.09930600	4.62607100	-2.47635300
H	11.90961400	5.89233300	-0.41861900
H	11.75485400	6.21959400	1.64567800
H	11.61661300	5.63991700	3.99495600
H	11.55096200	4.39365200	5.67761300
H	11.54805900	2.31834300	6.92914600
H	11.60865100	0.24824800	7.24458700
H	11.73799900	-2.10444100	6.67785500
H	12.24841300	2.93377000	-3.69977400
H	12.37723400	0.58190700	-4.26847400
H	12.43474200	-1.48690800	-3.95362000
H	12.42773500	-3.56351900	-2.70500600
H	12.35911700	-4.81146200	-1.02432900

H	12.22214100	-5.38536000	1.32634700
H	12.07166200	-5.05664700	3.38983700
H	11.88528600	-3.79575500	5.45111500
C	11.10731900	4.79946400	-2.06206700
C	10.99905000	5.52255900	-0.88754800
C	10.77831500	5.98638900	2.06725900
C	10.69943400	5.65539600	3.40823200
C	10.60523500	3.87258200	5.81825500
C	10.60362800	2.68776200	6.53257500
C	10.68932400	-0.27624700	6.98875700
C	10.76318100	-1.61939900	6.66526900
C	11.32071700	2.37569300	-3.81651800
C	11.39423800	1.03278300	-4.14128400
C	11.47639800	-1.93164100	-3.68994200
C	11.47236800	-3.11756300	-2.97735600
C	11.37478800	-4.89846100	-0.56678600
C	11.29668900	-5.22578300	0.77516800
C	11.08070400	-4.76045700	3.73043400
C	10.97434200	-4.04056300	4.90709900
C	9.97047600	4.17109200	-2.65422200
C	9.74595700	5.66956100	-0.21961900
C	9.63905500	5.89362300	1.21203800
C	9.47568800	5.20682700	3.99070900
C	9.43014100	4.34277700	5.15795200
C	9.42662300	1.88710300	6.63903500
C	9.46804100	0.45173000	6.86117600
C	9.62115500	-2.33249300	6.19080200
C	10.07393200	2.99661100	-3.50381000
C	10.22657900	0.21242100	-4.17765500
C	10.26635500	-1.22387500	-3.95965600
C	10.25805400	-3.68179000	-2.48222200
C	10.21069600	-4.54374300	-1.31320500
C	10.04857100	-5.22182800	1.46808200
C	9.94400000	-4.99729100	2.89993500
C	9.72343100	-3.50527100	5.33900200
C	8.68355500	4.56381000	-2.17200200



C	8.57097300	5.31513400	-0.95195400
C	8.36285800	5.75026500	1.83918900
C	8.28099900	5.40495300	3.23167500
C	8.19214100	3.72021900	5.50755400
C	8.19050300	2.48989300	6.25007500
C	8.27089000	-0.30888100	6.68532700
C	8.34747900	-1.70406800	6.34989300
C	8.88514100	2.27285700	-3.82908600
C	8.96153600	0.87770800	-4.16743200
C	9.03922800	-1.92391700	-3.74273500
C	9.03492100	-3.15614000	-3.00222800
C	8.94265100	-4.83428500	-0.72119200
C	8.86159900	-5.17335200	0.67336700
C	8.65756000	-4.73773900	3.46600500
C	8.54693200	-3.99034400	4.68846100
C	7.49495700	4.01995600	-2.76962100
C	7.27320100	5.50219400	-0.36277600
C	7.16842100	5.72044400	1.04039200
C	7.00701700	5.03680600	3.78610700
C	6.96260400	4.18958400	4.92958400
C	6.95909400	1.76350800	6.39634900
C	6.99937200	0.35739600	6.61622600
C	7.15042000	-2.39476700	5.95502400
C	7.59665800	2.86819900	-3.60176900
C	7.74771200	0.11474700	-4.27071000
C	7.78670400	-1.29343300	-4.05844800
C	7.77827200	-3.72314500	-2.59532800
C	7.73170200	-4.56542100	-1.44737000
C	7.57156800	-5.23481900	1.30426000
C	7.46888800	-5.01699400	2.70795200
C	7.25064300	-3.54365400	5.12005800
C	6.20587100	4.46787600	-2.33722300
C	6.09319300	5.21936400	-1.12136200
C	5.88496000	5.65170200	1.67036400
C	5.80340900	5.30348700	3.05864000
C	5.71490700	3.61739400	5.33447100

C	5.71329100	2.39133500	6.07722100
C	5.79332800	-0.40666600	6.51651800
C	5.86942400	-1.79844200	6.18240900
C	6.40780500	2.17506300	-3.99437400
C	6.48383400	0.78362200	-4.33391100
C	6.56194700	-2.01963700	-3.91234600
C	6.55766500	-3.24793500	-3.17171000
C	6.46468600	-4.92032900	-0.88439300
C	6.38374300	-5.25967400	0.50650600
C	6.17960200	-4.82886300	3.30067800
C	6.06872800	-4.08398900	4.52037600
C	5.02807700	3.93577600	-2.94310700
C	4.80598100	5.42749400	-0.53893500
C	4.70030800	5.64548500	0.87319500
C	4.53876400	4.95320600	3.62159000
C	4.49438000	4.10033600	4.77236800
C	4.49105100	1.67334200	6.24678900
C	4.53118900	0.25878500	6.47036000
C	4.68176700	-2.49708200	5.80761400
C	5.13133900	2.77801600	-3.78113200
C	5.28174200	0.02214900	-4.45240500
C	5.32168900	-1.39500200	-4.24358400
C	5.31318500	-3.82194500	-2.77298800
C	5.26555000	-4.66270500	-1.61450900
C	5.10564400	-5.34111900	1.13804500
C	5.00176500	-5.12583600	2.55069800
C	4.78253700	-3.65265500	4.96676900
C	3.73719700	4.37023100	-2.49736600
C	3.62467200	5.13201800	-1.29530900
C	3.41498200	5.56315900	1.50398700
C	3.33434200	5.21211900	2.88745500
C	3.24638900	3.52023800	5.17396700
C	3.24456400	2.30006100	5.91832300
C	3.32402400	-0.50756700	6.36426500
C	3.39942200	-1.89498000	6.02932900
C	3.94046000	2.07578500	-4.15657300

C	4.01557000	0.69134500	-4.49283700
C	4.09377000	-2.11491900	-4.07759600
C	4.08992800	-3.33515200	-3.33695600
C	3.99675200	-4.99799700	-1.04094700
C	3.91609300	-5.34925900	0.33955000
C	3.71006100	-4.92724700	3.14100700
C	3.59907500	-4.18642700	4.35785000
C	2.55801300	3.82992200	-3.09902400
C	2.33273600	5.33715000	-0.71265600
C	2.22783300	5.55078100	0.70117300
C	2.06750200	4.85304600	3.45161200
C	2.02333700	4.00073000	4.60434200
C	2.01960600	1.57773000	6.08984300
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C	2.20845000	-2.59467800	5.64832400
C	2.66056700	2.67777700	-3.93660200
C	2.80895000	-0.06940300	-4.59499700
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C	2.79481800	-4.73544600	-1.76934000
C	2.63388500	-5.42867500	0.97015400
C	2.52960400	-5.21813900	2.38300800
C	2.30926500	-3.74893000	4.80290600
C	1.27218900	4.28034000	-2.67787600
C	1.15807000	5.03370100	-1.46776700
C	0.94829800	5.45163800	1.32849200
C	0.86841300	5.09743900	2.71465000
C	0.78156000	3.41637000	4.99912300
C	0.77854600	2.19886000	5.75317000
C	0.85565700	-0.60066500	6.20460200
C	0.93120000	-1.99120900	5.86481600
C	1.47518600	1.98800600	-4.32867200
C	1.55033800	0.59792400	-4.64657800
C	1.62650400	-2.19410600	-4.21719000
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C	1.53215800	-5.09113800	-1.21168700

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C	1.24167800	-5.01273100	2.96531400
C	1.13078800	-4.27243300	4.18649300
C	0.09594100	3.75712800	-3.30230100
C	-0.13368100	5.21849600	-0.88242100
C	-0.23794000	5.41875000	0.52601400
C	-0.39705500	4.72657100	3.27234600
C	-0.44158300	3.88606600	4.42341100
C	-0.44776600	1.47901900	5.92108100
C	-0.40900600	0.06971300	6.14484400
C	-0.25966000	-2.68112000	5.46689400
C	0.19776100	2.60023200	-4.13224100
C	0.34631700	-0.16194600	-4.76032800
C	0.38478900	-1.56981300	-4.54560800
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C	0.33328700	-4.85359800	-1.95206800
C	0.16723000	-5.52007600	0.79715100
C	0.06262600	-5.29640900	2.20238800
C	-0.15899600	-3.82581300	4.61914400
C	-1.19556700	4.19836200	-2.86971000
C	-1.31044000	4.92606900	-1.64282700
C	-1.51929600	5.32601600	1.15592100
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C	-1.68839100	3.31792400	4.83442600
C	-1.69256500	2.10489800	5.59282700
C	-1.61658200	-0.69193900	6.03338200
C	-1.54010100	-2.07706900	5.68129900
C	-0.99006600	1.90380800	-4.52584500
C	-0.91541900	0.50800500	-4.83644700
C	-0.83823000	-2.29880900	-4.40401900
C	-0.84158900	-3.52893500	-3.67178900
C	-0.93322300	-5.22181900	-1.39681800
C	-1.01678100	-5.55496800	-0.00653000
C	-1.22736400	-5.09906600	2.78679600
C	-1.33894500	-4.35224600	4.00195100
C	-2.37042200	3.66973200	-3.48655600

C	-2.59607700	5.10452600	-1.05112100
C	-2.70187000	5.31263900	0.35974800
C	-2.86259800	4.63714900	3.10895600
C	-2.90827000	3.79828100	4.26877300
C	-2.91710100	1.39078500	5.76841000
C	-2.87815100	-0.02421700	5.98930700
C	-2.72649400	-2.76584400	5.28539500
C	-2.26776200	2.51062600	-4.32545800
C	-2.11524100	-0.25602800	-4.96359100
C	-2.07674600	-1.67446400	-4.74415200
C	-2.08443800	-4.11460800	-3.28479500
C	-2.13094000	-4.97089400	-2.13427000
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C	-2.40217400	-5.40015000	2.03216300
C	-2.62406700	-3.91536300	4.43991300
C	-3.66164900	4.09448900	-3.03507700
C	-3.77436100	4.81305000	-1.80790600
C	-3.98253600	5.23833400	0.99260200
C	-4.06443100	4.89871000	2.37757200
C	-4.15645800	3.23169600	4.68044100
C	-4.16069500	2.01790100	5.43489800
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C	-4.00516800	-2.16616400	5.50740100
C	-3.45608400	1.80490900	-4.70415900
C	-3.37953500	0.41394200	-5.02715300
C	-3.30188100	-2.39930700	-4.58794500
C	-3.30564100	-3.62639700	-3.85248000
C	-3.39999600	-5.31719600	-1.56706400
C	-3.48323900	-5.65227600	-0.17973400
C	-3.69194400	-5.19940800	2.61938400
C	-3.80286200	-4.45042400	3.83043000
C	-4.84329100	3.56101500	-3.64744800
C	-5.06504100	5.01245600	-1.21967200
C	-5.17077000	5.22786800	0.19289700
C	-5.33328000	4.55296700	2.94737100
C	-5.37970800	3.71255500	4.10698600

C	-5.38862500	1.29605100	5.59824600
C	-5.34863200	-0.11893600	5.81712800
C	-5.19397400	-2.86330400	5.11966400
C	-4.73989300	2.40645000	-4.48916000
C	-4.58601000	-0.35345500	-5.14025800
C	-4.54695700	-1.76914600	-4.91796400
C	-4.55623400	-4.20265100	-3.45266000
C	-4.60382200	-5.05364000	-2.30041900
C	-4.76777000	-5.72282900	0.45324000
C	-4.87292200	-5.49711900	1.86414200
C	-5.09272600	-4.01520800	4.27619600
C	-6.12972100	3.98753600	-3.19899200
C	-6.24193300	4.72325300	-1.97352500
C	-6.44949000	5.14396000	0.82221100
C	-6.53163200	4.80298600	2.21275400
C	-6.62434500	3.13778200	4.50556800
C	-6.62853900	1.91708400	5.25796100
C	-6.54882200	-0.88102300	5.69359200
C	-6.47088300	-2.26873400	5.34414600
C	-5.92574700	1.70526700	-4.86412200
C	-5.84812300	0.31223100	-5.19483000
C	-5.77063600	-2.48675200	-4.75475100
C	-5.77534300	-3.71425900	-4.01351000
C	-5.86979800	-5.39320500	-1.73352200
C	-5.95274800	-5.73166600	-0.34287800
C	-6.15914300	-5.29167400	2.44894800
C	-6.27018900	-4.54637200	3.66840000
C	-7.31008400	3.44780200	-3.80142800
C	-7.53196000	4.90802900	-1.38160800
C	-7.63632400	5.11904500	0.02314200
C	-7.79866500	4.44472800	2.77336900
C	-7.84519800	3.60780200	3.92484900
C	-7.85323300	1.19232700	5.40928000
C	-7.81307900	-0.21404600	5.62975700
C	-7.65899700	-2.96179900	4.95060800
C	-7.20750700	2.30092400	-4.63901500

C	-7.05405000	-0.45158600	-5.29857900
C	-7.01509300	-1.85775000	-5.07738700
C	-7.02492700	-4.28170600	-3.60754400
C	-7.07255600	-5.12457000	-2.46089000
C	-7.23579500	-5.79423000	0.28841000
C	-7.33965800	-5.57500900	1.69166800
C	-7.55847100	-4.10568500	4.10774100
C	-8.60711600	3.89081600	-3.36881500
C	-8.71967700	4.63169200	-2.14248000
C	-8.92701600	5.05325800	0.65231900
C	-9.00932300	4.71154000	2.04593600
C	-9.10196800	3.04409900	4.33577300
C	-9.10594000	1.81940500	5.08780200
C	-9.02626000	-0.97805100	5.52808100
C	-8.94827200	-2.37174600	5.18587600
C	-8.40336600	1.61003100	-5.03662400
C	-8.32545000	0.21504600	-5.37268900
C	-8.24785400	-2.58281400	-4.93355900
C	-8.25297800	-3.81069600	-4.18709000
C	-8.34769300	-5.48455700	-1.90365200
C	-8.43059000	-5.82386900	-0.50970500
C	-8.63642400	-5.39041500	2.28328600
C	-8.74736600	-4.64764900	3.50874100
C	-9.78225300	3.40710900	-4.02261000
C	-10.00701800	4.88623600	-1.57627200
C	-10.11327700	5.10300800	-0.14320800
C	-10.27745100	4.42118800	2.63774000
C	-10.32498900	3.56538100	3.81130600
C	-10.33264300	1.12081100	5.31059000
C	-10.29171100	-0.31397800	5.53767600
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C	-9.52235600	-0.54503300	-5.55210300
C	-9.48246500	-1.98003100	-5.32721000
C	-9.49282000	-4.42877900	-3.83570200
C	-9.54174400	-5.28592600	-2.66333400

C	-9.70686500	-5.96311500	0.11844200
C	-9.81232300	-5.74207500	1.55093300
C	-10.03366300	-4.26186100	3.99775400
C	-11.03423800	3.93850100	-3.58922100
C	-11.14266500	4.65224200	-2.40891800
C	-11.36194900	5.10242100	0.54847200
C	-11.44119400	4.77356800	1.89005000
C	-11.53915600	3.00486700	4.31073000
C	-11.54291100	1.82535600	5.03394600
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C	-11.38359000	-2.47772900	5.17696600
C	-10.81819100	1.52578200	-5.35833600
C	-10.74314800	0.18312000	-5.68362200
C	-10.66073200	-2.77876800	-5.22056000
C	-10.66582700	-3.96013400	-4.50050200
C	-10.76701800	-5.72637700	-2.07817000
C	-10.84676200	-6.05303800	-0.73603300
C	-11.06421100	-5.59976500	2.22179900
C	-11.17097000	-4.88618300	3.40240700
H	-11.94444200	3.69475500	-4.13498600
H	-12.13436100	4.94516700	-2.06767400
H	-12.28712100	5.26130300	-0.00333700
H	-12.42583700	4.68529000	2.34654000
H	-12.49454700	3.44842000	4.03476500
H	-12.50102700	1.38223800	5.30108000
H	-12.44175200	-0.68604700	5.63484700
H	-12.31053500	-3.03728700	5.06143900
H	-11.79298200	2.01089000	-5.37304100
H	-11.66161500	-0.34115600	-5.94299100
H	-11.60377900	-2.40963400	-5.62068600
H	-11.61264000	-4.47910300	-4.35924500
H	-11.68460100	-5.70840300	-2.66420700
H	-11.82416900	-6.28084500	-0.31357600
H	-11.97533500	-5.96729700	1.75221600
H	-12.16232300	-4.71730400	3.82001200
H	-4.24606500	-1.58228300	9.34644000



C	-1.50350600	0.20686500	9.57620900
H	-0.76830500	-0.11511700	8.83625600
C	-5.70948500	-2.87949700	8.58241400
H	-5.96224300	-3.82937200	8.10969600
H	-6.53329300	-2.19349700	8.78362300
H	-2.12612100	-0.56796100	10.02725600

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C	-1.04136700	0.38902500	-8.42675500
C	-3.10565100	1.63860700	-8.25529700
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C	-3.82163400	0.43399900	-8.25328100
H	-3.62912600	2.58678100	-8.14883600
H	-1.22594500	-1.76332600	-8.45311800
H	-4.90791200	0.45812200	-8.14753400
C	-3.05732500	-7.93456400	-3.73552200
C	-5.40497300	-8.34484900	-4.52042300
C	-4.24777200	-7.59440800	-4.55225500
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C	-5.03355000	-5.53619900	-5.83259700
C	-2.46934200	-5.15067300	-6.83117800
C	-4.79436400	-4.45966300	-6.69794100
H	-6.01748400	-5.60524800	-5.37337300
H	-1.45743100	-4.91941000	-7.15742400
H	-5.60558300	-3.77292100	-6.92769700
C	-3.15529400	-0.80201200	-8.30531500
C	-3.49076300	-4.24441600	-7.17105400
C	-3.96755700	-2.07528500	-8.15139300
H	-4.58804100	-2.27428700	-9.04481100
H	-4.64487500	-1.94743100	-7.29325200
O	-3.08386500	-3.18224000	-7.93498200
C	-2.72594000	-6.27666600	-6.03702600
C	-1.68757900	-7.28112800	-5.71832300
C	-0.80258200	-7.75811000	-6.66205500
S	-0.74442300	-7.20057200	-8.37210800

S	0.33472400	-9.12143500	-6.36946300
C	0.28593100	-8.50053900	-8.96095100
H	0.49565300	-8.52546800	-10.02845700
C	0.77487800	-9.36887700	-8.05511400
H	1.43967500	-10.20054500	-8.27985100
S	-6.81451900	-8.07183600	-5.60494400
C	-7.10102600	-10.37115200	-4.28978300
H	-7.51626800	-11.31965000	-3.95490000
S	-5.63526600	-9.80859900	-3.49560800
C	-7.63478200	-9.58615200	-5.24481600
H	-8.54604900	-9.80367700	-5.79832800
C	-2.00915300	-8.69913600	-1.65821400
C	-1.77216300	-7.81035100	-4.34130800
C	-0.63589600	-8.14209000	-3.57250400
H	0.35790100	-7.97141900	-3.98203700
C	-0.74189900	-8.60932600	-2.26598800
H	0.14320100	-8.83679700	-1.67525800
C	-3.15614000	-8.34577800	-2.38943300
H	-4.12523900	-8.33045700	-1.89955900
O	-2.00154000	-9.07565600	-0.34525000
C	-0.23841200	9.17595900	-1.19804600
C	-1.49172600	8.46572000	-3.64875900
C	0.53432400	8.86252800	-2.33099800
H	1.61474900	8.81417100	-2.21045300
C	-1.64152700	9.16293800	-1.29311300
H	-2.26461100	9.37311500	-0.42756100
C	-2.24102500	8.78201200	-2.49980600
H	-3.32166400	8.65891100	-2.51105700
C	-0.06546700	8.54738900	-3.55827100
C	0.72648200	8.24246500	-4.77014800
C	-2.09093100	7.98265800	-4.91495200
C	-1.25584400	6.99102500	-5.63642100
C	0.16800700	7.13951000	-5.57845200
C	-1.79536500	5.89501800	-6.32720700
H	-2.86076900	5.67949400	-6.28716700
C	0.96731300	6.19869100	-6.24966200

H	2.05036600	6.24870000	-6.15214800
C	0.42092300	5.14247500	-6.98883100
H	1.08701100	4.44165600	-7.48542400
C	-0.97359300	4.97628800	-7.00749300
O	-1.63487500	3.92937100	-7.59758600
C	-1.70263300	1.62417900	-8.31063400
C	-0.85832700	2.87579100	-8.18440900
C	-3.27483300	8.47022900	-5.42923200
C	1.81552800	8.99334300	-5.15456900
S	-3.98472400	7.96090200	-7.00232800
S	-4.22712200	9.79682200	-4.67390400
S	2.44036800	10.40743700	-4.23442800
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C	-5.29238800	10.07703600	-6.04540100
H	-6.00378000	10.89651300	-5.96495500
C	-5.18182400	9.24644500	-7.09965100
H	-5.79027700	9.29350900	-8.00059400
C	3.60752300	10.27158400	-6.62901000
H	4.23893200	10.51731500	-7.48049000
C	3.49175600	11.01194200	-5.50997200
H	4.01616600	11.94677500	-5.32208000
H	-0.46945000	3.21413600	-9.16343600
H	0.00635000	2.64001400	-7.54334200
O	0.47082400	9.42579600	-0.05710900
C	-0.24263200	9.48187400	1.19525900
H	-0.95009200	8.63998700	1.25273300
H	-0.82104900	10.42125000	1.25582400
C	0.79067000	9.36796200	2.31370000
H	1.44619900	10.25270000	2.31468400
H	1.42372900	8.49867400	2.08343400
C	0.13878900	9.15936000	3.69458400
H	-0.33013100	10.09300300	4.04815400
H	-0.67279700	8.42139000	3.59352200
C	1.14163700	8.62748400	4.73674100
H	1.86566300	9.41414100	5.00895300
H	1.72504700	7.82101900	4.26470500

C	0.47104000	8.05447300	5.99908900
H	0.03878200	8.86476100	6.61086100
H	-0.37207600	7.41749700	5.68566900
C	1.43356100	7.19894400	6.84186500
H	2.21212600	7.83536200	7.29695600
H	1.95920000	6.50475100	6.16652200
C	0.72775500	6.36762000	7.92574200
H	0.26940300	7.02865600	8.68164200
H	-0.10028600	5.81368000	7.45489700
C	-3.24125100	-9.08538000	0.39056500
H	-3.77733500	-8.13724900	0.22878100
H	-3.88339400	-9.90908300	0.03049200
C	-2.88095600	-9.22100100	1.86840900
H	-2.42886600	-10.20648600	2.05933600
H	-2.10856700	-8.46688800	2.07830700
C	-4.08675000	-8.97193200	2.79500600
H	-4.74673500	-9.85514000	2.82326300
H	-4.68867400	-8.14559800	2.38356200
C	-3.65379700	-8.57599800	4.21810700
H	-3.14139100	-9.41932500	4.71187600
H	-2.90918600	-7.76813000	4.13365900
C	-4.81847500	-8.07272600	5.08793900
H	-5.48576900	-8.90930500	5.35796100
H	-5.42520600	-7.37413400	4.48998300
C	-4.34713200	-7.34125800	6.35623000
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C	-5.49293300	-6.66124700	7.12277700
H	-6.19350700	-7.42343500	7.50688000
H	-6.06870600	-6.03616200	6.42227700
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H	-4.43776100	-6.40252100	9.00473100
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H	2.40442100	5.90182500	9.23467200

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H	0.19271700	3.78574800	8.83939100
H	0.33891300	4.86135300	10.24115500
C	1.85268800	3.33757000	10.12650000
H	2.64141500	3.77396300	10.75051300
C	-5.64401100	-4.19217900	10.14675100
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C	-8.11968700	-2.92062200	6.15924600
C	-7.92741900	-1.72451700	6.93145600
C	-6.59846300	-1.20552900	7.10134100
C	-9.43855500	-3.34986500	5.81424700
C	-10.52560500	-2.71243000	6.48283800
C	-10.34082400	-1.55885900	7.22476600
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C	-7.56539300	1.02426000	7.53850700
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C	-1.50416100	-0.40900200	7.10557000
C	-1.68834400	-1.79789300	6.80291400
C	-0.55880800	-2.59792500	6.44406500
C	-0.75245700	-3.78914700	5.67126600
C	-0.19314100	0.15693800	7.04122200
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C	0.76646700	-2.08492000	6.62902300
C	1.89863700	-2.88633800	6.26887900
C	1.70443900	-4.07998100	5.49954800
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C	-7.58930700	-4.16299000	-2.29725200

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C	-5.96885300	6.63666200	2.88999600
C	-6.29028100	6.36129800	-1.30058900
C	-6.14868400	6.77332200	0.05578500
C	-6.64447300	4.65856600	-3.54711800
C	-6.83608000	3.46400500	-4.29970700
C	11.67386000	-4.13269100	5.68649000
C	11.48616200	-5.28976000	4.95145500
C	12.05802900	-1.22196800	6.31031800
C	12.20267200	0.14023100	6.11575000
C	11.10678000	-7.09850800	2.58646700
C	10.96655900	-7.50829300	1.27243500
C	12.44518100	3.70679800	3.67737900
C	12.40966200	2.78142300	4.70533900
C	12.29666400	4.90729200	-0.47878700
C	12.38490500	4.84501800	0.90062200
C	11.99563000	4.01823300	-3.32998900
C	11.82260600	3.18466500	-4.42067700
C	10.77460400	-7.37568100	-1.71990200
C	10.74783500	-6.85165700	-3.00014600
C	10.82997000	-4.84147500	-5.22804900
C	10.92721300	-3.62405800	-5.87830800
C	11.24216500	-0.66911600	-6.30035000
C	11.41859000	0.67276600	-6.01310400
C	-8.16641200	2.95585500	-4.49601200
C	-8.35007900	1.56051700	-4.79009000
C	-7.78446800	5.33614600	-2.99306800
C	-7.60526600	6.19860600	-1.85708400
C	-8.64967400	-1.23830100	-4.39088200
C	-8.75100900	-2.50572600	-3.71947500
C	-7.23082800	6.95564600	2.28032100
C	-7.32171300	7.02448700	0.84724300
C	-7.21302000	4.92820600	5.98528400
C	-7.17490800	5.88324900	4.91199200
C	-7.41314200	2.43845000	7.33586600
C	-8.82925800	-4.41412200	-1.61540800

C	-8.80068200	-4.95480400	-0.28390600
C	-8.56620800	3.27941100	7.25834000
C	-8.46346500	4.55413300	6.56828800
C	-10.00193400	-5.02651400	0.48801100
C	-9.81618100	-0.43707400	-4.59302000
C	-9.66286300	0.99433900	-4.79653200
C	-10.01917800	-2.96961700	-3.25041400
C	-10.05902200	-3.94457500	-2.17264800
C	-8.38658800	6.46437600	4.42423400
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C	-8.74243300	6.72476500	-1.16893200
C	-8.59727000	7.14810300	0.21397500
C	-9.10084900	4.99985300	-3.43705200
C	-9.29638900	3.78205500	-4.20614200
C	-10.58707300	3.24395500	-4.48825800
C	-10.76366500	1.90134000	-4.77290300
C	-10.18362500	5.75743900	-2.89969300
C	-10.01102000	6.58879400	-1.80720100
C	-11.07982900	-1.05477300	-4.35514700
C	-11.17751100	-2.27444000	-3.70861900
C	-9.62295800	7.40182900	2.42648600
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C	-9.60086800	5.34957400	6.23874700
C	-9.56377000	6.26965100	5.20610300
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C	-9.95972000	1.35271800	7.85522600
C	-11.25948400	-4.28442200	-1.48108900
C	-11.23214300	-4.80579000	-0.19951200
H	12.70723400	2.82272000	-4.94203500
H	13.00988200	4.28104100	-3.03399200
H	12.42688500	1.08211900	-6.04717700
H	13.21837800	4.89793300	-1.05823500
H	11.73049900	-5.44318100	-5.11676200
H	11.90062900	-3.31330000	-6.25419600
H	11.67287000	-6.83795300	-3.57418100
H	12.11813800	-1.26563300	-6.54983200

H	12.09738800	-7.13138500	3.03700200
H	11.85214600	-7.84849800	0.73824900
H	12.36102100	-5.87538200	4.67391400
H	11.71968700	-7.75478100	-1.33460500
H	13.37279200	4.78919100	1.35483700
H	13.41444500	4.00196600	3.27895700
H	13.20899200	0.55071700	6.05122600
H	12.95583400	-1.83251700	6.39144100
H	13.35213600	2.38282700	5.07716200
H	12.68937000	-3.85084800	5.95977900
H	-10.95394400	0.96267700	8.06684800
H	-10.69812300	3.34573000	7.72602600
H	-11.21724300	-1.06062900	7.63594700
H	-10.54995600	5.17322000	6.74222600
H	-12.04275500	-5.04836900	2.39299100
H	-11.79934300	-4.32574300	4.69005200
H	-12.17771600	-4.95778000	0.31836600
H	-11.54063700	-3.07880800	6.33847200
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H	-12.16876400	-2.65575000	-3.46888500
H	-11.77895800	1.52509100	-4.88707900
H	-12.22565000	-4.04588200	-1.92274500
H	-10.48509100	6.78315400	4.93627300
H	-10.52664900	7.56509600	3.01130900
H	-10.88847600	7.07000100	-1.37836100
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H	-10.67996900	7.67833800	0.59896400
H	-11.47012700	3.87310800	-4.38903900
C	-5.84998500	-2.87248000	10.26608500
H	-6.43351700	-2.32243700	9.52569200
C	1.79981900	2.00568900	9.97809900
H	1.03266600	1.53538200	9.36032900
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C	1.62477100	-0.44129300	-6.31764200
C	4.04061300	-0.47895200	-6.17692100
C	1.62451800	0.93553000	-6.03860200
H	0.67593200	-0.96025900	-6.46753000
C	4.04262800	0.88718400	-5.89121000
H	4.97852500	-1.03434700	-6.20489000
H	0.68589000	1.47884400	-5.94719200
H	4.98748500	1.39633300	-5.69277000
C	0.39368000	7.33359400	-0.12069200
C	1.82230200	9.02869200	-1.30219900
C	1.27121600	7.77273000	-1.22780100
C	1.40676900	6.75341300	-2.29105700
C	2.63252800	6.46752900	-2.91633200
C	0.40446800	4.94048900	-3.57914800
C	2.76484900	5.45335800	-3.87281800
H	3.52460500	7.01580800	-2.61614800
H	-0.41295400	4.25748700	-3.79273200
H	3.73692400	5.26835200	-4.32370800
C	2.83544700	1.60929500	-5.81713100
C	1.64250000	4.66822600	-4.18853900
C	2.92530900	3.08033600	-5.46341500
H	3.27383900	3.67739500	-6.32725400
H	3.67143100	3.18772200	-4.66023200
O	1.65489200	3.57847900	-5.02694000
C	0.25799300	5.97096400	-2.63530600
C	-1.00336500	6.21621500	-1.88909900
C	-2.25726100	6.10435700	-2.45599000
S	-2.56892800	5.61133800	-4.15601000
S	-3.78460000	6.51714000	-1.60125400
C	-4.30901000	5.85190100	-4.12337200
H	-4.85826300	5.64119300	-5.03865200
C	-4.85962700	6.26118700	-2.96437300
H	-5.92228900	6.42598800	-2.79895100
S	2.75382400	9.63093800	-2.71945600
C	2.22721000	11.62895000	-1.03227200
H	2.18362500	12.62913700	-0.60569600



S	1.58372600	10.30859500	-0.06046400
C	2.75651200	11.32374400	-2.23262200
H	3.20372400	12.03997900	-2.91901700
C	-0.14434700	7.11086000	2.26245000
C	-0.78039400	6.59329700	-0.46986900
C	-1.60467800	6.15739200	0.58123700
H	-2.47122500	5.54097700	0.36342400
C	-1.31158100	6.40184000	1.92652200
H	-1.96723900	5.98272100	2.68537700
C	0.70167100	7.56254600	1.22950300
H	1.63181500	8.05364100	1.51019400
O	0.26348500	7.40734100	3.53749500
C	-0.01381000	5.31315800	4.83087700
H	0.96981200	5.28196600	5.32553400
H	0.11295400	4.84732500	3.84435100
C	-1.05350100	4.50723500	5.63630000
H	-1.91193100	4.29235300	4.97725600
H	-1.44839800	5.11465400	6.46985300
C	-0.49763600	3.18310000	6.19842600
H	0.13898500	3.39669000	7.07445000
H	0.15783800	2.71318500	5.45274700
C	-1.60326400	2.18913700	6.58386700
H	-2.22164300	1.97917800	5.69728100
H	-2.27531700	2.64840700	7.33014300
C	-0.43325300	6.77959000	4.63491800
H	-0.16564500	7.38411700	5.51221300
H	-1.52419200	6.86732400	4.49508500
C	-1.05847000	0.85847600	7.14661100
C	-2.16918900	-0.10016000	7.49713400
C	-2.24364200	-1.41528400	7.22256500
O	2.10989800	-5.85819000	3.30644600
C	2.71622100	-6.06573900	2.09661300
C	3.73761900	-6.30141000	-0.53606200
C	1.84347600	-6.21325400	1.00364900
H	0.77781000	-6.12874100	1.20093800
C	4.10666200	-6.06591600	1.88080100

H	4.80525400	-5.90313700	2.69688200
C	4.59250000	-6.16903800	0.57254800
H	5.66325800	-6.05715200	0.41162100
C	2.32582600	-6.33836000	-0.30772200
C	1.42814200	-6.40438200	-1.48653900
C	4.22163800	-6.30094300	-1.93363400
C	3.34163100	-5.55567300	-2.86236800
C	1.92584200	-5.64114800	-2.65421900
C	3.83772600	-4.76337600	-3.90752200
H	4.90821400	-4.61241000	-4.03056300
C	1.09117900	-4.93525100	-3.53772300
H	0.02014200	-4.90322500	-3.35402400
C	1.58899500	-4.17600400	-4.60502000
H	0.88792900	-3.61464700	-5.21763100
C	2.97647400	-4.09541600	-4.80100200
O	3.61485000	-3.42064500	-5.81179900
C	2.82796700	-1.16109400	-6.39313600
C	2.86464400	-2.63109300	-6.76196800
C	5.32611900	-7.00950300	-2.34985400
C	0.27114200	-7.15416100	-1.50307100
S	5.88370600	-7.11292900	-4.05707900
S	6.30061200	-8.06311000	-1.26448700
S	-0.30372200	-8.15524200	-0.12367100
S	-0.78033400	-7.35239300	-2.94818600
C	7.19668300	-8.87418300	-2.54423900
H	7.87662900	-9.67106600	-2.24961700
C	7.00717600	-8.44519300	-3.80679800
H	7.51104300	-8.84403300	-4.68500400
C	-1.76703300	-8.65400100	-2.29482500
H	-2.51951900	-9.08712500	-2.95067900
C	-1.55048900	-9.01685600	-1.01612800
H	-2.10197700	-9.78831500	-0.48246000
H	3.41944100	-2.76237100	-7.70321800
H	1.85221400	-3.03138300	-6.91608600
H	-3.01022900	0.35164500	8.03536600
H	-0.36375100	0.40569900	6.42434100

H	-0.46403600	1.08457200	8.05216800
C	-1.20716500	-2.28494800	6.55183200
H	-1.71740100	-3.01047700	5.89669500
H	-3.13029300	-1.95211300	7.57678500
C	-0.35058800	-3.05849600	7.59012900
H	0.42713900	-2.37912200	7.97714700
H	-0.98379800	-3.32379900	8.45318000
C	0.29537200	-4.35430700	7.06476100
H	-0.50157100	-5.07558900	6.81246400
H	0.86713500	-4.80706000	7.89413100
C	1.22733800	-4.21540900	5.84331900
H	0.64083100	-4.03848000	4.93027800
H	1.89140700	-3.34306000	5.96595300
C	2.08177200	-5.48825300	5.68606400
H	1.43189700	-6.37864000	5.69960400
H	-0.54693000	-1.69104300	5.90759700
C	2.95648700	-5.56813500	4.43670500
H	3.49949400	-4.62419700	4.25376800
H	3.69875400	-6.37755500	4.54979700
H	2.74811400	-5.57420800	6.56074200
C	10.28771000	3.88255600	-0.75252900
C	10.41563200	2.99430400	-1.80409900
C	9.29349200	2.21589000	-2.23914900
C	7.99817600	2.70566000	-1.89261200
C	7.86438800	3.63165300	-0.79559600
C	9.03108900	4.03777900	-0.08065700
C	6.82426500	1.99973400	-2.33247200
C	6.95026100	0.61865300	-2.67084000
C	8.24478300	0.00071500	-2.55686100
C	9.42196700	0.80760800	-2.58485500
C	8.31738500	-1.33488300	-2.01793200
C	9.56495600	-1.81947300	-1.52213500
C	10.74725500	-1.15933900	-1.99188200
C	10.67766300	0.12077900	-2.50961500
C	6.56504700	3.79861400	-0.19954000
C	5.38887500	3.45025700	-0.94025400

C	5.52394200	2.52364500	-2.03527800
C	4.36618900	1.81399100	-2.47393600
C	4.49434600	0.42482600	-2.81624200
C	5.77257000	-0.19582500	-2.70334700
C	5.84534500	-1.53234100	-2.16980600
C	7.09205600	-1.97801500	-1.62329300
C	4.10362700	3.62487100	-0.34320000
C	2.92838200	3.24913300	-1.07582800
C	3.06288100	2.32494800	-2.15884100
C	1.90470800	1.61748800	-2.61241300
C	2.03318700	0.23265500	-2.96056700
C	3.31407300	-0.38900700	-2.83488300
C	3.38493200	-1.71138400	-2.30107900
C	4.63541100	-2.17521300	-1.77311700
C	1.63796800	3.42322700	-0.48050800
C	-0.55351700	1.42916100	-2.77090400
C	-0.42749800	0.04629900	-3.11609000
C	0.85784800	-0.57533000	-2.98541900
C	0.92742400	-1.89425500	-2.43222900
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C	-0.81757500	3.19804700	-0.61644800
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C	-1.85615000	1.95048000	-2.47246600
C	-3.01603400	1.24968300	-2.92480800
C	-2.88907800	-0.14477900	-3.26293100
C	-1.60853900	-0.76689400	-3.13889300
C	-1.53674700	-2.09391900	-2.58317800
C	-0.28966900	-2.53610900	-2.03327400
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C	-5.48459500	1.05641200	-3.05538200
C	-5.35768800	-0.33668400	-3.39422900
C	-4.07020500	-0.95914500	-3.26591000
C	-3.99763800	-2.28133200	-2.71899400
C	-2.74724900	-2.74077700	-2.18688000

C	-5.74165900	2.84574400	-0.90534700
C	-6.91146700	2.48732000	-1.64047000
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C	-7.94461100	0.85434300	-3.17454100
C	-7.81892400	-0.52551000	-3.51190100
C	-6.53221600	-1.14769500	-3.40534200
C	-6.45915200	-2.47762200	-2.85838700
C	-5.21534600	-2.93170200	-2.32497600
C	-8.20174000	2.64242500	-1.03505500
C	-9.38670700	2.28859700	-1.77086100
C	-9.25426900	1.36723700	-2.87178700
C	-10.41272800	0.68851100	-3.35637800
C	-10.28438800	-0.71918100	-3.70151000
C	-9.00776000	-1.33541600	-3.53414800
C	-8.93462600	-2.66776500	-2.98869100
C	-7.67701600	-3.11363400	-2.45029900
C	-10.67366000	2.50217900	-1.19148400
C	-11.80964000	2.16528900	-1.99866000
C	-11.68251600	1.28113500	-3.05350300
C	-10.14058800	-3.34160200	-2.62933500
C	-11.35030000	-2.86949500	-3.23666500
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C	-7.68645100	-3.86815700	-1.24035400
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C	-6.47787400	-3.96254100	-0.47546600
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C	-7.85957800	-3.68306000	1.54905700
C	-9.04234300	-4.05186900	0.81749100
C	-10.32548300	-3.92367700	1.42958800
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C	-11.36979700	-4.44339100	-0.71866600
C	-7.99271100	-2.77369400	2.63921600
C	-9.30316400	-2.26814600	2.95138400
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C	-5.39839000	-3.50807900	1.69532100
C	-5.53256100	-2.59202500	2.79723800
C	-6.82874900	-2.07914900	3.10532800
C	-6.95661100	-0.68662500	3.44853500
C	-8.24062200	-0.06573600	3.30503200
C	-9.43083300	-0.87371400	3.29351500
C	-10.71240600	-0.25025600	3.21385700
C	-11.85499700	-1.11524600	3.25082200
C	-11.73266800	-2.45244700	2.92288400
C	-8.31100900	1.25134800	2.76304700
C	-9.56871000	1.70836600	2.23483600
C	-10.78417200	1.09472700	2.66339200
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C	-5.85365700	1.45210200	2.91944100
C	-7.09499600	1.90591500	2.38030200
C	-7.08314900	2.66649600	1.15738400
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C	-9.55749000	2.47179900	1.01206500
C	-10.76263300	2.59815300	0.25762600
C	-11.99128900	2.36398700	0.95804200
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C	-4.63417300	2.09333600	2.51862000
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C	-3.31460400	0.31392500	3.61531900
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C	-0.46960600	-3.11361800	1.97393700
C	-0.29855100	-3.29394800	-0.82056400
C	-0.85309100	0.50588600	3.73595700
C	-0.92409700	1.82259300	3.18827500
C	-0.90529800	3.28464400	0.80360700
C	0.56134700	-1.49889400	3.52300500
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C	0.82097700	-3.27495700	1.37448000
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C	0.29130700	2.46951400	2.78920900
C	0.29904300	3.23178300	1.57438200
C	1.85799000	-2.00649500	3.21104000
C	1.98939200	-2.91563400	2.10889000
C	2.15855900	-3.10247900	-0.68278200
C	1.60831500	0.70373400	3.88572600
C	1.53551700	2.02930000	3.33149600
C	1.54897800	3.52236400	0.95129600
C	3.02192800	-1.30071400	3.66203400
C	2.89551500	0.08359900	4.00371800
C	3.27705700	-3.08189700	1.50590600
C	3.36367400	-3.18134100	0.08414000
C	2.74917600	2.68130200	2.93391500
C	2.75599700	3.44398100	1.72106600
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C	4.45477600	-2.72942800	2.24526900
C	4.62368900	-2.92837600	-0.55026500
C	4.07621600	0.90074600	4.01913600
C	4.00125900	2.23076600	3.47364400
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C	5.21082300	2.87661500	3.07612500
C	5.21825000	3.64096600	1.85535500
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C	6.91270300	-2.53204700	2.37699500
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C	6.53768700	1.09178300	4.13218400
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C	7.68701400	3.06073700	3.20787100
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H	11.05169000	4.49370900	1.83865900
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H	11.60370600	0.66068100	-2.70502000
H	11.72629100	-1.59410500	-1.79265200
H	11.71149200	-2.75880000	0.05422100
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**(6,6)@Cycle-6**

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H	12.70552000	1.91916900	4.19743200
H	12.70731300	-0.47453900	4.62226900
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H	12.58414400	-3.61896200	-2.35331400
H	12.61838400	-4.44340200	-0.06613400
H	12.65440000	-4.06022700	2.04034600
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C	11.72522700	3.67952000	2.32107200
C	11.75206200	1.39438600	4.24334000
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C	11.61480200	-0.08701400	-3.98737000
C	11.61531900	-1.44875900	-3.74551900

C	11.63935700	-3.73464400	-1.82353000
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C	10.43011200	2.05191400	-3.34669700
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C	10.53441600	3.18688100	2.94242800
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C	10.54962700	-0.73328200	4.37683600
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C	10.43167800	-3.23584000	-2.40610300
C	10.47189100	-4.20203300	0.27612500
C	10.49627400	-3.94287400	1.70631900
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C	9.20472100	2.61336700	-2.87392200
C	9.22446700	3.54277200	-1.77590200
C	9.27027000	4.04362300	0.99061300
C	9.29118600	3.55615500	2.34395900
C	9.31640400	1.40534700	4.15483100
C	9.31759900	-0.01112800	4.40632800
C	9.18331200	-0.03162400	-3.82952400
C	9.18384700	-1.44823800	-3.57851300
C	9.20659800	-3.59897800	-1.76771700
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C	4.22382200	-1.43711400	-3.51618400

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C	3.10000900	3.17013400	3.03739600
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H	-11.41385500	1.96653200	4.56947700
H	-11.41261200	-0.42519100	5.00410800
H	-11.54313600	0.47528200	-3.78352000
H	-11.54208000	-1.91614000	-3.34814400
H	-11.52440800	-3.55159200	-1.96788800
H	-11.49081500	-4.37930500	0.31772600
H	-11.45698900	-4.00729800	2.42516700
H	-11.42588400	-2.44147400	4.28476700
C	0.19592800	0.31213000	-6.69294800
C	-2.09318000	1.08419000	-6.68010900
C	-0.23688700	-1.02099600	-6.67989300
H	1.26617300	0.52265700	-6.65667700
C	-2.52639700	-0.24873600	-6.66206900
H	-2.81893900	1.89386300	-6.62617200
H	0.48873700	-1.83140500	-6.63174500
H	-3.59631800	-0.45808200	-6.60680800
C	-1.71540600	-7.24439200	-0.70105400
C	-3.71536100	-8.25616400	-1.82143400
C	-2.67461800	-7.35474100	-1.82567600
C	-2.34463600	-6.48316200	-2.97518700
C	-3.32070500	-5.82891900	-3.74734000
C	-0.64709800	-5.27049100	-4.25507100
C	-2.99548100	-4.92306900	-4.76329500
H	-4.37370400	-5.96462700	-3.50816100
H	0.38273600	-4.95396800	-4.40266300
H	-3.80189400	-4.44651000	-5.31435900
C	-1.60990100	-1.31554100	-6.61631400
C	-1.64589600	-4.59328300	-4.98364300



C	-2.16453000	-2.72133600	-6.44304900
H	-2.46982300	-3.16172800	-7.40990300
H	-3.06096100	-2.63351900	-5.81235900
O	-1.19963400	-3.59766500	-5.82619800
C	-0.96782200	-6.22276600	-3.26817200
C	0.05503600	-6.92747600	-2.45022400
C	1.21832700	-7.42707000	-2.99818800
S	1.66981600	-7.26636800	-4.73235900
S	2.40654800	-8.43098300	-2.09594800
C	3.01250500	-8.40165700	-4.68958700
H	3.52119400	-8.60718900	-5.62931000
C	3.34720800	-8.92847000	-3.49626900
H	4.16697200	-9.62320100	-3.32503700
S	-4.78962500	-8.56221300	-3.23162900
C	-5.20827900	-10.38773400	-1.33519700
H	-5.60902500	-11.25433100	-0.81305900
S	-4.07519400	-9.36890300	-0.45438000
C	-5.53284800	-10.02347300	-2.59055700
H	-6.23452400	-10.55009000	-3.23428400
C	-1.19071900	-7.08827400	1.69499100
C	-0.32740400	-7.10733900	-1.02587000
C	0.58563700	-7.05727300	0.04504700
H	1.64323700	-6.90230200	-0.15550200
C	0.18101200	-7.07249800	1.38716400
H	0.93027000	-6.99171600	2.17163800
C	-2.12352800	-7.20358900	0.64236300
H	-3.18124900	-7.16827200	0.89646400
O	-1.72224500	-6.95447700	2.95066700
C	-1.79797900	-5.77043600	5.04893100
H	-2.42839400	-6.50987700	5.56717600
H	-2.47510600	-5.12966100	4.46923200
C	-1.04425400	-4.88395200	6.07076900
H	-0.28460700	-4.29319900	5.53589900
H	-0.49951100	-5.50538000	6.80138400
C	-2.00216400	-3.91108700	6.79978100
H	-2.63865200	-4.47274400	7.50490700

H	-2.68743800	-3.48283000	6.05428900
C	-1.31728600	-2.74536000	7.55111400
H	-0.51907500	-2.31386900	6.92529500
H	-0.83066300	-3.12066200	8.46709000
C	-0.88456900	-6.47740000	4.03642100
H	-0.34338900	-7.33039800	4.48146400
H	-0.14394800	-5.76458100	3.64558200
C	-2.33313600	-1.61968900	7.90920800
C	-1.88836500	-0.66520700	8.99592800
C	-1.50649700	0.62405300	8.89030700
O	-1.23736000	7.03330500	2.99064200
C	-1.69020100	7.13475100	1.70016100
C	-2.39601400	7.06288800	-1.06365900
C	-0.69898100	7.22733300	0.70095900
H	0.34214300	7.21080800	1.01715500
C	-3.04067700	7.09524200	1.31465500
H	-3.83382000	7.02688600	2.05591000
C	-3.36752500	7.02264900	-0.04630700
H	-4.40931000	6.84403400	-0.30185100
C	-1.02880100	7.23142200	-0.66507400
C	-0.01431600	7.36699000	-1.73747100
C	-2.69871900	6.87657200	-2.50411900
C	-1.61844800	6.20299600	-3.26990000
C	-0.26512900	6.50513100	-2.91387800
C	-1.86610000	5.25155900	-4.27654600
H	-2.87714300	4.90089800	-4.46981800
C	0.76355200	5.89467600	-3.65254100
H	1.80045300	6.05718400	-3.36536000
C	0.51117100	5.00097200	-4.69975500
H	1.35399600	4.55817200	-5.22402200
C	-0.81470900	4.63140300	-4.98205200
O	-1.19212800	3.64068400	-5.86079400
C	-0.72212000	1.37987700	-6.64462300
C	-0.18758700	2.79251800	-6.45509800
C	-3.83830800	7.35675300	-3.11599400
C	1.00423700	8.29343300	-1.67345500

S	-4.17933200	7.20326800	-4.87668900
S	-5.09918100	8.33095000	-2.28220900
S	1.27176000	9.40345500	-0.28311200
S	2.13596300	8.64035500	-3.02829300
C	-5.94692000	8.84086000	-3.73687300
H	-6.78098800	9.52858300	-3.61279500
C	-5.52927100	8.33040900	-4.91096000
H	-5.97537500	8.54393600	-5.88027300
C	2.80803300	10.11591300	-2.34381500
H	3.52498900	10.66568900	-2.95025600
C	2.41560300	10.46062400	-1.10250300
H	2.76816600	11.33259400	-0.55516700
H	0.13381700	3.24510100	-7.41093400
H	0.69326400	2.72096400	-5.80043200
H	-1.90071300	-1.09359700	10.00467500
H	-2.58653000	-1.07359600	6.99176700
H	-3.26604400	-2.10411800	8.25075400
C	-1.29836000	1.44466800	7.64039500
H	-0.21549300	1.65907700	7.56739000
H	-1.25418900	1.14536600	9.82137600
C	-2.06104300	2.80506400	7.57129300
H	-3.04777700	2.62943400	7.11332700
H	-2.25421300	3.18227300	8.58912800
C	-1.28345700	3.87555600	6.75617800
H	-0.65750100	3.36743300	6.01014600
H	-0.58203100	4.40446400	7.42363400
C	-2.15778300	4.89894200	6.00035900
H	-2.88058000	4.34168400	5.38243400
H	-2.75089300	5.50242300	6.70813500
C	-1.30798900	5.81297400	5.08283100
H	-0.56805200	5.19250200	4.55879800
H	-1.54934200	0.85195500	6.75527900
C	-2.13972800	6.52469400	4.00705800
H	-2.83395600	5.80397400	3.55234100
H	-2.73199300	7.35855700	4.42233800
H	-0.74425400	6.54705000	5.67933600

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C	-1.85997400	-0.45465000	-7.07885900
C	0.47703100	-0.94056900	-7.08591300
C	-1.59673600	0.93541800	-7.07560300
H	-2.90403200	-0.76969800	-7.03783500
C	0.73946900	0.44865000	-7.09058200
H	1.32005900	-1.63042100	-7.05413600
H	-2.43965600	1.62514500	-7.03519300
H	1.78389400	0.76373900	-7.05861100
C	0.09764100	7.60019300	-0.93503800
C	2.16038900	8.40034600	-2.11447900
C	1.03858700	7.59347000	-2.10017100
C	0.61606300	6.76970500	-3.27781500
C	1.51781700	6.12329500	-4.15223500
C	-1.16412500	5.61146200	-4.52375000
C	1.12646300	5.22391100	-5.16209400
H	2.58769000	6.21885000	-3.98340000
H	-2.20848100	5.32053400	-4.60980300
H	1.90546400	4.73475900	-5.74319200
C	-0.27922100	1.43061300	-6.99276400
C	-0.22897800	4.87683400	-5.30652700
C	0.16710300	2.92299000	-6.82193900
H	0.31089800	3.37977100	-7.81619100
H	1.14186300	2.88756700	-6.31732100
O	-0.73273500	3.81464900	-6.07168200
C	-0.77932600	6.55549800	-3.52748800
C	-1.73626200	7.31636600	-2.66146400
C	-2.90496600	7.84556600	-3.17929100
S	-3.45389800	7.61414500	-4.87704200
S	-3.99466500	8.96595900	-2.28765200
C	-4.73603400	8.81572900	-4.83963600
H	-5.28194900	8.99044500	-5.76458000
C	-4.98223900	9.42790600	-3.66578700
H	-5.75786200	10.17187000	-3.49563300
S	3.22871200	8.63686800	-3.54282200

C	3.87222600	10.36850500	-1.62600800
H	4.37026400	11.17701600	-1.09457100
S	2.65502500	9.45668000	-0.74412200
C	4.13363400	9.99795100	-2.89381900
H	4.87463200	10.45896900	-3.54371700
C	-0.40707100	7.55930300	1.51461000
C	-1.29823200	7.55699000	-1.24678700
C	-2.18862200	7.63721000	-0.14977400
H	-3.25910000	7.56278800	-0.32271600
C	-1.77473900	7.66546100	1.19207300
H	-2.53080000	7.65489100	1.97443500
C	0.51088800	7.58541800	0.42800200
H	1.56613100	7.47516200	0.66619300
O	0.10296000	7.34584100	2.79285400
C	-0.00618400	6.30973000	5.11097700
H	0.50232400	7.10378900	5.67919300
H	0.78709300	5.69311500	4.67733900
C	-0.86343500	5.41991800	6.12837700
H	-1.66707500	4.91057600	5.58028000
H	-1.36332600	6.09174900	6.84557000
C	-0.02604500	4.33265600	6.92530600
H	0.71839500	4.86744800	7.53751400
H	0.55733100	3.77390600	6.18919300
C	-0.78061200	3.27973000	7.88692000
H	-1.86845300	3.36043400	7.73190800
H	-0.59502700	3.57957200	8.93069500
C	-0.79702700	6.97247000	3.91583700
H	-1.31212900	7.88650900	4.25370200
H	-1.55173000	6.27891300	3.53453800
C	-0.36786500	1.74716600	7.67986400
C	-0.24833400	0.69752200	8.80149500
C	-0.43320700	-0.66190600	8.85653600
O	-1.14917700	-7.31913300	2.80613100
C	-0.63310300	-7.53918400	1.53210100
C	0.25685000	-7.54058400	-1.23128500
C	-1.55036300	-7.56894500	0.44607600

H	-2.60564600	-7.45611400	0.68382900
C	0.73459300	-7.65044600	1.20910000
H	1.49058200	-7.63819700	1.99165700
C	1.14826200	-7.62542000	-0.13398300
H	2.21869700	-7.55015300	-0.30590300
C	-1.13850600	-7.58733100	-0.91579800
C	-2.08522600	-7.58644700	-2.07418800
C	0.68662600	-7.29596400	-2.64893800
C	-0.28136700	-6.54447800	-3.51369900
C	-1.67439600	-6.76189000	-3.25299900
C	0.08893800	-5.60428800	-4.52019900
H	1.13123400	-5.31264700	-4.62330000
C	-2.58793200	-6.12125000	-4.11956000
H	-3.65544200	-6.22047500	-3.93811800
C	-2.21039700	-5.22543700	-5.13688000
H	-2.99668800	-4.74032400	-5.71139600
C	-0.85741400	-4.87485900	-5.29538600
O	-0.36675400	-3.81244000	-6.06700600
C	-0.83995400	-1.43558200	-6.99061700
C	-1.27735400	-2.92933800	-6.81610600
C	1.86089000	-7.81157000	-3.16991400
C	-3.20133600	-8.40205400	-2.08192900
S	2.40100800	-7.57786700	-4.86974600
S	2.96896000	-8.91406000	-2.27945900
S	-3.67783900	-9.46389900	-0.70975900
S	-4.27476800	-8.64788200	-3.50441100
C	3.96479200	-9.35899900	-3.65668600
H	4.75487400	-10.08730300	-3.48538500
C	3.70620600	-8.75377200	-4.83146800
H	4.25490400	-8.91894900	-5.75649400
C	-5.16117600	-10.01954600	-2.85238300
H	-5.90034100	-10.48806900	-3.49899300
C	-4.88926700	-10.38835400	-1.58620300
H	-5.37566700	-11.20272800	-1.05294100
H	-1.42060700	-3.39064600	-7.80820400
H	-2.25021900	-2.89917500	-6.30777400

H	0.23986300	1.09584400	9.70072500
H	-1.04292800	1.34427600	6.93371700
H	0.63974400	1.76636600	7.23532700
C	-1.13090400	-1.77222800	8.02526200
H	-1.95785600	-2.13128100	8.66635700
H	-0.06784500	-1.08535300	9.80149000
C	-0.27675300	-3.06731800	7.63536900
H	0.55132100	-2.75636400	6.98730000
H	0.18891800	-3.45542900	8.55701600
C	-1.08271400	-4.25338500	6.93536100
H	-1.81539300	-3.81817700	6.24892600
H	-1.67472500	-4.76876500	7.71005500
C	-0.24840700	-5.34796200	6.12955100
H	0.54706800	-4.83702900	5.57359000
H	0.26618000	-6.00336900	6.85113200
C	-1.08070100	-6.26828200	5.11738800
H	-1.89213700	-5.68102100	4.67681300
H	-1.61005700	-1.36044800	7.13589400
C	-0.26322100	-6.91191800	3.92755100
H	0.46988300	-6.19778300	3.54135400
H	0.28049100	-7.80650700	4.27267600
H	-1.56461800	-7.07702700	5.68621500
H	12.31203300	4.80921000	-0.86217400
H	12.33461200	4.80119900	1.56503700
H	12.33619100	3.86956700	3.46453400
H	12.32125700	1.95556200	4.95722400
H	12.29722100	-0.10738000	5.40785700
H	12.26171700	-2.47175900	4.86199100
H	12.22868300	-4.12662500	3.54732400
H	12.19482500	-5.18528400	1.36337700
H	12.27924000	3.89010000	-2.76615200
H	12.23790100	1.98795200	-4.27299900
H	12.20576600	-0.06979200	-4.74485300
H	12.17926800	-2.44048100	-4.22704200
H	12.16924400	-4.10931100	-2.92952000
H	12.17532200	-5.18175400	-0.75201700

C	11.36232400	4.75586600	-0.33168500
C	11.37528100	4.75131500	1.05181600
C	11.37864400	3.42917500	3.73907700
C	11.37010000	2.33794000	4.58952200
C	11.33576000	-0.58768700	5.23177000
C	11.31550700	-1.93567200	4.92067200
C	11.26851100	-4.28091900	3.05700200
C	11.24913900	-4.88471300	1.81231000
C	11.31684700	3.45204400	-3.02714100
C	11.29325400	2.36730200	-3.88581700
C	11.24730300	-0.55211200	-4.55807000
C	11.23217000	-1.90392000	-4.26312800
C	11.21810400	-4.26712700	-2.42292900
C	11.22160500	-4.87865500	-1.18184400
C	10.15338500	4.53305100	-1.05959200
C	10.17990700	4.52365000	1.80024700
C	10.18145000	3.87976100	3.10321000
C	10.16388700	1.62231100	4.86112200
C	10.14730200	0.20269700	5.17262600
C	10.10522800	-2.58598900	4.52979200
C	10.08240100	-3.72447700	3.62641000
C	10.04242800	-4.97299600	1.05266800
C	10.13130600	3.89772000	-2.36672800
C	10.08266000	1.65392300	-4.14221900
C	10.06039000	0.23747200	-4.46860000
C	10.02891100	-2.55877700	-3.85869700
C	10.02192800	-3.70651300	-2.96660500
C	10.02899200	-4.97039700	-0.40079700
C	8.92708400	4.65587300	-0.33673000
C	8.94058300	4.65120600	1.10066300
C	8.94388200	3.39792800	3.63037600
C	8.93501900	2.26253600	4.51198900
C	8.90266300	-0.49707500	5.11866800
C	8.88169100	-1.89801100	4.79686800
C	8.83722900	-4.11121100	3.04186700
C	8.81696500	-4.73923200	1.74893800



C	8.88432000	3.41903100	-2.87449200
C	8.86014500	2.29062600	-3.76503900
C	8.81669400	-0.46297200	-4.40080400
C	8.80083600	-1.86784400	-4.09550700
C	8.78747400	-4.09855800	-2.36332700
C	8.79091400	-4.73413700	-1.07399200
C	7.67094300	4.50605400	-1.01985500
C	7.69749300	4.49739100	1.80604900
C	7.69918800	3.86227800	3.08094900
C	7.68148000	1.62633900	4.81346600
C	7.66533100	0.23516600	5.11948800
C	7.62399700	-2.52259200	4.48880800
C	7.60149400	-3.63911600	3.60454000
C	7.56171600	-4.87358800	1.06055500
C	7.64943700	3.87916400	-2.29912100
C	7.60160400	1.65735300	-4.05086400
C	7.57970400	0.26916300	-4.37204600
C	7.54858800	-2.49630100	-3.77226700
C	7.54136500	-3.62277600	-2.89995000
C	7.54820800	-4.87180100	-0.36395300
C	6.44217300	4.70348900	-0.31246700
C	6.45566900	4.70025700	1.12307800
C	6.45865600	3.43548400	3.65325700
C	6.44963400	2.29858200	4.52974500
C	6.41755300	-0.46614400	5.14020000
C	6.39675100	-1.86596800	4.82270700
C	6.35208100	-4.08437800	3.06600000
C	6.33173000	-4.71093900	1.77421300
C	6.39900500	3.45601000	-2.85190000
C	6.37550600	2.32720600	-3.73946200
C	6.33192900	-0.43211300	-4.37917000
C	6.31583800	-1.83599400	-4.07620800
C	6.30193300	-4.07393300	-2.34362400
C	6.30512800	-4.70813900	-1.05524300
C	5.19745900	4.56714800	-0.99932900
C	5.22478100	4.56414700	1.83408200

C	5.22670100	3.91736100	3.11491700
C	5.20836600	1.66731700	4.84500400
C	5.19212900	0.26650000	5.15609700
C	5.15114900	-2.50101500	4.53219100
C	5.12874200	-3.62576500	3.64159000
C	5.08849500	-4.86038800	1.08756900
C	5.17617100	3.92944400	-2.28483500
C	5.12928800	1.69933200	-4.04168100
C	5.10704100	0.30122100	-4.36595200
C	5.07571100	-2.47427400	-3.76924200
C	5.06779500	-3.61000800	-2.89206100
C	5.07446300	-4.86017400	-0.34727800
C	3.96738800	4.75191900	-0.28451500
C	3.98071000	4.75599400	1.14513100
C	3.98413900	3.47273200	3.67603800
C	3.97552000	2.33513700	4.54253300
C	3.94333200	-0.43943300	5.16507700
C	3.92224600	-1.83494800	4.85373400
C	3.87782700	-4.05926100	3.08949500
C	3.85739700	-4.67921600	1.80136400
C	3.92457900	3.48539200	-2.82471900
C	3.90223500	2.36538600	-3.71435100
C	3.85781900	-0.40383300	-4.35366000
C	3.84149600	-1.80349500	-4.05890900
C	3.82647200	-4.04725800	-2.32050500
C	3.82957300	-4.67641200	-1.03703800
C	2.71903300	4.58747100	-0.96672700
C	2.74546800	4.60262500	1.85393200
C	2.74906800	3.94942300	3.12781200
C	2.73196300	1.69073200	4.83801900
C	2.71487400	0.29569200	5.15850900
C	2.67299400	-2.46592300	4.54694100
C	2.65097400	-3.58590700	3.65537200
C	2.61167500	-4.80999000	1.10860000
C	2.69985700	3.93423800	-2.23729400
C	2.65398800	1.72720400	-3.99871500

C	2.63139000	0.33142600	-4.31200000
C	2.59870500	-2.43447400	-3.73449300
C	2.58988500	-3.56396000	-2.85518100
C	2.59737100	-4.80611600	-0.32148700
C	1.49250800	4.73697300	-0.25654700
C	1.50473400	4.75083400	1.16488000
C	1.51245100	3.47470800	3.65288300
C	1.50593300	2.33298800	4.49821600
C	1.47090700	-0.40132300	5.13068400
C	1.44891200	-1.78995400	4.82415800
C	1.40642600	-3.98077300	3.08107200
C	1.38621900	-4.60178200	1.80351900
C	1.45497400	3.46845200	-2.74789800
C	1.43149800	2.36869300	-3.64216000
C	1.38864800	-0.36139900	-4.24945800
C	1.37122200	-1.75243800	-3.98076500
C	1.35579600	-3.95251800	-2.25680500
C	1.35767500	-4.58694600	-0.99007200
C	0.24357100	4.55033200	-0.92411600
C	0.26588700	4.56771100	1.85295800
C	0.26901100	3.92159700	3.10500200
C	0.25818700	1.69246700	4.75534400
C	0.24240200	0.32059500	5.06933800
C	0.19539300	-2.38802900	4.48435500
C	0.17214800	-3.49443900	3.61375500
C	0.13366600	-4.72398100	1.12309300
C	0.22598200	3.90934900	-2.17653500
C	0.17926800	1.73788100	-3.90564300
C	0.15798000	0.36180200	-4.19827700
C	0.12433500	-2.35500000	-3.63713100
C	0.11457400	-3.45769600	-2.76436200
C	0.12057600	-4.70944600	-0.28540800
C	-0.99284500	4.72693300	-0.23533300
C	-0.98143300	4.73392600	1.17683800
C	-0.97239100	3.48770100	3.65723600
C	-0.97811000	2.36146700	4.50975000

C	-1.01201600	-0.35426600	5.07985800
C	-1.03505000	-1.73109100	4.77601900
C	-1.08049800	-3.92012000	3.07949900
C	-1.10123100	-4.55406400	1.81932600
C	-1.02591200	3.49149800	-2.72001400
C	-1.04950200	2.39116000	-3.60194900
C	-1.09272800	-0.31644000	-4.19480800
C	-1.10964800	-1.69974500	-3.91931100
C	-1.12960200	-3.87872100	-2.20516200
C	-1.12695500	-4.52694800	-0.95325100
C	-2.23727800	4.59677100	-0.91598800
C	-2.21782300	4.59338800	1.87248100
C	-2.21350800	3.96550500	3.14540600
C	-2.22209900	1.76033800	4.85748000
C	-2.23937900	0.36704700	5.14348600
C	-2.28616900	-2.35511100	4.51490200
C	-2.30974700	-3.47769400	3.64786100
C	-2.34779300	-4.72582700	1.15309500
C	-2.25574400	3.97390100	-2.18704200
C	-2.29802200	1.79307300	-3.93015100
C	-2.31965900	0.40536700	-4.21399500
C	-2.35358500	-2.33018200	-3.64121000
C	-2.36296400	-3.43552300	-2.75235900
C	-2.36049000	-4.70767700	-0.26701500
C	-3.46950200	4.80128500	-0.22344100
C	-3.45904700	4.79776300	1.19882700
C	-3.45106300	3.56175100	3.73618700
C	-3.45586200	2.43959200	4.61367500
C	-3.48669200	-0.32704400	5.19876500
C	-3.51005300	-1.71350600	4.87494000
C	-3.55866600	-3.94613400	3.13878200
C	-3.57799500	-4.58281200	1.86463100
C	-3.50226500	3.58721400	-2.76826800
C	-3.52463100	2.47212700	-3.65509700
C	-3.56719100	-0.28763600	-4.26143100
C	-3.58501000	-1.68050400	-3.96534900

C	-3.60263000	-3.89914300	-2.21847500
C	-3.60110100	-4.55318400	-0.95551000
C	-4.71448400	4.68557600	-0.92046700
C	-4.69363400	4.67066800	1.91306500
C	-4.69041000	4.04301100	3.20105500
C	-4.70096100	1.80956300	4.94487400
C	-4.71640700	0.40785400	5.24358700
C	-4.76100900	-2.35648400	4.60156100
C	-4.78569100	-3.48589200	3.71972600
C	-4.82739100	-4.73993500	1.17882700
C	-4.73216800	4.06882300	-2.21346400
C	-4.77501800	1.84794400	-3.97205300
C	-4.79632000	0.44799300	-4.28145500
C	-4.83139000	-2.32237700	-3.66968800
C	-4.83931400	-3.45069400	-2.78473000
C	-4.83914000	-4.72705300	-0.25415400
C	-5.94178800	4.86095800	-0.21142300
C	-5.93118100	4.85164000	1.22438500
C	-5.92546900	3.60527100	3.76774500
C	-5.93083800	2.47360000	4.65142500
C	-5.95992500	-0.29422200	5.25154200
C	-5.98253000	-1.69314600	4.92720000
C	-6.03219000	-3.92049900	3.17637600
C	-6.05312700	-4.55390900	1.88761600
C	-5.97709600	3.63807200	-2.76453400
C	-5.99918700	2.51116700	-3.65461600
C	-6.04069700	-0.25294000	-4.27806900
C	-6.05816900	-1.65503800	-3.96549200
C	-6.07596300	-3.89248800	-2.22593600
C	-6.07551200	-4.53716000	-0.94212200
C	-7.18727500	4.70721500	-0.89930800
C	-7.16545100	4.68939800	1.93080300
C	-7.16258700	4.06098200	3.21013000
C	-7.17446600	1.83183500	4.95344100
C	-7.18914700	0.43962500	5.25743900
C	-7.23268700	-2.31903100	4.62005700

C	-7.25752800	-3.43790400	3.73745400
C	-7.29927300	-4.67658000	1.19422200
C	-7.20507200	4.09051000	-2.18430800
C	-7.24776300	1.87219800	-3.94148900
C	-7.26886400	0.48182500	-4.25620100
C	-7.30267800	-2.28253300	-3.63865500
C	-7.31137500	-3.40838000	-2.76427700
C	-7.31064600	-4.66920700	-0.23082600
C	-8.42633800	4.88709100	-0.19207500
C	-8.41541800	4.87788000	1.24593200
C	-8.40986100	3.63115300	3.78138700
C	-8.41582700	2.49920600	4.66802900
C	-8.44502900	-0.26039100	5.27644100
C	-8.46715700	-1.66133900	4.95313800
C	-8.51638000	-3.87558400	3.19786200
C	-8.53745700	-4.50312300	1.90441600
C	-8.46188300	3.66491800	-2.73808900
C	-8.48371900	2.53825100	-3.63148900
C	-8.52521400	-0.21774400	-4.25788300
C	-8.54236900	-1.62137300	-3.94440300
C	-8.56087000	-3.85115700	-2.20742600
C	-8.56038300	-4.49030200	-0.91918100
C	-9.66810600	4.80160800	-0.89379600
C	-9.64566400	4.78450000	1.96697500
C	-9.64277900	4.14260600	3.27131600
C	-9.65492000	1.89115900	5.03763100
C	-9.66969500	0.47209600	5.35241700
C	-9.71364500	-2.31615700	4.70930500
C	-9.73924600	-3.45378900	3.80462800
C	-9.78120000	-4.69785100	1.22878400
C	-9.68639200	4.17284500	-2.20436800
C	-9.72934300	1.93314900	-3.98429500
C	-9.75066700	0.51570300	-4.30701700
C	-9.78459300	-2.27794600	-3.68397900
C	-9.79402800	-3.42395600	-2.78951600
C	-9.79288000	-4.69168700	-0.22494000

C	-10.85757800	5.05418400	-0.14402800
C	-10.84689400	5.04601900	1.23953900
C	-10.84084300	3.72430800	3.92714000
C	-10.84666000	2.63603600	4.78152600
C	-10.87720400	-0.28645900	5.43476100
C	-10.89840000	-1.63444900	5.12387200
C	-10.95094500	-3.97423800	3.25544500
C	-10.97127300	-4.57532600	2.00939000
C	-10.89523300	3.76041900	-2.84375900
C	-10.91599100	2.67755900	-3.70487000
C	-10.95988500	-0.24186000	-4.37220100
C	-10.97630800	-1.59227400	-4.07125700
C	-10.99620400	-3.95040700	-2.22516800
C	-10.99576500	-4.56310800	-0.98470100
H	-11.81458000	5.13505900	-0.65767400
H	-11.79560100	5.12114400	1.76915300
H	-11.79134100	4.18719500	3.66548800
H	-11.80156100	2.27865900	5.16432100
H	-11.82208800	0.21895700	5.62933300
H	-11.85931300	-2.14551600	5.08406900
H	-11.89754600	-3.79270900	3.76250100
H	-11.93325000	-4.84636400	1.57655700
H	-11.84097500	4.22216800	-2.56339900
H	-11.87736800	2.32342500	-4.07434100
H	-11.90806800	0.26535800	-4.54492900
H	-11.93685000	-2.10278000	-4.01737200
H	-11.95117200	-3.76471800	-2.71477300
H	-11.95028300	-4.83882600	-0.53848600

**(5,5)@Cycle-8**

C	-1.45498200	1.90266900	7.13082000
C	0.79586700	2.38696400	6.37068600
C	-1.26323900	0.54503500	6.85410000
H	-2.41388700	2.24810200	7.52406200
C	0.98490300	1.02913600	6.08330500
H	1.58240200	3.11158700	6.16127800

H	-2.06814500	-0.17128900	7.01493200
H	1.92660400	0.69130400	5.64998800
C	-2.04396400	-7.10771000	2.06564800
C	-0.92559100	-8.29631300	3.97449700
C	-1.34030600	-7.13735800	3.36473400
C	-1.21599200	-5.79870500	3.97693800
C	-0.03801200	-5.35871700	4.60539200
C	-2.18486700	-3.60447800	4.39312700
C	0.08226000	-4.07396100	5.15111100
H	0.82739600	-6.01994900	4.63302100
H	-2.95261500	-2.84969800	4.24919300
H	1.01748700	-3.76575700	5.61274000
C	-0.03656300	0.09680500	6.33181400
C	-1.00741200	-3.19593900	5.04248300
C	0.18732600	-1.37057600	6.05671000
H	0.40435800	-1.92711300	6.98819700
H	1.04008000	-1.50964300	5.37234800
O	-1.01312800	-1.89467700	5.46826400
C	-2.31791900	-4.89125600	3.85066500
C	-3.50474700	-5.32727000	3.06882300
C	-4.79785500	-4.94456400	3.36815500
S	-5.25115300	-3.84040000	4.71228400
S	-6.25372300	-5.56522900	2.51239300
C	-6.98989500	-3.94427200	4.48837700
H	-7.61431800	-3.35369700	5.15547200
C	-7.44366500	-4.72345800	3.48822700
H	-8.48977800	-4.85102700	3.21845400
S	-0.20037700	-8.35732100	5.62014300
C	-0.75018100	-10.81884000	4.75064900
H	-0.84752700	-11.90243700	4.72709500
S	-1.16831600	-9.93939400	3.28336200
C	-0.31290200	-10.10530600	5.80608600
H	-0.00485900	-10.52679800	6.76085000
C	-2.26420900	-7.76345500	-0.27927800
C	-3.15951100	-6.22443100	1.93378600
C	-3.81368900	-6.17726500	0.68624400



H	-4.65033100	-5.50278800	0.54328500
C	-3.38874900	-6.93154700	-0.40835200
H	-3.91238100	-6.85968200	-1.36105000
C	-1.60133200	-7.84740300	0.95272800
H	-0.70339900	-8.45986500	1.01354800
O	-1.80011800	-8.52759100	-1.32797300
C	0.75830700	6.59763600	-1.76184400
C	0.61153800	7.43520600	0.93123600
C	-0.42943500	6.42602000	-1.02771900
H	-1.24262900	5.90148200	-1.51802600
C	1.88265300	7.18098700	-1.15131600
H	2.82028100	7.29698900	-1.68979400
C	1.79092600	7.59165200	0.18429000
H	2.67556200	8.00495400	0.66833400
C	-0.51956200	6.80676900	0.31886900
C	-1.68916900	6.49471100	1.18279900
C	0.50759500	7.82053200	2.35512500
C	-0.19192800	6.80405700	3.16784500
C	-1.30590000	6.13242200	2.57197100
C	0.23719200	6.43946200	4.45136000
H	1.11886300	6.89751400	4.89607300
C	-1.92213800	5.10304900	3.30723300
H	-2.72325200	4.52356400	2.85534000
C	-1.51034100	4.75513400	4.60050500
H	-1.99783000	3.92884500	5.11111200
C	-0.43001300	5.44199400	5.18208100
O	0.07277700	5.21321300	6.44214500
C	-0.42446300	2.83207700	6.90555700
C	-0.63102900	4.28835000	7.28169600
C	0.93680800	9.02973000	2.84291800
C	-2.99923700	6.57323300	0.76497600
S	0.71924900	9.57139600	4.54493600
S	1.66446500	10.31455700	1.81384300
S	-3.51314700	7.02033700	-0.89713400
S	-4.40889700	6.34530800	1.85862000
C	1.57222500	11.59155400	3.02354300

H	1.88322400	12.58951500	2.72097000
C	1.14484800	11.25625600	4.25613800
H	1.05989200	11.94316700	5.09586900
C	-5.64748400	6.62999400	0.64828400
H	-6.68417500	6.51708500	0.95747800
C	-5.24259000	6.93443600	-0.59999400
H	-5.90384600	7.11126500	-1.44547700
H	-0.22669000	4.48319300	8.28653300
H	-1.70884900	4.52891900	7.29414200
O	0.73761600	6.11135800	-3.04263400
C	2.01352300	5.89654300	-3.67795600
H	2.67818300	5.37118100	-2.97028500
H	2.48067300	6.86586100	-3.92884800
C	1.79481500	5.03151600	-4.91684500
H	1.29607500	5.61062700	-5.70909700
H	1.11038500	4.22105900	-4.63198700
C	3.11963100	4.41964600	-5.41733200
H	3.69892700	5.15890500	-5.99535300
H	3.73832100	4.15470000	-4.54422600
C	2.90983200	3.13868400	-6.24173900
H	2.41254000	3.37169800	-7.19871600
H	2.22021500	2.48215900	-5.68627600
C	4.21679900	2.36823300	-6.49344100
H	4.86814900	2.93280000	-7.18288900
H	4.76780800	2.28631400	-5.54165100
C	3.96710200	0.95293300	-7.03148600
H	3.42516400	1.00221800	-7.99206300
H	3.29581100	0.43397200	-6.32853200
C	5.24404400	0.11291600	-7.20997800
H	5.80283900	0.46082300	-8.09565500
H	5.90924800	0.25118700	-6.34227600
C	4.90469400	-1.38739800	-7.34891600
H	4.06035100	-1.48266400	-8.05843900
H	4.53345100	-1.74873200	-6.37861100
C	-1.38330600	-7.78528300	-2.49791500
H	-1.41999900	-8.50531500	-3.32852200

H	-2.09508500	-6.97029600	-2.71629000
C	0.03458900	-7.23396500	-2.33155500
H	0.06166000	-6.54909300	-1.46878800
H	0.70505100	-8.07683400	-2.09766000
C	0.52254300	-6.50889600	-3.59719200
H	-0.00919100	-5.54856000	-3.70127500
H	0.26761500	-7.10765900	-4.49017100
C	2.03844100	-6.25952900	-3.58721700
H	2.31345100	-5.70437200	-2.67723300
H	2.56229200	-7.22966600	-3.53104700
C	2.52267500	-5.49046600	-4.82441100
H	1.98954100	-4.52596200	-4.88605700
H	2.24903800	-6.05573900	-5.73312300
C	4.03520400	-5.22161400	-4.82055000
H	4.27706000	-4.56118300	-3.97396200
H	4.58244700	-6.16372500	-4.64233400
C	4.52879500	-4.57800900	-6.12747100
H	3.83631400	-3.77344500	-6.42013800
H	4.50311600	-5.31831600	-6.94435200
C	5.95101900	-3.98589200	-5.99250800
H	6.63485200	-4.77156600	-5.63310100
H	5.91827900	-3.22162300	-5.20239600
C	6.49742200	-3.37342900	-7.26681200
C	6.04405500	-2.24370000	-7.84028400
H	6.51893300	-1.90222900	-8.76682800
H	7.31583500	-3.90628300	-7.75998300
C	11.26439600	-3.79642800	-0.54293100
C	11.11745400	-3.95302300	0.82243500
C	9.85163200	-3.70986500	1.45029300
C	8.69662400	-3.76816500	0.61387000
C	8.85010200	-3.60612600	-0.81035200
C	10.15299300	-3.38955500	-1.35191300
C	7.38944200	-3.57493700	1.18354100
C	7.28528400	-2.87004400	2.41864600
C	8.49296500	-2.38959200	3.03576200
C	9.74530900	-2.99322000	2.71191400

C	8.47726700	-1.07806900	3.63356000
C	9.71432200	-0.41259200	3.88777500
C	10.88556200	-1.23513400	3.97054000
C	10.90063800	-2.49278700	3.39755400
C	7.68747600	-3.26156500	-1.58368100
C	6.37909700	-3.53334300	-1.06545500
C	6.22494800	-3.69425400	0.35658300
C	4.93104700	-3.50760600	0.93048500
C	4.82600200	-2.79491900	2.17620200
C	6.02007900	-2.30550800	2.78735100
C	6.00465200	-0.99566700	3.38526800
C	7.25470100	-0.32166000	3.58093900
C	5.23176200	-3.19389900	-1.84221600
C	3.92001200	-3.44557500	-1.31751100
C	3.76626700	-3.60610400	0.09640000
C	2.46516400	-3.42246500	0.67096700
C	2.36067400	-2.70649500	1.91573200
C	3.56105100	-2.21390700	2.52810400
C	3.54684500	-0.91013700	3.12222600
C	4.79603900	-0.23737400	3.34332000
C	2.76858400	-3.11212500	-2.10388500
C	0.00798500	-3.32429800	0.40879300
C	-0.09352300	-2.60558000	1.64245800
C	1.10421100	-2.12605200	2.26612100
C	1.09068300	-0.81758800	2.86475100
C	2.33310400	-0.14778700	3.08182800
C	0.31123100	-3.03295700	-2.37066300
C	-1.00078900	-3.28970700	-1.84834900
C	-1.15454300	-3.43258600	-0.42430600
C	-2.44452200	-3.21825300	0.14625800
C	-2.54571200	-2.50500100	1.38671800
C	-1.35164300	-2.02370500	2.00026000
C	-1.36768800	-0.72795600	2.61854400
C	-0.12113400	-0.05502800	2.83016000
C	-2.14746900	-2.95380600	-2.63312200
C	-3.45864700	-3.18536800	-2.09870000

C	-3.60687300	-3.30681600	-0.68402100
C	-4.90394900	-3.11596100	-0.10339600
C	-5.00620900	-2.42427300	1.14982900
C	-3.80440500	-1.93472500	1.75805600
C	-3.82349900	-0.64785900	2.38238600
C	-2.57790300	0.02671100	2.60281800
C	-4.61636100	-2.85488900	-2.88108400
C	-5.91711200	-3.09759400	-2.34615400
C	-6.06427500	-3.23844100	-0.92120500
C	-7.35914500	-3.04410900	-0.34065800
C	-7.45985500	-2.34713700	0.89922300
C	-6.26370200	-1.86743900	1.52370700
C	-6.28356200	-0.56624600	2.13947900
C	-5.04441000	0.10806400	2.35604000
C	-7.07401700	-2.74553500	-3.11396400
C	-8.38853400	-2.99949000	-2.58690700
C	-8.53528800	-3.15818400	-1.16145900
C	-9.82841400	-3.02283300	-0.57281100
C	-9.93158100	-2.31104600	0.69324900
C	-8.73373200	-1.79046300	1.26937300
C	-8.75330800	-0.48086000	1.87286500
C	-7.49849400	0.19152700	2.08090900
C	-9.53896900	-2.70231200	-3.37775200
C	-10.81445300	-3.02675900	-2.81024800
C	-10.95521600	-3.18421300	-1.44394300
C	-9.96826700	0.26858000	1.87295600
C	-11.18398100	-0.47301100	1.70873800
C	-11.16599400	-1.73088800	1.13539400
C	-7.42308000	1.58798000	1.80076900
C	-8.60513200	2.25460700	1.32340100
C	-9.89123800	1.69342200	1.58550300
C	-4.96863600	1.51763500	2.07727500
C	-6.13528500	2.18111400	1.59137200
C	-5.99128700	3.13969100	0.52710100
C	-7.14311000	3.46665300	-0.25866800
C	-8.46113200	3.22409000	0.26568700

C	-9.60912300	3.60443500	-0.49293400
C	-10.88875800	3.36657500	0.10808000
C	-11.02633300	2.43466800	1.12001300
C	-6.99198900	3.62289600	-1.66851100
C	-8.16466200	3.53278700	-2.49667100
C	-9.45435900	3.76750700	-1.93102300
C	-4.68923800	3.38581400	0.00075800
C	-4.53657900	3.54085300	-1.41837000
C	-5.69339800	3.44602800	-2.24750000
C	-5.59027800	2.73911100	-3.49803100
C	-6.79271200	2.24576800	-4.10128900
C	-8.06208400	2.82451600	-3.74833100
C	-9.25257300	2.37339400	-4.39353200
C	-10.47461500	3.02583800	-4.02516000
C	-10.57299100	3.70490600	-2.82509000
C	-6.77907300	0.95233200	-4.70180300
C	-8.03676500	0.28784100	-4.91947000
C	-9.23981100	1.05150200	-5.00170400
C	-4.33450100	2.16487100	-3.86061300
C	-4.31928100	0.86113500	-4.46902100
C	-5.56296900	0.19320500	-4.68201000
C	-5.64249100	-1.21832500	-4.40886500
C	-6.93437700	-1.78985900	-4.16283600
C	-8.11706200	-1.12382800	-4.63953900
C	-9.39754300	-1.72465200	-4.44642700
C	-10.52665800	-1.02665900	-4.98736800
C	-10.44949400	0.32649300	-5.25886900
C	-4.47411400	-1.89150000	-3.93933100
C	-3.23677300	3.34336100	-1.99335000
C	-3.13319000	2.64327600	-3.23728700
C	-3.53575700	3.05152200	0.78451500
C	-3.67710300	2.10178400	1.84608700
C	-3.10268800	0.09752000	-4.42789200
C	-3.18032200	-1.30692100	-4.15983500
C	-2.07578500	3.44725100	-1.16145500
C	-2.22762200	3.31142600	0.26139400

C	-2.50293000	1.43918600	2.33479100
C	-1.87024700	2.07212600	-3.60383200
C	-1.85286500	0.76943800	-4.21642900
C	-2.00507300	-1.98567500	-3.68973900
C	-0.78337000	3.25311500	-1.73288700
C	-0.67850700	2.55146000	-2.98024300
C	-1.08050300	2.98343500	1.04383500
C	-1.22086000	2.02391000	2.10424900
C	-0.64284800	0.01015000	-4.17841300
C	-0.71963200	-1.40186700	-3.91015600
C	0.37713200	3.36601100	-0.90131800
C	0.22707700	3.23431200	0.51450700
C	-0.04524800	1.35018500	2.57265400
C	0.58454700	1.97398500	-3.33322300
C	0.60397400	0.68221900	-3.94792200
C	0.45416000	-2.07126500	-3.42355900
C	1.67524200	3.18840400	-1.47810400
C	1.78055500	2.46725500	-2.71655500
C	1.38243400	2.91227100	1.30009900
C	1.24221800	1.94112200	2.35311400
C	1.82106700	-0.07402500	-3.91233600
C	1.74512900	-1.48597700	-3.64728100
C	2.83484500	3.31024200	-0.65377900
C	2.68491100	3.16512500	0.77060000
C	2.41079000	1.26567300	2.81908000
C	3.03844000	1.90268600	-3.07844000
C	3.05881700	0.60122500	-3.68590100
C	2.91300100	-2.15032800	-3.16290500
C	4.13303200	3.11553700	-1.23209100
C	4.23642900	2.39891900	-2.46777100
C	3.84119500	2.81706200	1.54518000
C	3.70114200	1.84743300	2.58991600
C	4.27558400	-0.15261500	-3.64483500
C	4.20065400	-1.55537700	-3.37383200
C	5.30170800	3.22890300	-0.40557600
C	5.15154400	3.07290800	1.01716300

C	4.87497500	1.17339800	3.06800100
C	5.50260500	1.83436100	-2.83796800
C	5.52150600	0.52675600	-3.43794600
C	5.37464500	-2.22070400	-2.88969700
C	6.59341400	3.03821400	-0.98329900
C	6.69681300	2.32598800	-2.23054400
C	6.30052600	2.72793200	1.79083200
C	6.15880500	1.75489100	2.84243200
C	6.73219000	-0.22712800	-3.39773600
C	6.65631800	-1.63511700	-3.11339900
C	7.75828500	3.12496300	-0.15221400
C	7.60921700	2.96567500	1.25684800
C	7.33302300	1.07490800	3.30400400
C	7.95901300	1.74311100	-2.58090200
C	7.97700400	0.44612900	-3.17365700
C	7.82823400	-2.29772700	-2.62521600
C	9.06506800	2.94509900	-0.72656900
C	9.16847900	2.23471100	-1.97668000
C	8.77251900	2.63077600	2.03419500
C	8.63035800	1.65802300	3.08834600
C	9.20158300	-0.30778200	-3.13640300
C	9.12499600	-1.71942600	-2.85400500
C	10.22630800	3.09030200	0.09074500
C	10.07413100	2.92551800	1.52813700
C	9.79431400	1.01183100	3.60295800
C	10.42975800	1.69313300	-2.36887500
C	10.44712800	0.36941500	-2.97209500
C	10.29607300	-2.40796300	-2.41631500
C	11.49608600	2.94150200	-0.55802700
C	11.59528400	2.26097900	-1.75683500
C	11.18506200	2.60389500	2.37536300
C	11.04869500	1.67146200	3.38648400
C	11.62998600	-0.44061700	-2.98697800
C	11.55642100	-1.79397900	-2.71616200
C	1.30826200	-3.52651800	-0.16180600
C	1.46334200	-3.36880700	-1.58387700



H	-11.37851700	2.85301500	-4.60844400
H	-11.55214600	4.04943400	-2.49378300
H	-11.49772700	-1.51876700	-5.03225900
H	-11.36180200	0.86607000	-5.51116500
H	-11.95730300	-3.26834500	-1.02450500
H	-11.70898600	-2.99088400	-3.43126100
H	-11.78563100	3.79426600	-0.33898000
H	-12.02786500	2.15265600	1.44350000
H	-12.14354600	0.01351900	1.88143800
H	-12.11216400	-2.20237800	0.87135900
H	12.40916600	3.21922700	-0.03239100
H	12.58399800	2.01964700	-2.14577100
H	12.60979700	0.03174800	-3.04957200
H	12.48004300	-2.35373700	-2.57229900
H	12.26549200	-3.82529500	-0.97195400
H	12.00655300	-4.10115100	1.43452300
H	11.84621500	-3.02978900	3.32957600
H	11.81965500	-0.81278100	4.33961500
H	11.94072900	1.32460200	3.90712800
H	12.18099800	2.96792800	2.12498200

**(6,6)@Cycle-8**

C	0.52073400	-0.88525600	-7.03535200
C	2.85430100	-0.25150900	-6.91296600
C	0.14045400	0.43371900	-6.73940700
H	-0.24695800	-1.64527500	-7.19574000
C	2.48064700	1.05918800	-6.61496500
H	3.90899900	-0.52479100	-6.95813900
H	-0.91081000	0.69872100	-6.64660800
H	3.24755200	1.81224900	-6.42625800
C	-3.51066400	7.04022700	-1.93322500
C	-2.16547900	8.77586700	-3.14237300
C	-2.48589400	7.45731400	-2.91270300
C	-1.94211200	6.33531800	-3.70347500
C	-0.58863300	6.24833700	-4.06962500
C	-2.30052600	4.18005300	-4.78891400

C	-0.08556700	5.18536200	-4.82897300
H	0.10685700	7.01358900	-3.72761100
H	-2.90444000	3.30005600	-4.99284300
H	0.96792200	5.17711100	-5.09568800
C	1.12057300	1.41696100	-6.53518300
C	-0.95140700	4.13805400	-5.18426900
C	0.79969900	2.86149700	-6.22084600
H	1.02273400	3.51461500	-7.08580000
H	1.44808100	3.17854700	-5.38919200
O	-0.57726500	3.00442800	-5.86372300
C	-2.82558000	5.26993200	-4.07496200
C	-4.24378300	5.35632100	-3.64349500
C	-5.29317100	4.91418500	-4.42705400
S	-5.10485200	4.14985500	-6.04428100
S	-7.02678600	5.14495400	-4.00960600
C	-6.80833000	4.16926400	-6.47609900
H	-7.07631700	3.79666100	-7.46267500
C	-7.67947200	4.61897000	-5.55271900
H	-8.75941300	4.66401400	-5.67790000
S	-1.06294500	9.32865300	-4.45283200
C	-2.32483800	11.40848200	-3.36105500
H	-2.65054500	12.42944900	-3.17188500
S	-2.91194000	10.15965300	-2.26773800
C	-1.48898800	11.03426000	-4.34858900
H	-1.03844700	11.70664700	-5.07592200
C	-4.58293300	7.17988800	0.26253000
C	-4.43225100	6.01960000	-2.32923700
C	-5.43561400	5.65427700	-1.41053100
H	-6.12627100	4.85260400	-1.65624800
C	-5.53463100	6.23084900	-0.14149000
H	-6.31745800	5.90851200	0.54320700
C	-3.57813400	7.57603100	-0.63474300
H	-2.82590900	8.28012700	-0.28359500
O	-4.61651500	7.77955500	1.50000700
C	3.06503100	-6.78813000	1.07522900
C	3.91181200	-6.52888300	-1.61337000

C	2.13050700	-6.84518900	0.02611200
H	1.07905500	-6.88379800	0.29895100
C	4.42788800	-6.60096300	0.78580600
H	5.16335400	-6.51060400	1.58149600
C	4.82566600	-6.45339500	-0.54766400
H	5.86773800	-6.21414000	-0.75367700
C	2.52645300	-6.73229200	-1.31515900
C	1.55914200	-6.72926300	-2.43857800
C	4.30466600	-6.34126200	-3.02579500
C	3.31016000	-5.58936400	-3.82115600
C	1.92114600	-5.80711000	-3.53947600
C	3.67563900	-4.67860100	-4.82187000
H	4.72112600	-4.43559700	-4.99975800
C	0.97902100	-5.08823300	-4.29588900
H	-0.07503500	-5.14686600	-4.03538800
C	1.34685600	-4.21270100	-5.32618700
H	0.57604700	-3.64865700	-5.84518900
C	2.70903600	-4.02298000	-5.60746100
O	3.21899500	-3.23698900	-6.60942400
C	1.87532500	-1.23794900	-7.13889900
C	2.31262700	-2.62720400	-7.55336000
C	5.43055500	-6.91467100	-3.57434500
C	0.46174800	-7.56531100	-2.48280400
S	5.88077500	-6.81473400	-5.31364400
S	6.55106600	-7.98383000	-2.65739100
S	0.05028300	-8.76612800	-1.20848900
S	-0.66043600	-7.67964700	-3.88372600
C	7.41178300	-8.60411800	-4.06194200
H	8.16413500	-9.37077500	-3.88761600
C	7.10805500	-8.07616600	-5.26308500
H	7.57805100	-8.35227500	-6.20492800
C	-1.49759000	-9.13044000	-3.34695000
H	-2.25174000	-9.54626200	-4.01204600
C	-1.17471100	-9.62197100	-2.13546900
H	-1.62868200	-10.49604800	-1.67284000
H	2.90385400	-2.56829000	-8.47916600

H	1.44648600	-3.27992200	-7.74488800
O	2.53990200	-6.84859200	2.33742900
C	3.34998000	-6.33714300	3.41791200
H	3.85991300	-5.42053100	3.08175800
H	4.12228400	-7.07739400	3.69328500
C	2.42579800	-6.00463700	4.58791900
H	2.03485200	-6.92559300	5.04713700
H	1.56479000	-5.46195300	4.17268900
C	3.12623600	-5.10898300	5.63243200
H	3.78916000	-5.70674900	6.27995000
H	3.77336600	-4.39073600	5.10301100
C	2.12429100	-4.30077500	6.47670600
H	1.57375000	-4.96514100	7.16423500
H	1.37363700	-3.87371600	5.79367400
C	2.77170000	-3.14202000	7.25467600
H	3.39494500	-3.52693900	8.08020700
H	3.45216200	-2.60213700	6.57538100
C	1.73126800	-2.14586000	7.79067100
H	1.08917200	-2.63640500	8.54294200
H	1.06560200	-1.85746300	6.96198800
C	2.34890600	-0.87532300	8.39559300
H	2.87914900	-1.12774200	9.33005600
H	3.10661700	-0.46443000	7.70786700
C	1.28585600	0.21428700	8.67444700
H	0.41690600	-0.26738700	9.15991100
H	0.92435100	0.61841200	7.71667300
C	-4.58904300	6.90484900	2.65510900
H	-5.15581600	7.42878300	3.43938500
H	-5.09881800	5.95164600	2.43804200
C	-3.14790000	6.65883300	3.10723800
H	-2.60730400	6.12194100	2.31209800
H	-2.65474600	7.63633900	3.23207200
C	-3.06815100	5.86385200	4.42155400
H	-3.49172200	4.85777900	4.27251600
H	-3.68995300	6.35528400	5.19073600
C	-1.62485700	5.73931500	4.93440100

H	-0.99911300	5.30508300	4.13945700
H	-1.21926400	6.74749400	5.12853300
C	-1.48796900	4.87745100	6.19917500
H	-1.94679300	3.89206400	6.01361800
H	-2.05255000	5.33514000	7.03038000
C	-0.01950400	4.67449100	6.60247800
H	0.52450800	4.26824300	5.73752000
H	0.44548100	5.65123100	6.82285500
C	0.18108600	3.73387100	7.80227400
H	-0.46989800	2.84923600	7.70238200
H	-0.12387600	4.24003300	8.73343200
C	1.64929600	3.24935900	7.91823900
H	2.31968900	4.11199700	7.76581600
H	1.84763500	2.54972200	7.09148400
C	1.96113200	2.60868500	9.25107200
C	1.79225800	1.31375900	9.57243100
H	2.05462700	0.99619500	10.58773500
H	2.31963200	3.28604700	10.03284900
H	-12.31867800	0.33502100	4.30711300
H	-12.61302600	1.75408300	2.35538800
H	-12.68818800	2.00862700	0.23192900
H	-12.54694900	1.07001900	-2.00602000
H	-12.25436500	-0.61813300	-3.29165100
H	-11.81488400	-2.99088900	-3.58577700
H	-11.94021500	-1.59457000	5.15991200
H	-11.49545500	-3.96661000	4.86278700
H	-11.19754500	-5.64843900	3.57202600
H	-11.05666800	-6.58846100	1.33448500
H	-11.13846100	-6.34343300	-0.79102200
H	-11.43773600	-4.92313800	-2.74128300
C	-11.43714600	0.76983200	3.83761400
C	-11.60446400	1.57665400	2.72670300
C	-11.70978300	1.92181900	-0.23902000
C	-11.62936500	1.38847100	-1.51269300
C	-11.22056900	-0.96106800	-3.31076300
C	-10.97059200	-2.31106400	-3.47790700

C	-10.91067300	-1.92142500	5.01912100
C	-10.65767700	-3.27050800	4.84987600
C	-10.24234700	-5.61647000	3.04939800
C	-10.16218900	-6.15116500	1.77641100
C	-10.27522300	-5.81183800	-1.18959000
C	-10.44542200	-5.00399500	-2.29921400
C	-10.13252000	0.35928500	4.25733000
C	-10.47774200	2.02254300	1.96629100
C	-10.52810600	2.18714300	0.52227100
C	-10.36241300	1.08796100	-2.10523600
C	-10.16384700	-0.05390400	-2.98333100
C	-9.64856100	-2.83696500	-3.32757500
C	-9.87593700	-0.95154700	4.83131300
C	-9.35477100	-3.73246600	4.48143800
C	-9.15276200	-4.87369200	3.60397800
C	-8.98730800	-5.97701300	0.97910600
C	-9.04207400	-5.81311500	-0.46434800
C	-9.39296700	-4.14753600	-2.75252200
C	-9.02510400	1.10884100	3.75574300
C	-9.19935500	1.94583900	2.59851200
C	-9.29639700	2.25796900	-0.19761800
C	-9.21288400	1.70539500	-1.52414500
C	-8.82889100	-0.50043400	-3.22586200
C	-8.56865400	-1.90489600	-3.39956000
C	-8.52933600	-1.42695200	4.86237300
C	-8.26636000	-2.82993400	4.68379100
C	-7.87577000	-5.03708600	2.98529100
C	-7.79231600	-5.59397500	1.66140500
C	-7.89781200	-5.27848500	-1.13147900
C	-8.07461400	-4.43898700	-2.28639900
C	-7.68892200	0.78646700	4.17982800
C	-8.02924700	2.42263100	1.91246800
C	-8.07732700	2.57406900	0.49625700
C	-7.91473100	1.49372100	-2.10520200
C	-7.72014900	0.37882100	-2.97054100
C	-7.21069900	-2.37058800	-3.31070300

C	-7.43725600	-0.49956800	4.73849400
C	-6.92262800	-3.24635300	4.38569300
C	-6.72499600	-4.36368500	3.52420700
C	-6.56114100	-5.45622900	0.93143700
C	-6.61424400	-5.29770200	-0.48334900
C	-6.96033800	-3.65426300	-2.74557600
C	-6.58395500	1.57913100	3.73080000
C	-6.75841300	2.41019300	2.57240900
C	-6.85188800	2.70011900	-0.23237200
C	-6.77029000	2.15896700	-1.56062200
C	-6.38597100	-0.04352000	-3.27701900
C	-6.12560000	-1.44599900	-3.44981300
C	-6.08624500	-0.96598500	4.83414300
C	-5.82400600	-2.36656400	4.65150500
C	-5.43276300	-4.57921000	2.94562300
C	-5.34914300	-5.13709900	1.62442300
C	-5.45394700	-4.82505100	-1.17724200
C	-5.63023000	-3.98762700	-2.33141500
C	-5.26030800	1.25939200	4.16143300
C	-5.60211100	2.88747400	1.88570700
C	-5.64789500	3.01848700	0.46058800
C	-5.48664300	1.95335000	-2.14747500
C	-5.29117900	0.83754000	-3.02749800
C	-4.77977300	-1.91731800	-3.37018400
C	-5.00696200	-0.03738900	4.72268500
C	-4.49181300	-2.79078700	4.36219800
C	-4.29289900	-3.91638800	3.49312200
C	-4.12810200	-5.01590300	0.89481600
C	-4.18107600	-4.85893900	-0.53162400
C	-4.52742600	-3.21145600	-2.80038000
C	-4.15124700	2.04121400	3.69251400
C	-4.32477700	2.86621900	2.53778200
C	-4.42126300	3.13864500	-0.26764500
C	-4.33945500	2.60160000	-1.58535900
C	-3.95255800	0.40882200	-3.31474500
C	-3.69347500	-0.98694700	-3.49044600

C	-3.65362900	-0.50847300	4.80078800
C	-3.39311400	-1.90309400	4.61569300
C	-3.00138500	-4.12162900	2.90304400
C	-2.91753500	-4.68044400	1.58818300
C	-3.02144300	-4.37219800	-1.22220800
C	-3.19705300	-3.53663500	-2.37098800
C	-2.82246900	1.71994700	4.12190500
C	-3.16898700	3.35160300	1.84401300
C	-3.22174500	3.50277700	0.41868200
C	-3.05249800	2.41007000	-2.17701800
C	-2.85442200	1.29364000	-3.05624900
C	-2.34249400	-1.45968100	-3.41057200
C	-2.57008600	0.42461600	4.69029900
C	-2.05589000	-2.32983900	4.32484200
C	-1.85752600	-3.45589100	3.45375600
C	-1.69140900	-4.56351200	0.85534900
C	-1.74422300	-4.40812500	-0.57280500
C	-2.09054100	-2.75527200	-2.84017600
C	-1.71990100	2.49382500	3.64375900
C	-1.89644100	3.32547400	2.48900600
C	-2.00595700	3.64440600	-0.31524300
C	-1.91908000	3.08288600	-1.63208500
C	-1.52225100	0.86809900	-3.34066300
C	-1.26269000	-0.53122800	-3.52337100
C	-1.22357300	-0.04533700	4.76912300
C	-0.96307800	-1.44477700	4.57863700
C	-0.57294600	-3.65916200	2.86316800
C	-0.48763800	-4.22423200	1.54566200
C	-0.59143600	-3.91794000	-1.25840700
C	-0.76828200	-3.07460200	-2.40601400
C	-0.39037200	2.16861800	4.06535400
C	-0.74128800	3.81457400	1.79551800
C	-0.79771000	3.98460800	0.37669700
C	-0.62740500	2.87483800	-2.21414300
C	-0.42570500	1.74749900	-3.06706400
C	0.08731700	-1.00162400	-3.42870300



C	-0.13937300	0.88516400	4.64232000
C	0.37166000	-1.86173500	4.26804300
C	0.56765300	-2.97881100	3.40006700
C	0.73466600	-4.08856000	0.81200200
C	0.68271900	-3.93735400	-0.60661200
C	0.33688300	-2.28541000	-2.86072100
C	0.71519400	2.94776400	3.59130200
C	0.53655900	3.79045000	2.44457900
C	0.42732700	4.11895600	-0.35679500
C	0.51252200	3.55393000	-1.67320700
C	0.90984600	1.32073600	-3.35376600
C	1.17127400	-0.07419600	-3.54304000
C	1.21245800	0.41535000	4.72346900
C	1.47157500	-0.98155700	4.53017600
C	1.85797600	-3.18473600	2.81327400
C	1.94230900	-3.75005400	1.50098400
C	1.84029400	-3.45513500	-1.29632800
C	1.66454700	-2.61453800	-2.43984700
C	2.03944000	2.63201300	4.02405500
C	1.68894600	4.28569500	1.76039900
C	1.63332500	4.45251900	0.33450000
C	1.79961300	3.34323700	-2.25466000
C	2.00140700	2.20583700	-3.10783700
C	2.51429600	-0.54700600	-3.46927300
C	2.29259700	1.34222700	4.60185100
C	2.80171300	-1.40675800	4.23741900
C	2.99709400	-2.52634400	3.36319000
C	3.16228600	-3.63432100	0.77171700
C	3.11246800	-3.49249100	-0.65327500
C	2.76636900	-1.84498400	-2.91388400
C	3.14404000	3.41568600	3.55700100
C	2.96694000	4.25175300	2.40944300
C	2.86035300	4.57266500	-0.39724600
C	2.94427300	4.01101000	-1.71023100
C	3.33725600	1.77665900	-3.39908300
C	3.59695500	0.38291200	-3.57940600

C	3.64364000	0.86939600	4.67770900
C	3.90172500	-0.52506600	4.49410600
C	4.28642200	-2.73445700	2.77439500
C	4.36910400	-3.29327400	1.46225400
C	4.26923200	-3.00857600	-1.34379900
C	4.09443000	-2.17448000	-2.49027500
C	4.47470000	3.09398400	3.98828300
C	4.12585300	4.74419800	1.72137200
C	4.07194600	4.90520200	0.29562900
C	4.23643200	3.79955100	-2.29842700
C	4.43562600	2.66674700	-3.15858600
C	4.94808200	-0.09121600	-3.51226800
C	4.72873000	1.79953100	4.55559900
C	5.23873000	-0.95626800	4.20285600
C	5.43447700	-2.08070100	3.33124400
C	5.59774100	-3.18626500	0.73293900
C	5.54694200	-3.04150000	-0.69445100
C	5.20131300	-1.39271200	-2.95892400
C	5.57643500	3.87165400	3.51961300
C	5.39904000	4.71070400	2.36696100
C	5.29345300	5.02446000	-0.43420200
C	5.37724100	4.46229300	-1.75365800
C	5.76672000	2.23841600	-3.44776300
C	6.02707900	0.83620200	-3.62724200
C	6.07421600	1.32689500	4.62851700
C	6.33385200	-0.07483800	4.44973300
C	6.71845000	-2.29125200	2.74419800
C	6.80127000	-2.85404400	1.42428400
C	6.70070300	-2.55716500	-1.38046700
C	6.52465400	-1.71660600	-2.53297100
C	6.90727500	3.53765900	3.93157300
C	6.55907700	5.18492000	1.67328400
C	6.50590500	5.34242300	0.25841100
C	6.66976300	4.24003100	-2.32997500
C	6.86648200	3.11772200	-3.18559500
C	7.37750800	0.36743100	-3.53500000

C	7.15886300	2.25167200	4.49043100
C	7.66751900	-0.49743200	4.14163500
C	7.86195700	-1.61712600	3.28200800
C	8.02523000	-2.72228000	0.69219700
C	7.97383000	-2.57052300	-0.72384500
C	7.62851100	-0.92142400	-2.98136400
C	8.02081600	4.32388200	3.47377800
C	7.84291700	5.16558200	2.32080100
C	7.73751200	5.47657400	-0.47185900
C	7.82126900	4.91350200	-1.79316600
C	8.20955100	2.69776600	-3.48236600
C	8.47027300	1.29388200	-3.66028500
C	8.51663900	1.78529100	4.57481500
C	8.77645100	0.38152100	4.39666900
C	9.16085400	-1.83221100	2.70359900
C	9.24405800	-2.39638000	1.38237200
C	9.14197300	-2.09033800	-1.41134800
C	8.96553400	-1.24743100	-2.56407500
C	9.33975500	4.03057900	3.93709300
C	8.98699000	5.69996800	1.65326500
C	8.93263200	5.86042300	0.20955700
C	9.09853900	4.74450800	-2.40990300
C	9.29922400	3.59945900	-3.28278100
C	9.81633700	0.81672500	-3.63307000
C	9.59633200	2.71757300	4.50544000
C	10.11131200	-0.06513800	4.15406600
C	10.31000900	-1.20991700	3.28047000
C	10.47507100	-2.32709000	0.66126200
C	10.42208800	-2.16754800	-0.78263500
C	10.07232900	-0.49703100	-3.06585400
C	10.39162900	4.88905100	3.48604100
C	10.22041900	5.69894500	2.37824900
C	10.10841300	6.02945700	-0.58771900
C	10.18883600	5.48822600	-1.85787600
C	10.60141200	3.13510100	-3.65088200
C	10.85214500	1.78566100	-3.82053300

C	10.91858500	2.19117500	4.65230800
C	11.16826200	0.84167900	4.48182200
C	11.57723900	-1.51304400	2.68973700
C	11.65712600	-2.05459400	1.41971100
C	11.54759800	-1.72251500	-1.54567600
C	11.37795300	-0.91194400	-2.65319100
H	11.38392000	4.80806800	3.92806200
H	11.08289800	6.23228600	1.98041500
H	11.00317100	6.46734800	-0.14700300
H	11.14460600	5.51608800	-2.37970500
H	11.44031000	3.82985500	-3.66426400
H	11.88117600	1.45755300	-3.96223400
H	11.76285100	2.87069100	4.76197200
H	12.20184200	0.49830600	4.46276900
H	12.49462600	-1.19102100	3.18093900
H	12.63511200	-2.14272300	0.94811100
H	12.55691000	-1.90308800	-1.17788300
H	12.25860000	-0.47776400	-3.12498600

**(7,7)@Cycle-8**

C	-0.19309800	-0.30686900	-7.27087600
C	2.15985500	-0.85295900	-7.19181100
C	0.10910100	1.06126100	-7.25394000
H	-1.23856000	-0.62047000	-7.26762800
C	2.46104000	0.51538500	-7.16372000
H	2.95766100	-1.58974600	-7.11870300
H	-0.69304700	1.79660500	-7.22711800
H	3.50269000	0.82818900	-7.07402500
C	0.72407900	8.05564700	-1.74571600
C	2.38442700	9.23697700	-3.20862300
C	1.58598700	8.14682800	-2.94351500
C	1.40237500	7.02988600	-3.89314100
C	2.47374800	6.44799600	-4.59190400
C	-0.06757900	5.39013400	-4.94072700
C	2.30319800	5.37420600	-5.47427700
H	3.48561600	6.80667600	-4.40814200

H	-1.01890600	4.87254600	-5.01761200
H	3.17287300	4.96005500	-5.97806600
C	1.44308800	1.48794500	-7.15155700
C	1.02259400	4.81933000	-5.62842300
C	1.83346600	2.94066100	-6.92990000
H	2.13400300	3.43903600	-7.87046500
H	2.70143100	2.94904700	-6.25137100
O	0.74097300	3.67395700	-6.34130700
C	0.08868400	6.48571300	-4.07013200
C	-1.02255200	7.06375200	-3.26341200
C	-2.31678300	7.15756100	-3.74154800
S	-2.84056700	6.61489800	-5.37563200
S	-3.67192900	7.93105700	-2.84724500
C	-4.46400800	7.28105200	-5.30256300
H	-5.09144700	7.16018000	-6.18332400
C	-4.84172500	7.87764800	-4.15600300
H	-5.82118000	8.31216800	-3.96686200
S	3.28654100	9.46560600	-4.74962200
C	3.32373900	11.71004500	-3.31102400
H	3.51869000	12.73943500	-3.01670500
S	2.53227900	10.67033000	-2.13073300
C	3.66562300	11.16614200	-4.49466100
H	4.17806200	11.68933000	-5.29954400
C	0.31860100	8.39813700	0.65528100
C	-0.61159600	7.56534000	-1.92283300
C	-1.43416900	7.53602900	-0.77953700
H	-2.42441200	7.09436200	-0.84243100
C	-1.00354200	7.95430500	0.48817200
H	-1.68077800	7.86924300	1.33546200
C	1.17273400	8.42109800	-0.46682900
H	2.21142100	8.70443600	-0.30663400
O	0.88763000	8.82115300	1.82687400
C	1.76008200	-7.92495500	0.66346500
C	2.63835900	-7.43965800	-2.01106000
C	0.84647300	-7.93844900	-0.40833400
H	-0.21192700	-8.03144700	-0.17257100

C	3.12633200	-7.74156700	0.38798800
H	3.85900900	-7.71294100	1.19126600
C	3.53565700	-7.47069300	-0.92537400
H	4.57474100	-7.18791100	-1.07532100
C	1.26550500	-7.74196400	-1.73412600
C	0.32777900	-7.79210700	-2.87807700
C	3.01346500	-7.03748600	-3.39180800
C	1.93354600	-6.34371900	-4.14492000
C	0.58288800	-6.76077200	-3.90499800
C	2.16529900	-5.28015500	-5.03868200
H	3.15799200	-4.84816500	-5.13841600
C	-0.44627000	-6.12934200	-4.62313300
H	-1.48289900	-6.38506600	-4.41146400
C	-0.20162400	-5.11388100	-5.55489800
H	-1.04680800	-4.66316400	-6.06807300
C	1.10993100	-4.64146500	-5.72346000
O	1.45547600	-3.52033600	-6.44872700
C	0.82182500	-1.27999300	-7.19907300
C	0.40410500	-2.73347900	-7.04329000
C	4.22916200	-7.34718500	-3.96902800
C	-0.61677300	-8.78679400	-3.01162300
S	4.68346500	-6.93148400	-5.66008500
S	5.50364500	-8.33327900	-3.16948300
S	-0.86693500	-10.10383500	-1.81149000
S	-1.64349100	-9.01359700	-4.47159700
C	6.49759500	-8.57039500	-4.60043200
H	7.37718000	-9.20263500	-4.49723500
C	6.12521300	-7.93603500	-5.72841400
H	6.65831100	-7.97832900	-6.67611700
C	-2.21942800	-10.62315000	-4.05122100
H	-2.85127200	-11.13212100	-4.77634100
C	-1.86706000	-11.11527600	-2.84816200
H	-2.17177700	-12.08333100	-2.45540800
H	0.12219600	-3.18774500	-8.01114500
H	-0.48614000	-2.73915200	-6.39585700
O	1.21288500	-8.03791600	1.91532000

C	2.00357900	-7.62951500	3.05933400
H	2.59780100	-6.74352000	2.79228000
H	2.70079800	-8.43968700	3.33710300
C	1.04208400	-7.27990400	4.20383300
H	0.53795500	-8.18983600	4.56483800
H	0.26310500	-6.63027600	3.78111400
C	1.73831700	-6.53364100	5.37015900
H	2.33769600	-7.23585500	5.97347000
H	2.44783600	-5.80490000	4.94866100
C	0.73935200	-5.76460400	6.27023000
H	0.15073900	-6.47420700	6.87600300
H	0.01897000	-5.25308200	5.61487300
C	1.39725600	-4.70357200	7.18468300
H	1.93596200	-5.19387300	8.01372800
H	2.15804600	-4.16123000	6.60195600
C	0.39320200	-3.67152000	7.74663600
H	-0.32179000	-4.17128700	8.42325700
H	-0.20462900	-3.27266700	6.91286000
C	1.06297000	-2.49467700	8.48966800
H	1.54694300	-2.86924000	9.40822200
H	1.86569600	-2.07358900	7.86313300
C	0.06706500	-1.35829000	8.85583700
H	-0.83125700	-1.82633800	9.30058500
H	-0.26218900	-0.86016000	7.93301700
C	0.13943200	8.79298400	3.06651500
H	0.68837700	9.49028900	3.71561900
H	-0.87467400	9.19731100	2.90732800
C	0.11191700	7.39169900	3.69209400
H	-0.64459800	6.77377700	3.18829000
H	1.08388100	6.92325100	3.47781900
C	-0.11554900	7.34555300	5.22489400
H	-1.06154100	7.84366600	5.49821800
H	0.69621700	7.89872200	5.72847900
C	-0.12239400	5.86953300	5.67585700
H	-1.01458000	5.38824400	5.24916400
H	0.73756400	5.38399100	5.18961100

C	-0.05534400	5.50616300	7.17952200
H	-0.98143500	5.80760900	7.69811400
H	0.77791700	6.04157200	7.66692600
C	0.16455500	3.97724100	7.27930400
H	-0.63163000	3.48181600	6.70162900
H	1.10072100	3.75333500	6.74450500
C	0.24895600	3.28320900	8.65260300
H	-0.69824300	3.38959700	9.20750500
H	1.03769600	3.74659100	9.27065400
C	0.57819700	1.78113700	8.43484000
H	1.48403500	1.73912500	7.80331200
H	-0.21822200	1.32340000	7.82953500
C	0.82946800	0.96407800	9.68165300
C	0.63131900	-0.35998500	9.84334800
H	0.91898800	-0.79429500	10.80771200
H	1.26886000	1.51356400	10.52194000
H	11.88898700	-0.89897300	-4.07630600
H	11.80110000	1.52568200	-4.12089400
H	11.70934800	3.44448600	-3.24260500
H	11.60232800	4.99954600	-1.38224600
H	11.52452800	5.51725000	0.66770500
H	11.47495600	5.01656200	3.04226500
H	11.47574300	3.72883800	4.71720800
H	11.53154400	1.56155800	5.80844900
H	11.93455200	-2.78726700	-3.12979200
H	11.93940000	-4.27138800	-1.20949700
H	11.90087700	-4.70480300	0.85886000
H	11.81899100	-4.11536100	3.21173000
H	11.72803300	-2.75604000	4.82857200
H	11.61671300	-0.55071000	5.83504600
C	10.91563100	-0.41159100	-4.04178100
C	10.86554800	0.97072000	-4.06705000
C	10.73425300	3.69385400	-2.82653200
C	10.67333400	4.58060000	-1.76646200
C	10.56447800	5.30690100	1.13702100
C	10.53618900	5.02122200	2.49021800



C	10.53863400	3.19311900	4.86175600
C	10.57051600	1.95795000	5.48378200
C	10.97986600	-3.08908600	-2.70123500
C	10.98266400	-3.93525000	-1.60679200
C	10.92864900	-4.54696000	1.32364500
C	10.88205100	-4.21064900	2.66475400
C	10.75175800	-2.29204600	4.96156800
C	10.68831600	-1.03482900	5.53538400
C	9.73881500	-1.19015000	-3.81810500
C	9.63526100	1.66984400	-3.87022200
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C	9.44525700	4.82680200	-1.07905300
C	9.39253300	5.17768500	0.33012600
C	9.33433900	4.58454700	3.12784100
C	9.33559700	3.69575600	4.27748500
C	9.40103100	1.14147900	5.56523400
C	9.76994800	-2.49041000	-3.16927400
C	9.77551200	-4.23985100	-0.90574300
C	9.74931000	-4.53540200	0.51711700
C	9.65261100	-3.84017200	3.29127800
C	9.58944500	-2.91109600	4.40727800
C	9.45821300	-0.31041200	5.59406000
C	8.48198200	-0.52557800	-3.96238100
C	8.42983700	0.91136700	-3.98847300
C	8.30564800	3.48432800	-2.82637900
C	8.24224200	4.40765800	-1.72612200
C	8.14023100	5.08653700	1.01213100
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C	8.54550500	-3.93400200	-1.56555300
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C	7.25763200	-1.26465000	-3.81454500
C	7.15495200	1.56477100	-3.86616900
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C	6.96760400	4.68191000	-1.12041900
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C	5.75906400	4.32761600	-1.80088200
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C	-11.61631100	1.10309900	4.87058300
C	-11.20245100	-3.91094300	-3.29242400
C	-11.20167900	-4.75757900	-2.19832100
C	-11.25973200	-5.38632400	0.72975700
C	-11.30906400	-5.05920800	2.07294700
C	-11.44393900	-3.14892700	4.37478800
C	-11.50688300	-1.88978500	4.94420800
H	-12.19512000	-1.79883400	-4.73155500
H	-12.28516400	0.62576500	-4.79188900
H	-12.38357600	2.55004700	-3.92033700
H	-12.49451800	4.09899100	-2.05490700
H	-12.56914200	4.60001600	-0.00014900
H	-12.61399300	4.08935900	2.37196500
H	-12.61106800	2.79705600	4.04346600
H	-12.56076700	0.63357500	5.14202100
H	-12.15208000	-3.68147400	-3.77374600
H	-12.15063900	-5.16636900	-1.85407400
H	-12.19152600	-5.61130800	0.21274100
H	-12.27801800	-5.03695200	2.56970500
H	-12.37322100	-3.68798600	4.19594300
H	-12.48363300	-1.47889000	5.19561500

**(8,8)@Cycle-8**

C	-1.94728400	-0.28980600	-7.69818400
C	0.38350900	-0.84078700	-7.72788000
C	-1.64590000	1.08916600	-7.68209100
H	-2.99734600	-0.58368000	-7.65084400
C	0.68379400	0.53712000	-7.71889500
H	1.20037200	-1.56147700	-7.70650100
H	-2.46223500	1.80863100	-7.62417900
H	1.73475200	0.83005000	-7.68846400
C	0.06571500	8.11159300	-1.96255300
C	2.10286300	8.81754800	-3.23896800
C	0.99877200	7.99445900	-3.12157200
C	0.58026900	7.04297400	-4.19279800



C	1.48842500	6.32209100	-4.99575100
C	-1.19709200	5.77660000	-5.32586600
C	1.09923300	5.35066600	-5.93414300
H	2.55695400	6.43517700	-4.82852600
H	-2.23922100	5.47213900	-5.38878900
H	1.87795800	4.82052000	-6.47757300
C	-0.31282300	1.53826400	-7.62309800
C	-0.25735200	5.00223100	-6.05757200
C	0.16397100	3.00724000	-7.46193000
H	0.36756800	3.44921800	-8.45334900
H	1.11314100	2.95808500	-6.91068200
O	-0.75583000	3.90483700	-6.76370800
C	-0.81549000	6.79845200	-4.41456600
C	-1.77694700	7.63001400	-3.62723800
C	-2.94933700	8.10158500	-4.19103700
S	-3.49509900	7.71749600	-5.86208400
S	-4.04659000	9.29072600	-3.40357800
C	-4.77222000	8.92302200	-5.93821900
H	-5.31190200	9.01800100	-6.87833300
C	-5.02306800	9.63575800	-4.82366300
H	-5.79690300	10.39421000	-4.72371400
S	3.15386700	8.90948500	-4.69681600
C	3.75783000	10.87884300	-3.01016600
H	4.23425000	11.76045800	-2.58592800
S	2.58239100	10.03935900	-2.00749600
C	4.01806900	10.36800600	-4.22847200
H	4.73638700	10.77152400	-4.93925600
C	-0.41516600	8.39622800	0.46507100
C	-1.33363200	8.01326100	-2.25029100
C	-2.21639200	8.20644900	-1.16364900
H	-3.28615900	8.08555500	-1.31402400
C	-1.78811400	8.42610000	0.15565000
H	-2.53328200	8.50744000	0.94415200
C	0.49262100	8.27339800	-0.61903000
H	1.55064300	8.20474500	-0.37690700
O	0.11833000	8.38999300	1.74509800

C	-0.51748500	-8.37467600	0.25299400
C	0.30321400	-7.89292900	-2.48049200
C	-1.46304500	-8.21362900	-0.79393000
H	-2.51163600	-8.15266200	-0.51178500
C	0.84225500	-8.39775700	-0.10800600
H	1.61628200	-8.50951000	0.64854400
C	1.22326700	-8.12856900	-1.43402400
H	2.28722300	-8.00199100	-1.61646600
C	-1.08575000	-8.00310400	-2.14448300
C	-2.06138300	-7.85644000	-3.26368700
C	0.69357100	-7.46854700	-3.86192600
C	-0.30004300	-6.62094000	-4.59182200
C	-1.68628500	-6.87597100	-4.32373500
C	0.04183800	-5.58025500	-5.49807400
H	1.07955600	-5.27144200	-5.59752300
C	-2.62710200	-6.14247500	-5.07633100
H	-3.68797900	-6.26421300	-4.87114800
C	-2.27758200	-5.15265900	-6.01087300
H	-3.07868600	-4.61427800	-6.51201200
C	-0.92868300	-4.79378100	-6.17578000
O	-0.46345200	-3.67395500	-6.86849900
C	-0.94820700	-1.29158100	-7.64939400
C	-1.41020100	-2.76791700	-7.51940700
C	1.84681600	-7.91831900	-4.48156300
C	-3.16557400	-8.68282000	-3.36343200
S	2.32463900	-7.49201400	-6.16318300
S	2.98240900	-9.11632200	-3.76581000
S	-3.59105100	-9.94345200	-2.15161100
S	-4.26884800	-8.74112900	-4.78346400
C	3.90658300	-9.41985900	-5.22946300
H	4.68993500	-10.17325200	-5.17654100
C	3.60754700	-8.68365000	-6.31650000
H	4.11179200	-8.75134000	-7.27839000
C	-5.10364500	-10.22047800	-4.32785100
H	-5.84409200	-10.60940500	-5.02390500
C	-4.79515400	-10.76427200	-3.13531100

H	-5.24866900	-11.66212300	-2.72011000
H	-1.63067700	-3.18396900	-8.51826600
H	-2.34711400	-2.74393800	-6.94633100
O	-1.00878900	-8.40497300	1.54942100
C	-0.09365500	-8.28223800	2.70154800
H	0.66385600	-7.52567000	2.46663700
H	0.41966900	-9.24846200	2.84032100
C	-0.88048900	-7.87493300	3.99607600
H	-1.42403200	-8.75442500	4.37487000
H	-1.64254800	-7.14682700	3.70096800
C	-0.00651600	-7.25120600	5.15947800
H	0.57485100	-8.05207600	5.64585400
H	0.73336300	-6.57080700	4.71715300
C	-0.82173500	-6.46065100	6.26419300
H	-1.33236300	-7.18818900	6.91716400
H	-1.62008800	-5.89880000	5.76311700
C	0.00772700	-5.45447800	7.15815900
H	0.62858600	-6.02984900	7.86570600
H	0.71382000	-4.92155400	6.51108400
C	-0.81988300	-4.37478200	7.96109200
H	-1.37580600	-4.87250800	8.77368400
H	-1.58476100	-3.96014300	7.29137500
C	0.02161300	-3.18441400	8.58352600
H	0.48402900	-3.53378400	9.52248000
H	0.85490900	-2.93841400	7.91093100
C	-0.78353300	-1.85533200	8.88932500
H	-1.66991200	-2.14571500	9.48560100
H	-1.17491500	-1.44394500	7.95741900
C	-0.76079500	8.20262400	2.91642200
H	-1.30157100	9.14631900	3.09951900
H	-1.49840500	7.42893000	2.67739400
C	0.07438700	7.78419400	4.17325700
H	0.83670500	7.07306500	3.83764500
H	0.61945600	8.66442000	4.54864200
C	-0.73778200	7.13353900	5.36857400
H	-1.48992600	6.43965100	4.96749800

H	-1.29683300	7.92352200	5.89770500
C	0.18156600	6.36650500	6.39381000
H	0.76550100	5.63352800	5.82469100
H	0.91751200	7.09277600	6.77587500
C	-0.46901600	5.62327900	7.65684400
H	-1.55584300	5.80998100	7.67906800
H	-0.05968700	6.08723200	8.56885700
C	-0.22269800	4.06747700	7.68804000
H	-0.90821700	3.65760600	6.94711100
H	0.79423800	3.87761600	7.31230800
C	-0.39277600	3.18401200	8.98805100
H	-1.33193500	3.43461900	9.50832500
H	0.42899000	3.40183500	9.69175700
C	-0.38200100	1.63732100	8.61995100
H	0.34188700	1.53847700	7.80315200
H	-1.36034900	1.37443000	8.19622200
C	0.05965900	0.58508900	9.65087300
C	-0.03627700	-0.77703700	9.69690000
H	0.48873600	-1.21746300	10.55448400
H	0.66521700	1.01064100	10.46091700
H	-12.00625000	-3.76213400	-3.52465700
H	-11.99600400	-5.19237500	-1.56866600
H	-11.97213600	-5.68280600	0.46761500
H	-11.93148700	-5.28579700	2.85839300
H	-11.89104000	-4.16207200	4.62595600
H	-11.84404400	-2.17618600	6.01387900
H	-11.80835900	-0.13500400	6.47425600
H	-11.78254800	2.25451200	6.07308200
H	-11.99919200	-1.98052700	-4.61976900
H	-11.97515500	0.40804300	-5.02357200
H	-11.94381700	2.45034800	-4.57262000
H	-11.89969200	4.43700300	-3.18579000
H	-11.86014000	5.55451200	-1.41407500
H	-11.81923000	5.94677100	0.97718000
H	-11.79242100	5.45915500	3.01481100
H	-11.77821400	4.03358600	4.97414300

C	-11.04861500	-4.02336600	-3.07697800
C	-11.04282500	-4.84053400	-1.96042600
C	-11.00879900	-5.53990700	0.95480900
C	-10.98564500	-5.31322600	2.31952200
C	-10.92726800	-3.70805600	4.85119100
C	-10.90049100	-2.57391500	5.64343500
C	-10.85038600	0.35259100	6.30035900
C	-10.83557500	1.71702500	6.07122100
C	-11.03877500	-1.46816400	-4.64841000
C	-11.02500000	-0.10385900	-4.87913700
C	-10.97990400	2.82414300	-4.23071700
C	-10.95470900	3.95894700	-3.43933900
C	-10.89790700	5.55842900	-0.90424600
C	-10.87463600	5.78213800	0.46104500
C	-10.83685700	5.08331400	3.37732400
C	-10.82870800	4.26891800	4.49591200
C	-9.84976000	-3.41700000	-3.55915400
C	-9.83766500	-5.11105300	-1.24502700
C	-9.82117800	-5.45066200	0.16809000
C	-9.77312200	-4.98063800	2.99517000
C	-9.74503600	-4.20218800	4.22226000
C	-9.68943000	-1.85161900	5.86412800
C	-9.66506300	-0.43316300	6.18046500
C	-9.63460400	2.39563100	5.70486800
C	-9.84513200	-2.17788400	-4.31929600
C	-9.81659600	0.65124000	-4.79796600
C	-9.79471100	2.07073500	-4.48524000
C	-9.74236300	4.42283600	-2.84603200
C	-9.71483000	5.19898000	-1.61745100
C	-9.66630100	5.66216400	1.21129400
C	-9.64809200	5.32185300	2.62428800
C	-9.63139100	3.63298900	4.94238200
C	-8.61352100	-3.91813400	-3.04568100
C	-8.60739300	-4.76867100	-1.88646500
C	-8.57520500	-5.43078800	0.86798200
C	-8.55108300	-5.19458800	2.28553200

C	-8.49610400	-3.67805700	4.67790000
C	-8.46854900	-2.49924700	5.49993900
C	-8.42140900	0.26826500	6.11458000
C	-8.40583600	1.68574000	5.87565600
C	-8.60437300	-1.49947400	-4.52765900
C	-8.58988600	-0.08180300	-4.76812400
C	-8.54721400	2.68766200	-4.15916600
C	-8.52075900	3.86811400	-3.33902900
C	-8.46707100	5.38148800	-0.94499500
C	-8.44302100	5.61290300	0.47360100
C	-8.40777400	4.94839700	3.22836500
C	-8.39926400	4.10047100	4.38917000
C	-7.36726600	-3.39729200	-3.53736400
C	-7.35557500	-5.07719800	-1.25030200
C	-7.33897100	-5.41108900	0.13469400
C	-7.29114200	-4.94405300	2.93099800
C	-7.26400000	-4.18146900	4.13424300
C	-7.20949800	-1.85547100	5.75679200
C	-7.18572800	-0.46414200	6.06310300
C	-7.15507300	2.33445100	5.58945600
C	-7.36309800	-2.18101800	-4.28050800
C	-7.33450200	0.61897700	-4.75526300
C	-7.31277500	2.01137200	-4.45096900
C	-7.26089900	4.34184100	-2.83403600
C	-7.23400900	5.10326200	-1.62978500
C	-7.18624500	5.55928600	1.16909200
C	-7.16873600	5.22432200	2.55408100
C	-7.15196800	3.54875300	4.84389600
C	-6.12935600	-3.94954200	-3.07733300
C	-6.12321100	-4.80217800	-1.92311800
C	-6.09042000	-5.46627400	0.83269900
C	-6.06612900	-5.22769100	2.24718800
C	-6.01195800	-3.71203900	4.64327700
C	-5.98493900	-2.53577500	5.46395300
C	-5.93736900	0.23542500	6.06960600
C	-5.92111600	1.64965800	5.82854900

C	-6.12050800	-1.52764100	-4.55851300
C	-6.10567400	-0.11283600	-4.79853500
C	-6.06292700	2.65999300	-4.19402800
C	-6.03624400	3.84042900	-3.37886600
C	-5.98287800	5.35409700	-0.98264100
C	-5.95903500	5.58345400	0.43314800
C	-5.92401300	4.91860900	3.19034500
C	-5.91498800	4.06926200	4.34629100
C	-4.89472600	-3.43414900	-3.57374300
C	-4.88349700	-5.12427900	-1.29289900
C	-4.86577600	-5.46127600	0.09870700
C	-4.81731700	-4.98696900	2.89706800
C	-4.79051500	-4.22406900	4.10876600
C	-4.73727700	-1.89860600	5.73645100
C	-4.71366700	-0.49874500	6.03621700
C	-4.68117700	2.30219900	5.55238600
C	-4.89119900	-2.21431000	-4.32490900
C	-4.86133800	0.58809600	-4.79515400
C	-4.83937100	1.98872100	-4.49570500
C	-4.78739200	4.32219000	-2.88118700
C	-4.76053500	5.08589600	-1.67071700
C	-4.71343100	5.54108500	1.12958800
C	-4.69607200	5.20800600	2.52200300
C	-4.67792800	3.52636400	4.80902800
C	-3.65574400	-3.96047800	-3.08632400
C	-3.64914200	-4.81959300	-1.95272200
C	-3.61372200	-5.48257800	0.79714900
C	-3.59013900	-5.24097400	2.20156000
C	-3.53720900	-3.73589300	4.60337600
C	-3.51093700	-2.57148200	5.42421300
C	-3.46412700	0.20101800	6.00790100
C	-3.44718100	1.60296900	5.75689600
C	-3.64663500	-1.55086300	-4.57448300
C	-3.63111100	-0.14519000	-4.80286300
C	-3.58736300	2.62508600	-4.21198700
C	-3.56028300	3.79665000	-3.40100200

C	-3.50882000	5.30699400	-1.01174200
C	-3.48539300	5.53402600	0.39298500
C	-3.44957400	4.87768200	3.14587800
C	-3.44024500	4.03239900	4.29242700
C	-2.41809900	-3.42816800	-3.55859600
C	-2.40520900	-5.11846400	-1.31908400
C	-2.38666400	-5.44203700	0.06597700
C	-2.33935000	-4.96209400	2.83430000
C	-2.31150800	-4.21208400	4.04246900
C	-2.26064000	-1.92435700	5.66498800
C	-2.23875000	-0.53083100	5.94728800
C	-2.20556900	2.23120800	5.43170600
C	-2.41345100	-2.22515400	-4.31361100
C	-2.38365500	0.54869500	-4.75529000
C	-2.36169000	1.93986400	-4.47592600
C	-2.30971600	4.24372000	-2.87338400
C	-2.28242600	5.01660000	-1.68403800
C	-2.23716600	5.46792400	1.08189900
C	-2.21927500	5.13291800	2.46290500
C	-2.20004900	3.46129000	4.71600700
C	-1.18275300	-3.95098400	-3.08990300
C	-1.17581500	-4.81072500	-1.96782700
C	-1.13794700	-5.43602800	0.75114000
C	-1.11338400	-5.19439200	2.14388000
C	-1.05932100	-3.72540000	4.52225200
C	-1.03247500	-2.57576500	5.34760200
C	-0.99061300	0.15156100	5.89390700
C	-0.97656200	1.53282700	5.59990700
C	-1.17169600	-1.57245800	-4.55190300
C	-1.15685500	-0.17427000	-4.76282500
C	-1.11219000	2.55555300	-4.18102600
C	-1.08390900	3.71482900	-3.37225000
C	-1.03244500	5.24706600	-1.03875400
C	-1.00877500	5.47669800	0.35787000
C	-0.97229400	4.79992300	3.06713100
C	-0.96457300	3.94450600	4.19562000



C	0.05678600	-3.45065800	-3.59030100
C	0.07348900	-5.12086300	-1.35111700
C	0.09182300	-5.42384900	0.02707600
C	0.13993400	-4.95049600	2.78137900
C	0.16837000	-4.21165800	3.98355200
C	0.22149200	-1.95043500	5.62067700
C	0.24291400	-0.56672400	5.90789900
C	0.27127200	2.16531400	5.32549500
C	0.06206100	-2.25272900	-4.33391700
C	0.09202800	0.50906500	-4.76031900
C	0.11408600	1.88984300	-4.47115100
C	0.17047600	4.18655600	-2.87989400
C	0.19748300	4.97496400	-1.71020500
C	0.24377100	5.44089400	1.04274000
C	0.26076600	5.08876800	2.40926400
C	0.27645000	3.38219100	4.61616400
C	1.29944400	-4.01294400	-3.16376300
C	1.30699100	-4.85790700	-2.02431700
C	1.34453400	-5.47155400	0.71183400
C	1.37001700	-5.23720800	2.11184400
C	1.42555000	-3.76936600	4.50254300
C	1.45272800	-2.61956000	5.33880100
C	1.49302000	0.12529700	5.92343900
C	1.50630100	1.51731500	5.62794300
C	1.30628000	-1.61819200	-4.62961500
C	1.32164400	-0.21384800	-4.82976000
C	1.36640500	2.53185700	-4.23479100
C	1.39479200	3.69171400	-3.41687700
C	1.45091000	5.24952100	-1.08271400
C	1.47524700	5.49137000	0.31903100
C	1.51043100	4.79002600	3.03751100
C	1.51729800	3.92151600	4.16231000
C	2.53141500	-3.53838500	-3.70260800
C	2.54933700	-5.19236300	-1.41138800
C	2.56802600	-5.50264100	-0.01717700
C	2.61878300	-5.04747700	2.77438600

C	2.64722300	-4.29743100	3.99076800
C	2.70151400	-1.99623300	5.63742500
C	2.72224900	-0.59791000	5.93853300
C	2.74523200	2.18734600	5.40541800
C	2.53569300	-2.31624700	-4.44605000
C	2.56416500	0.48154800	-4.88096600
C	2.58766300	1.87828500	-4.57524000
C	2.64413100	4.20104000	-2.95881200
C	2.67278900	4.99591800	-1.77251000
C	2.72254700	5.47730300	1.01212200
C	2.74023900	5.12065400	2.39755300
C	2.75068400	3.40513700	4.65547100
C	3.77087100	-4.09223000	-3.25016600
C	3.77928000	-4.92767600	-2.09175800
C	3.81582900	-5.56267800	0.67899600
C	3.84217400	-5.33177900	2.08855900
C	3.90039900	-3.83288600	4.50417200
C	3.92776300	-2.66895900	5.33183300
C	3.96753900	0.10901900	5.93325800
C	3.97922100	1.51420900	5.67289400
C	3.77697900	-1.66253800	-4.72746000
C	3.79119100	-0.25050800	-4.94875700
C	3.83773400	2.52750700	-4.32683000
C	3.86544700	3.70151500	-3.51158100
C	3.92646300	5.25362900	-1.13075700
C	3.95158300	5.49502800	0.27723000
C	3.98275000	4.79774700	3.03248600
C	3.98808800	3.93761400	4.17366800
C	5.00945900	-3.57925600	-3.75943700
C	5.02599200	-5.24271400	-1.45717800
C	5.04443000	-5.56471900	-0.06059400
C	5.09620900	-5.09964700	2.74308200
C	5.12548100	-4.34169000	3.95934300
C	5.17998700	-2.02270300	5.59796200
C	5.20013100	-0.62245000	5.90258500
C	5.22259800	2.17619900	5.40384700

C	5.01284500	-2.35375400	-4.50328800
C	5.03995700	0.45411300	-4.95534400
C	5.06322300	1.85293500	-4.64060700
C	5.12085500	4.19140100	-3.02375900
C	5.15128500	4.97082300	-1.82078700
C	5.20212500	5.44155000	0.97775100
C	5.21807200	5.09274900	2.36806200
C	5.22697700	3.39530100	4.64924200
C	6.24636600	-4.11425000	-3.28756600
C	6.25458700	-4.95563100	-2.12555500
C	6.29079200	-5.59899600	0.63552700
C	6.31697300	-5.36278800	2.05044900
C	6.37547400	-3.85917500	4.45298300
C	6.40284700	-2.68708200	5.27908300
C	6.44277000	0.08100500	5.88780700
C	6.45439800	1.49378800	5.64021600
C	6.25182300	-1.69350100	-4.76450600
C	6.26569800	-0.27711600	-4.99420400
C	6.31178400	2.49092800	-4.37090400
C	6.34062300	3.67085100	-3.55500300
C	6.40161600	5.20179000	-1.17054300
C	6.42701800	5.43817900	0.24386300
C	6.45728800	4.76027500	2.99516100
C	6.46219400	3.90693500	4.14817500
C	7.48337900	-3.59201500	-3.78265900
C	7.49981400	-5.25582000	-1.48730100
C	7.51809000	-5.58051800	-0.10042000
C	7.56976300	-5.11293000	2.69567700
C	7.59914700	-4.35618200	3.90200500
C	7.65301800	-2.03879300	5.53350900
C	7.67310200	-0.64832900	5.84108500
C	7.69669900	2.14696000	5.35982200
C	7.48631400	-2.37634600	-4.52538800
C	7.51334800	0.42369000	-4.98341900
C	7.53640600	1.81360800	-4.67075600
C	7.59471500	4.14245700	-3.05269400

C	7.62518000	4.90997300	-1.85301900
C	7.67533500	5.37484100	0.94121500
C	7.69073400	5.03685800	2.32462300
C	7.70063300	3.35882200	4.61112300
C	8.73101600	-4.14108600	-3.32651300
C	8.73931300	-4.98508200	-2.16329600
C	8.77562300	-5.63288800	0.59412100
C	8.80187600	-5.39543600	2.01128700
C	8.85996000	-3.88728900	4.40862700
C	8.88727000	-2.71222900	5.23544800
C	8.92756500	0.05310800	5.85306400
C	8.93950700	1.46980500	5.61174600
C	8.73630000	-1.72519200	-4.80821700
C	8.74998400	-0.30694300	-5.04155000
C	8.79602000	2.45862400	-4.41913400
C	8.82550500	3.63776000	-3.59785000
C	8.88608800	5.15783800	-1.20898600
C	8.91152600	5.39346300	0.20832400
C	8.94199600	4.72948000	2.96148800
C	8.94716100	3.88152200	4.12181400
C	9.96299200	-3.67295300	-3.87934500
C	9.97973300	-5.35635400	-1.55827700
C	9.99825900	-5.68938800	-0.14376400
C	10.05046000	-5.21570500	2.68320400
C	10.08044500	-4.44066500	3.91220800
C	10.13465100	-2.09628900	5.56260500
C	10.15507200	-0.67851300	5.88149900
C	10.17943800	2.14955300	5.40384100
C	9.96566600	-2.43455300	-4.64022500
C	9.99301400	0.39545200	-5.10791000
C	10.01654800	1.81328800	-4.78907900
C	10.07580200	4.16293800	-3.14635600
C	10.10710300	4.94075000	-1.91909300
C	10.15751700	5.41091700	0.90811800
C	10.17284200	5.07304500	2.32144200
C	10.18340000	3.38601900	4.64027100

C	11.16043300	-4.30806900	-3.43214500
C	11.16858400	-5.12060100	-2.31217400
C	11.20683800	-5.80911200	0.60618600
C	11.23211500	-5.58058000	1.97056100
C	11.29380900	-3.97860100	4.50521500
C	11.32000900	-2.84740700	5.30163900
C	11.36236500	0.07796900	5.96552100
C	11.37394000	1.44233400	5.73579500
C	11.16579100	-1.75407500	-5.00548900
C	11.17890600	-0.38897800	-5.23138400
C	11.22751600	2.53698100	-4.57274900
C	11.25623900	3.67047600	-3.77964800
C	11.32085000	5.26955400	-1.24359100
C	11.34528800	5.49648500	0.12113500
C	11.37705500	4.80707600	3.03996200
C	11.38204700	3.99376100	4.15927900
H	12.10997800	-4.07261900	-3.91036500
H	12.12416600	-5.49527700	-1.94848900
H	12.15040800	-5.97903400	0.08988000
H	12.19450600	-5.57878200	2.48003400
H	12.23845600	-4.45526600	4.24798600
H	12.28427300	-2.47424700	5.64321200
H	12.31290100	-0.43283900	6.11134800
H	12.33326400	1.95677800	5.70920700
H	12.11335800	-2.29061700	-5.00872700
H	12.13634400	0.09994600	-5.40458400
H	12.17001900	2.14080900	-4.94755800
H	12.22028900	4.12564900	-3.55780000
H	12.26656700	5.23818800	-1.78250600
H	12.30923600	5.63582800	0.60813700
H	12.33012000	5.16076600	2.64959100
H	12.33899900	3.73689800	4.61086400

**(9,9)@Cycle-8**

C	-0.72259600	-0.75075800	-8.26007400
C	1.63190100	-0.98473600	-8.19755900

C	-0.60517000	0.66957300	-8.28794600
H	-1.73625400	-1.15509100	-8.24816900
C	1.74697600	0.43426000	-8.22445300
H	2.55519400	-1.56139100	-8.14152300
H	-1.53030400	1.24664300	-8.29965800
H	2.75962700	0.83950300	-8.17796700
C	0.74654000	8.32314300	-2.54083500
C	2.85600500	8.91423000	-3.77512000
C	1.72186200	8.12500700	-3.67790700
C	1.33314400	7.15354200	-4.77218200
C	2.25426500	6.43058200	-5.57178600
C	-0.39492700	5.84345300	-5.96272400
C	1.90263000	5.42876200	-6.50706500
H	3.31990000	6.54904600	-5.39486200
H	-1.43617700	5.54591600	-6.05328100
H	2.70982700	4.89487900	-7.00631900
C	0.64236700	1.33140300	-8.17031800
C	0.56186600	5.03363700	-6.66139700
C	0.98224100	2.90809700	-8.06250600
H	1.05147400	3.30269900	-9.08834500
H	1.97757500	2.95071500	-7.60261400
O	0.08649000	3.87127400	-7.33088300
C	-0.05224000	6.88688500	-5.03555700
C	-1.03574400	7.74605500	-4.27946300
C	-2.19013600	8.20022700	-4.89694900
S	-2.68125700	7.75721300	-6.57135200
S	-3.31698200	9.41509500	-4.19441100
C	-3.96059800	8.95014400	-6.73363800
H	-4.47009500	9.00566500	-7.69354100
C	-4.24957200	9.70276100	-5.65541300
H	-5.02926500	10.46023300	-5.60696200
S	3.96417000	8.94778000	-5.19338300
C	4.58810900	10.91356900	-3.51323900
H	5.08503800	11.77991300	-3.08120700
S	3.33398800	10.14552400	-2.55218700
C	4.87546200	10.37061300	-4.71120400

H	5.64042600	10.72788100	-5.39764600
C	0.13713100	8.78445800	-0.11497600
C	-0.64069300	8.20485900	-2.89283600
C	-1.56141900	8.50353200	-1.85768800
H	-2.62572300	8.38545500	-2.04275400
C	-1.20725600	8.81480000	-0.52504600
H	-2.00650300	8.94887300	0.20312300
C	1.09414400	8.60378800	-1.17505800
H	2.13881600	8.55476300	-0.87859700
O	0.60511300	8.81510000	1.21593300
C	0.66921200	-8.77827200	0.20329300
C	1.53884500	-8.33698700	-2.57752000
C	-0.24901000	-8.63189700	-0.89379200
H	-1.30056100	-8.54753500	-0.63100600
C	2.02634200	-8.84124500	-0.16379600
H	2.80155400	-8.95653000	0.59297800
C	2.42394600	-8.60367100	-1.50117000
H	3.49513300	-8.50863800	-1.65859100
C	0.14184300	-8.42313000	-2.26081900
C	-0.80196800	-8.26357500	-3.42745000
C	1.97531700	-7.94087900	-3.97310300
C	1.02086400	-7.10238200	-4.79118300
C	-0.37254400	-7.35041800	-4.55376800
C	1.39416000	-6.09107200	-5.74348900
H	2.43983700	-5.80660600	-5.82297900
C	-1.26981500	-6.64938200	-5.39691200
H	-2.33995000	-6.75541600	-5.24156300
C	-0.88960700	-5.68686400	-6.35805000
H	-1.68166800	-5.16392600	-6.89158400
C	0.45569800	-5.30097400	-6.49072000
O	0.93617600	-4.14609300	-7.17234200
C	0.37992000	-1.64160900	-8.11253900
C	0.05085200	-3.21747300	-7.96235100
C	3.13776500	-8.43454400	-4.54107400
C	-1.95043800	-9.03497700	-3.51183900
S	3.68021100	-8.06010700	-6.21616400

S	4.22978600	-9.63355700	-3.76057600
S	-2.48037500	-10.19559300	-2.24224600
S	-3.02436400	-9.12148800	-4.95405400
C	5.20396100	-9.98163400	-5.18092400
H	5.97466100	-10.74328900	-5.08129600
C	4.95378700	-9.26777600	-6.29464700
H	5.49074200	-9.36405100	-7.23618900
C	-3.97214900	-10.50308800	-4.42550000
H	-4.72699700	-10.88078000	-5.11220600
C	-3.72414500	-10.98997000	-3.19507700
H	-4.24748700	-11.82452000	-2.73273100
H	0.01671000	-3.64367500	-8.97719100
H	-0.95763700	-3.25517800	-7.53236600
O	0.14473000	-8.76291700	1.51315600
C	0.96641000	-8.69337500	2.79325700
H	1.81817900	-8.02647000	2.62327000
H	1.34778300	-9.71044800	2.96722600
C	0.09211600	-8.20874300	4.07778200
H	-0.48333600	-9.08421800	4.41428900
H	-0.64404700	-7.49736700	3.70401600
C	0.83170500	-7.56853700	5.40142600
H	1.29197900	-8.40645900	5.94876500
H	1.66279700	-6.93998200	5.07059200
C	-0.05570100	-6.71493800	6.49567600
H	-0.60044100	-7.45183200	7.10714700
H	-0.82894200	-6.15656300	5.95910300
C	0.70773200	-5.69790900	7.54870700
H	1.12520400	-6.32987400	8.34903100
H	1.57279300	-5.25620900	7.04396000
C	-0.14368200	-4.49243600	8.27535400
H	-0.76117900	-4.96454700	9.05633700
H	-0.85259800	-4.09909500	7.54759900
C	0.62973200	-3.22692100	8.97839200
H	1.02830600	-3.58693700	9.94034600
H	1.50730400	-2.97486000	8.37645900
C	-0.17374100	-1.81273900	9.33449200



H	-0.66003500	-1.99139300	10.30987700
H	-0.99915600	-1.64572500	8.63378800
C	-0.28663500	8.81938400	2.44918000
H	-0.63741500	9.85508700	2.56980900
H	-1.15237600	8.17955400	2.25119900
C	0.48289800	8.34343100	3.79880900
H	1.18846100	7.56654600	3.50765700
H	1.09824200	9.19339800	4.13041300
C	-0.37759800	7.82151800	5.09874300
H	-1.24264200	7.25248100	4.74330100
H	-0.78899100	8.71543600	5.59472000
C	0.39565000	6.94706700	6.25698600
H	1.05219000	6.22855500	5.77550400
H	1.07193100	7.65421200	6.76138100
C	-0.47556000	6.23955600	7.48050500
H	-1.53587500	6.39504400	7.22453000
H	-0.28434600	6.89055300	8.34551600
C	-0.64680000	4.68843000	8.20240500
H	-1.26577900	5.00653000	9.05760300
H	-1.33634900	4.14390900	7.55858300
C	0.38961100	3.60141300	8.81378200
H	0.85693300	4.03757500	9.71114500
H	1.20665100	3.41872700	8.11418000
C	-0.26552600	2.14520400	9.29426300
H	-1.11892900	1.89665000	8.65770300
H	-0.70006600	2.34789000	10.28950600
C	0.69258700	0.88858300	9.50167600
C	0.71959600	-0.50399300	9.52487600
H	1.72683300	-0.83876500	9.80465900
H	1.68456400	1.27345400	9.77177300
C	-11.16734900	-6.17829600	-1.19946700
C	-9.98272000	-6.22694200	-0.40689100
C	-8.73752300	-6.02639800	-1.07961700
C	-8.71803200	-5.52723800	-2.42738800
C	-9.94373800	-5.22994900	-3.09999200
C	-11.14854700	-5.69806600	-2.49724100

C	-7.50226000	-6.13348700	-0.35223700
C	-6.25323600	-6.01257100	-1.03948600
C	-6.23415500	-5.51155000	-2.38395800
C	-7.46372900	-5.14465900	-3.01628500
C	-5.02866200	-6.14190400	-0.31646900
C	-3.77788800	-5.99517300	-1.00115800
C	-3.75960400	-5.49241500	-2.33571300
C	-4.99070900	-5.14415500	-2.98149900
C	-2.55128100	-6.07877100	-0.27261700
C	-1.30805400	-5.86472200	-0.93175200
C	-1.28899900	-5.39290100	-2.25780000
C	-2.51636000	-5.08684900	-2.90901300
C	-5.05225600	-6.14692300	1.11607200
C	-3.82429000	-6.00967800	1.84287700
C	-2.57485500	-6.09192200	1.15258700
C	-6.29948800	-6.02414800	1.80065000
C	-6.32395800	-5.54039500	3.15121400
C	-5.10044000	-5.18422100	3.79523500
C	-3.84929800	-5.52457600	3.18458500
C	-7.52560200	-6.13967900	1.07272600
C	-8.78357100	-6.04071200	1.76120600
C	-8.80799900	-5.55919400	3.11536000
C	-7.57375000	-5.18487900	3.75007600
C	-10.00626900	-6.23462800	1.04664800
C	-11.21582600	-6.19596300	1.80114400
C	-11.23932100	-5.73381900	3.10536700
C	-10.05497300	-5.27451100	3.75365100
C	-7.59656600	-4.28249000	4.85292600
C	-8.85341200	-3.76059800	5.31541800
C	-10.07811600	-4.35504500	4.87938800
C	-6.36926100	-3.73898100	5.34854500
C	-5.12323400	-4.27408100	4.90152400
C	-3.89478100	-3.71205000	5.38034800
C	-2.64670000	-4.21711900	4.89956800
C	-2.62426700	-5.12812100	3.80575100
C	-1.37714200	-5.40374700	3.17730600

C	-1.35268800	-5.89548400	1.85338900
C	-1.42270700	-3.62313100	5.31604400
C	-0.16684500	-4.10763300	4.84938100
C	-0.14486400	-5.00082000	3.77340700
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C	1.20030300	-5.34084800	-2.20732500
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C	2.38681500	-5.96099800	1.22421200
C	3.65938500	-5.86959500	-0.86843300
C	3.67874700	-5.41178100	-2.20858500
C	2.44715400	-5.02775000	-2.81475100
C	2.45987000	-4.10014600	-3.87899100
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C	-0.02565700	-4.06845400	-3.86468200
C	-1.26344200	-3.56458200	-4.35930500
C	-2.50320900	-4.15173200	-3.98012500
C	4.92754600	-5.08292200	-2.82628500
C	4.94006900	-4.15891500	-3.91672000
C	3.70305900	-3.59107400	-4.36178200
C	3.70811900	-2.34723200	-5.04566000
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C	1.22942500	-2.31378200	-4.98178700
C	-0.01378400	-1.66176800	-5.21389000
C	-1.25698200	-2.34482100	-5.06547100
C	-0.01960700	-0.27658200	-5.40196400
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C	2.46457700	-0.26703800	-5.41421600
C	3.69710800	0.44809800	-5.46831700
C	4.94181600	-0.25825100	-5.50144500
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C	-1.27973000	1.80098000	-5.25126900
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C	-0.06551400	3.63069500	-4.20021400
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C	1.09334900	5.96013100	-0.04643900
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C	6.09285800	5.23682500	-2.66321300
C	6.11733200	4.32301300	-3.76854500
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C	1.07421900	5.96667600	1.35630900

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C	2.28844300	5.40467300	3.39385800
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C	4.77802900	6.01197900	2.13328300
C	6.02278000	6.15915600	1.44977400
C	6.04390000	6.18027100	0.01542500
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C	2.26655200	3.61543000	5.54880000
C	1.03346100	4.09144700	5.02572500
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C	9.70158700	-0.35234200	6.94609200
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C	9.76905300	-5.16755300	4.07736900
C	9.69621100	3.74827300	5.76688900



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C	9.81707400	-6.12565600	1.36882600
C	9.88169900	-5.11757600	-2.77722000
C	9.89552900	-4.17042900	-3.88014700
C	9.89741400	-0.22447100	-5.50550000
C	9.90335900	-1.66033600	-5.27669900
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C	11.00124500	-6.07536900	2.16225200
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C	10.89378600	0.42301700	7.05433900
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C	10.89529300	4.40360200	5.35861400

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C	11.09906600	-3.61618700	-4.40813200
C	11.10277800	-2.40706600	-5.08121300
C	11.09044200	0.55547800	-5.55683400
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C	11.03355300	4.50028300	-3.77632500
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C	-9.95497700	2.46839800	-5.30883100
C	-9.97534300	3.71444400	-4.56017700
C	-9.92729200	-0.35135300	-5.85126200
C	-9.92205400	-1.78608400	-5.61716600
C	-10.14036800	2.36825300	6.18472700
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H	11.95622200	5.77514400	-2.34196200
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H	11.99732200	4.23460400	-4.20758800
H	11.99900900	-6.30135700	-0.36178200
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**(5,5)@Cycle-9**

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C	4.57035800	0.78520400	-5.51515100
H	4.91416100	2.91640200	-5.67708300
H	6.99108300	-1.56681300	-5.04739900
H	3.48547500	0.87774800	-5.59499000
C	2.51015700	-6.83226700	-0.68997900
C	0.95487000	-7.59843900	-2.50912600
C	1.97613600	-6.79018900	-2.07080600
C	2.70447600	-5.83757300	-2.93521700
C	2.06910600	-4.99132700	-3.85995600
C	4.81308400	-4.71601800	-3.45056700
C	2.77362300	-4.01801100	-4.57966900
H	0.98696400	-5.03430800	-3.97209300
H	5.85946600	-4.51008200	-3.23881600
H	2.23740000	-3.35404000	-5.25363000
C	5.14851400	-0.48888000	-5.36528000
C	4.14859900	-3.85783300	-4.34265400
C	4.22981800	-1.69287700	-5.37470200
H	3.87715000	-1.90680000	-6.40149700

H	3.34137300	-1.47505400	-4.75892500
O	4.91453500	-2.84218500	-4.85704700
C	4.11761800	-5.70632000	-2.74335400
C	4.76505900	-6.55665000	-1.71525800
C	6.00525600	-7.12867700	-1.88832500
S	7.01360500	-6.93234300	-3.36477000
S	6.75362400	-8.26826900	-0.71614200
C	8.18082600	-8.18685100	-2.96575500
H	8.95297200	-8.40185100	-3.70175400
C	8.06408700	-8.79078600	-1.76742200
H	8.72752100	-9.56647200	-1.39025100
S	0.37458500	-7.64647000	-4.21099700
C	-0.72236300	-9.62646100	-2.80037600
H	-1.31392200	-10.50498400	-2.55061400
S	0.13108700	-8.82761100	-1.48377300
C	-0.61215300	-9.09360200	-4.03238500
H	-1.10134200	-9.47741400	-4.92538400
C	2.18635500	-6.82013600	1.73377000
C	3.92279600	-6.76046800	-0.51502300
C	4.42725200	-6.77827500	0.80316700
H	5.49526100	-6.66035100	0.97392200
C	3.58422800	-6.82407500	1.91191600
H	3.98582600	-6.77117800	2.92249100
C	1.65999000	-6.85148100	0.43114600
H	0.58704100	-6.82035400	0.26793200
O	1.44087300	-6.71050400	2.87471200
C	2.06313200	6.32488200	1.17377800
C	3.47889000	6.81207200	-1.23030500
C	3.45382500	6.10252600	1.10471800
H	3.92913700	5.66094300	1.97708200
C	1.36994900	6.75001600	0.02697900
H	0.29253900	6.89183800	0.03292800
C	2.08360500	6.95918200	-1.15861500
H	1.52876600	7.21996600	-2.05920100
C	4.18557000	6.36268100	-0.06711100
C	5.65550200	6.17467400	-0.18267500

C	4.24467900	7.06900800	-2.46715900
C	5.35632200	6.11815200	-2.67414100
C	6.10081300	5.71064300	-1.52180800
C	5.67567500	5.58987000	-3.93456000
H	5.06932200	5.82991800	-4.80633700
C	7.18034000	4.83094200	-1.72671800
H	7.76161600	4.48033000	-0.87972900
C	7.51452400	4.32340300	-2.98744200
H	8.33535100	3.61481200	-3.06431200
C	6.75109100	4.70048700	-4.10162100
O	6.98789400	4.29557400	-5.39760300
C	6.76446800	1.83221100	-5.42474600
C	7.65859600	3.04672900	-5.61927500
C	4.02876100	8.15663200	-3.28152000
C	6.53570000	6.48131200	0.83635600
S	5.03074700	8.55221300	-4.72361400
S	2.80482700	9.43344900	-2.94663500
S	6.04726300	7.05069500	2.46976600
S	8.32450600	6.47961600	0.64713100
C	3.41514200	10.58983800	-4.12649500
H	2.93428500	11.56532500	-4.16396600
C	4.42068200	10.19144400	-4.92898500
H	4.87340300	10.79742700	-5.71133300
C	8.69208200	7.21076200	2.20040700
H	9.73931500	7.40091400	2.42654400
C	7.66019100	7.47283900	3.02550700
H	7.74664500	7.90863200	4.01878500
H	7.97365600	3.10514100	-6.67256000
H	8.57590700	2.96013700	-5.01372300
O	1.47404100	6.05176400	2.38023500
C	0.04679900	6.22331500	2.47110800
H	-0.44218400	5.68516200	1.64283500
H	-0.20316800	7.29534200	2.37476200
C	-0.44564200	5.64588000	3.79338900
H	-0.00330700	6.19432800	4.63930000
H	-0.09850800	4.60499700	3.86375700

C	-1.98529800	5.67715000	3.85420000
H	-2.34061800	6.71295300	3.98904000
H	-2.38385700	5.33476300	2.88487200
C	-2.56787400	4.76854000	4.94849500
H	-2.26484400	5.12727300	5.94707200
H	-2.13010500	3.76392200	4.83153900
C	-4.10002500	4.64967500	4.86949100
H	-4.57073100	5.60538200	5.15827500
H	-4.38683400	4.46631900	3.82059600
C	-4.65690500	3.50735700	5.73260100
H	-4.41645300	3.68636400	6.79531300
H	-4.14256700	2.57237600	5.45065300
C	-6.17059700	3.30392400	5.56565300
H	-6.70905100	4.22144800	5.86089000
H	-6.39181900	3.14608200	4.49919400
C	0.01083300	-6.56878500	2.75441700
H	-0.23583100	-5.91626800	1.90478200
H	-0.44272500	-7.55946200	2.57235700
C	-0.52791600	-5.91709200	4.02347400
H	-0.30184700	-6.54008400	4.90287200
H	-0.00900800	-4.95585200	4.15824700
C	-2.04229600	-5.67296900	3.89808500
H	-2.57956700	-6.63704300	3.89968100
H	-2.25075200	-5.20371600	2.92193800
C	-2.60747600	-4.75698000	4.99381900
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H	-2.07181200	-3.79458400	4.95322100
C	-4.11501200	-4.50267000	4.82261500
H	-4.67847700	-5.41871800	5.07111400
H	-4.32378400	-4.29050600	3.76180700
C	-4.63298100	-3.32917200	5.66816600
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H	-4.04050400	-2.42895000	5.42980900
C	-6.11877800	-3.02569100	5.42198400
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C	-6.65704900	-1.88578400	6.29951100
H	-5.99015900	-1.01088300	6.22814500
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C	-6.70275200	2.11323200	6.37868800
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C	-8.14812000	1.70558400	5.99378800
H	-8.12872300	1.25212400	4.99157600
H	-8.76729300	2.61612400	5.92008700
C	-8.75271600	0.76317000	7.00685400
H	-9.19783400	1.24068500	7.88609900
C	-8.72604000	-0.58144500	6.97033800
H	-9.15189700	-1.12333500	7.82151200
C	-8.09127100	-1.44524100	5.90762300
H	-8.70634900	-2.34863800	5.75209200
H	-8.04727400	-0.91972400	4.94287700
C	-12.72586300	-2.02245700	0.46411400
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C	-11.23699900	-2.93696900	-1.24589400
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C	-10.32543300	-2.05460000	0.87940300
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C	-8.79824500	-3.02744400	-0.80402300
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C	-9.36757100	-1.63049400	-4.14183200
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C	1.18218700	-3.47989000	-0.39474400
C	0.11205700	-3.13551900	-1.27397100
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C	10.29344300	1.30304000	-0.65695200
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C	1.04284000	2.81572300	2.27047000
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H	-13.01749200	-2.82668300	-3.43495800
H	-12.59158700	-1.24092000	-5.23439000
H	-12.38260000	0.88141400	-5.70392400
H	-12.43087400	3.12370800	-4.75310900

**(6,6)@Cycle-9**

C	1.41357000	1.10734600	-7.05016700
C	-0.58812200	2.46697800	-7.13459200
C	0.63019500	-0.04801500	-6.89656900
H	2.50230700	1.02104000	-7.06783500
C	-1.36810000	1.32000800	-6.96764900
H	-1.05589000	3.44753500	-7.21753500
H	1.10140200	-1.02231600	-6.78218700
H	-2.45464300	1.40848000	-6.90732200
C	-2.72891100	-6.78353200	-2.35541900
C	-4.62095600	-7.25200100	-3.93962300
C	-3.50078800	-6.52978900	-3.59545400
C	-2.89555700	-5.49353800	-4.46139300
C	-3.64808700	-4.53970900	-5.17047300
C	-0.87104000	-4.32605400	-5.17984200
C	-3.04637700	-3.49801700	-5.88609700
H	-4.73422100	-4.55309100	-5.10270900
H	0.20173500	-4.15762800	-5.11994900
H	-3.67053700	-2.76305600	-6.38798600
C	-0.76976900	0.04857800	-6.87695000
C	-1.64659200	-3.36847900	-5.85435000
C	-1.68435400	-1.15415200	-6.78160300
H	-2.16923800	-1.34894100	-7.75716500
H	-2.48350500	-0.94412900	-6.05344000
O	-0.94507100	-2.31433800	-6.38120800

C	-1.46866800	-5.39750000	-4.50005600
C	-0.68175000	-6.38926500	-3.73029900
C	0.47824400	-6.95430600	-4.21370100
S	1.20341100	-6.55927900	-5.81189200
S	1.37525900	-8.27330700	-3.38382100
C	2.36101200	-7.88419500	-5.82906800
H	2.97293400	-7.99991400	-6.72139200
C	2.43949200	-8.65949000	-4.73059000
H	3.12437500	-9.49509700	-4.60128400
S	-5.48633400	-7.07416600	-5.50687800
C	-6.40112700	-9.19900700	-4.18191300
H	-6.97287000	-10.09347900	-3.94274300
S	-5.31106200	-8.58388200	-2.94425200
C	-6.48056600	-8.51692200	-5.34046800
H	-7.12599000	-8.77731400	-6.17696800
C	-2.59025100	-7.22458600	0.04929200
C	-1.30385700	-6.75930200	-2.43995500
C	-0.56538700	-7.01630400	-1.26535100
H	0.51941600	-6.93374100	-1.28308100
C	-1.18631200	-7.26832200	-0.04368200
H	-0.60204400	-7.41486300	0.86338300
C	-3.35284700	-6.99578900	-1.11027300
H	-4.43327800	-6.90797500	-1.04038400
O	-3.10491100	-7.36154400	1.30760900
C	-1.30897900	7.34982700	0.52764000
C	-0.60470000	7.74266000	-2.18418200
C	-0.01831700	7.02009300	0.07042800
H	0.65369800	6.55600600	0.78572300
C	-2.26409400	7.84760200	-0.37696000
H	-3.27813000	8.07889600	-0.06043600
C	-1.89932600	8.02487900	-1.71697100
H	-2.65727800	8.36160800	-2.42372300
C	0.35842300	7.20350000	-1.26998500
C	1.68110900	6.80342200	-1.81708500
C	-0.20903800	7.92935000	-3.59728300
C	0.64117600	6.83305700	-4.10539300

C	1.60862400	6.28366300	-3.20718500
C	0.49404000	6.28602400	-5.38905200
H	-0.27891700	6.65033100	-6.06343800
C	2.37887900	5.20069300	-3.66347700
H	3.08611300	4.72858900	-2.99049000
C	2.23843600	4.65643600	-4.94472900
H	2.83156200	3.78530800	-5.21158600
C	1.29858400	5.21697400	-5.82412100
O	1.08987500	4.82375700	-7.12575700
C	0.81460600	2.36815600	-7.20238900
C	1.64904100	3.58085500	-7.57796600
C	-0.51269200	9.05424800	-4.32543400
C	2.87209700	6.93093000	-1.13146900
S	0.05693300	9.35438500	-6.00607000
S	-1.41060800	10.46446900	-3.65825900
S	3.02577200	7.51215700	0.56136600
S	4.48291200	6.62795000	-1.87358300
C	-1.04404300	11.56128400	-4.98690700
H	-1.38869400	12.58939300	-4.89517200
C	-0.38128200	11.05990700	-6.04683400
H	-0.11114700	11.62295400	-6.93803100
C	5.44064700	7.07524700	-0.47383800
H	6.52141700	6.98302100	-0.55887200
C	4.78123400	7.47886500	0.62934900
H	5.24895900	7.77047400	1.56741700
H	1.66130400	3.68801100	-8.67353300
H	2.69531600	3.46305900	-7.25183900
O	-1.54473400	7.11020500	1.85508300
C	-2.90072600	7.24804600	2.32144200
H	-3.57654400	6.71080400	1.63615300
H	-3.18913800	8.31478000	2.31926900
C	-3.00148600	6.63324300	3.71409500
H	-2.43969000	7.23802500	4.44279900
H	-2.52578700	5.64387100	3.68003200
C	-4.47145700	6.47347400	4.14343300
H	-4.92411100	7.46039700	4.34048400



H	-5.03773500	6.03354500	3.30570000
C	-4.64846800	5.55734100	5.36552400
H	-4.15072800	5.99490400	6.24773100
H	-4.13589200	4.60349300	5.16049800
C	-6.12802600	5.26909300	5.67451400
H	-6.61536000	6.17741900	6.06937900
H	-6.64333300	5.02752500	4.73131900
C	-6.32941700	4.09693300	6.64777600
H	-5.89133000	4.33926000	7.63185100
H	-5.77246700	3.22546500	6.26515700
C	-7.80566900	3.70281100	6.81553200
H	-8.36752900	4.53740000	7.27074400
H	-8.24810100	3.53848000	5.82096200
C	-4.50177200	-7.07554500	1.52367100
H	-4.79527900	-6.18518700	0.94647500
H	-5.11582500	-7.92724300	1.17979800
C	-4.68616700	-6.79073400	3.01144400
H	-4.34986900	-7.65594600	3.60324700
H	-4.02176100	-5.95036800	3.26410600
C	-6.14201000	-6.41578400	3.36282300
H	-6.76067000	-7.32411000	3.45481200
H	-6.57622900	-5.82284900	2.54246300
C	-6.21451400	-5.57665900	4.65013200
H	-5.83138700	-6.16227500	5.50364600
H	-5.52745700	-4.72369500	4.53107400
C	-7.61277200	-5.02534300	4.98114900
H	-8.28071800	-5.83986200	5.31067700
H	-8.06125800	-4.60313000	4.06757200
C	-7.54091700	-3.92786400	6.05683900
H	-7.12958300	-4.35245900	6.98960900
H	-6.81776300	-3.16492300	5.72340700
C	-8.87679900	-3.23030300	6.35385200
H	-9.61098600	-3.96201800	6.73478100
H	-9.29364500	-2.82854200	5.41855900
C	-8.71461000	-2.09015900	7.37274400
H	-7.88506300	-1.43251300	7.06385400

H	-8.42504400	-2.51464700	8.34960900
C	-7.99119300	2.43962400	7.67101900
H	-7.34757000	1.63075200	7.28698700
H	-7.64838800	2.64565300	8.69981500
C	-9.45631700	1.93414700	7.70439400
H	-9.70372800	1.48521300	6.73107700
H	-10.12126000	2.80783400	7.83342600
C	-9.68714700	0.96714900	8.83828000
H	-9.61542800	1.41590900	9.83545400
C	-9.91261500	-0.35726100	8.77041500
H	-10.00654800	-0.90106100	9.71697400
C	-9.98801200	-1.22469600	7.53899400
H	-10.86092600	-1.89735200	7.62077000
H	-10.13134700	-0.62509000	6.62824400
H	-10.52729200	3.62958100	-3.70183700
H	-10.61202900	1.42919300	-4.73234000
H	-10.79133600	-0.69673900	-4.55569500
H	-11.06431000	-2.67575000	-3.17013600
H	-11.30065100	-3.56707500	-1.23586900
H	-11.49143200	-3.34401200	1.17802600
H	-10.57851000	4.85152900	-1.94374200
H	-10.76376200	5.05871600	0.47159800
H	-10.99124600	4.19024900	2.42241600
H	-11.26947700	2.21794100	3.82137200
H	-11.46184000	0.07368200	3.99140500
H	-11.54548300	-2.12051400	2.94107900
C	-9.60541000	3.05590700	-3.78921200
C	-9.65360500	1.80422600	-4.37541500
C	-9.90519900	-1.16087100	-4.12446000
C	-10.06047200	-2.28668100	-3.33622000
C	-10.38982900	-3.52937800	-0.63953900
C	-10.49869900	-3.40229700	0.73345200
C	-9.67657400	4.76166100	-1.33958000
C	-9.78218700	4.87949400	0.03455200
C	-10.10444000	3.64382900	2.74110000
C	-10.26324500	2.52300900	3.53689500

C	-10.52749500	-0.44703700	3.78610000
C	-10.57446400	-1.69279500	3.18668800
C	-8.41566500	3.51897100	-3.14351500
C	-8.51511700	0.93812800	-4.35145500
C	-8.63772900	-0.50533700	-4.22741900
C	-8.95797400	-2.82695800	-2.60191600
C	-9.11868400	-3.43126300	-1.28906800
C	-9.34251400	-3.16712600	1.54253500
C	-8.45044300	4.34896000	-1.95040600
C	-8.66804300	4.59056000	0.88362100
C	-8.82608000	3.98330700	2.19547400
C	-9.15274100	1.67315000	3.83614100
C	-9.28122500	0.23187900	3.96767100
C	-9.37925800	-2.33353800	2.73174000
C	-7.19905000	2.84288200	-3.46461300
C	-7.24980200	1.53977900	-4.07288300
C	-7.48750000	-1.25317200	-3.82956600
C	-7.64920400	-2.42502900	-3.00945300
C	-7.95984100	-3.59427000	-0.47055900
C	-8.07268700	-3.45772100	0.95732800
C	-7.26612200	4.44754700	-1.15792200
C	-7.37715500	4.56498100	0.27163700
C	-7.68417500	3.38055000	2.80423200
C	-7.84886300	2.21907300	3.63453600
C	-8.09646900	-0.56164200	3.89427700
C	-8.14489000	-1.85069200	3.26262200
C	-5.95604600	3.29179000	-2.89652300
C	-6.05549900	0.73892300	-4.08468100
C	-6.17647100	-0.67577600	-3.95800700
C	-6.49313100	-2.97059600	-2.35053200
C	-6.65103000	-3.56258600	-1.06404000
C	-6.87260000	-3.29357500	1.73086300
C	-5.98994700	4.10427000	-1.72673300
C	-6.20682000	4.32715200	1.07240400
C	-6.36346000	3.72192300	2.35166600
C	-6.68725100	1.45229600	3.98870300

C	-6.81235900	0.04121400	4.12603800
C	-6.90922500	-2.48554400	2.90015400
C	-4.72680500	2.65768400	-3.26954000
C	-4.77932200	1.35461300	-3.87291500
C	-5.01918600	-1.44661700	-3.61615800
C	-5.18042100	-2.61498000	-2.79603100
C	-5.49290400	-3.78677300	-0.25299800
C	-5.60536900	-3.65106000	1.17175100
C	-4.79390000	4.26291500	-0.95452200
C	-4.90672300	4.36812000	0.47342700
C	-5.21870300	3.17464000	3.01140400
C	-5.38289400	2.02496300	3.85285600
C	-5.62935200	-0.76560100	4.11925800
C	-5.67956200	-2.05508900	3.49206900
C	-3.49453300	3.11399200	-2.70889600
C	-3.59762700	0.55364900	-3.88963400
C	-3.72220300	-0.86912700	-3.74886400
C	-4.03895600	-3.16090900	-2.13739000
C	-4.19707800	-3.75798900	-0.84584400
C	-4.42139600	-3.51291100	1.95486600
C	-3.52892800	3.92975900	-1.52750800
C	-3.75157100	4.13287200	1.27780500
C	-3.91155100	3.52820500	2.56728500
C	-4.23332300	1.26217400	4.21893900
C	-4.35772100	-0.16106900	4.35486800
C	-4.45813900	-2.70236700	3.13749400
C	-2.26628500	2.46327800	-3.06818700
C	-2.31981200	1.16471000	-3.66321800
C	-2.56534200	-1.63471200	-3.38797500
C	-2.72665000	-2.79166600	-2.57139200
C	-3.03764000	-3.97339700	-0.03113500
C	-3.15087800	-3.85688200	1.38708800
C	-2.33542400	4.06473100	-0.74198600
C	-2.44968700	4.16376200	0.67915300
C	-2.76533400	2.97962000	3.23005300
C	-2.92684600	1.83326200	4.06799400

C	-3.17054700	-0.96720900	4.32929400
C	-3.22217700	-2.25854500	3.71607700
C	-1.03016900	2.91396800	-2.49965100
C	-1.13758900	0.35596800	-3.68242600
C	-1.26308300	-1.06360700	-3.53962300
C	-1.58286100	-3.34791400	-1.92089700
C	-1.73950400	-3.94203000	-0.62954700
C	-1.96155100	-3.72511300	2.17466500
C	-1.06682100	3.72449900	-1.31445100
C	-1.29487400	3.94166600	1.49454800
C	-1.45289100	3.34580100	2.79018800
C	-1.77018800	1.06797900	4.43049800
C	-1.89363700	-0.35737500	4.56172400
C	-1.99624200	-2.91046300	3.35755100
C	0.18785500	2.25539100	-2.85067700
C	0.13545600	0.95968900	-3.46232400
C	-0.11431600	-1.83587500	-3.19669500
C	-0.27681300	-2.99435500	-2.37049200
C	-0.58502300	-4.16341800	0.17583100
C	-0.69677100	-4.05796400	1.59986900
C	0.11440200	3.84709100	-0.52422400
C	-0.00014000	3.96415900	0.89924400
C	-0.31011000	2.80443900	3.45396400
C	-0.47047800	1.64279500	4.28268700
C	-0.71123900	-1.15992200	4.53453600
C	-0.76358600	-2.45918500	3.92431600
C	1.41776900	2.68308400	-2.25838500
C	1.31577300	0.14704700	-3.48320800
C	1.19078500	-1.27153800	-3.35456700
C	0.86855200	-3.55726300	-1.72391300
C	0.71266000	-4.14352200	-0.42940200
C	0.49823400	-3.91457700	2.37841600
C	1.38162700	3.49458500	-1.08544300
C	1.15898700	3.75476800	1.71440200
C	1.00311600	3.16597100	3.00801800
C	0.68878900	0.87364300	4.62996700

C	0.56686300	-0.54659100	4.75532700
C	0.46484100	-3.10186100	3.55512000
C	2.64321800	2.03686600	-2.62020500
C	2.59398400	0.75017200	-3.25049800
C	2.34608400	-2.05046500	-3.01187700
C	2.18219000	-3.21259600	-2.18262900
C	1.87348600	-4.38151700	0.37446300
C	1.76510900	-4.26029800	1.80224500
C	2.57148100	3.65187200	-0.30639000
C	2.46054200	3.79215600	1.11685000
C	2.15303500	2.62104500	3.66831700
C	1.99333800	1.45332900	4.48938000
C	1.75385700	-1.35094600	4.73276600
C	1.70188600	-2.65005400	4.12249200
C	3.87131500	2.48555800	-2.04856700
C	3.77442800	-0.05437200	-3.27576500
C	3.64888800	-1.48117000	-3.15619100
C	3.32511200	-3.77098100	-1.53127900
C	3.16798700	-4.36493900	-0.23130100
C	2.95587900	-4.11500100	2.57753000
C	3.83518800	3.31006300	-0.87330400
C	3.61774200	3.58425700	1.92722400
C	3.46169400	2.98597600	3.22405100
C	3.14796600	0.68640900	4.83599500
C	3.02601900	-0.74003800	4.95820100
C	2.92375100	-3.29453800	3.75686700
C	5.09823400	1.84322500	-2.41193400
C	5.04884100	0.55405500	-3.02977600
C	4.80374500	-2.25127300	-2.79742700
C	4.63992600	-3.41195300	-1.97672100
C	4.33049500	-4.58320400	0.57887700
C	4.22323100	-4.45460100	1.99986500
C	5.02687800	3.46502600	-0.09505900
C	4.91759000	3.60618100	1.32295500
C	4.61149300	2.42818200	3.87393800
C	4.45251700	1.26302200	4.68837400

C	4.21277400	-1.54340100	4.92602800
C	4.16090500	-2.83665600	4.31742800
C	6.33289900	2.30204600	-1.84428200
C	6.23598300	-0.25033700	-3.05356800
C	6.11149700	-1.67591000	-2.93639200
C	5.78899300	-3.97050600	-1.32293100
C	5.63179500	-4.56590000	-0.02589400
C	5.41911600	-4.30892000	2.77900400
C	6.29662400	3.12777100	-0.66957300
C	6.08167100	3.39420200	2.13419200
C	5.92619900	2.79459500	3.42963700
C	5.61216700	0.49296600	5.03630900
C	5.49035900	-0.93237900	5.15606500
C	5.38765800	-3.48607700	3.95497100
C	7.55483200	1.65639300	-2.20064800
C	7.50521000	0.35769300	-2.81355200
C	7.26266000	-2.44269400	-2.58375100
C	7.09862300	-3.61163700	-1.76501900
C	6.78957300	-4.78334500	0.78124400
C	6.68152100	-4.65163200	2.20753500
C	7.48560100	3.28252900	0.10523900
C	7.37605900	3.41682900	1.53207300
C	7.07113500	2.23824600	4.07628900
C	6.91140400	1.06713100	4.89277600
C	6.67180600	-1.73315000	5.12629800
C	6.61945900	-3.03224000	4.51577200
C	8.78733000	2.10187500	-1.62306000
C	8.68912700	-0.44754900	-2.82088900
C	8.56660200	-1.86220500	-2.70552600
C	8.24626900	-4.15686600	-1.10383900
C	8.09009200	-4.74977700	0.18202100
C	7.87733800	-4.48980900	2.97922700
C	8.75252700	2.92396600	-0.45968300
C	8.53754200	3.18530300	2.33766200
C	8.38353700	2.58994400	3.62289500
C	8.07009100	0.29256600	5.22320400

C	7.94913600	-1.12196100	5.34066300
C	7.84626000	-3.67079400	4.14436700
C	10.02323500	1.46121700	-1.98409500
C	9.97297000	0.15931200	-2.59449600
C	9.73175600	-2.63319500	-2.36605200
C	9.56806900	-3.80634700	-1.54962700
C	9.25973300	-4.97883500	0.98691300
C	9.15123300	-4.84531000	2.41516800
C	9.95540200	3.08376200	0.31218900
C	9.84556200	3.21736300	1.74061800
C	9.54136400	2.04180500	4.27648600
C	9.38137100	0.86810800	5.09295700
C	9.14226600	-1.92445000	5.32393900
C	9.08963100	-3.22619000	4.71370900
C	11.25928900	1.94885900	-1.46026400
C	11.15903100	-0.63302500	-2.66859500
C	11.03428900	-2.07670600	-2.55090200
C	10.71053100	-4.40276700	-0.93396600
C	10.55090900	-5.01013400	0.37702100
C	10.33547300	-4.74529000	3.20762600
C	11.22412400	2.78847000	-0.27401400
C	11.00637200	3.05298600	2.55653600
C	10.84920000	2.44458600	3.86743100
C	10.53197500	0.11781900	5.48478300
C	10.40852900	-1.32577000	5.60369600
C	10.30408500	-3.90689600	4.39478800
C	12.45378000	1.29843800	-1.90385300
C	12.40517500	0.04636900	-2.48939900
C	12.14895900	-2.92023800	-2.24683700
C	11.99183400	-4.04884700	-1.46306000
C	11.66392200	-5.29891900	1.22824000
C	11.55950700	-5.17027400	2.60125000
C	12.38199300	3.02427000	0.53255000
C	12.27642000	3.15269300	1.90547900
C	11.95346000	1.90149000	4.59712700
C	11.79962500	0.77277900	5.38136000



C	11.54588300	-2.19332000	5.62479900
C	11.49518700	-3.44502900	5.03872600
H	13.42569500	1.72412500	-1.65739800
H	13.34021800	-0.47655800	-2.68648700
H	13.15643200	-2.60390300	-2.51437100
H	12.88027100	-4.58783200	-1.13633600
H	12.64424900	-5.48779100	0.79247600
H	12.46054900	-5.26189200	3.20650700
H	13.37398200	2.96506600	0.08638600
H	13.18830500	3.19066700	2.50014300
H	12.95704300	2.29065200	4.42988100
H	12.68645600	0.30645600	5.80874600
H	12.50517200	-1.81983800	5.98100500
H	12.41606700	-4.02022000	4.95090900

**(7,7)@Cycle-9**

C	2.69159000	1.09638500	-7.36850400
C	0.33829700	1.65234900	-7.50573200
C	2.36858100	-0.26340800	-7.23561400
H	3.73859700	1.40598200	-7.35428000
C	0.01476700	0.30202500	-7.36250900
H	-0.44821800	2.40210600	-7.58816500
H	3.15203400	-1.00611200	-7.09950100
H	-1.03262300	-0.00337700	-7.32996100
C	1.82693600	-7.55040700	-2.37238200
C	-0.12701300	-8.52682800	-3.60330500
C	0.80956600	-7.52919300	-3.44881200
C	0.97473100	-6.40188200	-4.39062400
C	-0.10359500	-5.72088800	-4.97883800
C	2.47475400	-4.78633300	-5.45164800
C	0.07847500	-4.61502600	-5.81819200
H	-1.12346100	-6.01177200	-4.73390300
H	3.45830800	-4.33617200	-5.56716900
H	-0.79623900	-4.12369800	-6.23539800
C	1.02553700	-0.67062700	-7.24151900
C	1.37432200	-4.10969300	-6.00888100

C	0.58828500	-2.11282700	-7.10073900
H	0.21273100	-2.50949000	-8.06286100
H	-0.24509500	-2.14233500	-6.38204600
O	1.67279100	-2.92889600	-6.64453400
C	2.30199300	-5.94136100	-4.67423400
C	3.43380700	-6.69327200	-4.08286900
C	4.58673800	-6.96893300	-4.78602200
S	4.89716400	-6.42533100	-6.47326200
S	5.90252500	-8.03555700	-4.17956800
C	6.29668600	-7.45571900	-6.75083400
H	6.73930200	-7.43813000	-7.74478600
C	6.75219100	-8.18350700	-5.71326800
H	7.61824300	-8.84171000	-5.74200100
S	-1.26933200	-8.63209800	-4.98960400
C	-1.33906400	-10.88273700	-3.56273800
H	-1.60172000	-11.88892400	-3.24209700
S	-0.25759300	-9.96193400	-2.52302100
C	-1.79629700	-10.28261100	-4.67821400
H	-2.48358300	-10.73013900	-5.39337300
C	2.50447900	-7.91308000	-0.05065900
C	3.16444200	-7.19385100	-2.71682900
C	4.14709700	-7.25780700	-1.70615400
H	5.16096300	-6.92508000	-1.91783200
C	3.83949200	-7.63934000	-0.40312300
H	4.59995400	-7.64009100	0.37527900
C	1.50572700	-7.87337700	-1.03850500
H	0.46628200	-8.03919800	-0.76810500
O	2.28403700	-8.14950100	1.27670900
C	0.23049300	7.85829500	0.61003400
C	-0.03654800	7.71298100	-2.20603900
C	1.36589100	7.72026100	-0.20882200
H	2.32091400	7.57463400	0.28899000
C	-1.04711400	7.91142500	0.02389500
H	-1.94590100	7.97603000	0.63152000
C	-1.16040400	7.81275400	-1.36739500
H	-2.15743600	7.76215300	-1.80260100

C	1.26309200	7.66474800	-1.60728100
C	2.43941400	7.49115400	-2.49375200
C	-0.13670500	7.60744200	-3.67629100
C	0.86205500	6.69642200	-4.27440500
C	2.17233400	6.66329700	-3.69301600
C	0.57450100	5.87781000	-5.37519000
H	-0.43337700	5.82694800	-5.78218100
C	3.12202800	5.81080400	-4.28148100
H	4.09744000	5.69165200	-3.81794500
C	2.84563000	5.02654600	-5.40942400
H	3.62082600	4.36228600	-5.78345100
C	1.56311300	5.07419400	-5.97648400
O	1.14904800	4.42296100	-7.11117500
C	1.68449600	2.06241400	-7.52218100
C	2.02123400	3.51201500	-7.80837300
C	-0.98931100	8.38598200	-4.42800600
C	3.65076200	8.11141800	-2.25632600
S	-1.04983700	8.38474500	-6.22657200
S	-2.07223000	9.64137100	-3.72688100
S	3.97484300	9.20718600	-0.86634500
S	5.06150500	8.02933300	-3.36930000
C	-2.46612700	10.42451800	-5.25351200
H	-3.08435000	11.31902000	-5.21039200
C	-2.00316200	9.85678200	-6.38354000
H	-2.19087100	10.22389800	-7.39062100
C	6.00264800	9.29489900	-2.59210100
H	6.94882100	9.56825000	-3.05473500
C	5.50931000	9.82809700	-1.45822200
H	5.99648100	10.59892900	-0.86440200
H	1.83696300	3.72758400	-8.87295300
H	3.08269500	3.72076200	-7.61460700
O	0.47323500	7.85946400	1.95739900
C	-0.66231400	7.69046600	2.82943700
H	-1.30513200	6.89149400	2.42879900
H	-1.25516600	8.62247000	2.85693200
C	-0.17351800	7.28418900	4.21900000

H	0.34235700	8.12228500	4.71202400
H	0.56330400	6.47937100	4.08941700
C	-1.35342000	6.76358000	5.06755300
H	-1.94376200	7.60478400	5.46766600
H	-2.03207600	6.20025500	4.40559900
C	-0.93881200	5.81123800	6.20471800
H	-0.41437000	6.35951400	7.00537000
H	-0.21826200	5.08286000	5.80011000
C	-2.14902000	5.04330600	6.76859300
H	-2.78787000	5.71951800	7.36227700
H	-2.76578900	4.70919100	5.91880800
C	-1.78255100	3.80337300	7.60085900
H	-1.31182600	4.10343400	8.55309000
H	-1.02889500	3.21459200	7.05324600
C	-3.00392600	2.91131100	7.87494000
H	-3.76533600	3.48393900	8.43348800
H	-3.46860700	2.64112600	6.91381300
C	0.93126600	-8.12019500	1.77726200
H	0.36867300	-7.31402000	1.28039000
H	0.42827300	-9.07877700	1.55725600
C	1.01320300	-7.82914000	3.27417200
H	1.51209400	-8.66030700	3.79604300
H	1.65560400	-6.94390100	3.39030000
C	-0.36643100	-7.53125400	3.89325400
H	-0.92632000	-8.46523200	4.06766800
H	-0.96087900	-6.94028600	3.17790400
C	-0.25129400	-6.72076300	5.19618500
H	0.24627500	-7.32149700	5.97682600
H	0.40761100	-5.85826000	5.00381900
C	-1.60100500	-6.19257500	5.70951800
H	-2.23265100	-7.02766700	6.05840800
H	-2.13931500	-5.72868100	4.86816500
C	-1.43813200	-5.14937700	6.82720800
H	-0.98842900	-5.62142200	7.71823800
H	-0.71994500	-4.38434600	6.48977000
C	-2.74882900	-4.44917400	7.21831400

H	-3.46316100	-5.18539700	7.62681500
H	-3.21934200	-4.03041100	6.31605900
C	-2.52635000	-3.32823500	8.24473100
H	-1.75321600	-2.63521000	7.87372200
H	-2.12913000	-3.76589600	9.17727300
C	-2.66498700	1.63262900	8.65419000
H	-1.85441000	1.08650400	8.14454900
H	-2.27683200	1.90895300	9.65004900
C	-3.88320300	0.69066200	8.81911800
H	-4.11476200	0.21836100	7.85339800
H	-4.76071500	1.30881600	9.08624300
C	-3.66166700	-0.33376000	9.90215200
H	-3.48145900	0.09550300	10.89443900
C	-3.63583600	-1.67399700	9.79592900
H	-3.43420600	-2.24663800	10.70844300
C	-3.80783200	-2.52109300	8.56108900
H	-4.63607200	-3.23541000	8.72452600
H	-4.08268000	-1.91418400	7.68618800
H	11.55247300	5.29748500	1.93330300
H	11.34240400	4.61945500	4.25401400
H	11.22146200	3.21054300	5.82450300
H	11.18095800	0.96774200	6.75153100
H	11.23883300	-1.14342500	6.62377300
H	11.39434400	-3.25819100	5.44259000
H	11.58083900	-4.46937600	3.71944000
H	11.81344300	-4.86183500	1.33597000
H	11.76118000	4.95037800	-0.14061900
H	11.98093700	3.55998800	-2.11741300
H	12.11718700	1.71686400	-3.14402400
H	12.17738700	-0.70492800	-3.28952800
H	12.13588800	-2.66263000	-2.49230900
H	11.99381600	-4.27841300	-0.68675200
C	10.56165000	5.06538500	2.32134000
C	10.44202000	4.67890200	3.64419900
C	10.27057500	2.68148500	5.86924800
C	10.24756100	1.40333300	6.39778800

C	10.32797200	-1.58529900	6.22228600
C	10.41659000	-2.79043700	5.54895200
C	10.68153000	-4.50395300	3.10611900
C	10.81403700	-4.72748800	1.74736500
C	10.85672900	4.57740500	-0.61920900
C	10.98205600	3.78487400	-1.74612200
C	11.17475100	1.17400900	-3.20152500
C	11.20908300	-0.20641900	-3.28470200
C	11.15108100	-2.97611200	-2.14869700
C	11.07010500	-3.89661800	-1.11932000
C	9.44434400	5.01445200	1.43229000
C	9.19683100	4.21409600	4.16852600
C	9.11368900	3.24538800	5.24852900
C	9.06574200	0.60226800	6.34218800
C	9.10455800	-0.84794300	6.25888300
C	9.28792300	-3.34042200	4.86688900
C	9.41661900	-4.16990800	3.68055500
C	9.69115200	-4.63121400	0.86900000
C	9.58744400	4.77907300	0.00528700
C	9.84659000	3.13991900	-2.32615800
C	9.94026000	1.87350700	-3.03317400
C	10.01128300	-0.98152400	-3.20496200
C	9.98282000	-2.32501500	-2.65159500
C	9.81525800	-4.22808600	-0.52179000
C	8.14915500	4.88616100	2.02225800
C	8.02478500	4.48309400	3.39672000
C	7.86309000	2.60029700	5.49655200
C	7.83894800	1.27277100	6.04726100
C	7.91380400	-1.54514300	5.88807800
C	8.00593100	-2.79755800	5.18879200
C	8.25629300	-4.40760200	2.88144500
C	8.39423500	-4.63756100	1.46878200
C	8.42713000	4.43058600	-0.75229500
C	8.55745800	3.60737300	-1.92426200
C	8.73944500	1.14617000	-3.29968500
C	8.77495200	-0.28860200	-3.38653800

C	8.71983500	-2.89773000	-2.30754400
C	8.63577100	-3.85236000	-1.23568100
C	6.97676300	4.89355600	1.19061300
C	6.73204700	4.09832900	3.89495200
C	6.65047800	3.14963100	4.95405100
C	6.60272600	0.53909300	6.03945200
C	6.64026500	-0.88214100	5.96068600
C	6.82134000	-3.34527600	4.58636000
C	6.94811600	-4.15520800	3.42200700
C	7.21974800	-4.60255900	0.64105400
C	7.11718900	4.66485500	-0.20840000
C	7.37342900	3.04559600	-2.51526600
C	7.46520100	1.80545100	-3.21058600
C	7.53506800	-1.01680800	-3.37987900
C	7.50708400	-2.33199200	-2.83354800
C	7.34125100	-4.20717000	-0.72186900
C	5.67576900	4.83505000	1.78585800
C	5.55112800	4.43006000	3.15688800
C	5.38918500	2.54557800	5.26162000
C	5.36471800	1.22182600	5.81416200
C	5.43900700	-1.60029900	5.65876000
C	5.53087700	-2.85028300	4.96102400
C	5.78255600	-4.45669500	2.64845500
C	5.92064600	-4.67699200	1.23774800
C	5.95458900	4.38088900	-0.99350200
C	6.08448200	3.55873200	-2.16282800
C	6.26720400	1.09720800	-3.54844100
C	6.30170600	-0.33512100	-3.63352400
C	6.24597200	-2.94413500	-2.54430500
C	6.16207500	-3.89032400	-1.46935600
C	4.51523600	4.85664400	0.95557700
C	4.26898400	4.05747900	3.66418200
C	4.18644800	3.10373100	4.73217100
C	4.13826400	0.49042700	5.82668400
C	4.17568700	-0.94079700	5.74847100
C	4.35685900	-3.40743600	4.36932900

C	4.48541900	-4.22019300	3.19555000
C	4.75931200	-4.65032900	0.41162400
C	4.65743000	4.62519900	-0.45180200
C	4.91355700	3.00326400	-2.76063900
C	5.00606000	1.76145800	-3.47158900
C	5.07333600	-1.06425000	-3.63407300
C	5.04500600	-2.38623000	-3.07846600
C	4.88138400	-4.25339300	-0.95806600
C	3.21258100	4.77520900	1.54922100
C	3.08818800	4.37408700	2.91525400
C	2.92481600	2.49021900	5.03273100
C	2.89966600	1.17313700	5.58866700
C	2.97358600	-1.65755300	5.43324300
C	3.06519700	-2.90127800	4.73452500
C	3.32028500	-4.50812300	2.41136700
C	3.45949000	-4.72496700	1.00776500
C	3.49464400	4.32075200	-1.23065800
C	3.62323900	3.49879100	-2.38796900
C	3.80371700	1.04979300	-3.79340500
C	3.83677600	-0.37658900	-3.86979200
C	3.78155300	-2.98825100	-2.76661800
C	3.70072500	-3.93671200	-1.70321800
C	2.05132300	4.78739800	0.71297800
C	1.80315300	3.99218100	3.41935100
C	1.71893200	3.04554000	4.49385500
C	1.66901100	0.43802200	5.60322800
C	1.70613700	-0.99452900	5.52437700
C	1.88811500	-3.45629900	4.13344400
C	2.01810100	-4.26714300	2.95749800
C	2.29782200	-4.72062900	0.17358500
C	2.19387800	4.56877100	-0.69402200
C	2.44896200	2.95868300	-3.00056100
C	2.53984600	1.71972900	-3.71014300
C	2.60339600	-1.10367800	-3.84782200
C	2.57546000	-2.42120800	-3.28841200
C	2.41978800	-4.32308800	-1.19695300



C	0.75494800	4.70740300	1.30016300
C	0.62986400	4.29758700	2.66444800
C	0.46267800	2.43265500	4.78929200
C	0.43555400	1.11769300	5.35996300
C	0.50890500	-1.70750600	5.20454000
C	0.60182600	-2.94848200	4.49190400
C	0.86008900	-4.55576800	2.17322200
C	1.00228900	-4.79375100	0.76759700
C	1.03830200	4.29324800	-1.48348900
C	1.16747300	3.48044800	-2.65436700
C	1.34105600	1.01297700	-4.02273000
C	1.37418700	-0.41662200	-4.07995700
C	1.32102400	-3.02471000	-2.97824700
C	1.24259300	-3.99994900	-1.93523500
C	-0.40472800	4.73921500	0.46318600
C	-0.65489700	3.91784800	3.16517600
C	-0.74002200	2.97728600	4.23421100
C	-0.79527200	0.38333600	5.36527500
C	-0.75834700	-1.04346500	5.28734000
C	-0.57271800	-3.49184800	3.87692800
C	-0.44243100	-4.30595800	2.71203400
C	-0.16266600	-4.78602800	-0.06596500
C	-0.26339500	4.53944800	-0.94307600
C	-0.00871400	2.93692400	-3.26293600
C	0.07923700	1.68470300	-3.94513100
C	0.14274800	-1.14120300	-4.04483000
C	0.11643200	-2.45575800	-3.49468000
C	-0.04089600	-4.38225600	-1.43015700
C	-1.70595400	4.66386500	1.05479700
C	-1.83147200	4.24572000	2.41942200
C	-2.00125200	2.37427300	4.53745400
C	-2.03077900	1.06406600	5.11340000
C	-1.95811500	-1.75633500	4.96032200
C	-1.86294000	-2.99070600	4.24069100
C	-1.60549000	-4.61435100	1.93415100
C	-1.46443400	-4.86186800	0.52875200

C	-1.42667100	4.26652200	-1.73324700
C	-1.29825800	3.45459500	-2.90892900
C	-1.12293600	0.97018100	-4.25305900
C	-1.08965500	-0.46109300	-4.30488400
C	-1.14192900	-3.07433000	-3.21202700
C	-1.22185500	-4.05233400	-2.16975600
C	-2.86693800	4.71082500	0.22630400
C	-3.11433600	3.88378400	2.92902700
C	-3.19958800	2.93220100	3.99844500
C	-3.25869200	0.33540400	5.12299600
C	-3.22205400	-1.09649700	5.04659700
C	-3.03413300	-3.54535900	3.64087100
C	-2.90446600	-4.37134800	2.47612200
C	-2.62735100	-4.84711100	-0.30244000
C	-2.72563500	4.50858300	-1.18803900
C	-2.47285000	2.89818500	-3.50435500
C	-2.38335000	1.63731500	-4.18638300
C	-2.31358200	-1.19582600	-4.30894300
C	-2.33952600	-2.52108200	-3.75548700
C	-2.50372400	-4.43666400	-1.67197100
C	-4.16705400	4.63408600	0.82424500
C	-4.29185400	4.21808600	2.18694800
C	-4.46194100	2.33115200	4.30332300
C	-4.49156400	1.01852800	4.86800300
C	-4.41987300	-1.80877300	4.71569600
C	-4.32524200	-3.04763900	4.00957000
C	-4.06843300	-4.67232800	1.69708700
C	-3.92847500	-4.90875900	0.29414000
C	-3.89112900	4.21650000	-1.96885700
C	-3.76343300	3.40177800	-3.13737000
C	-3.58355100	0.91543400	-4.49123700
C	-3.54832900	-0.51323700	-4.55680100
C	-3.59993900	-3.13749100	-3.46733800
C	-3.68284700	-4.10127200	-2.41393100
C	-5.33492000	4.66702500	-0.00700900
C	-5.57974600	3.84853000	2.69766600

C	-5.66551100	2.89521400	3.76568400
C	-5.72437700	0.28713200	4.87413900
C	-5.68820300	-1.14436200	4.79794800
C	-5.50195300	-3.60851500	3.41210600
C	-5.37203800	-4.42805200	2.24271900
C	-5.09521300	-4.88584800	-0.53989500
C	-5.19518200	4.45322500	-1.41829400
C	-4.94236000	2.83733100	-3.72936300
C	-4.85150100	1.58093500	-4.41503000
C	-4.77939800	-1.24945700	-4.55273300
C	-4.80542400	-2.57443400	-4.00331000
C	-4.97104000	-4.47759100	-1.90882500
C	-6.63100400	4.58806700	0.58789000
C	-6.75514600	4.17476700	1.95647500
C	-6.92375100	2.28996800	4.06217900
C	-6.95313600	0.96853700	4.62101700
C	-6.88249000	-1.85441900	4.47064100
C	-6.78849600	-3.10405300	3.77157400
C	-6.53233800	-4.71932800	1.46313800
C	-6.39202000	-4.94860200	0.05379600
C	-6.35694700	4.15731000	-2.19371400
C	-6.22874400	3.33791600	-3.36439800
C	-6.04805100	0.86366100	-4.72003800
C	-6.01165300	-0.56907100	-4.79123000
C	-6.06309500	-3.18272200	-3.70834400
C	-6.14688800	-4.14464900	-2.64692100
C	-7.79694300	4.60347000	-0.24228900
C	-8.04081800	3.79290900	2.45749000
C	-8.12558300	2.84378500	3.51622000
C	-8.18254300	0.23575700	4.60942900
C	-8.14693400	-1.18598200	4.53414900
C	-7.96326200	-3.65169800	3.16352400
C	-7.83423600	-4.46469200	2.00130200
C	-7.55726200	-4.91366300	-0.77702800
C	-7.65873300	4.38487500	-1.64266300
C	-7.40612500	2.76917000	-3.94736700

C	-7.31519100	1.52343900	-4.63113400
C	-7.24290500	-1.29958500	-4.77634000
C	-7.26884800	-2.61510100	-4.23131700
C	-7.43386000	-4.50869800	-2.13673900
C	-9.10515200	4.54268200	0.35101900
C	-9.22921300	4.13144000	1.72290900
C	-9.39668800	2.24503200	3.82038200
C	-9.42544500	0.91872500	4.37421800
C	-9.35525200	-1.90008600	4.22417200
C	-9.26200000	-3.15470200	3.52882200
C	-9.00610400	-4.76855100	1.22566200
C	-8.86530300	-4.99577700	-0.18676000
C	-8.83144400	4.10324400	-2.42509100
C	-8.70297100	3.28092800	-3.59695700
C	-8.52209700	0.81282000	-4.95532200
C	-8.48530500	-0.62225900	-5.03020800
C	-8.53662800	-3.23174100	-3.94942200
C	-8.62057300	-4.19349500	-2.88426400
C	-10.26847500	4.62787000	-0.47431900
C	-10.51533200	3.81166600	2.25743400
C	-10.60151100	2.84030700	3.33500800
C	-10.65805700	0.19861800	4.43359300
C	-10.62184500	-1.25215000	4.35659700
C	-10.43695300	-3.74983700	2.97495300
C	-10.30527100	-4.58076000	1.79002700
C	-10.02460500	-5.03311900	-1.02123100
C	-10.12777900	4.39997500	-1.90265000
C	-9.87211000	2.76226700	-4.23381700
C	-9.77887500	1.49221900	-4.93391700
C	-9.70547300	-1.36382100	-5.08602700
C	-9.73189700	-2.70624900	-4.52993800
C	-9.89872000	-4.62038300	-2.40898700
C	-11.53565900	4.62762600	0.18552000
C	-11.65500100	4.23324900	1.50612400
C	-11.83223300	2.22784800	3.72444100
C	-11.85971800	0.95056100	4.25507100

C	-11.78516300	-2.03957200	4.09578100
C	-11.69566800	-3.24771600	3.42795800
C	-11.42436800	-4.96154300	0.98748400
C	-11.28865700	-5.17994800	-0.37180100
C	-11.24566900	4.15212400	-2.75734600
C	-11.12207300	3.35989200	-3.88463400
C	-10.92958200	0.74367900	-5.33002800
C	-10.89398800	-0.63728500	-5.40389800
C	-10.94836500	-3.40463900	-4.25831400
C	-11.02911400	-4.32979000	-3.23290700
H	-12.44261200	4.82589400	-0.38390300
H	-12.65196300	4.13448200	1.93320300
H	-12.77740200	2.71757100	3.49446900
H	-12.82539500	0.47638200	4.42465900
H	-12.77270300	-1.63603100	4.31488800
H	-12.61577700	-3.75596400	3.14303600
H	-12.42408400	-4.96599600	1.41948800
H	-12.18599000	-5.34937900	-0.96528100
H	-12.23877700	4.48685000	-2.46100900
H	-12.02189300	3.09656600	-4.43883700
H	-11.88532400	1.24899800	-5.46185500
H	-11.82288100	-1.17379500	-5.59207200
H	-11.86138000	-3.12595100	-4.78257600
H	-12.00296700	-4.74888500	-2.98373200

**(8,8)@Cycle-9**

C	2.41694900	0.51339800	-7.75856400
C	0.06866700	1.05603500	-7.85690400
C	2.12046700	-0.85751100	-7.77420400
H	3.45893300	0.82628400	-7.67086600
C	-0.22965600	-0.31574900	-7.86470800
H	-0.73775200	1.78757900	-7.83788300
H	2.92192000	-1.59038500	-7.69839900
H	-1.27567400	-0.62794100	-7.86519000
C	1.34470000	-7.96244900	-2.47062100
C	-0.78545700	-8.75563200	-3.52791200

C	0.27432900	-7.86803200	-3.49827600
C	0.50966400	-6.84695300	-4.55180700
C	-0.52066600	-6.15619100	-5.21492900
C	2.09319800	-5.43012000	-5.78480400
C	-0.28130100	-5.14464000	-6.15613300
H	-1.55715300	-6.33894100	-4.94085600
H	3.10466100	-5.06003500	-5.93810900
H	-1.13659200	-4.64739800	-6.60577700
C	0.78303600	-1.29145600	-7.78111900
C	1.03538300	-4.71322600	-6.38482400
C	0.35241800	-2.74896600	-7.64717000
H	0.04990100	-3.16976400	-8.62361900
H	-0.52964300	-2.75574100	-6.98993500
O	1.39318200	-3.58006700	-7.09083000
C	1.85770600	-6.50808400	-4.90800900
C	2.94084800	-7.32143800	-4.30494400
C	4.03174200	-7.74203100	-5.04019100
S	4.32449300	-7.29649400	-6.75931800
S	5.25309400	-8.92426300	-4.44857700
C	5.58232500	-8.49059600	-7.05669700
H	5.97453000	-8.55946000	-8.06942800
C	6.00326900	-9.22691700	-6.01078500
H	6.78775400	-9.98009600	-6.04914200
S	-2.00881200	-8.83343900	-4.84510800
C	-2.26672000	-10.93975700	-3.23733500
H	-2.62847700	-11.87722900	-2.81962300
S	-1.02713600	-10.08134100	-2.33245300
C	-2.71159600	-10.37570600	-4.37610500
H	-3.48757800	-10.78594700	-5.01922200
C	2.14020000	-8.40465300	-0.18318400
C	2.68817500	-7.75104400	-2.90824400
C	3.72165900	-7.90518800	-1.95775500
H	4.74629800	-7.66625200	-2.23415100
C	3.46757400	-8.25964900	-0.63636800
H	4.27784400	-8.33535500	0.08644600
C	1.08713400	-8.24879800	-1.10367200

H	0.06111700	-8.27875200	-0.74467900
O	2.03074900	-8.63992900	1.16276700
C	-0.31077200	8.45603200	-0.12011200
C	-0.86218700	7.85967300	-2.86580800
C	0.72978000	8.38821400	-1.07325800
H	1.75299300	8.45853900	-0.70877200
C	-1.63714700	8.30955300	-0.56241600
H	-2.46927500	8.35408000	0.13676100
C	-1.88537700	7.98678100	-1.90548900
H	-2.90904000	7.73496200	-2.17263800
C	0.47591600	8.13634800	-2.43366000
C	1.54518600	8.10803500	-3.46055500
C	-1.08181000	7.40022500	-4.26360200
C	0.05642700	6.64469800	-4.85520900
C	1.37847000	7.05100600	-4.48464900
C	-0.10267000	5.54173400	-5.72128800
H	-1.09017100	5.12707500	-5.90965900
C	2.46275100	6.37312300	-5.06991700
H	3.47700200	6.61326300	-4.75724300
C	2.29918400	5.32500900	-5.98319600
H	3.18636900	4.84615200	-6.38810600
C	1.00399400	4.86528500	-6.28018600
O	0.71395000	3.73987400	-7.02729400
C	1.39905200	1.48997400	-7.75417400
C	1.80241600	2.94751500	-7.55273800
C	-2.20038200	7.72905100	-5.00367300
C	2.53625200	9.06574700	-3.51075800
S	-2.45673600	7.24894800	-6.71920900
S	-3.51794400	8.80501200	-4.41847600
S	2.70134000	10.40729500	-2.32310900
S	3.72959400	9.21491800	-4.84930500
C	-4.30851600	9.01518100	-5.97538700
H	-5.16199800	9.68905400	-6.01409600
C	-3.82690700	8.31072100	-7.01701200
H	-4.23206500	8.32949100	-8.02678200
C	4.32108000	10.81125300	-4.40283700

H	5.05208200	11.27470000	-5.06233400
C	3.85461800	11.34996800	-3.26013100
H	4.15217500	12.31612700	-2.85735600
H	2.14843400	3.40919600	-8.49586300
H	2.64625000	2.94812100	-6.84730300
O	0.08370600	8.61467000	1.18486000
C	-0.88359100	8.46794700	2.25935100
H	-1.57317600	7.64397900	2.02508600
H	-1.47367900	9.39702600	2.34604700
C	-0.11298000	8.14745400	3.55316100
H	0.48252400	9.02221700	3.85794200
H	0.60011000	7.34787700	3.31262900
C	-1.02325100	7.67142300	4.71832700
H	-1.61627800	8.51512400	5.10947800
H	-1.74679900	6.94403800	4.32080900
C	-0.23142100	6.99123600	5.87052400
H	0.30872300	7.75462100	6.45561700
H	0.54158000	6.35175000	5.41936700
C	-1.09055600	6.10405000	6.81450100
H	-1.72595500	6.73530500	7.45856000
H	-1.77833700	5.50941700	6.19545400
C	-0.24466100	5.13192300	7.68229400
H	0.25545200	5.69020500	8.49226300
H	0.56266800	4.72762300	7.05280700
C	-1.01951200	3.92673200	8.28185000
H	-1.72961200	4.27339800	9.05229900
H	-1.62881300	3.46951500	7.48847700
C	0.79318100	-8.49314900	1.90715300
H	0.21198000	-7.64802900	1.51312700
H	0.18815000	-9.41058300	1.80189500
C	1.23147700	-8.23798700	3.36673900
H	1.76723400	-9.12931900	3.72932500
H	1.97448300	-7.43027700	3.32009900
C	0.12979900	-7.82980700	4.38483000
H	-0.45726700	-8.71087000	4.69315600
H	-0.57739600	-7.13619200	3.90790800



C	0.75353500	-7.12938100	5.62661400
H	1.33810100	-7.86345200	6.20717200
H	1.48107900	-6.39250600	5.25498800
C	-0.23359000	-6.38213900	6.56415100
H	-0.81976600	-7.10291400	7.15902900
H	-0.95800400	-5.83367500	5.94504000
C	0.48230000	-5.36692700	7.49970300
H	1.05760200	-5.90964100	8.26926200
H	1.22658100	-4.82347600	6.89741500
C	-0.43930600	-4.31669400	8.18280400
H	-1.01684300	-4.78881500	8.99608600
H	-1.17761600	-3.96064900	7.45035400
C	0.35282300	-3.10505600	8.73719300
H	1.03951400	-2.74469500	7.95889000
H	0.99438600	-3.44740800	9.56815800
C	-0.06883200	2.85936800	8.88347700
H	0.75784500	2.68764900	8.17878500
H	0.39584500	3.26752600	9.79807500
C	-0.70569400	1.48272700	9.23284500
H	-1.17439900	1.03775800	8.34476100
H	-1.52495200	1.64982200	9.95780900
C	0.31618400	0.53177300	9.83644900
H	1.10985500	1.04663100	10.39140000
C	0.40089000	-0.81675200	9.83523700
H	1.25468700	-1.22888400	10.38687000
C	-0.48897700	-1.89564600	9.23866000
H	-1.18813200	-2.25502600	10.01794500
H	-1.11356200	-1.49536100	8.42688500
H	-11.94792700	-4.07467800	-4.40101000
H	-11.96360400	-5.61472800	-2.53003400
H	-12.01837200	-6.23445000	-0.52921200
H	-12.12275300	-6.00642300	1.88130200
H	-12.23464900	-5.02846800	3.73042000
H	-12.37341600	-3.15505400	5.26197200
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H	-11.97868800	-2.23360900	-5.39627100
H	-12.06215200	0.17542800	-5.64882200
H	-12.16446400	2.18119000	-5.05342600
H	-12.29927600	4.05525500	-3.52234100
H	-12.41180600	5.04013000	-1.67659500
H	-12.52066700	5.26492400	0.73412100
H	-12.58136400	4.64316900	2.73228900
H	-12.60026700	3.10689100	4.60644000
C	-11.00262200	-4.31253800	-3.91566900
C	-11.01160500	-5.19203300	-2.84749300
C	-11.09089100	-6.07505800	0.01862300
C	-11.15049600	-5.94501200	1.39484500
C	-11.31191800	-4.53952100	4.03897700
C	-11.39117300	-3.47009700	4.91318200
C	-11.54463800	-0.59815000	5.76453100
C	-11.59450500	0.77716700	5.62153700
C	-11.04743200	-1.67217800	-5.33884800
C	-11.09505100	-0.29692800	-5.48335000
C	-11.24141300	2.57471100	-4.63046400
C	-11.31832000	3.64454400	-3.75642600
C	-11.48028900	5.05079500	-1.11275000
C	-11.54250100	5.17876400	0.26349500
C	-11.62880400	4.29515000	3.12879100
C	-11.63966400	3.41797800	4.19878700
C	-9.81455900	-3.61910900	-4.29649500
C	-9.83287600	-5.44230700	-2.08243000
C	-9.87131400	-5.86966200	-0.69390800
C	-9.99487900	-5.59885900	2.15793200
C	-10.07303900	-4.91670700	3.43858700
C	-10.23703100	-2.70093200	5.25043700
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C	-10.41479100	1.54033500	5.36977900
C	-9.83630300	-2.33963100	-4.98537000
C	-9.93497100	0.51069800	-5.28509900
C	-10.00583200	1.90230200	-4.87265900
C	-10.16520000	4.11868900	-3.06139600

C	-10.24361900	4.79865400	-1.77951900
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C	-10.41424300	4.63691700	2.46128700
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C	-8.59116300	-4.99841800	-2.63356300
C	-8.66638500	-5.83026300	0.07377200
C	-8.72823700	-5.69335800	1.50289700
C	-8.88106600	-4.36142000	3.99840900
C	-8.96343100	-3.25119800	4.90703800
C	-9.10817600	-0.54135900	5.72045500
C	-9.16000600	0.88717700	5.57319200
C	-8.62449000	-1.58820300	-5.08447900
C	-8.67382300	-0.15989400	-5.23559100
C	-8.81196300	2.55299200	-4.43234900
C	-8.89180600	3.66378200	-3.52413600
C	-9.04491200	4.98719400	-1.02442700
C	-9.10969000	5.11908300	0.40526700
C	-9.19125100	4.29005700	3.11441800
C	-9.20250300	3.38019000	4.22689100
C	-7.34125600	-3.47335700	-4.13446000
C	-7.35938100	-5.27823800	-1.94761100
C	-7.39712400	-5.69630700	-0.58673500
C	-7.51924000	-5.42201100	2.23176800
C	-7.59599300	-4.75129200	3.48567600
C	-7.75837200	-2.56242300	5.27986100
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C	-7.93363100	1.61711000	5.40320800
C	-7.36267500	-2.21852100	-4.80807500
C	-7.46017200	0.59963400	-5.10702700
C	-7.52945900	1.96395200	-4.70445100
C	-7.68692000	4.15350800	-2.91220800
C	-7.76396800	4.81739200	-1.65440900
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C	-6.10088300	-3.98744600	-3.63935800
C	-6.10990400	-4.90210800	-2.53463000
C	-6.18518300	-5.73267900	0.17353700
C	-6.24674000	-5.59108100	1.59912700
C	-6.39953500	-4.25354600	4.09322400
C	-6.48195800	-3.14735000	5.00204000
C	-6.62748400	-0.43932800	5.82440900
C	-6.67923200	0.98629300	5.68007900
C	-6.14357100	-1.48863900	-4.97934700
C	-6.19237100	-0.06345900	-5.13251800
C	-6.33060000	2.65162700	-4.33278200
C	-6.41036100	3.75897600	-3.42512000
C	-6.56328000	5.07670300	-0.92053500
C	-6.62827900	5.20757600	0.50641400
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C	-5.21605600	4.26289300	-2.82635100
C	-5.29382700	4.92426000	-1.55710200
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C	-3.63769600	-4.81637400	-2.44329800
C	-3.71237700	-5.65047200	0.27393100
C	-3.77386600	-5.50096300	1.69448800

C	-3.92760600	-4.14781300	4.19327000
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C	-2.57241600	-5.23046400	2.42610300
C	-2.65034600	-4.54268900	3.68075700
C	-2.81443700	-2.36208900	5.48971000
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C	-2.51316100	0.79544400	-4.91941000
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C	-1.16419600	-3.77423600	-3.41099000
C	-1.17034900	-4.70174000	-2.32854700
C	-1.24077700	-5.53392200	0.36771100
C	-1.30324000	-5.37208600	1.78690000
C	-1.45846900	-4.01466900	4.26292300
C	-1.53991600	-2.92085200	5.17553500
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C	-1.73606000	1.18074300	5.87749600

C	-1.20439000	-1.29025100	-4.75856500
C	-1.25154700	0.12903000	-4.90277400
C	-1.38568700	2.84343200	-4.12423600
C	-1.46608200	3.94136600	-3.21399600
C	-1.62317200	5.21563700	-0.70469300
C	-1.68751400	5.35522900	0.70957400
C	-1.76698100	4.54650700	3.40913600
C	-1.77689000	3.64919200	4.51695600
C	0.06878200	-3.16989700	-3.80715200
C	0.05590200	-4.98674100	-1.65299500
C	0.02054700	-5.39250600	-0.29202500
C	-0.10197000	-5.07554100	2.50647500
C	-0.17951500	-4.39809200	3.75262500
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C	-0.41343400	-0.89272100	6.00436400
C	-0.51378500	1.90443100	5.70528400
C	0.04863900	-1.92226000	-4.48432500
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C	-0.11083100	2.24660900	-4.37693400
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C	-0.35013700	5.07621900	-1.33486900
C	-0.47653300	5.33584300	1.46874900
C	-0.51676300	4.92162800	2.82617000
C	-0.53511600	3.14559500	5.01567200
C	1.30867400	-3.68181600	-3.32112600
C	1.30228600	-4.59823700	-2.23332000
C	1.23295500	-5.38996300	0.46494900
C	1.17104500	-5.23096700	1.87767100
C	1.01550300	-3.90031400	4.35694100
C	0.93515700	-2.81268800	5.27307000
C	0.79229200	-0.13581700	6.14680400
C	0.74133500	1.28093500	5.98809800
C	1.26814800	-1.19870400	-4.65318700
C	1.21960900	0.21781000	-4.77610200
C	1.08716500	2.91732600	-3.97997900
C	1.00776100	4.02091000	-3.08464900

C	0.84757200	5.34954800	-0.60317900
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C	2.53964800	-3.09918500	-3.74568700
C	2.52686000	-4.89313500	-1.56578900
C	2.49073000	-5.28231000	-0.19494000
C	2.36842000	-4.98291500	2.61128100
C	2.29078100	-4.31210100	3.86875300
C	2.13108800	-2.15242500	5.68798100
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C	1.95620000	2.01641600	5.83578200
C	2.51946000	-1.84171000	-4.41885300
C	2.42431800	0.97019400	-4.66707800
C	2.35733200	2.33566800	-4.26097600
C	2.19799200	4.52949600	-2.48764900
C	2.11825000	5.21186500	-1.23577800
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C	1.95116200	5.05760700	2.94314700
C	1.93391400	3.26769800	5.14205600
C	3.78160100	-3.61963200	-3.26261500
C	3.77398800	-4.51994200	-2.15699200
C	3.70019700	-5.30334500	0.56548700
C	3.63957400	-5.15811600	1.98161300
C	3.48652900	-3.82836600	4.48700400
C	3.40614600	-2.73738000	5.40395500
C	3.26439800	-0.03247600	6.25578900
C	3.21234600	1.38718500	6.10937500
C	3.73885700	-1.11344700	-4.58968900
C	3.69037600	0.30702000	-4.70961600
C	3.55543500	3.01898400	-3.88352900
C	3.47512400	4.12338900	-2.98633600
C	3.31666400	5.48373600	-0.50202100
C	3.25222600	5.62239300	0.91841000
C	3.17364600	4.78319200	3.63507300
C	3.16484000	3.87989300	4.74194400

C	5.01739100	-3.02456500	-3.67929000
C	5.00016900	-4.81065700	-1.47655100
C	4.96269700	-5.20374800	-0.10048700
C	4.84104800	-4.91002700	2.72076300
C	4.76433100	-4.23884000	3.98369500
C	4.60640100	-2.06247300	5.80164300
C	4.53472300	-0.69668300	6.22799300
C	4.43056900	2.12526100	5.94339100
C	4.99597300	-1.75706700	-4.34710200
C	4.89830300	1.06921700	-4.59998800
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C	4.67137200	4.63769400	-2.39158600
C	4.59220200	5.32367700	-1.13621800
C	4.46312500	5.60121500	1.68590800
C	4.42341100	5.17994300	3.05535800
C	4.40658800	3.38329600	5.25757000
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C	6.24597500	-4.43154400	-2.06127500
C	6.16974900	-5.22108400	0.66035400
C	6.10871000	-5.07047500	2.08526600
C	5.95834000	-3.73844800	4.58470800
C	5.87836700	-2.63836400	5.50107200
C	5.73726300	0.06516500	6.33816200
C	5.68444400	1.49095500	6.19652000
C	6.21138000	-1.02195900	-4.49733600
C	6.16224700	0.40577400	-4.62520200
C	6.02539800	3.11498400	-3.79294900
C	5.94497200	4.22530800	-2.88876100
C	5.78931400	5.57390300	-0.40019000
C	5.72409100	5.71546500	1.02552200
C	5.64442400	4.89033400	3.73659400
C	5.63585600	3.98329900	4.84745700
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C	7.46977900	-4.70652900	-1.37120300
C	7.43175300	-5.10390900	-0.00373100
C	7.30989700	-4.80391000	2.81557000



C	7.23440200	-4.13374500	4.07036800
C	7.07737500	-1.95453400	5.87878200
C	7.00625200	-0.59572000	6.29902800
C	6.90191700	2.22316900	6.02328700
C	7.46613000	-1.65808700	-4.23452100
C	7.36800600	1.16558700	-4.49067700
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C	8.72735800	-4.33842300	-1.96154700
C	8.65092900	-5.13411300	0.75708000
C	8.58936300	-4.98120600	2.18521100
C	8.43969600	-3.64426000	4.68127100
C	8.36005000	-2.53914500	5.59679500
C	8.21864100	0.16457000	6.43185100
C	8.16555400	1.59395100	6.29409300
C	8.69287100	-0.92693600	-4.39989600
C	8.64331800	0.50388900	-4.52948300
C	8.50590800	3.21075000	-3.69662000
C	8.42576700	4.32203100	-2.78807000
C	8.27061700	5.66724000	-0.29834800
C	8.20525800	5.81381700	1.12988600
C	8.12521300	4.99882000	3.84212300
C	8.11673000	4.08982500	4.95514900
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C	9.95146600	-4.67939100	-1.30719000
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C	9.78917900	-4.78439000	2.93653300
C	9.71258000	-4.09762600	4.21510500
C	9.55386200	-1.89049900	6.04022200
C	9.48126700	-0.50390800	6.46885000
C	9.37541800	2.34820400	6.19634900

C	9.94751300	-1.58400200	-4.20805100
C	9.84841200	1.27027600	-4.46844400
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C	9.61841300	4.87378200	-2.22610000
C	9.53875800	5.56381300	-0.94952900
C	9.40840600	5.85886500	1.89980300
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C	9.34999500	3.62955300	5.51176500
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C	11.08410200	-5.18987200	0.89575600
C	11.02474700	-5.04343700	2.27027100
C	10.86666300	-3.62267800	4.90798500
C	10.79020200	-2.55790300	5.78815700
C	10.64023900	0.30421400	6.67256000
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C	11.12775700	-0.81981000	-4.45465300
C	11.07992200	0.55719600	-4.58025200
C	10.93450900	3.42043100	-3.69677700
C	10.85749200	4.48914900	-2.82133900
C	10.69315700	5.91329900	-0.18615300
C	10.63023000	6.05634800	1.18854100
C	10.54450000	5.20251800	4.06186700
C	10.53637100	4.32738000	5.13333400
H	12.13354200	-3.15945100	-3.46276700
H	12.11808400	-4.69123100	-1.58433400
H	12.06146300	-5.28118400	0.42441100
H	11.95748000	-5.02568300	2.83185900
H	11.84779100	-4.03045700	4.66974000
H	11.71374000	-2.16519200	6.21072200
H	11.60876700	-0.16757300	6.83097700
H	11.51918200	2.24363500	6.60110900
H	12.10145200	-1.30711700	-4.44094900
H	12.01769100	1.10463300	-4.66171000
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H	11.78181200	4.97258700	-2.50883700

H	11.66684000	5.96865300	-0.67053500
H	11.55660100	6.21890600	1.73725700
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H	11.48087900	4.09583600	5.62325100

**(9,9)@Cycle-9**

C	0.47749600	0.08470100	-8.32268000
C	-1.85440100	0.58361900	-8.29670300
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H	1.52469500	0.39315700	-8.30820900
C	-2.12453100	-0.80534000	-8.25965100
H	-2.69447700	1.27749900	-8.26745200
H	1.04834400	-1.99631800	-8.24328300
H	-3.17050300	-1.11123800	-8.19982200
C	-1.15078000	-8.48696100	-2.43946600
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C	-1.86284300	-7.33965600	-4.61655400
C	-2.80393300	-6.60125300	-5.37108500
C	-0.14814200	-6.11284100	-5.90979100
C	-2.46431800	-5.63873000	-6.34438100
H	-3.86159900	-6.67721700	-5.13547800
H	0.89762500	-5.84933600	-6.05191100
H	-3.27390300	-5.09081000	-6.82217800
C	-1.11094100	-1.79321100	-8.17160500
C	-1.11691800	-5.30055000	-6.56472100
C	-1.57183600	-3.28041800	-7.97314300
H	-1.79393000	-3.72768200	-8.95737500
H	-2.50911000	-3.22881200	-7.40260100
O	-0.64356600	-4.19632900	-7.28924900
C	-0.48817300	-7.13421400	-4.97701500
C	0.49992600	-8.03626700	-4.32038600
C	1.55330200	-8.58291700	-5.03293500
S	1.93161100	-8.17806800	-6.74478700
S	2.61811300	-9.90042100	-4.42260400
C	3.05863600	-9.50018400	-7.01807500

H	3.46607100	-9.60807300	-8.02130600
C	3.37020700	-10.27996000	-5.96550800
H	4.06950100	-11.11345900	-5.98643300
S	-4.63816000	-8.97908400	-4.75518100
C	-5.19829000	-10.89409900	-2.99649000
H	-5.69743200	-11.72693800	-2.50518900
S	-3.80654700	-10.19865400	-2.18140900
C	-5.57635200	-10.34205300	-4.16469900
H	-6.42787700	-10.65738100	-4.76422800
C	-0.35177500	-8.92694000	-0.10250000
C	0.19731200	-8.43217500	-2.91110600
C	1.21748500	-8.69843700	-1.96763200
H	2.25923800	-8.59453100	-2.26170000
C	0.96130800	-8.97321400	-0.62699100
H	1.78932200	-9.10808800	0.06675300
C	-1.40286700	-8.71945300	-1.03747100
H	-2.41945900	-8.62114700	-0.66564700
O	-0.33525300	-8.99529100	1.29231500
C	-0.56244200	8.88237200	-0.73686700
C	-1.45949600	8.12267800	-3.40026600
C	0.35170700	8.59287300	-1.79530400
H	1.40402900	8.53382000	-1.52783400
C	-1.92614800	8.90104000	-1.07516900
H	-2.68400100	9.11123400	-0.32216400
C	-2.34150800	8.49797700	-2.36022000
H	-3.41279200	8.37938200	-2.50076000
C	-0.05735500	8.23451400	-3.11290100
C	0.87848200	7.95291500	-4.25014600
C	-1.90610400	7.59718900	-4.73422100
C	-0.96186400	6.66984500	-5.43993100
C	0.43790200	6.91434600	-5.23999600
C	-1.36244800	5.57919600	-6.26738500
H	-2.41157600	5.29774300	-6.30624100
C	1.32500300	6.10757600	-5.98772800
H	2.39651500	6.20840800	-5.83568200
C	0.91617900	5.06740600	-6.84567800

H	1.68773600	4.47721800	-7.33572400
C	-0.44330800	4.72187200	-6.93912000
O	-0.96172400	3.55590200	-7.53237400
C	-0.53414100	1.07845700	-8.25655700
C	-0.07011800	2.57977900	-8.18784500
C	-3.06157500	8.04202500	-5.35486200
C	2.01602200	8.71901200	-4.44166100
S	-3.60101400	7.51080500	-6.98794100
S	-4.13852700	9.32799100	-4.70324000
S	2.54046500	10.04017800	-3.33765900
S	3.07524000	8.62771900	-5.89402400
C	-5.08707500	9.56061600	-6.16437800
H	-5.84025700	10.34581600	-6.14922800
C	-4.84251400	8.73621700	-7.20038000
H	-5.36729700	8.75283800	-8.15350500
C	3.99525800	10.08954200	-5.56790000
H	4.73188300	10.39022700	-6.31020500
C	3.75150600	10.72955900	-4.40873900
H	4.26097500	11.62934000	-4.06962400
H	0.10411600	2.94535900	-9.21442200
H	0.89408900	2.56861300	-7.66234700
O	-0.03507700	9.03731400	0.54419300
C	-0.89341700	9.14670600	1.75544400
H	-1.74698900	8.46623200	1.64869200
H	-1.27763500	10.17865400	1.79956600
C	-0.07527400	8.79410900	3.06445700
H	0.60937300	9.62915400	3.27972800
H	0.55879700	7.93722500	2.82693200
C	-0.91847000	8.45604600	4.37818000
H	-1.37756900	9.38569200	4.75321900
H	-1.75333700	7.80337400	4.09447500
C	-0.11694700	7.76655300	5.58295400
H	0.46865200	8.54785100	6.09506100
H	0.62154700	7.07693400	5.15834200
C	-0.97526800	6.97538700	6.67775400
H	-1.48668900	7.71315300	7.31841900

H	-1.77291200	6.43175500	6.15855800
C	-0.19455700	5.94487800	7.62000900
H	0.39404400	6.52126800	8.35350500
H	0.54139300	5.40657400	7.01140600
C	-1.06105200	4.85807100	8.40976500
H	-1.61836400	5.36658900	9.21427300
H	-1.82376500	4.46455800	7.72716400
C	-1.39463400	-8.87793500	2.31220500
H	-2.12256600	-8.11422700	2.01877200
H	-1.91691300	-9.84658100	2.37810600
C	-0.68093300	-8.52933400	3.69588400
H	-0.15355200	-9.43938800	4.02168900
H	0.09919200	-7.79832300	3.46276500
C	-1.54732000	-7.97062600	4.91690200
H	-2.11456600	-8.80520800	5.36058300
H	-2.29738700	-7.27225100	4.53108500
C	-0.72634600	-7.24214100	6.08587800
H	-0.22378400	-8.01772100	6.68768600
H	0.07947800	-6.65513500	5.62839500
C	-1.53787400	-6.28092500	7.07094200
H	-2.18477400	-6.90082100	7.71436000
H	-2.21988800	-5.66956900	6.46891100
C	-0.67304100	-5.31017900	8.00231900
H	-0.18026700	-5.92170200	8.77673300
H	0.14047600	-4.89439100	7.39505500
C	-1.43040800	-4.09699600	8.72910600
H	-1.98613000	-4.50349900	9.59038400
H	-2.19270800	-3.70355300	8.04860600
C	-0.51642600	-2.88859200	9.23889800
H	0.26826900	-2.71841900	8.49408900
H	0.01203800	-3.21852500	10.14903500
C	-0.24170200	3.64212200	9.04795200
H	0.55606700	3.36542300	8.35017200
H	0.27472500	4.01654900	9.94761500
C	-1.01439800	2.29512000	9.47381500
H	-1.81232500	2.06696000	8.76019900

H	-1.53216900	2.50022100	10.42834500
C	-0.08228100	1.06301200	9.69583800
H	0.93711500	1.41361300	9.90346500
C	-0.14506700	-0.31055800	9.74008200
H	0.83740500	-0.73798300	9.97848100
C	-1.18458400	-1.46365200	9.58603900
H	-1.71320300	-1.57620200	10.55038500
H	-1.96389900	-1.20411200	8.85935400
C	-10.97776700	-5.98453500	1.98107300
C	-9.76234200	-5.71966300	2.67900900
C	-8.54309200	-5.87085000	1.94810600
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C	-9.81973100	-5.99422000	-0.17945000
C	-11.00551800	-6.11601000	0.60381000
C	-7.28078200	-5.68127800	2.60938900
C	-6.05954300	-5.90439400	1.89747600
C	-6.08808100	-6.05468800	0.47167400
C	-7.33794900	-5.96516000	-0.21893200
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C	-1.10390400	-5.84441600	1.77689400
C	-1.13099800	-6.01202900	0.37900300
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C	-1.04191700	-4.65211900	4.29087600
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C	1.37580200	-5.95781100	1.75233500
C	2.62336200	-5.83794400	2.43335100
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C	2.57245500	-6.09897900	-0.38937500
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C	1.31271900	-5.41228100	-2.38712500
C	0.07958000	-5.66168300	-1.71036900
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C	1.30548900	-4.58990800	-3.54306500
C	0.06432600	-4.02647900	-3.97388500
C	-1.17725500	-4.48985500	-3.44396600
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C	1.31760200	-2.26242900	-5.12010600
C	2.54596100	-2.95338100	-4.89975000
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C	1.33705500	-0.87806500	-5.42781800
C	0.11083400	-0.14724500	-5.39680300
C	-1.14215000	-0.81692400	-5.32402100
C	-1.16112100	-2.19183100	-5.01309100
C	-2.40645700	-2.81482400	-4.72635300
C	-2.41356200	-3.97126700	-3.91220000
C	0.13881800	1.25299900	-5.26788300
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C	3.86472900	1.89965100	-5.27537700
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C	6.26521800	-2.36427400	-5.26337700
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C	1.50392900	5.21928900	-2.59637900
C	2.72071200	4.81320400	-3.21709800
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C	6.33873000	1.85315400	-5.32942100
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C	1.53903700	5.80871000	-1.30781800
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C	6.29343900	-6.24322000	0.26027600
C	6.31983200	-6.10940400	1.68792700
C	5.09961400	-5.90410300	2.40033500

C	-6.12895100	-4.47988600	-3.42956000
C	-6.12416100	-5.32173000	-2.26879200
C	-4.88379600	-5.65018100	-1.64409900
C	8.77721800	-6.29706700	0.21848300
C	8.80357300	-6.16695900	1.64955000
C	7.57307100	-5.93784500	2.35631000
C	7.60629900	-5.33765000	3.64789200
C	8.86992700	-4.97100600	4.22607400
C	8.90733600	-3.96252000	5.24914800
C	10.25953800	0.72412000	6.59939100
C	10.28004500	2.12991300	6.23128700
C	10.19809700	-2.13384700	6.32637300
C	10.16087100	-3.44515100	5.70101000
C	10.28951100	5.32567000	3.40498000
C	10.29525900	4.48842800	4.59300000
C	10.15090400	4.73952400	-3.41756200
C	10.11125300	3.71421100	-4.44708000
C	10.22380600	5.95127300	-0.81471600
C	10.25306900	6.07582700	0.63311300
C	10.05221100	-6.07281500	2.33890900
C	10.08606200	-5.46172900	3.65720500
C	9.99973900	-6.32895000	-0.52152700
C	9.98318200	-5.95623500	-1.92630300
C	9.97682100	-3.10940200	-5.10131100
C	9.97141200	-4.30574700	-4.27592300
C	10.01131100	-0.32806400	-5.81521700
C	10.03959300	1.11838100	-5.67483300
C	-7.08753000	1.05625100	6.82431900
C	-7.06621500	2.43698500	6.47224200
C	-7.35598700	-5.59702900	-1.59558200
C	-7.31922000	0.00084000	-5.40459600
C	-7.29054800	1.42008800	-5.27130400
C	-7.35830200	-2.75637000	-4.70171000
C	-7.36558500	-3.93783000	-3.90398900
C	-7.04753900	4.77550500	4.85678000
C	-7.05224400	5.59487900	3.69065700

C	-7.11474600	6.20010100	-0.47690600
C	-7.08700600	6.32628400	0.94276200
C	-7.18487200	5.00114400	-3.05564600
C	-7.22174700	3.99538300	-4.06506900
C	11.33747000	-4.14722700	5.30495000
C	11.30132700	-5.11881000	4.32038400
C	11.41434500	-1.43783100	6.59263400
C	11.44404300	-0.06068700	6.72392700
C	11.23146800	-6.37913700	1.59729900
C	11.20622600	-6.50188700	0.21923400
C	11.49373700	3.97882500	5.17477300
C	11.48647800	2.84233100	5.96413100
C	11.46433600	6.06888800	1.38619900
C	11.48191400	5.70772500	2.72188300
C	11.40396500	5.81033200	-1.60313400
C	11.36874000	5.22663300	-2.85731900
C	11.17220800	-5.72681800	-2.68003400
C	11.16654600	-4.93128200	-3.81229900
C	11.17760000	-2.46372700	-5.52013700
C	11.19408300	-1.12366000	-5.86472800
C	11.25220600	1.86289700	-5.57826000
C	11.28677700	3.11330600	-4.98653500
C	-8.48569100	3.43975100	-4.46525800
C	-8.52060700	2.13831600	-5.07605000
C	-8.41154400	5.44747300	-2.45395500
C	-8.37620200	6.05540100	-1.15106100
C	-8.57731800	-0.69231100	-5.34416300
C	-8.59705200	-2.08592300	-4.98910500
C	-8.30297100	5.93722200	3.06964400
C	-8.32050400	6.30712100	1.68025200
C	-8.30388300	3.11923400	6.20974100
C	-8.29436200	4.30295400	5.39409700
C	-8.34549700	0.36548500	6.90937900
C	-8.61261800	-4.43997100	-3.39521600
C	-8.60763200	-5.27778500	-2.22650800
C	-9.56641500	1.10798000	6.94195800

C	-9.54483200	2.51731700	6.58569900
C	-9.83801600	-5.61851800	-1.58381300
C	-9.80113700	0.03974500	-5.44458700
C	-9.77218200	1.48690900	-5.30656400
C	-9.84021100	-2.74475800	-4.73596200
C	-9.84812600	-3.94800900	-3.91984100
C	-9.52587700	4.88321000	4.95813500
C	-9.53029300	5.71983300	3.76928100
C	-9.59375900	6.33014800	-0.45399000
C	-9.56517400	6.45948100	0.99385200
C	-9.66445900	5.11359800	-3.05582600
C	-9.70248600	4.08620600	-4.08387400
C	-10.91956200	3.52503100	-4.57169300
C	-10.95311400	2.27337100	-5.16095900
C	-10.84101800	5.64640700	-2.45058600
C	-10.80706800	6.23285000	-1.19765200
C	-11.01270300	-0.71304100	-5.44840900
C	-11.03158900	-2.05403700	-5.10737800
C	-10.73102700	6.14521800	3.12741100
C	-10.74770600	6.50141800	1.79038300
C	-10.73135300	3.27711300	6.36380100
C	-10.72212400	4.41736300	5.57988300
C	-10.77566700	0.36766600	7.09658900
C	-10.80323700	-1.00877200	6.95568800
C	-11.04824000	-4.53473100	-3.41939200
C	-11.04345300	-5.33940000	-2.29362900
H	12.31052500	5.05721100	-3.37670900
H	12.37205300	6.07804400	-1.18295100
H	12.25289200	3.59770900	-4.85462000
H	12.41360600	6.25945800	0.88817200
H	12.12375000	-3.00118800	-5.48263800
H	12.15265100	-0.65710600	-6.08581000
H	12.11704600	-4.70961000	-4.29485700
H	12.19240200	1.41071600	-5.88966300
H	12.19366700	-6.42835400	2.10435700
H	12.14951500	-6.64268000	-0.30594600



H	12.24157500	-5.55777000	3.99084100
H	12.12688700	-6.10142600	-2.31436100
H	12.44429600	5.62780800	3.22470800
H	12.45250900	4.42977800	4.92419800
H	12.41038100	0.42925700	6.83131900
H	12.35847500	-1.97997100	6.60179600
H	12.43968100	2.44143900	6.30489300
H	12.30463500	-3.85786000	5.71269500
H	-11.76730800	-1.51343400	6.99045700
H	-11.71904100	0.89297700	7.23601900
H	-11.81332800	-3.39263400	6.10648100
H	-11.68706500	2.91127600	6.73553800
H	-11.97157800	-6.22016200	0.11252700
H	-11.92304200	-5.99145300	2.52123300
H	-11.99796100	-5.68152100	-1.89687900
H	-11.87247800	-5.10349900	4.39680300
H	-11.96172500	-0.21217900	-5.63253900
H	-11.99465600	-2.55686300	-5.03583300
H	-11.92092800	1.85364600	-5.43028900
H	-12.00642600	-4.27474700	-3.86629300
H	-11.67105300	4.90559500	5.36415800
H	-11.67720400	6.10344500	3.66443100
H	-11.74803500	6.53769700	-0.74260900
H	-11.80757200	5.51245100	-2.93359300
H	-11.70643700	6.72678400	1.32619900
H	-11.86225600	4.04196600	-4.39974000

**(9,9)@Cycle-10**

C	1.06809100	-0.47973600	-8.79897500
C	3.40985100	-0.68724500	-8.63097800
C	1.16529400	0.94526700	-8.76573300
H	0.05714900	-0.88834400	-8.85406300
C	3.50910700	0.73903000	-8.59513300
H	4.34310700	-1.24607600	-8.55348400
H	0.23014200	1.50401400	-8.80718600
H	4.51571900	1.14678800	-8.48634300

C	1.86584500	8.77554300	-2.90281400
C	4.19994400	9.18825400	-3.76939800
C	3.00020100	8.49856900	-3.88032300
C	2.73506400	7.55641000	-5.05575800
C	3.72852100	6.81622300	-5.75417400
C	1.14208100	6.23177900	-6.43292500
C	3.47693900	5.81117900	-6.71943700
H	4.77154800	6.92116700	-5.47192300
H	0.11029300	5.95159700	-6.62961900
H	4.33419200	5.27138100	-7.11938100
C	2.39221900	1.62763900	-8.55733800
C	2.16159400	5.40466200	-7.01755700
C	2.70766100	3.23246900	-8.38760500
H	2.84065300	3.63327100	-9.40352000
H	3.66829500	3.27217400	-7.86007100
O	1.76077500	4.21347400	-7.70827200
C	1.39499300	7.29886800	-5.49533100
C	0.35331100	8.20822000	-4.90020600
C	-0.66289300	8.71392600	-5.69634000
S	-0.94245000	8.22191900	-7.40498200
S	-1.77388200	10.04813600	-5.21804400
C	-2.07810800	9.50201600	-7.80463700
H	-2.43538600	9.54766000	-8.83147100
C	-2.45538700	10.33045600	-6.81268400
H	-3.16657200	11.14810400	-6.91174500
S	5.51970600	9.17189800	-4.99561200
C	6.06320500	10.97966900	-3.12400400
H	6.57056400	11.76424700	-2.56629800
S	4.58535100	10.33187300	-2.43344900
C	6.48815400	10.45278700	-4.28761800
H	7.39338200	10.74229100	-4.81748500
C	0.87100100	9.33640100	-0.60176400
C	0.56103700	8.69087100	-3.48128900
C	-0.51489300	9.04709400	-2.62604300
H	-1.53610000	8.94670600	-2.98515800
C	-0.37706700	9.38576400	-1.27443300

H	-1.27382600	9.57221800	-0.68539600
C	1.99209300	9.08046800	-1.47148400
H	2.97602600	8.97920700	-1.01936200
O	0.66813500	9.49086000	0.81578100
C	1.70344300	-9.28593100	-0.75425000
C	2.77680200	-8.55395800	-3.41707000
C	0.87095600	-9.01115200	-1.90223800
H	-0.19748400	-8.94965700	-1.71163900
C	3.08300700	-9.31158000	-1.03293900
H	3.80541200	-9.51001400	-0.24175300
C	3.57565700	-8.93531700	-2.30708400
H	4.65547500	-8.83187300	-2.37206100
C	1.35979300	-8.65817300	-3.21504400
C	0.51063400	-8.36397200	-4.43614500
C	3.32652200	-8.03336800	-4.73488800
C	2.44859600	-7.11638800	-5.56029700
C	1.03857400	-7.36362900	-5.45267700
C	2.90662600	-6.04366000	-6.41032300
H	3.95853500	-5.77250000	-6.38151200
C	0.22539400	-6.58630500	-6.31794300
H	-0.85518100	-6.68236900	-6.26082500
C	0.69118300	-5.56152200	-7.17808800
H	-0.05267400	-4.99254600	-7.73446000
C	2.04581700	-5.18487800	-7.18284900
O	2.60565900	-3.99796000	-7.76024700
C	2.16683800	-1.37425800	-8.63282600
C	1.81644100	-2.97835000	-8.57342400
C	4.52826300	-8.49509000	-5.24797300
C	-0.64348000	-9.09459300	-4.67601900
S	5.21202300	-7.98572800	-6.83355900
S	5.54105700	-9.77716700	-4.49206100
S	-1.29429900	-10.34761800	-3.55902600
S	-1.60972900	-9.02336900	-6.19371800
C	6.62453600	-10.01730700	-5.85397500
H	7.37578900	-10.79889800	-5.76020400
C	6.47442900	-9.20425000	-6.91645800

H	7.08532400	-9.22700900	-7.81667600
C	-2.63245900	-10.41146700	-5.85838700
H	-3.34558600	-10.70124200	-6.62747400
C	-2.48811400	-11.01213000	-4.66231800
H	-3.06642100	-11.86541500	-4.31364500
H	1.87004800	-3.35209400	-9.60665000
H	0.77458500	-3.01681300	-8.23319000
O	1.08625800	-9.42229400	0.51951500
C	1.81362000	-9.51308400	1.87781700
H	2.65532600	-8.81427800	1.85835700
H	2.20749000	-10.53779000	1.92961900
C	0.84795900	-9.24964100	3.19840000
H	0.34474600	-10.20778900	3.39473100
H	0.06432000	-8.55902400	2.88411700
C	1.48826700	-8.73482600	4.65883000
H	1.98860100	-9.61281100	5.09612900
H	2.28179500	-8.01529000	4.45406800
C	0.52147500	-8.10114700	5.86785400
H	0.02229300	-8.95865200	6.34540600
H	-0.27812200	-7.51908700	5.40134500
C	1.19317000	-7.20436300	7.12282700
H	1.61947700	-7.94395200	7.81844700
H	2.04717400	-6.64354800	6.73339300
C	0.25995000	-6.17126900	8.05617300
H	-0.28695200	-6.81471300	8.76297700
H	-0.50348700	-5.72997700	7.41235100
C	0.94187600	-4.94860100	8.98192400
H	1.37662600	-5.44292300	9.86478800
H	1.78890600	-4.52774900	8.43791700
C	1.49234000	9.41172600	2.10602400
H	2.24684200	8.63571000	1.99935300
H	1.99586900	10.38455500	2.19568500
C	0.57184900	9.17341400	3.47316900
H	0.12938500	10.15304500	3.70603700
H	-0.26162400	8.52787400	3.18946700
C	1.25532200	8.61517000	4.90934000

H	1.70757800	9.50219100	5.37825600
H	2.09257200	7.95488200	4.66971900
C	0.32461900	7.89343800	6.11535100
H	-0.14920300	8.72527100	6.65926800
H	-0.49387600	7.34574200	5.64136800
C	1.02400000	6.90790900	7.27860000
H	1.56369400	7.58199300	7.96239200
H	1.79465500	6.30858400	6.79490400
C	0.11683000	5.88884900	8.25113200
H	-0.37046900	6.53041000	9.00183200
H	-0.69568100	5.47043700	7.65071300
C	0.84518200	4.64170800	9.12523800
H	1.25443900	5.12113700	10.02773800
H	1.71623800	4.28823900	8.56802500
C	-0.02748600	3.31446500	9.67829800
H	-0.82880500	3.10349400	8.96684800
H	-0.53027800	3.65494100	10.59663300
C	0.01873600	-3.68523500	9.56495600
H	-0.75617300	-3.45416800	8.82979800
H	-0.51970700	-4.07819500	10.44141000
C	0.70823900	-2.22923600	10.10542900
H	1.65414200	-2.04053800	9.59021900
H	0.98455500	-2.43867800	11.15352600
C	-0.20697400	-0.89529700	10.19628700
H	-1.23054900	-1.24548000	10.38248300
C	-0.21239900	0.50796000	10.21437800
H	-1.23894200	0.84652100	10.40453800
C	0.69919300	1.84241900	10.10265600
H	1.09479000	2.01036000	11.11926300
H	1.57858900	1.66433100	9.48136000
C	-11.65839200	6.76017700	1.36834200
C	-10.52177300	6.44294000	2.16799800
C	-9.23453800	6.58787300	1.56324000
C	-9.12114000	6.80061500	0.14642300
C	-10.29502400	6.86790100	-0.66649800
C	-11.54915900	6.96456500	0.00410600

C	-8.04648400	6.35375200	2.33733200
C	-6.75796700	6.57789800	1.75780300
C	-6.64482400	6.79002600	0.34423900
C	-7.82205400	6.77531400	-0.46791900
C	-5.58036800	6.37368400	2.53921100
C	-4.29019000	6.59208200	1.95476200
C	-4.17721300	6.80353700	0.54594100
C	-5.35553200	6.79500100	-0.27012000
C	-3.11030600	6.35903000	2.73003000
C	-1.82392200	6.52158300	2.13587500
C	-1.71149600	6.73729600	0.73776500
C	-2.88601100	6.77945300	-0.07012400
C	-5.68212300	5.73728400	3.81865200
C	-4.49251300	5.32181900	4.50200600
C	-3.21113300	5.71941400	4.00390000
C	-6.96021100	5.31707900	4.29743100
C	-7.04155900	4.31957200	5.32405000
C	-5.84398600	3.75558800	5.86007900
C	-4.57349100	4.32862000	5.52563300
C	-8.14796900	5.72208400	3.61053800
C	-9.43736000	5.32535900	4.10608100
C	-9.51901300	4.32393900	5.13366400
C	-8.30964200	3.74086300	5.64656600
C	-10.62532000	5.79761100	3.46625700
C	-11.87240800	5.42636300	4.04854200
C	-11.95111000	4.46135900	5.03708900
C	-10.78866100	3.79286700	5.52067400
C	-8.36177400	2.48298200	6.31362900
C	-9.62275500	1.80949600	6.46211300
C	-10.84165400	2.50765600	6.19736000
C	-7.14603200	1.81218800	6.65792700
C	-5.89681100	2.49303600	6.53492000
C	-4.67946700	1.81656100	6.87407300
C	-3.42537400	2.48835200	6.71895200
C	-3.37239100	3.74417100	6.03994000
C	-2.10314100	4.27225000	5.66130500

C	-2.02310000	5.25901400	4.64523300
C	-2.20839000	1.80156100	7.00362900
C	-0.94796300	2.43054600	6.78081000
C	-0.89545700	3.65860200	6.10995200
C	0.38308900	4.17980400	5.75497900
C	0.46134100	5.14843200	4.75168000
C	-0.73852400	5.58843600	4.12003800
C	-0.64019000	6.22090000	2.87345300
C	-0.42253600	6.64047400	0.13874600
C	0.76169300	6.61194000	0.92637700
C	0.65450600	6.38547600	2.30072700
C	1.84093100	6.18487200	3.05138500
C	1.74293000	5.55299000	4.29827400
C	3.13025000	6.46409800	2.51637100
C	3.23927900	6.68818800	1.12991100
C	2.05523400	6.61282400	0.34241700
C	2.16360100	6.37584800	-1.03160300
C	0.97683100	6.14973400	-1.77980400
C	-0.31240900	6.39785900	-1.23743400
C	-1.49138300	6.25163000	-2.02713800
C	-2.77339900	6.53699100	-1.47448400
C	4.53037600	6.77359500	0.52749600
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H	-12.65175300	6.76315200	1.81364000
H	-12.29876100	6.77778800	-2.60203800
H	-12.79915100	5.84319400	3.65807500
H	-11.91938600	2.00819100	-7.24083000
H	-12.00992400	4.17752100	-6.17668300
H	-11.88943700	-0.03763200	-7.53327700
H	-12.12674800	5.66024800	-4.73934000
H	-12.78648100	-5.75405700	3.95171600
H	-12.60763000	-6.87407600	1.81633800
H	-12.91222000	-4.27005600	5.38528000
H	-12.44302300	-7.21784900	-0.21485200
H	-12.11237600	-5.94281600	-4.44383000
H	-11.98253700	-4.25186100	-6.16708600
H	-12.25425000	-6.86590400	-2.59947600
H	-11.91386500	-2.42054500	-7.12367900