

## Supporting information

### Understanding the Axial Chirality Control of Quinidine-derived Ammonium Cation-directed O-alkylation: A Computational Study

Han Li<sup>a</sup>, Wu Fan<sup>b,\*</sup> and Xin Hong<sup>a,\*</sup>

<sup>a</sup> Department of Chemistry, Zhejiang University, Hangzhou, 310027, China.

<sup>b</sup> Key Laboratory of Tobacco Flavor Basic Research, Zhengzhou Tobacco Research Institute of CNTC, No.2 Fengyang Street High-Tech Zone, Zhengzhou 450001, China

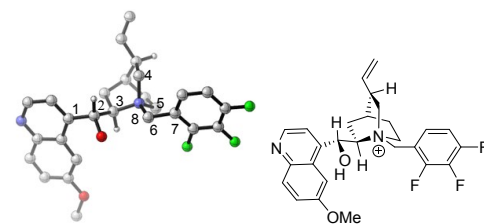
Email: hxchem@zju.edu.cn; fanwu2015@126.com

### CONTENTS

Conformational search of ammonium catalyst .....	S2
Conformational search of ammonium-enolate complex .....	S7
Conformational search of O-alkylation transition state .....	S16
Boltzmann distribution of transition states .....	S22
Procedure of Independent Gradient Model analysis.....	S23
Table of energies .....	S24
Cartesian coordinates of the DFT-computed stationary points .....	S28

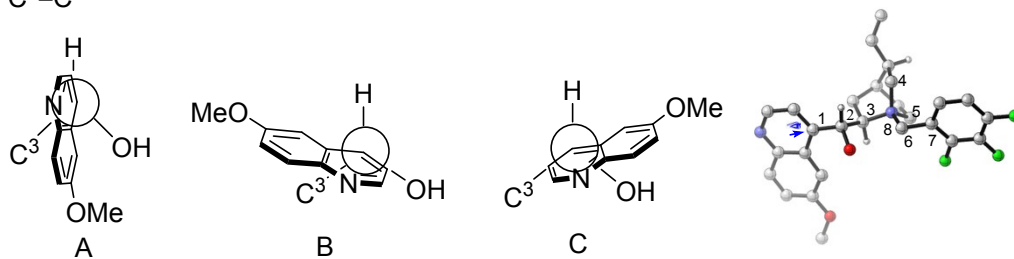
## Conformational search of ammonium catalyst.

We first identified the possible conformational flexibilities based on the initial conformation of the quinidine-derived ammonium catalyst **1**.

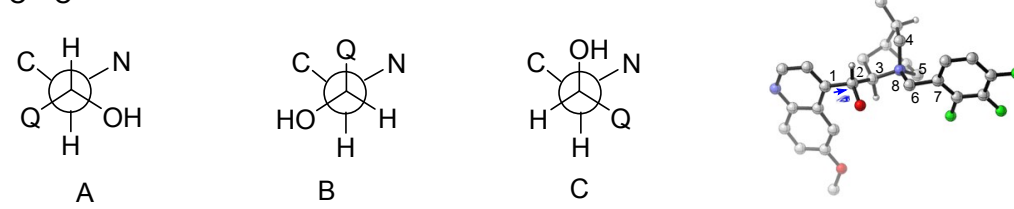


The conformers based on the Newman projection of  $C^1-C^2$ ,  $C^2-C^3$ ,  $C^6-N^8$ ,  $C^7-C^6$  are the following, where Q stands for the quinoline group and Ar stands for the fluoroaryl group. The structures and relative free energies of the unfavorable conformers are shown in Figure S2 and S3.

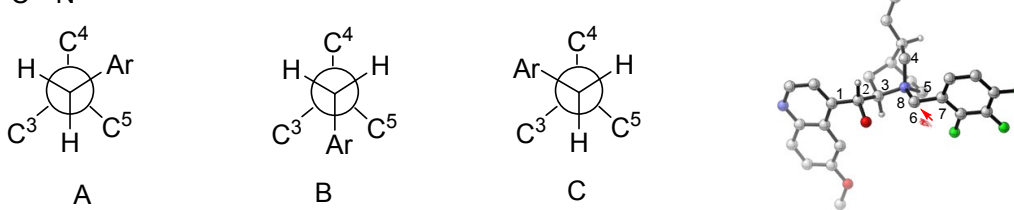
$C^1-C^2$



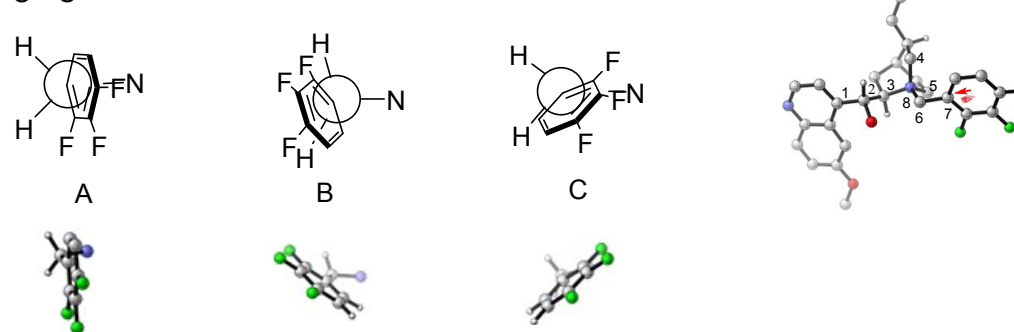
$C^2-C^3$



$C^6-N^8$



$C^7-C^6$



**Figure S1.** Conformational flexibilities of quinidine-derived ammonium catalyst **1**.

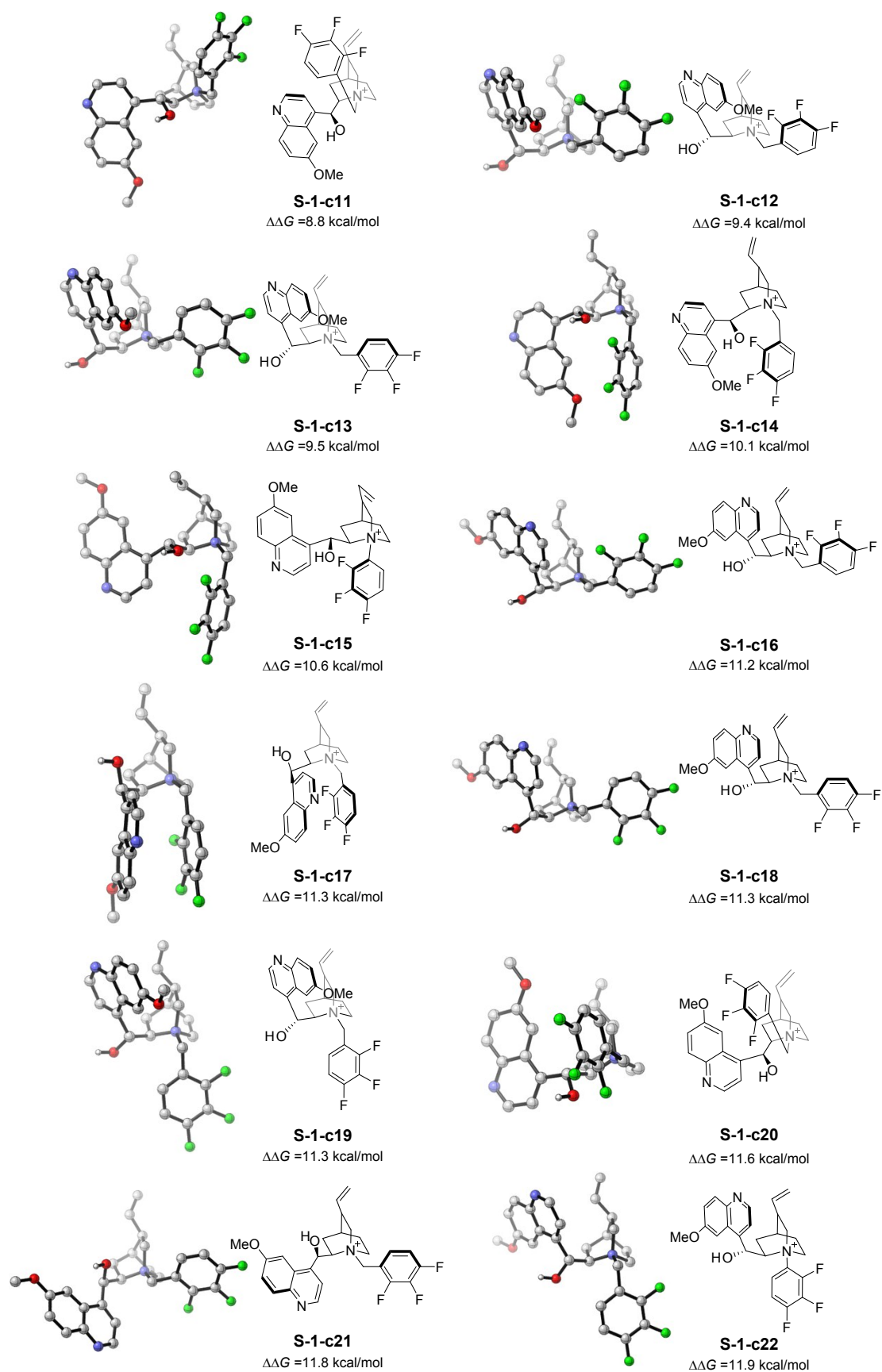
**Table S1.** Results of conformational search of ammonium catalyst **1**.

Entry of studied conformations	Newman projection of C <sup>1</sup> -C <sup>2</sup>	Newman projection of C <sup>2</sup> -C <sup>3</sup>	Newman projection of C <sup>6</sup> -N <sup>8</sup>	Newman projection of C <sup>7</sup> -C <sup>6</sup>	Optimized conformation of catalyst
1	A	A	A	A	1-c1
2	A	A	A	B	1-c5
3	A	A	A	C	1-c5
4	A	A	B	A	S-1-c14
5	A	A	B	B	1-c8
6	A	A	B	C	1-c8
7	A	A	C	A	S-1-c11
8	A	A	C	B	S-1-c24
9	A	A	C	C	*
10	A	B	A	A	S-1-c18
11	A	B	A	B	S-1-c16
12	A	B	A	C	S-1-c16
13	A	B	B	A	S-1-c27
14	A	B	B	B	S-1-c22
15	A	B	B	C	S-1-c33
16	A	B	C	A	S-1-c29
17	A	B	C	B	*
18	A	B	C	C	*
19	A	C	A	A	*
20	A	C	A	B	*
21	A	C	A	C	*
22	A	C	B	A	*
23	A	C	B	B	*
24	A	C	B	C	*
25	A	C	C	A	*
26	A	C	C	B	*
27	A	C	C	C	*
28	B	A	A	A	*
29	B	A	A	B	*
30	B	A	A	C	*
31	B	A	B	A	*
32	B	A	B	B	*
33	B	A	B	C	*
34	B	A	C	A	*
35	B	A	C	B	*
36	B	A	C	C	*
37	B	B	A	A	*
38	B	B	A	B	S-1-c35
39	B	B	A	C	1-c9
40	B	B	B	A	S-1-c23

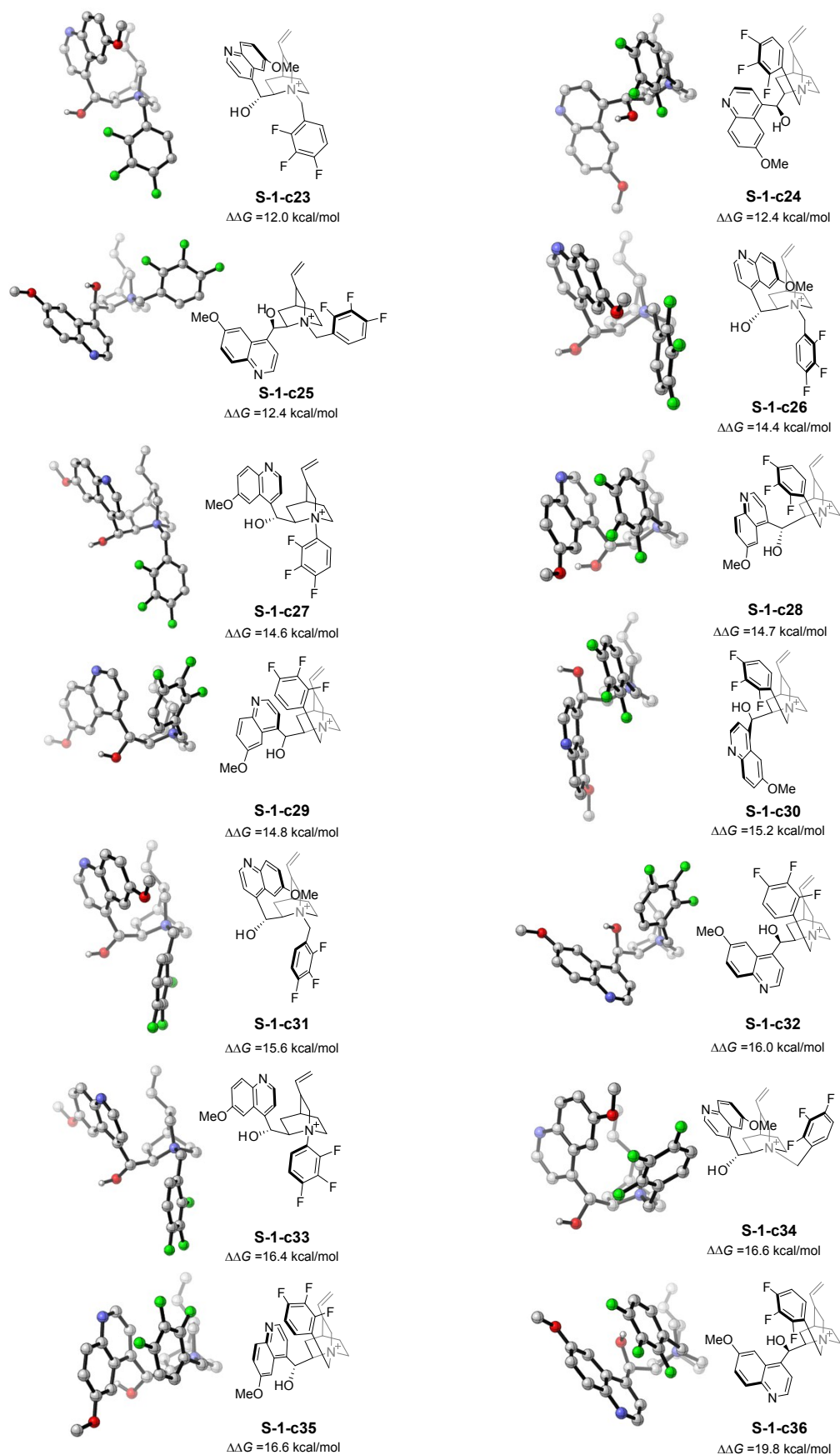
41	B	B	B	B	*
42	B	B	B	C	*
43	B	B	C	A	*
44	B	B	C	B	*
45	B	B	C	C	*
46	B	C	A	A	1-c2
47	B	C	A	B	1-c4
48	B	C	A	C	1-c4
49	B	C	B	A	*
50	B	C	B	B	*
51	B	C	B	C	S-1-c17
52	B	C	C	A	*
53	B	C	C	B	S-1-c30
54	B	C	C	C	*
55	C	A	A	A	1-c6
56	C	A	A	B	1-c3
57	C	A	A	C	1-c3
58	C	A	B	A	S-1-c15
59	C	A	B	B	1-c7
60	C	A	B	C	1-c7
61	C	A	C	A	1-c10
62	C	A	C	B	S-1-c20
63	C	A	C	C	*
64	C	B	A	A	S-1-c13
65	C	B	A	B	S-1-c12
66	C	B	A	C	S-1-c12
67	C	B	B	A	S-1-c26
68	C	B	B	B	S-1-c19
69	C	B	B	C	S-1-c31
70	C	B	C	A	S-1-c34
71	C	B	C	B	S-1-c28
72	C	B	C	C	*
73	C	C	A	A	S-1-c21
74	C	C	A	B	S-1-c25
75	C	C	A	C	S-1-c25
76	C	C	B	A	*
77	C	C	B	B	*
78	C	C	B	C	*
79	C	C	C	A	S-1-c32
80	C	C	C	B	S-1-c36
81	C	C	C	C	*

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\*Cannot be located.



**Figure S2.** Optimized structures and relative free energies of the unfavorable conformers of ammonium catalyst **1**. The hydrogens are hidden except for the one of the hydroxyl group.

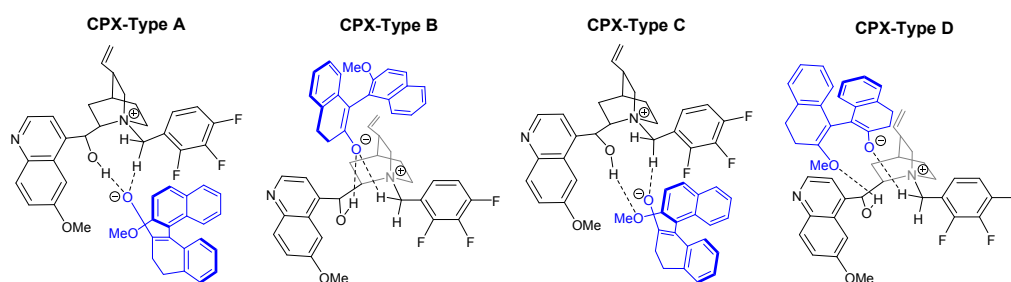


**Figure S3.** Optimized structures and relative free energies of the unfavorable conformers of ammonium catalyst **1**. The hydrogens are hidden except for the one of the hydroxyl group.

## Conformation search of ammonium-enolate complex.

The considered conformational flexibilities and labelling of the ammonium-enolate complex are described in Figure S4-S6. These conformations of the ammonium-enolate complex are all attempted for optimization, and the results are summarized in Table S2. In addition to the low-energy conformers shown in Figure 4, the optimized structures and relative free energies of all the rest conformers that are considered in transition state conformational search are included in Figure S7.

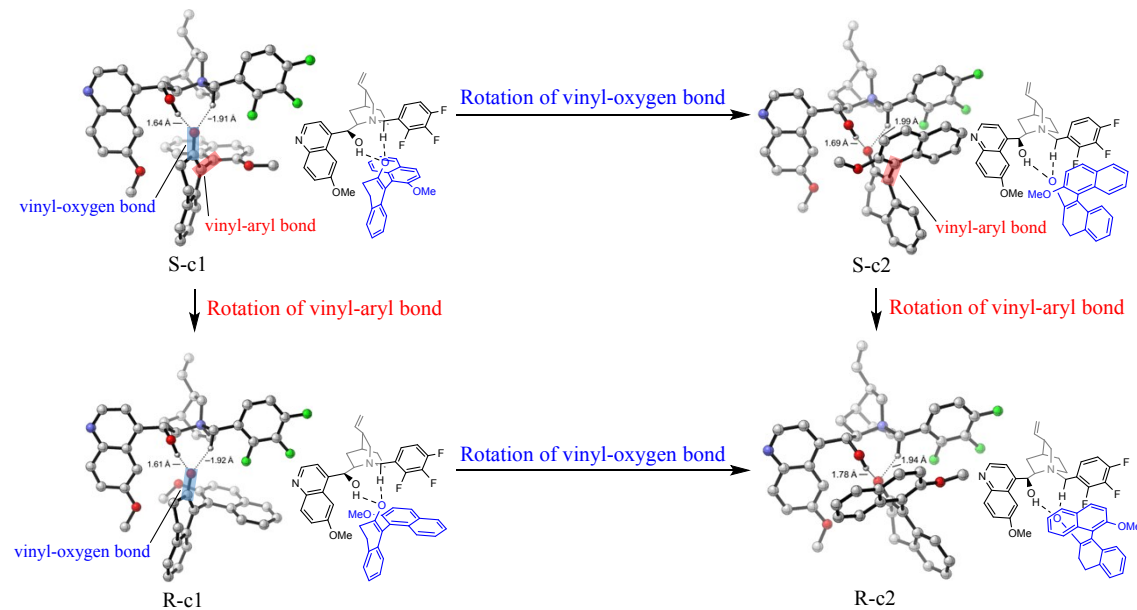
We want to emphasize that some conformers with reasonable stabilities are not considered in the transition state conformational search because the enolate oxygen is shielded from electrophilic attack. The optimized structures and relative free energies of these complexes are included in Figure S8 and S9. All the located high-energy conformers are illustrated in Figure S10-S12.



**Figure S4.** Four proposed complexation patterns between the ammonium catalyst and enolate substrate.



**Figure S5.** Chirality of enolate.



**Figure S6.** Illustration of rotations of vinyl-oxygen and vinyl-aryl bonds and related conformers.

**Table S2.** Results of conformational search of ammonium-enolate complex.

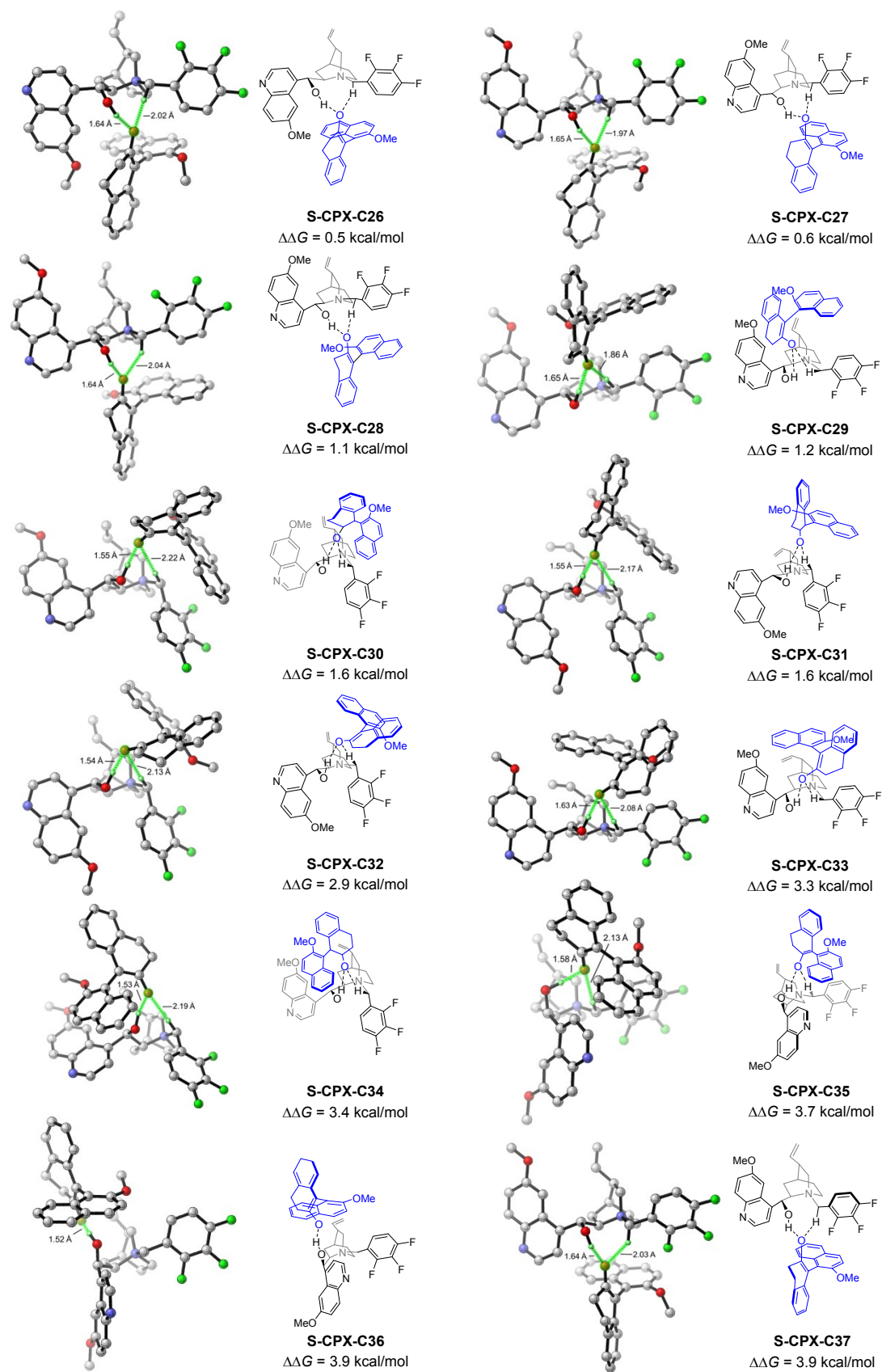
Entry of studied conformations	Conformation of catalyst	Complex type	Chirality of enolate	Optimized conformations of complex
1	1-c1	CPX-Type A	S	S-CPX-C19, S-CPX-C12
2	1-c1	CPX-Type A	R	S-CPX-C39, S-CPX-C46
3	1-c1	CPX-Type B	S	CPX-C2, S-CPX-C11
4	1-c1	CPX-Type B	R	S-CPX-C9, S-CPX-C10
5	1-c1	CPX-Type C	S	*
6	1-c1	CPX-Type C	R	*
7	1-c1	CPX-Type D	S	*
8	1-c1	CPX-Type D	R	*
9	1-c3	CPX-Type A	S	S-CPX-C6, S-CPX-C13
10	1-c3	CPX-Type A	R	S-CPX-C22, S-CPX-C28
11	1-c3	CPX-Type B	S	S-CPX-C55, S-CPX-C57
12	1-c3	CPX-Type B	R	S-CPX-C51
13	1-c3	CPX-Type C	S	S-CPX-C8, S-CPX-C27
14	1-c3	CPX-Type C	R	S-CPX-C15, S-CPX-C20
15	1-c3	CPX-Type D	S	*
16	1-c3	CPX-Type D	R	*
17	1-c6	CPX-Type A	S	S-CPX-C18, S-CPX-C37
18	1-c6	CPX-Type A	R	S-CPX-C23
19	1-c6	CPX-Type B	S	S-CPX-C29, S-CPX-C47
20	1-c6	CPX-Type B	R	S-CPX-C5, S-CPX-C33
21	1-c6	CPX-Type C	S	*
22	1-c6	CPX-Type C	R	*
23	1-c6	CPX-Type D	S	*
24	1-c6	CPX-Type D	R	*
25	1-c5	CPX-Type A	S	CPX-C1, S-CPX-C16
26	1-c5	CPX-Type A	R	CPX-C3, S-CPX-C45
27	1-c5	CPX-Type B	S	S-CPX-C59
28	1-c5	CPX-Type B	R	S-CPX-C25, S-CPX-C52
29	1-c5	CPX-Type C	S	S-CPX-C26
30	1-c5	CPX-Type C	R	S-CPX-C17, S-CPX-C21
31	1-c5	CPX-Type D	S	*
32	1-c5	CPX-Type D	R	*
33	1-c7	CPX-Type A	S	S-CPX-C38, S-CPX-C49
34	1-c7	CPX-Type A	R	S-CPX-C53, S-CPX-C60
35	1-c7	CPX-Type B	S	S-CPX-C30, S-CPX-C42
36	1-c7	CPX-Type B	R	CPX-C4, S-CPX-C34
37	1-c7	CPX-Type C	S	S-CPX-C7, S-CPX-C48
38	1-c7	CPX-Type C	R	*
39	1-c7	CPX-Type D	S	*
40	1-c7	CPX-Type D	R	*



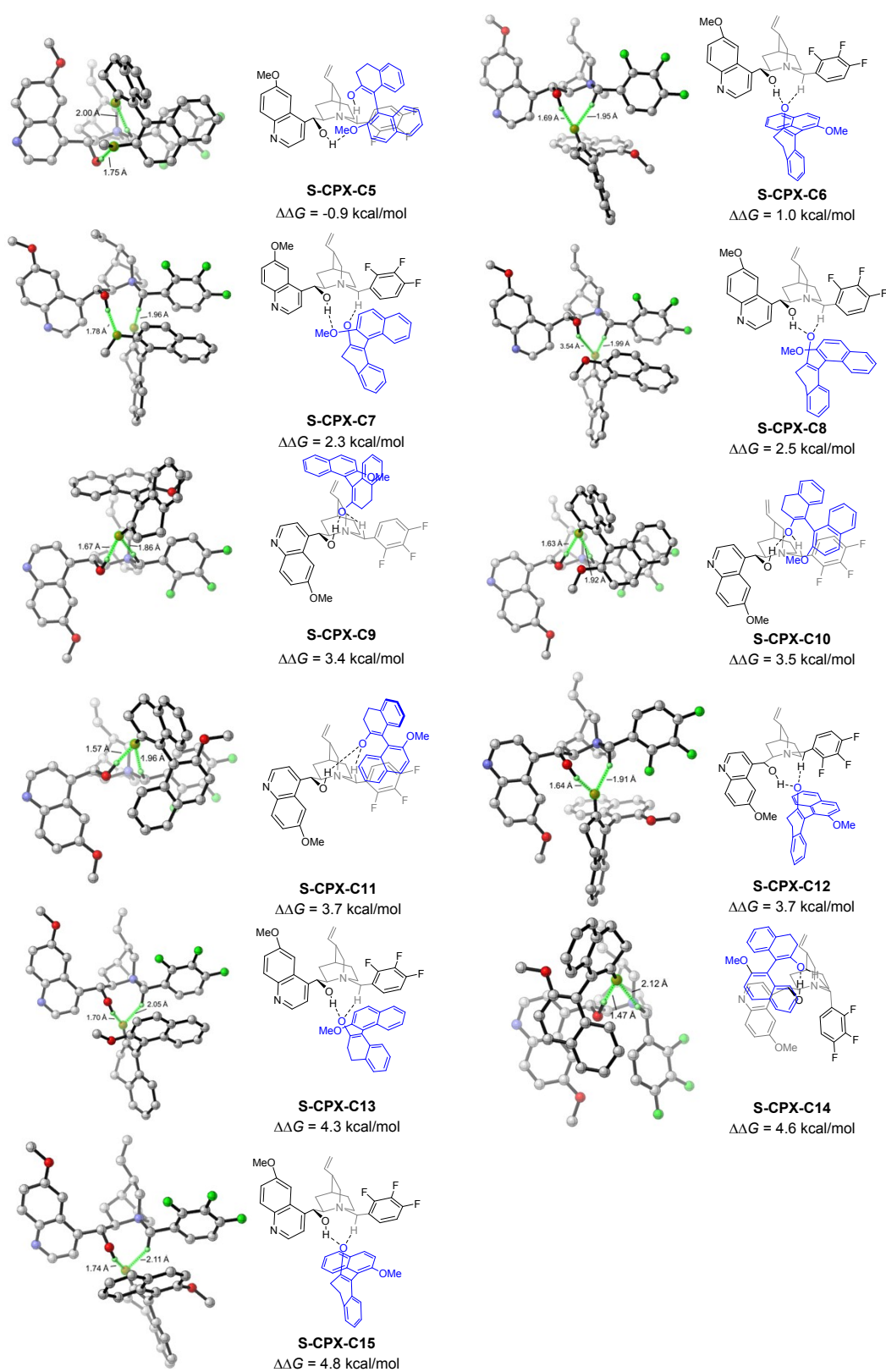
41	1-c8	CPX-Type A	S	S-CPX-C56, S-CPX-C65
42	1-c8	CPX-Type A	R	S-CPX-C54, S-CPX-C58
43	1-c8	CPX-Type B	S	S-CPX-C31, S-CPX-C41
44	1-c8	CPX-Type B	R	S-CPX-C14, S-CPX-C32
45	1-c8	CPX-Type C	S	*
46	1-c8	CPX-Type C	R	*
47	1-c8	CPX-Type D	S	*
48	1-c8	CPX-Type D	R	*
49	1-c4	CPX-Type A	S	*
50	1-c4	CPX-Type A	R	*
51	1-c4	CPX-Type B	S	S-CPX-C62, S-CPX-C63
52	1-c4	CPX-Type B	R	S-CPX-C61, S-CPX-C64
53	1-c4	CPX-Type C	S	*
54	1-c4	CPX-Type C	R	*
55	1-c4	CPX-Type D	S	*
56	1-c4	CPX-Type D	R	*
57	1-c2	CPX-Type A	S	*
58	1-c2	CPX-Type A	R	*
59	1-c2	CPX-Type B	S	S-CPX-C24, S-CPX-C44
60	1-c2	CPX-Type B	R	S-CPX-C40, S-CPX-C50
61	1-c2	CPX-Type C	S	*
62	1-c2	CPX-Type C	R	*
63	1-c2	CPX-Type D	S	S-CPX-C35, S-CPX-C36
64	1-c2	CPX-Type D	R	S-CPX-C43

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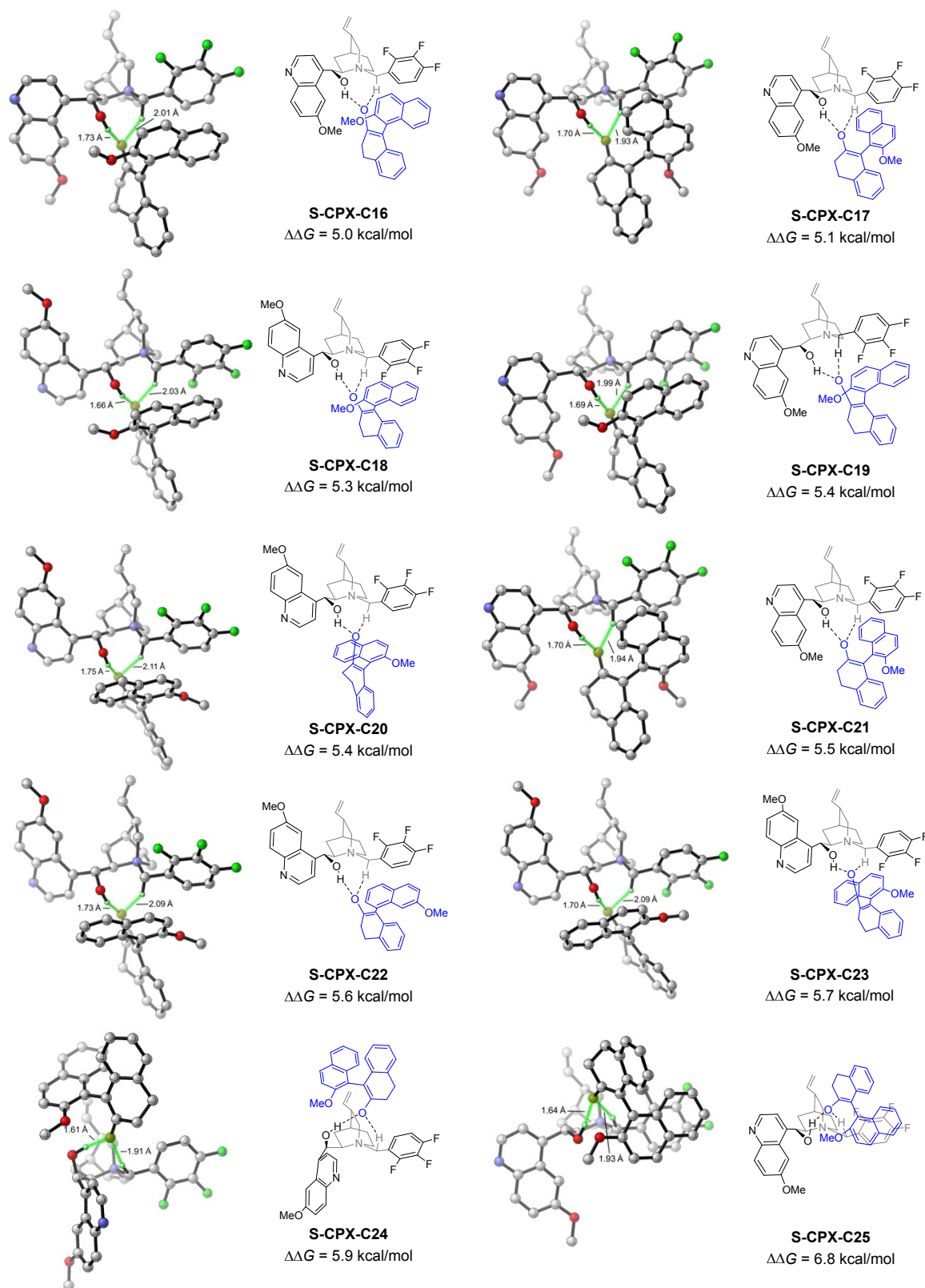
\*Cannot be located.



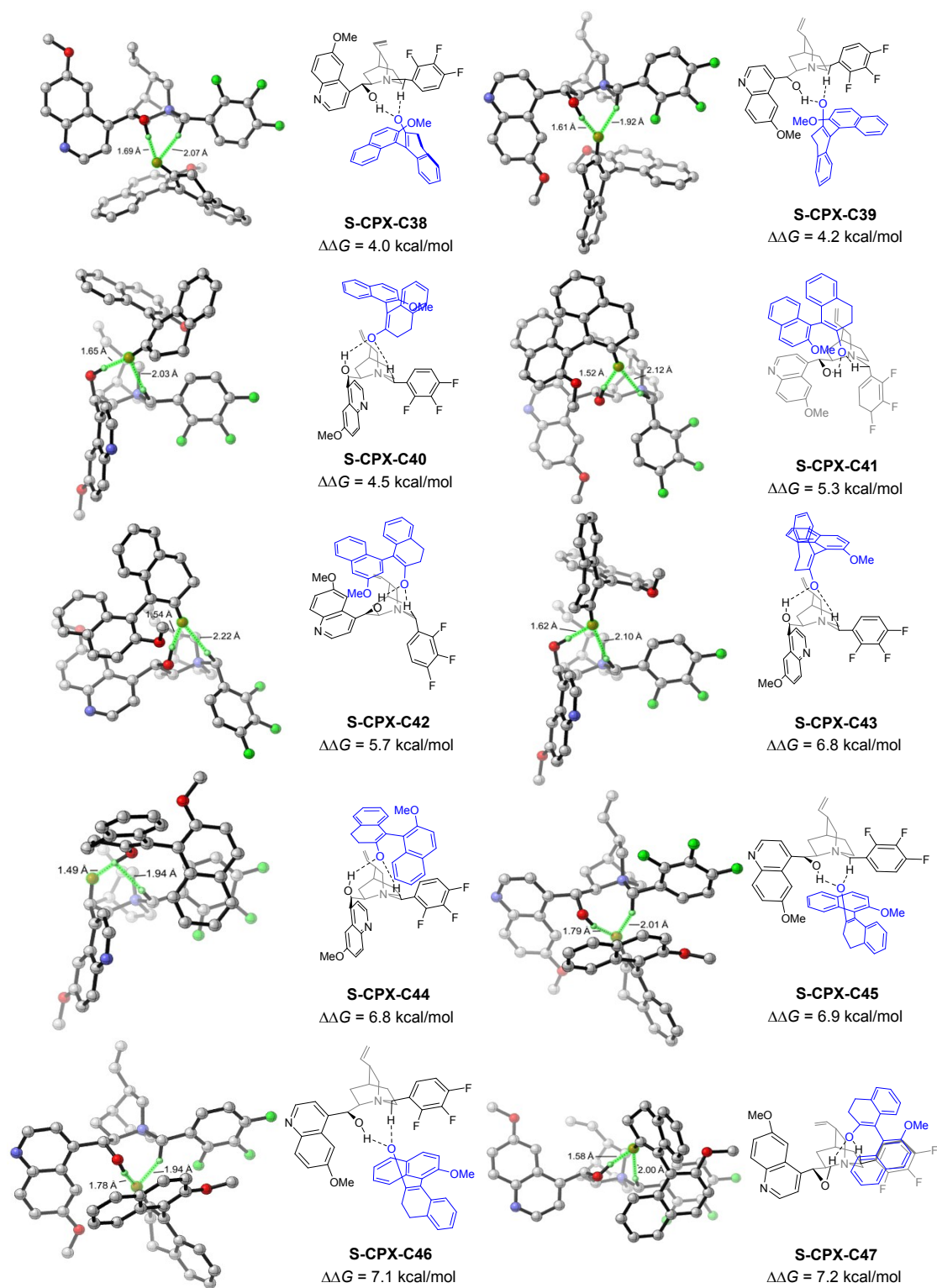
**Figure S7.** Optimized structures and relative free energies of low energy conformers of ammonium-enolate complex. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.



**Figure S8.** Optimized structures and relative free energies of conformers of ammonium-enolate complex that have reasonable stabilities but are not considered for transition state calculations. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.

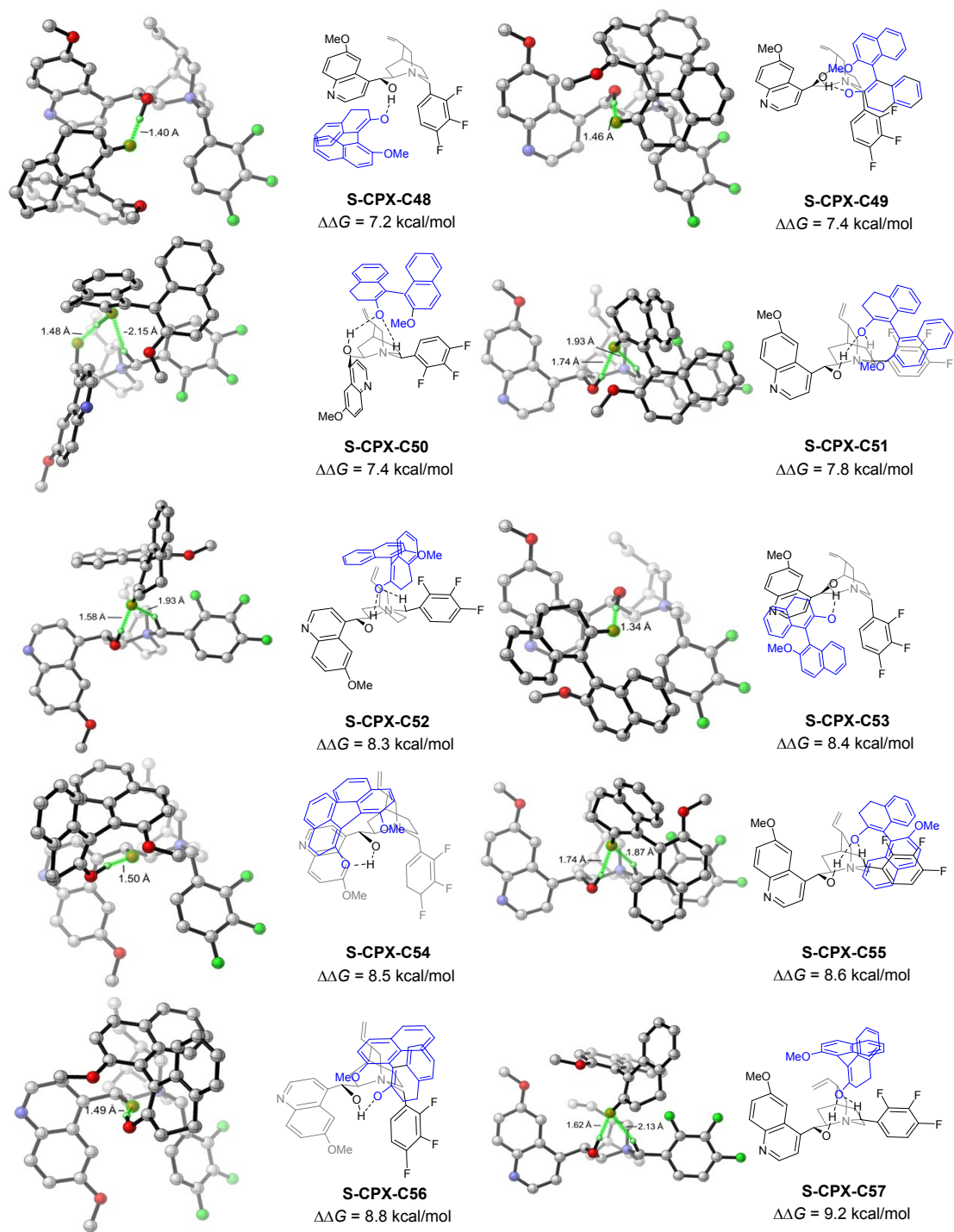


**Figure S9.** Optimized structures and relative free energies of conformers of ammonium-enolate complex that have reasonable stabilities but are not considered for transition state calculations. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.

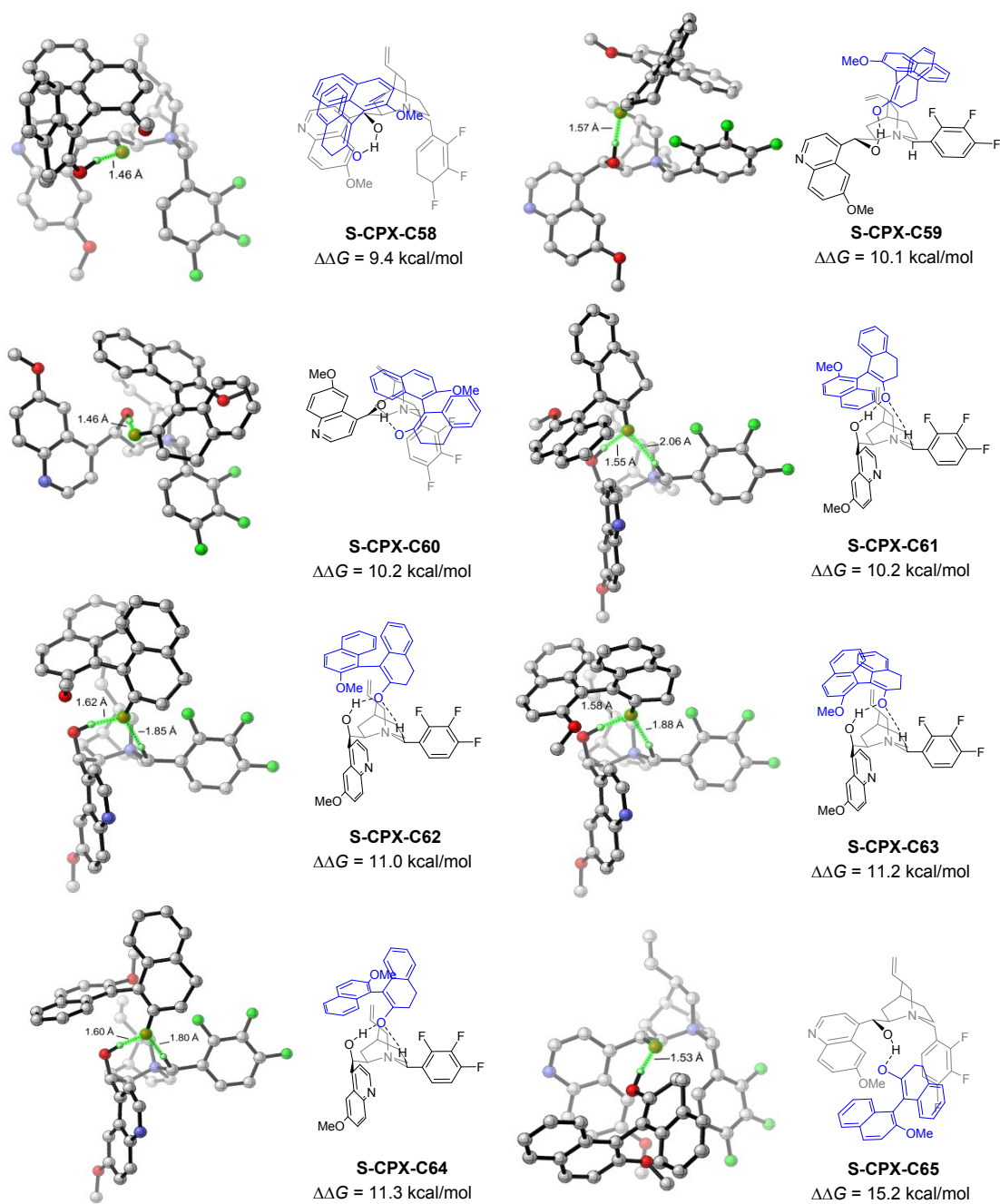


**Figure S10.** Optimized structures and relative free energies of high energy conformers of ammonium-enolate complex. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.





**Figure S11.** Optimized structures and relative free energies of high energy conformers of ammonium-enolate complex. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.



**Figure S12.** Optimized structures and relative free energies of high energy conformers of ammonium-enolate complex. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.

### Conformational search of O-alkylation transition state.

The considered conformational flexibilities and labelling of the O-alkylation transition state are described in Figure S13. These transition states are all attempted for optimization, and the results are summarized in Table S3. The optimized structures and relative free energies of all located transition states are included in Figure S14-S17.

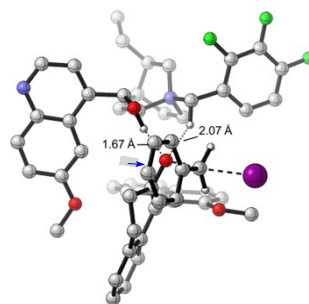
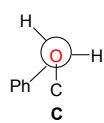
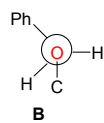
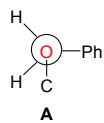
**Table S3.** Results of conformational search of O-alkylation transition state.

Entry of studied conformations	Conformations of complex	Optimized conformations of transition state
1	CPX-C2	S-TS-C7, S-TS-C10, S-TS-C18, S-TS-C28
2	S-CPX-C27	S-TS-C13, S-TS-C14, S-TS-C20
3	S-CPX-C28	TS-C3, S-TS-C31
4	S-CPX-C29	S-TS-C8, S-TS-C9, S-TS-C11, S-TS-C22
5	S-CPX-C33	S-TS-C37
6	CPX-C1	TS-C1, S-TS-C21, S-TS-C30
7	CPX-C3	S-TS-C33
8	S-CPX-C30	S-TS-C12, S-TS-C17
9	S-CPX-C34	S-TS-C35, S-TS-C36
10	CPX-C4	S-TS-C32, S-TS-C34
11	S-CPX-C31	TS-C2, S-TS-C5, S-TS-C6, S-TS-C27, S-TS-C29
12	S-CPX-C32	TS-C4
13	S-CPX-C35	*
14	S-CPX-C36	S-TS-C15, S-TS-C24, S-TS-C25
15	S-CPX-C37	S-TS-C16, S-TS-C19, S-TS-C23, S-TS-C26
16	S-CPX-C26	TS-C1, S-TS-C21, S-TS-C30

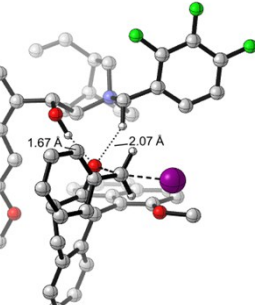
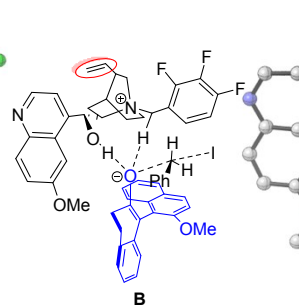
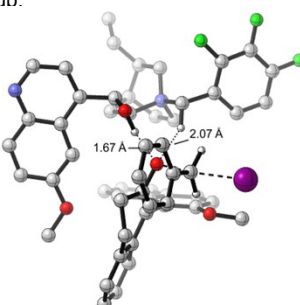
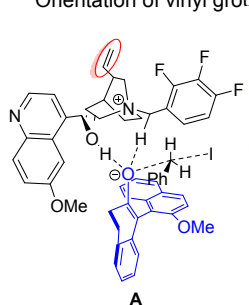
\*Cannot be located.



Newman projection of I-C bond:



Orientation of vinyl group:



6 types of transition states:

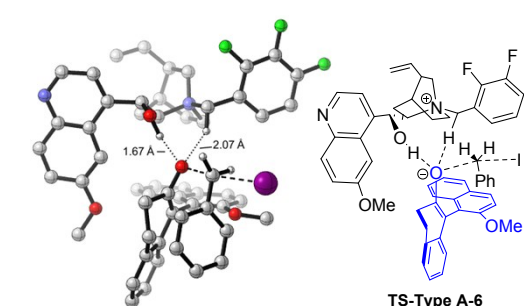
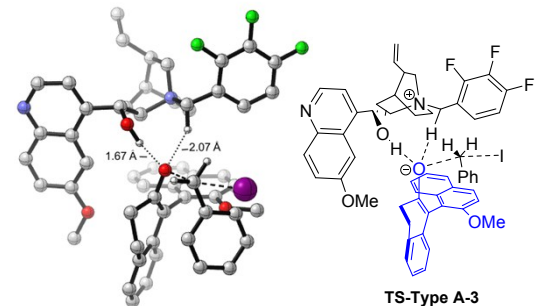
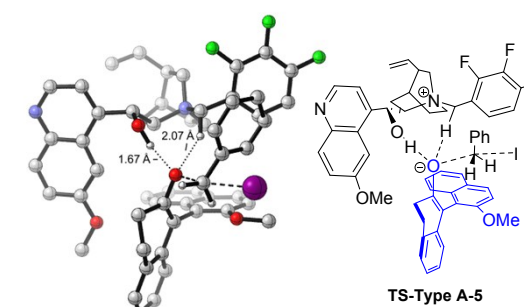
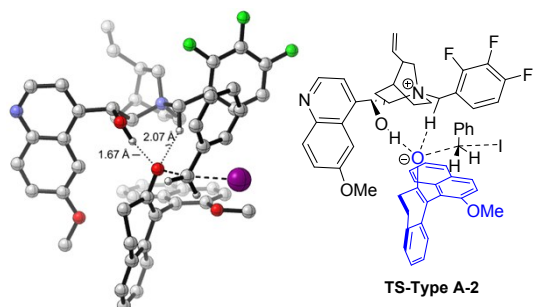
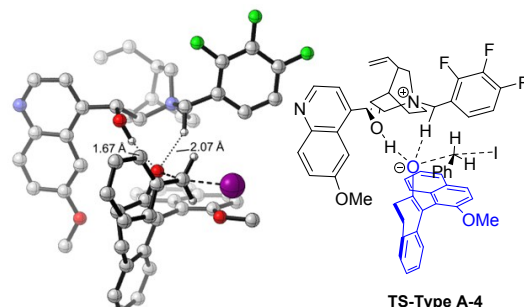
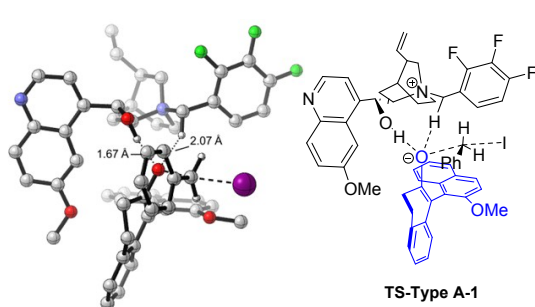
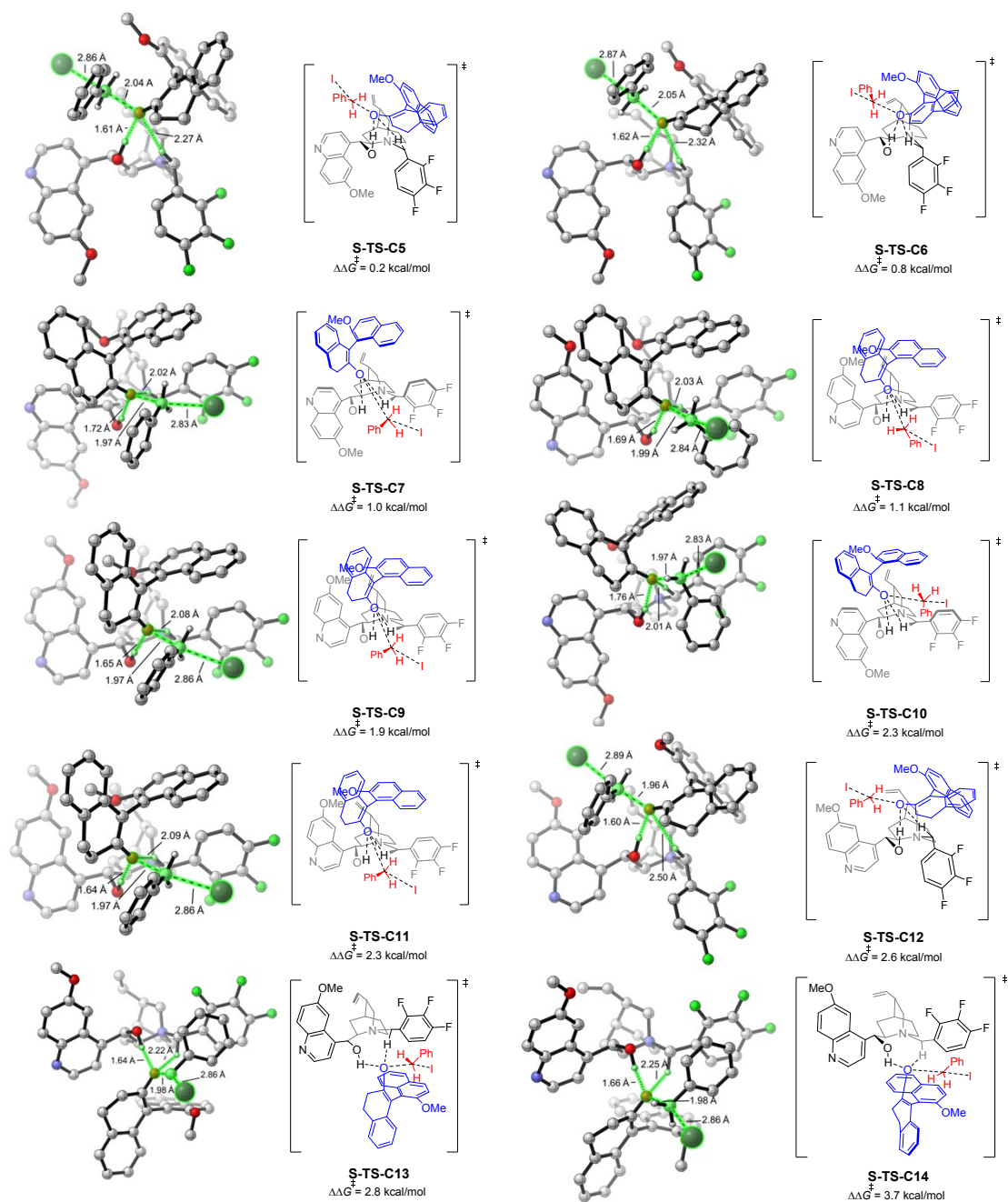
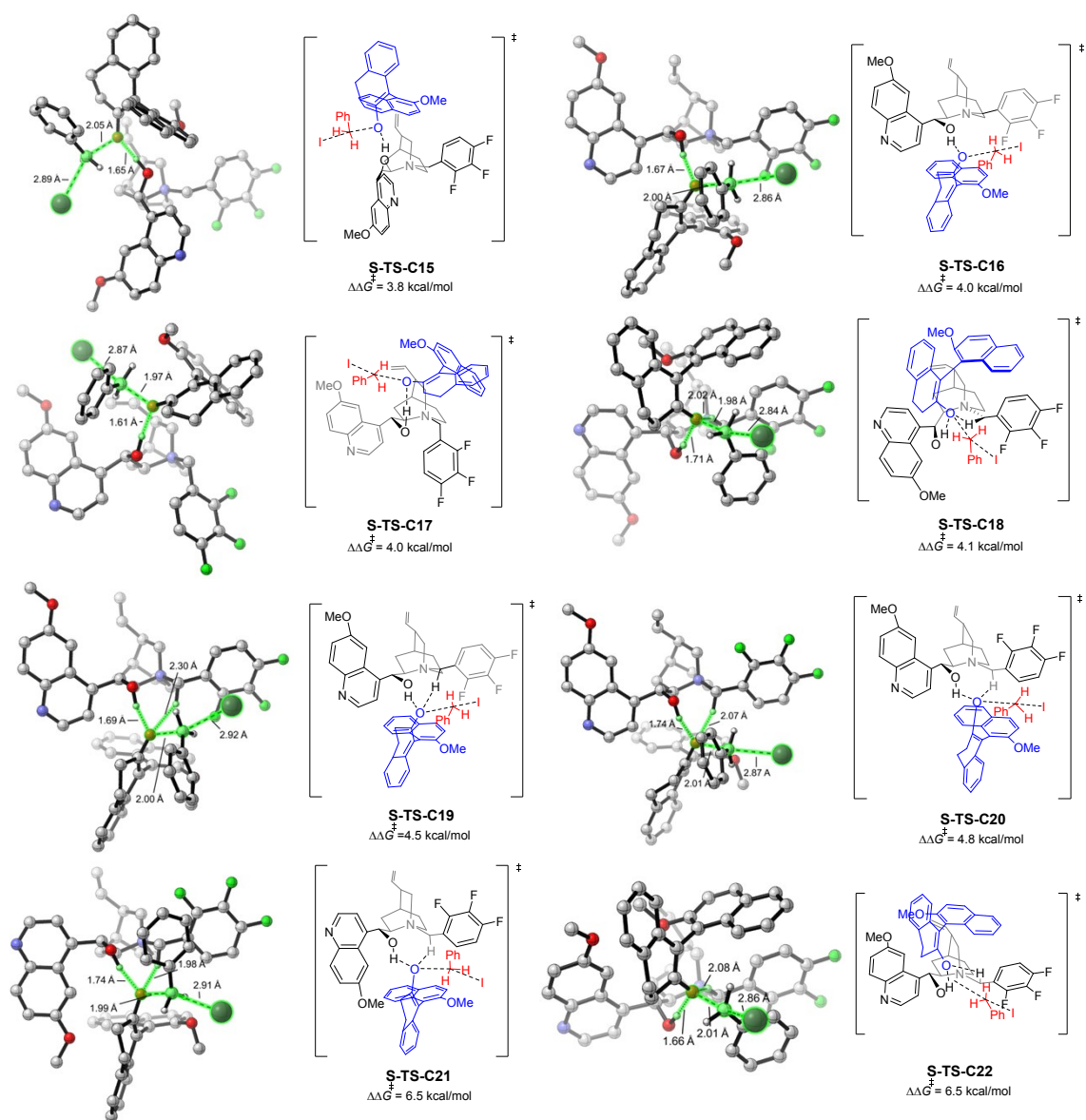


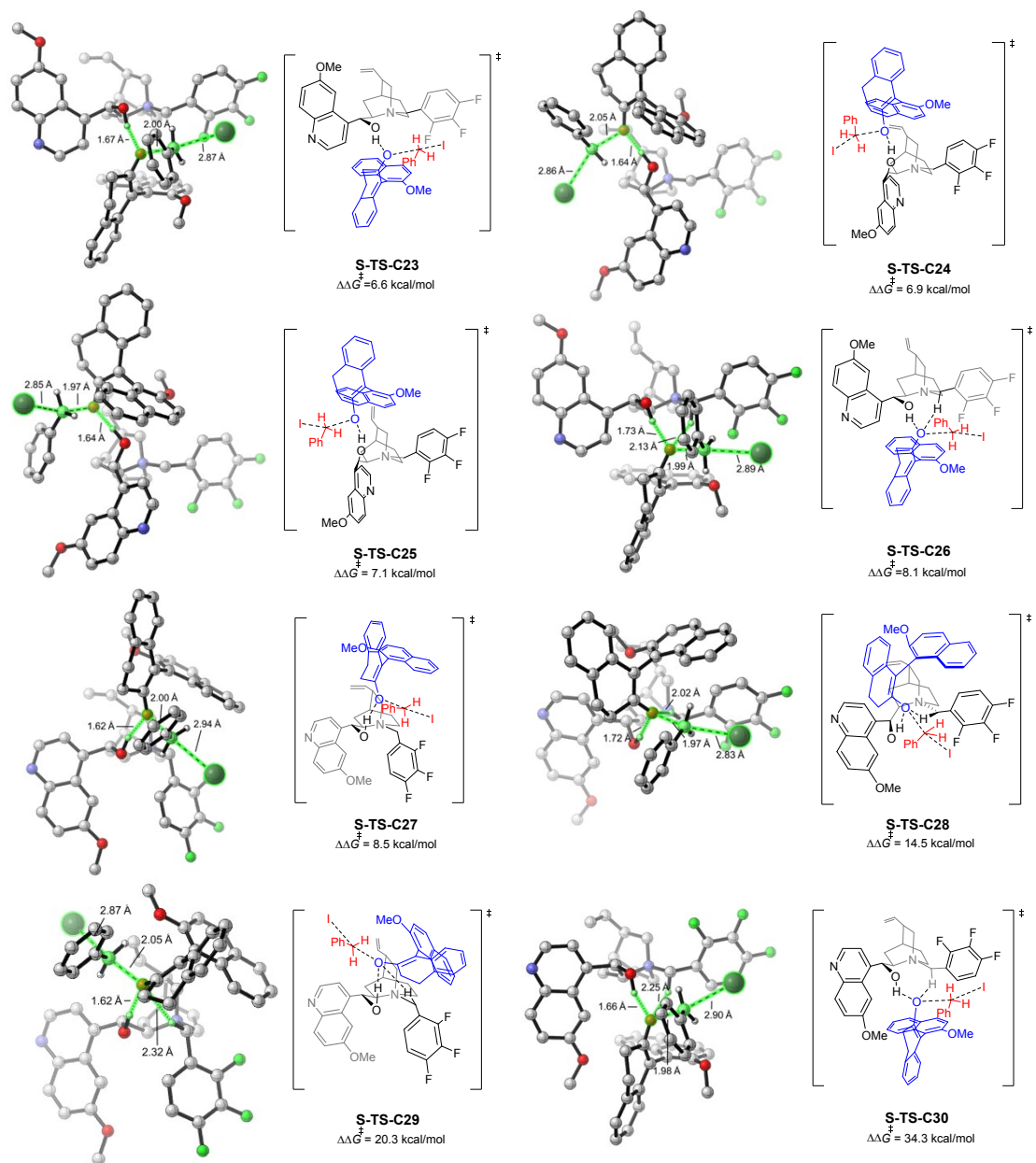
Figure S13. Conformational search of O-alkylation transition states



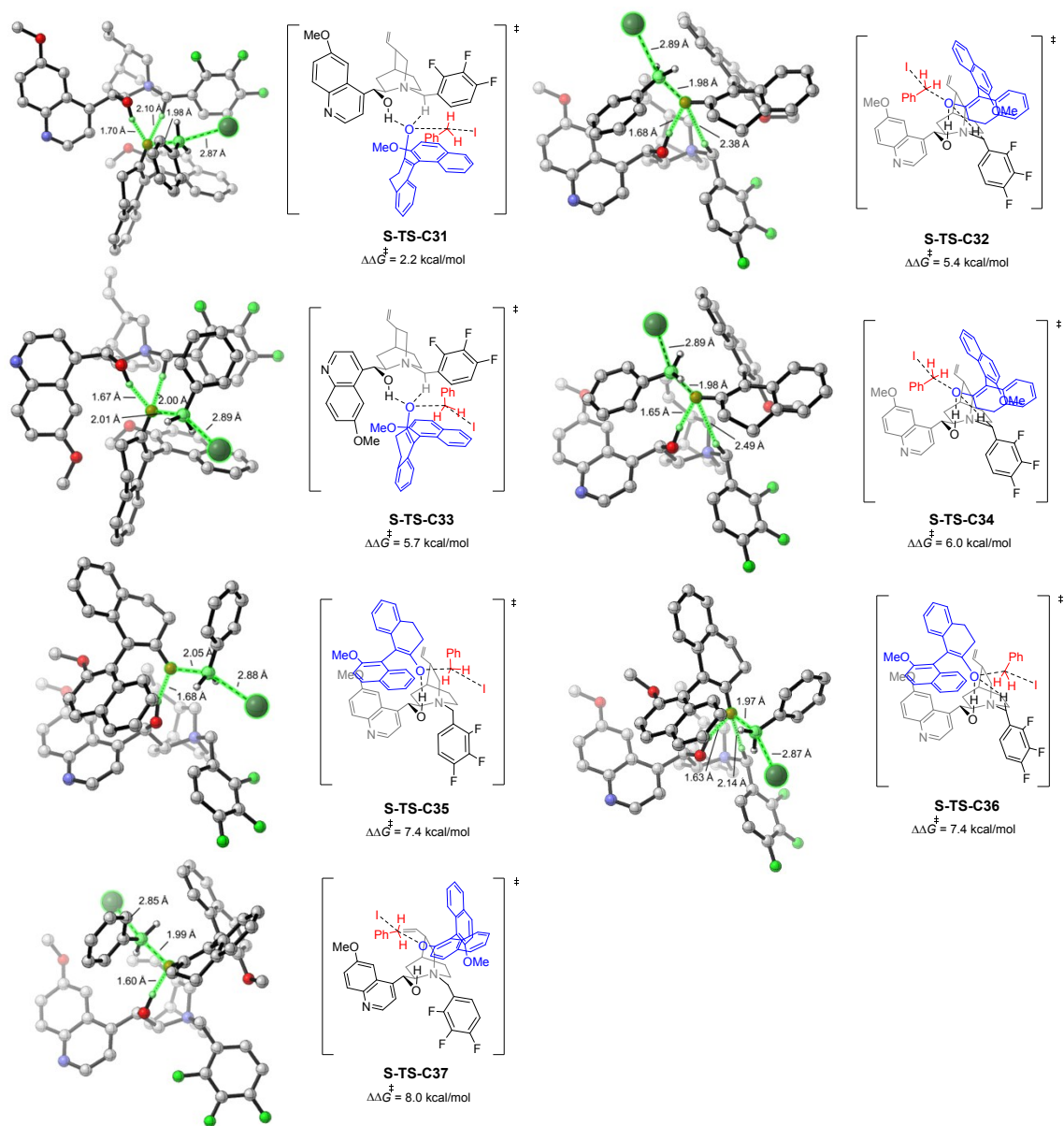
**Figure S14.** Optimized structures and relative free energies of conformers of transition state leading to major enantiomer. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.



**Figure S15.** Optimized structures and relative free energies of conformers of transition state leading to major enantiomer. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.



**Figure S16.** Optimized structures and relative free energies of conformers of transition state leading to major enantiomer. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.



**Figure S17.** Optimized structures and relative free energies of conformers of transition state leading to minor enantiomer. The hydrogens are hidden except for the ones that are involved in hydrogen-bonding.

**Boltzmann distribution of transition states.**

$$p_i = \frac{e^{-\varepsilon_i/kT}}{\sum_{j=1}^M e^{-\varepsilon_j/kT}}$$

$P_i$  is the probability of state  $i$ ,  $\varepsilon_i$  the energy of state  $i$ ,  $k$  is the Boltzmann constant,  $T$  is the temperature of the system and  $M$  is the number of all states accessible to the system. The sum is over all states accessible to the system of interest.

**Table S4.**

$\Delta\Delta G^\ddagger$ of major enantiomers	Probability	$\Delta\Delta G^\ddagger$ of major enantiomers	Probability
0.0	1.000	1.9	0.040
0.2	0.731	2.2	0.024
0.8	0.245	3.1	0.005
1.0	0.186	5.4	0.000
1.1	0.165	5.7	0.000
1.1	0.158	6	0.000
1.9	0.041	7.4	0.000
2.3	0.022	7.4	0.000
2.3	0.021	8	0.000
2.6	0.013		
2.8	0.008		
3.7	0.002		
3.8	0.002		
4	0.001		
4	0.001		
4.1	0.001		
4.5	0.001		
4.8	0.000		
6.5	0.000		
6.5	0.000		
6.6	0.000		
6.9	0.000		
7.1	0.000		
8.1	0.000		
8.5	0.000		
14.5	0.000		
20.3	0.000		
34.3	0.000		

$\Delta\Delta G^\ddagger$  in kcal/mol

Computationally e.e.% = 95%, favoring the major enantiomer, which is consistent with the observed enantioselectivity (e.e.% = 92%)



### **Procedure of Independent Gradient Model analysis**

Based on the gas phase-optimized geometry of the transition states TS-C1 and TS-C2, we performed the Independent Gradient Model analysis between the two fragments of the O-alkylation transition states using Multiwfn 3.5. One fragment is the interacting hydrogen of the iodobenzene, and the other fragment is the oxygen of methoxy group. This allows the generation of a cube file, which can be further visualized with VMD software.



**Table of Energies.****Table S5. Zero-point correction (ZPE), thermal correction to enthalpy (TCH), thermal correction to Gibbs free energy (TCG), energies (E), enthalpies (H), and Gibbs free energies (G) (in Hartree) of the structures calculated at the  $\omega$ B97XD/6-311+G(d,p)-SMD(Benzene)// $\omega$ B97XD/6-31G(d) level of theory**

Structures	ZPE	TCH	TCG	E	H	G	Imaginary Frequency
1-c1	0.518464	0.548223	0.457804	-1604.930919	-1604.382696	-1604.473115	
1-c2	0.518882	0.548552	0.45779	-1604.931114	-1604.382562	-1604.473324	
1-c3	0.518109	0.547827	0.458126	-1604.930304	-1604.382477	-1604.472178	
1-c4	0.518668	0.548289	0.458553	-1604.93063	-1604.382341	-1604.472077	
1-c5	0.518247	0.548075	0.457422	-1604.929342	-1604.381267	-1604.47192	
1-c6	0.51873	0.548298	0.459343	-1604.930452	-1604.382154	-1604.471109	
1-c7	0.519147	0.548776	0.459883	-1604.930759	-1604.381983	-1604.470876	
1-c8	0.519259	0.54895	0.459165	-1604.92864	-1604.37969	-1604.469475	
1-c9	0.518521	0.548249	0.457242	-1604.924845	-1604.376596	-1604.467603	
1-c10	0.518716	0.548275	0.459503	-1604.926792	-1604.378517	-1604.467289	
S-1-c11	0.518436	0.548149	0.458406	-1604.925384	-1604.377235	-1604.466978	
S-1-c12	0.51888	0.548542	0.459165	-1604.925092	-1604.37655	-1604.465927	
S-1-c13	0.519396	0.548967	0.459815	-1604.925635	-1604.376668	-1604.46582	
S-1-c14	0.518929	0.548589	0.45933	-1604.924164	-1604.375575	-1604.464834	
S-1-c15	0.518442	0.54813	0.459035	-1604.923032	-1604.374902	-1604.463997	
S-1-c16	0.519074	0.548729	0.459105	-1604.922233	-1604.373504	-1604.463128	
S-1-c17	0.51972	0.54878	0.463266	-1604.926254	-1604.377474	-1604.462988	
S-1-c18	0.519305	0.548844	0.459846	-1604.922811	-1604.373967	-1604.462965	
S-1-c19	0.519419	0.548882	0.460786	-1604.923746	-1604.374864	-1604.46296	
S-1-c20	0.519225	0.548712	0.460073	-1604.922564	-1604.373852	-1604.462491	
S-1-c21	0.518883	0.548428	0.459378	-1604.921461	-1604.373033	-1604.462083	
S-1-c22	0.51919	0.548777	0.459478	-1604.921402	-1604.372625	-1604.461924	
S-1-c23	0.518939	0.548602	0.458927	-1604.920773	-1604.372171	-1604.461846	
S-1-c24	0.519011	0.548532	0.459591	-1604.920864	-1604.372332	-1604.461273	
S-1-c25	0.518785	0.548341	0.459268	-1604.920395	-1604.372054	-1604.461127	
S-1-c26	0.518931	0.54843	0.460982	-1604.918947	-1604.370517	-1604.457965	
S-1-c27	0.519302	0.548919	0.459776	-1604.917482	-1604.368563	-1604.457706	
S-1-c28	0.518947	0.548566	0.461194	-1604.918686	-1604.37012	-1604.457492	
S-1-c29	0.519306	0.548988	0.459472	-1604.916816	-1604.367828	-1604.457344	
S-1-c30	0.518961	0.548583	0.459166	-1604.915848	-1604.367265	-1604.456682	
S-1-c31	0.519734	0.549156	0.461429	-1604.917506	-1604.36835	-1604.456077	
S-1-c32	0.518686	0.548445	0.458073	-1604.913489	-1604.365044	-1604.455416	
S-1-c33	0.519116	0.548766	0.459371	-1604.914136	-1604.36537	-1604.454765	
S-1-c34	0.518893	0.548519	0.460974	-1604.915518	-1604.366999	-1604.454544	
S-1-c35	0.519213	0.548726	0.460104	-1604.914557	-1604.365831	-1604.454453	
S-1-c36	0.519843	0.548857	0.463112	-1604.912468	-1604.363611	-1604.451445	

CPX-C1	0.847018	0.896287	0.763128	-2565.970343	-2565.074056	-2565.207215
CPX-C2	0.848663	0.897324	0.768643	-2565.977077	-2565.079753	-2565.208434
CPX-C3	0.848109	0.896762	0.767865	-2565.973068	-2565.076306	-2565.205203
CPX-C4	0.847544	0.896242	0.764616	-2565.973427	-2565.077185	-2565.208811
S-CPX-C5	0.84836	0.897229	0.766941	-2565.977235	-2565.080006	-2565.210294
S-CPX-C6	0.847788	0.896906	0.764223	-2565.971483	-2565.074577	-2565.20726
S-CPX-C7	0.849355	0.898186	0.766877	-2565.972042	-2565.073856	-2565.205165
S-CPX-C8	0.849122	0.898033	0.766083	-2565.970888	-2565.072855	-2565.204805
S-CPX-C9	0.847386	0.896295	0.764481	-2565.967897	-2565.071602	-2565.203416
S-CPX-C10	0.847395	0.89617	0.764094	-2565.967456	-2565.071286	-2565.203362
S-CPX-C11	0.846919	0.895836	0.762301	-2565.965285	-2565.069449	-2565.202984
S-CPX-C12	0.84853	0.896992	0.768382	-2565.971376	-2565.074384	-2565.202994
S-CPX-C13	0.848095	0.896908	0.764716	-2565.966775	-2565.069867	-2565.202059
S-CPX-C14	0.846391	0.895157	0.763562	-2565.965071	-2565.069914	-2565.201509
S-CPX-C15	0.847579	0.89676	0.76313	-2565.964333	-2565.067573	-2565.201203
S-CPX-C16	0.848727	0.897208	0.767535	-2565.968366	-2565.071158	-2565.200831
S-CPX-C17	0.847169	0.896279	0.763697	-2565.964493	-2565.068214	-2565.200796
S-CPX-C18	0.848044	0.896647	0.765652	-2565.966117	-2565.06947	-2565.200465
S-CPX-C19	0.848139	0.896605	0.76657	-2565.966892	-2565.070287	-2565.200322
S-CPX-C20	0.848304	0.897208	0.764763	-2565.964951	-2565.067743	-2565.200188
S-CPX-C21	0.847642	0.896631	0.764701	-2565.964817	-2565.068186	-2565.200116
S-CPX-C22	0.847384	0.896494	0.763302	-2565.963215	-2565.066721	-2565.199913
S-CPX-C23	0.847606	0.896637	0.762883	-2565.962665	-2565.066028	-2565.199782
S-CPX-C24	0.84873	0.897161	0.766086	-2565.965543	-2565.068382	-2565.199457
S-CPX-C25	0.847704	0.896286	0.765457	-2565.963426	-2565.06714	-2565.197969
S-CPX-C26	0.848029	0.896893	0.767094	-2565.975105	-2565.078212	-2565.208011
S-CPX-C27	0.847864	0.896778	0.764171	-2565.972123	-2565.075345	-2565.207952
S-CPX-C28	0.847605	0.896677	0.76349	-2565.970664	-2565.073987	-2565.207174
S-CPX-C29	0.847934	0.896949	0.764915	-2565.971891	-2565.074942	-2565.206976
S-CPX-C30	0.848114	0.896749	0.76647	-2565.972765	-2565.076016	-2565.206295
S-CPX-C31	0.847781	0.896547	0.764825	-2565.971131	-2565.074584	-2565.206306
S-CPX-C32	0.847769	0.896583	0.765059	-2565.9693	-2565.072717	-2565.204241
S-CPX-C33	0.847647	0.896436	0.765847	-2565.969427	-2565.072991	-2565.20358
S-CPX-C34	0.847362	0.895919	0.766675	-2565.970169	-2565.07425	-2565.203494
S-CPX-C35	0.8476	0.896641	0.764172	-2565.967079	-2565.070438	-2565.202907
S-CPX-C36	0.846787	0.895479	0.764543	-2565.967257	-2565.071778	-2565.202714
S-CPX-C37	0.847593	0.896737	0.763252	-2565.965845	-2565.069108	-2565.202593
S-CPX-C38	0.848611	0.897551	0.766459	-2565.968904	-2565.071353	-2565.202445
S-CPX-C39	0.847754	0.896449	0.765947	-2565.968093	-2565.071644	-2565.202146
S-CPX-C40	0.847727	0.896753	0.764196	-2565.965808	-2565.069055	-2565.201612
S-CPX-C41	0.84822	0.89641	0.766893	-2565.967348	-2565.070938	-2565.200455
S-CPX-C42	0.848343	0.896584	0.768668	-2565.968454	-2565.07187	-2565.199786
S-CPX-C43	0.8476	0.896641	0.764172	-2565.964052	-2565.067411	-2565.19988
S-CPX-C44	0.847009	0.895598	0.765287	-2565.963238	-2565.06764	-2565.197951

S-CPX-C45	0.848581	0.897187	0.766508	-2565.964326	-2565.067139	-2565.197818	
S-CPX-C46	0.84741	0.896222	0.764655	-2565.962226	-2565.066004	-2565.197571	
S-CPX-C47	0.848292	0.896868	0.766612	-2565.964056	-2565.067188	-2565.197444	
S-CPX-C48	0.845718	0.89466	0.760561	-2565.958025	-2565.063365	-2565.197464	
S-CPX-C49	0.84673	0.895007	0.766688	-2565.963721	-2565.068714	-2565.197033	
S-CPX-C50	0.846666	0.895188	0.765648	-2565.962649	-2565.067461	-2565.197001	
S-CPX-C51	0.848268	0.896804	0.76634	-2565.962734	-2565.06593	-2565.196394	
S-CPX-C52	0.847443	0.896257	0.763675	-2565.959271	-2565.063014	-2565.195596	
S-CPX-C53	0.845714	0.894496	0.763061	-2565.958483	-2565.063987	-2565.195422	
S-CPX-C54	0.846371	0.895321	0.761544	-2565.956885	-2565.061564	-2565.195341	
S-CPX-C55	0.847117	0.896077	0.763403	-2565.958511	-2565.062434	-2565.195108	
S-CPX-C56	0.846178	0.895071	0.762892	-2565.957683	-2565.062612	-2565.194791	
S-CPX-C57	0.847599	0.896346	0.765058	-2565.959277	-2565.062931	-2565.194219	
S-CPX-C58	0.847599	0.896346	0.765058	-2565.955511	-2565.059165	-2565.190453	
S-CPX-C59	0.84848	0.896492	0.768502	-2565.96134	-2565.064848	-2565.192838	
S-CPX-C60	0.847568	0.895888	0.766546	-2565.959202	-2565.063314	-2565.192656	
S-CPX-C61	0.847461	0.896305	0.763219	-2565.955783	-2565.059478	-2565.192564	
S-CPX-C62	0.847785	0.896579	0.764073	-2565.955399	-2565.05882	-2565.191326	
S-CPX-C63	0.847798	0.896366	0.765287	-2565.956271	-2565.059905	-2565.190984	
S-CPX-C64	0.846999	0.895828	0.763836	-2565.954685	-2565.058857	-2565.190849	
S-CPX-C65	0.846744	0.895653	0.763733	-2565.948318	-2565.052665	-2565.184585	
TS-C1	0.970647	1.027852	0.877439	-2848.339489	-2847.311637	-2847.46205	422.7i
TS-C2	0.970556	1.027604	0.876377	-2848.340128	-2847.312524	-2847.463751	430.6i
TS-C3	0.97031	1.027889	0.874178	-2848.33483	-2847.306941	-2847.460652	431.2i
TS-C4	0.970556	1.027735	0.875595	-2848.334401	-2847.306666	-2847.458806	410.8i
S-TS-C5	0.971312	1.028233	0.877487	-2848.340942	-2847.312709	-2847.463455	426.5i
S-TS-C6	0.971153	1.028012	0.877514	-2848.339938	-2847.311926	-2847.462424	424.1i
S-TS-C7	0.97097	1.028059	0.876872	-2848.339035	-2847.310976	-2847.462163	432.8i
S-TS-C8	0.970258	1.026929	0.878793	-2848.340804	-2847.313875	-2847.462011	448.9i
S-TS-C9	0.970481	1.027518	0.876129	-2848.336866	-2847.309348	-2847.460737	433.2i
S-TS-C10	0.970822	1.027771	0.877668	-2848.337825	-2847.310054	-2847.460157	443.8i
S-TS-C11	0.970577	1.027462	0.877503	-2848.337586	-2847.310124	-2847.460083	432.5i
S-TS-C12	0.97006	1.027106	0.876343	-2848.336007	-2847.308901	-2847.459664	404.7i
S-TS-C13	0.970503	1.027791	0.875787	-2848.335021	-2847.30723	-2847.459234	427.9i
S-TS-C14	0.970558	1.027612	0.876745	-2848.334593	-2847.306981	-2847.457848	422.5i
S-TS-C15	0.968566	1.026065	0.873077	-2848.330731	-2847.304666	-2847.457654	410.0i
S-TS-C16	0.970481	1.027518	0.876129	-2848.336866	-2847.309348	-2847.460737	433.2i
S-TS-C17	0.970772	1.027744	0.877114	-2848.334266	-2847.306522	-2847.457152	427.2i
S-TS-C18	0.970342	1.027391	0.876788	-2848.334011	-2847.30662	-2847.457223	448.8i
S-TS-C19	0.970281	1.027661	0.874924	-2848.331537	-2847.303876	-2847.456613	411.4i
S-TS-C20	0.970276	1.027618	0.875609	-2848.331776	-2847.304158	-2847.456167	426.7i
S-TS-C21	0.970925	1.027861	0.879198	-2848.33265	-2847.304789	-2847.453452	430.5i
S-TS-C22	0.972295	1.02849	0.882571	-2848.335899	-2847.307409	-2847.453328	461.8i
S-TS-C23	0.970284	1.026572	0.877789	-2848.331038	-2847.304466	-2847.453249	425.6i

S-TS-C24	0.96935	1.026518	0.873803	-2848.326633	-2847.300115	-2847.45283	420.9i
S-TS-C25	0.969847	1.026829	0.875677	-2848.328151	-2847.301322	-2847.452474	436.1i
S-TS-C26	0.969845	1.027454	0.873889	-2848.324731	-2847.297277	-2847.450842	419.7i
S-TS-C27	0.971003	1.028118	0.875741	-2848.325916	-2847.297798	-2847.450175	424.2i
S-TS-C28	0.969557	1.026918	0.875058	-2848.315705	-2847.288787	-2847.440647	420.9i
S-TS-C29	0.971322	1.028239	0.877482	-2848.308884	-2847.280645	-2847.431402	426.6i
S-TS-C30	0.971157	1.028115	0.879273	-2848.288412	-2847.260297	-2847.409139	424.8i
S-TS-C31	0.970188	1.027667	0.874128	-2848.334445	-2847.306778	-2847.460317	429.0i
S-TS-C32	0.971374	1.028077	0.87884	-2848.33397	-2847.305893	-2847.45513	404.2i
S-TS-C33	0.970018	1.026937	0.878124	-2848.332761	-2847.305824	-2847.454637	453.2i
S-TS-C34	0.971077	1.028046	0.87721	-2848.331332	-2847.303286	-2847.454122	426.6i
S-TS-C35	0.971168	1.028025	0.8786	-2848.331697	-2847.303672	-2847.453097	413.5i
S-TS-C36	0.970091	1.027285	0.875517	-2848.327455	-2847.30017	-2847.451938	415.2i
S-TS-C37	0.969834	1.027134	0.873661	-2848.32431	-2847.297176	-2847.450649	429.8i

### Cartesian coordinates of the DFT-computed stationary points

1-c1

C	2.620419	0.815498	-1.235992
C	3.559112	-0.110970	-0.677797
C	3.085933	2.020738	-1.698427
C	3.231335	-1.404215	-0.209773
C	4.913521	0.329796	-0.593211
C	4.460640	2.340541	-1.587993
H	2.407721	2.745055	-2.142752
C	4.193607	-2.219176	0.354407
H	2.234892	-1.810909	-0.331545
C	5.876931	-0.530024	-0.011714
H	4.825734	3.296040	-1.957931
C	5.535882	-1.770316	0.459087
H	6.898414	-0.169468	0.044335
H	6.298746	-2.403755	0.895865
C	-1.479374	1.949184	0.048379
C	-0.004773	1.990477	2.046599
C	-1.124137	2.759163	1.313531
H	-1.000918	2.358748	-0.844991
H	-2.555704	1.930897	-0.121057
H	-2.002114	2.791490	1.969746
C	0.523975	0.460207	0.117640
H	0.759150	-0.522313	0.531794
C	1.062926	1.575924	1.034044
H	1.960007	1.199953	1.532571
H	1.381493	2.436195	0.437851
H	0.429712	2.617757	2.827744
C	-0.613664	0.718262	2.641638
H	0.175408	0.064185	3.024962
H	-1.277520	0.952909	3.478068
C	-1.419231	0.006883	1.543646
H	-1.267574	-1.072211	1.539126
H	-2.489576	0.200556	1.632640
N	5.341848	1.540549	-1.044572
N	-1.017239	0.517653	0.173105
O	3.773115	-3.429555	0.773909
C	4.719936	-4.336701	1.311756
H	5.179194	-3.940652	2.224975
H	4.159975	-5.239715	1.553670
H	5.499170	-4.580106	0.580567
O	0.849841	-0.688993	-1.967827
H	1.512853	-0.822082	-2.657885
C	-0.766077	4.174067	0.949174

H	0.109051	4.308330	0.312510
C	-1.445956	5.241193	1.357197
H	-2.325736	5.152977	1.990619
H	-1.145364	6.246015	1.078298
C	-1.652519	-0.346508	-0.910869
H	-1.391039	0.116144	-1.861577
H	-1.141497	-1.307213	-0.865192
C	-3.142316	-0.510963	-0.806804
C	-3.683607	-1.592992	-0.112728
C	-4.029499	0.332098	-1.484898
C	-5.052151	-1.812795	-0.046297
C	-5.403438	0.133260	-1.435249
H	-3.636987	1.150453	-2.081352
C	-5.906730	-0.937996	-0.711880
H	-6.092119	0.782968	-1.962236
F	-2.878660	-2.456358	0.517189
F	-5.530811	-2.843412	0.632485
F	-7.210556	-1.156311	-0.644307
C	1.131663	0.524922	-1.301059
H	0.664505	1.366102	-1.839954

1-c2

C	-1.860642	-0.034562	1.714741
C	-2.905275	-0.541781	0.878525
C	-1.421891	-0.815017	2.753226
C	-3.519576	0.186034	-0.167530
C	-3.346842	-1.871599	1.138832
C	-1.958290	-2.112158	2.937898
H	-0.646657	-0.462033	3.426086
C	-4.505407	-0.384156	-0.949974
H	-3.281062	1.225557	-0.368254
C	-4.350454	-2.433629	0.311909
H	-1.600913	-2.730353	3.758549
C	-4.916514	-1.721325	-0.711854
H	-4.661078	-3.450579	0.526047
H	-5.684919	-2.181164	-1.321792
C	1.844745	2.033448	0.491215
C	0.591808	3.333346	-1.220740
C	1.883732	3.309608	-0.376993
H	1.526104	2.239555	1.512583
H	2.815813	1.538386	0.509336
H	2.733775	3.249393	-1.067153
C	-0.585972	1.543522	0.091226
H	-1.143377	0.945471	-0.632825

C	-0.603841	3.027618	-0.317166
H	-1.547192	3.227656	-0.835417
H	-0.586465	3.655935	0.578911
H	0.476538	4.307708	-1.700142
C	0.688677	2.217427	-2.266579
H	-0.271217	2.090490	-2.776805
H	1.432729	2.459223	-3.030041
C	1.099091	0.916454	-1.557375
H	0.543111	0.048088	-1.910715
H	2.164899	0.709420	-1.668947
N	-2.865396	-2.638210	2.155103
N	0.853044	1.031595	-0.065317
O	-5.022902	0.400797	-1.915305
C	-6.077477	-0.101965	-2.718643
H	-6.949909	-0.368012	-2.111002
H	-6.344728	0.708475	-3.396122
H	-5.754752	-0.970587	-3.304339
O	-0.393506	1.783028	2.470072
H	-0.889833	1.910907	3.289125
C	2.073778	4.525579	0.488185
H	1.322938	4.696672	1.259926
C	3.086719	5.377242	0.360602
H	3.861751	5.239127	-0.390092
H	3.177517	6.249203	1.000304
C	1.020354	-0.317744	0.611590
H	0.942710	-0.116472	1.679168
H	0.159529	-0.915467	0.308611
C	2.299968	-1.041511	0.305925
C	2.349586	-1.956139	-0.745676
C	3.438800	-0.911269	1.107594
C	3.492870	-2.689689	-1.028003
C	4.596233	-1.633704	0.845792
H	3.414120	-0.243613	1.963697
C	4.616201	-2.517099	-0.223652
H	5.480476	-1.537405	1.464722
F	1.273774	-2.147512	-1.518543
F	3.507333	-3.542600	-2.040276
F	5.702940	-3.221391	-0.498894
C	-1.279760	1.348162	1.462094
H	-2.132322	2.043092	1.398338
1-c3			
C	2.443946	-1.703726	-0.694264
C	3.359599	-0.607214	-0.717685

C	2.945290	-2.976973	-0.589040
C	2.979639	0.751353	-0.813034
C	4.743999	-0.925390	-0.611163
C	4.344144	-3.174961	-0.500444
H	2.278585	-3.833653	-0.581624
C	3.921522	1.759835	-0.782890
H	1.943399	1.054784	-0.916854
C	5.690020	0.130049	-0.603963
H	4.741093	-4.184294	-0.418563
C	5.300638	1.441159	-0.681394
H	6.737726	-0.139920	-0.526836
H	6.049679	2.223935	-0.665535
C	-0.947052	0.664982	0.759765
C	0.286445	-0.145076	2.761864
C	-0.357631	1.100012	2.118841
H	-0.312399	0.959528	-0.078585
H	-1.930787	1.101684	0.599947
H	-1.177739	1.431294	2.767170
C	0.301579	-1.491541	0.631040
H	0.111539	-2.542358	0.870813
C	1.170350	-0.836796	1.726059
H	1.782826	-1.616317	2.186015
H	1.863027	-0.114876	1.291158
H	0.879044	0.149758	3.630494
C	-0.828704	-1.111125	3.168049
H	-0.401463	-2.066417	3.487913
H	-1.407068	-0.715689	4.007388
C	-1.760124	-1.311930	1.962702
H	-2.025693	-2.360329	1.810037
H	-2.682689	-0.736962	2.054754
N	5.215291	-2.197443	-0.506155
N	-1.097095	-0.837634	0.686644
O	3.440738	3.019265	-0.845527
C	4.355495	4.102238	-0.872481
H	5.021257	4.039884	-1.740595
H	3.745362	5.001654	-0.951590
H	4.949453	4.146751	0.047799
O	0.314497	-2.548541	-1.484114
H	0.785042	-2.676112	-2.318939
C	0.585184	2.259227	1.933502
H	1.450223	2.096244	1.289903
C	0.410937	3.449281	2.499787
H	-0.440823	3.662591	3.141790
H	1.118467	4.257058	2.343148



C	-1.950281	-1.246044	-0.508826
H	-1.434548	-0.882155	-1.394639
H	-1.919654	-2.335310	-0.538357
C	-3.366159	-0.744472	-0.486655
C	-3.686900	0.449618	-1.131840
C	-4.416356	-1.488285	0.061415
C	-4.990387	0.920827	-1.202485
C	-5.729144	-1.038992	0.004580
H	-4.206163	-2.444923	0.529732
C	-6.007670	0.165426	-0.626355
H	-6.546162	-1.612298	0.426525
F	-2.719463	1.180718	-1.698537
F	-5.255772	2.065142	-1.812869
F	-7.248966	0.619902	-0.697731
C	0.940298	-1.497698	-0.775331
H	0.744932	-0.538373	-1.275036

1-c4

C	-1.842736	-0.514088	1.527895
C	-3.002968	-0.813145	0.745685
C	-1.309511	-1.508737	2.306666
C	-3.708126	0.134949	-0.032099
C	-3.471895	-2.158377	0.778634
C	-1.872212	-2.807814	2.276271
H	-0.444033	-1.321463	2.934577
C	-4.818071	-0.231470	-0.768791
H	-3.441874	1.186955	-0.045491
C	-4.605913	-2.506944	0.004296
H	-1.438156	-3.595769	2.887843
C	-5.265942	-1.577992	-0.756115
H	-4.940164	-3.538114	0.045248
H	-6.134861	-1.877026	-1.330275
C	1.767036	1.776115	0.397594
C	0.370730	3.418970	-0.845854
C	1.737955	3.214327	-0.161699
H	1.566906	1.738906	1.467062
H	2.725096	1.298058	0.201802
H	2.515322	3.315970	-0.928615
C	-0.704012	1.379947	0.155354
H	-1.347649	0.953734	-0.617608
C	-0.735412	2.917291	0.083525
H	-1.721377	3.222898	-0.281311
H	-0.616768	3.335472	1.087764
H	0.226454	4.474922	-1.083878

C	0.345694	2.564667	-2.118001
H	-0.659183	2.556422	-2.551597
H	1.022819	2.970057	-2.874531
C	0.790945	1.136869	-1.756752
H	0.169885	0.373726	-2.231408
H	1.830858	0.947299	-2.026443
N	-2.897358	-3.135883	1.531935
N	0.700788	0.919389	-0.260756
O	-5.416248	0.752682	-1.468875
C	-6.616371	0.466284	-2.167619
H	-7.395908	0.106757	-1.486487
H	-6.932401	1.410037	-2.611095
H	-6.450977	-0.269360	-2.963322
O	-0.252940	1.088562	2.490295
H	-0.649514	1.020509	3.368711
C	2.031693	4.207342	0.929766
H	1.359333	4.202346	1.787821
C	3.048332	5.063388	0.898925
H	3.749914	5.091501	0.068229
H	3.218214	5.771204	1.703830
C	0.901384	-0.548174	0.071990
H	0.876710	-0.602100	1.158265
H	0.026117	-1.067403	-0.323723
C	2.162625	-1.167028	-0.458397
C	3.301642	-1.210558	0.345206
C	2.219335	-1.805791	-1.701371
C	4.472782	-1.826830	-0.073758
C	3.378896	-2.428830	-2.143348
H	1.334931	-1.829726	-2.330830
C	4.500745	-2.433208	-1.326103
H	3.427841	-2.926112	-3.104828
F	3.285307	-0.642885	1.555815
F	5.538713	-1.839853	0.711399
F	5.620672	-3.019700	-1.719255
C	-1.253422	0.888157	1.517759
H	-2.089493	1.581826	1.701072

1-e5

C	2.446716	0.767721	-1.283000
C	3.562235	0.025882	-0.777345
C	2.678889	1.998563	-1.843199
C	3.476891	-1.269867	-0.218654
C	4.835601	0.664996	-0.846621
C	3.993407	2.523804	-1.882631

H	1.861192	2.586914	-2.252147
C	4.598267	-1.898602	0.286150
H	2.546560	-1.824200	-0.224749
C	5.966669	-0.006629	-0.321746
H	4.172089	3.499368	-2.329012
C	5.860555	-1.252388	0.238405
H	6.923031	0.501191	-0.384046
H	6.746130	-1.738552	0.630183
C	-1.594297	1.457384	0.370248
C	0.035102	1.680019	2.232824
C	-1.214059	2.319648	1.591985
H	-1.243158	1.893234	-0.567669
H	-2.672370	1.332563	0.294967
H	-2.030903	2.278021	2.322361
C	0.551171	0.178436	0.281542
H	0.922031	-0.765246	0.687317
C	1.048416	1.361262	1.133794
H	2.020614	1.090048	1.553473
H	1.219438	2.239104	0.504225
H	0.467483	2.360779	2.969109
C	-0.388587	0.363610	2.889824
H	0.492961	-0.200673	3.209322
H	-0.998332	0.545723	3.778808
C	-1.209293	-0.443180	1.871280
H	-0.940927	-1.501805	1.863506
H	-2.282429	-0.364889	2.051107
N	5.031841	1.896664	-1.392771
N	-0.978859	0.079828	0.468576
O	4.405502	-3.130793	0.799886
C	5.523807	-3.860027	1.274648
H	6.000181	-3.355913	2.123721
H	5.130272	-4.821497	1.603776
H	6.261551	-4.023669	0.480708
O	0.861126	-1.020444	-1.766300
H	1.433292	-1.080420	-2.542604
C	-1.030971	3.756660	1.186245
H	-0.252658	3.962383	0.450679
C	-1.753432	4.762093	1.670432
H	-2.542325	4.601333	2.401742
H	-1.580154	5.786712	1.357895
C	-1.605178	-0.872697	-0.543019
H	-1.424470	-0.440654	-1.524919
H	-1.027774	-1.795418	-0.481409
C	-3.071085	-1.138163	-0.348706

C	-4.010330	-0.374720	-1.041416
C	-3.543696	-2.207028	0.419992
C	-5.372624	-0.624323	-0.951508
C	-4.901549	-2.477387	0.527564
H	-2.835992	-2.850005	0.934141
C	-5.808491	-1.681419	-0.158018
H	-5.272363	-3.305006	1.120662
F	-3.604285	0.639756	-1.814407
F	-6.235814	0.128950	-1.614650
F	-7.109084	-1.914161	-0.075670
C	1.019310	0.259987	-1.187957
H	0.385112	0.992325	-1.714610

1-c6

C	2.380594	-1.813527	-0.458366
C	3.441630	-0.862243	-0.562566
C	2.689557	-3.110921	-0.134292
C	3.264637	0.504261	-0.880210
C	4.758280	-1.339574	-0.302006
C	4.038661	-3.474405	0.093799
H	1.909710	-3.862390	-0.060089
C	4.336505	1.372646	-0.920613
H	2.289545	0.923043	-1.105061
C	5.842223	-0.428649	-0.369453
H	4.282699	-4.503407	0.347996
C	5.647939	0.894811	-0.664145
H	6.834443	-0.819842	-0.171993
H	6.497769	1.566104	-0.699506
C	-0.744871	1.153394	0.363355
C	0.242114	0.512232	2.551679
C	-0.199788	1.716415	1.694133
H	-0.010008	1.234438	-0.441612
H	-1.649199	1.675740	0.052181
H	-1.015249	2.228725	2.218764
C	0.209410	-1.131603	0.640179
H	-0.133228	-2.101112	1.014803
C	1.090231	-0.423872	1.692675
H	1.572858	-1.191026	2.303154
H	1.891811	0.139078	1.212072
H	0.815038	0.860043	3.413882
C	-1.008387	-0.247056	2.998481
H	-0.726729	-1.191583	3.473656
H	-1.579464	0.328310	3.732096
C	-1.887762	-0.503245	1.765830

H	-2.296561	-1.512874	1.737047
H	-2.717852	0.202722	1.706305
N	5.037955	-2.631713	0.019162
N	-1.090331	-0.310943	0.490402
O	4.044595	2.659752	-1.204336
C	5.104766	3.595537	-1.308957
H	5.812236	3.310221	-2.095446
H	4.636356	4.543362	-1.572804
H	5.634544	3.706406	-0.355789
O	0.210714	-2.483346	-1.303100
H	0.718053	-2.800663	-2.062310
C	0.887649	2.723029	1.427958
H	1.779613	2.363303	0.913728
C	0.807730	4.004053	1.774601
H	-0.064881	4.409755	2.281675
H	1.616357	4.697128	1.565975
C	-1.911836	-0.774306	-0.708128
H	-1.324222	-0.533120	-1.593259
H	-1.964417	-1.859431	-0.634250
C	-3.280597	-0.164391	-0.820105
C	-4.382653	-0.811170	-0.260623
C	-3.520235	0.994337	-1.566648
C	-5.670980	-0.312256	-0.390517
C	-4.800165	1.514459	-1.711600
H	-2.690574	1.491074	-2.061302
C	-5.868706	0.858193	-1.118157
H	-4.988719	2.411920	-2.288777
F	-4.215868	-1.945662	0.428324
F	-6.691617	-0.946480	0.164440
F	-7.100949	1.326681	-1.236874
C	0.928553	-1.429835	-0.693946
H	0.903149	-0.537329	-1.335752

1-c7

C	-1.399271	1.371308	-0.311669
C	-2.810048	1.361856	-0.081790
C	-0.701644	2.524173	-0.041958
C	-3.654234	0.255067	-0.325092
C	-3.383923	2.561372	0.436567
C	-1.377316	3.658237	0.464442
H	0.369395	2.582929	-0.213613
C	-5.006957	0.319522	-0.061236
H	-3.276769	-0.675908	-0.728323
C	-4.777171	2.598312	0.693124

H	-0.821298	4.568226	0.678743
C	-5.576839	1.511695	0.456514
H	-5.188015	3.522022	1.086076
H	-6.638581	1.575436	0.663171
C	0.431141	-2.678070	-0.723493
C	-0.430403	-2.411871	1.606880
C	-0.650088	-3.155565	0.275205
H	0.013454	-2.337790	-1.672548
H	1.161032	-3.461712	-0.937718
H	-0.464177	-4.219147	0.473005
C	0.267388	-0.383890	0.248282
H	0.937762	0.413705	0.574825
C	-0.609963	-0.903398	1.418713
H	-0.351465	-0.377343	2.341683
H	-1.659447	-0.678818	1.216196
H	-1.144050	-2.778127	2.349678
C	0.999790	-2.670938	2.070196
H	1.157868	-2.270038	3.074740
H	1.205345	-3.744684	2.111956
C	1.950966	-1.978090	1.086583
H	2.405795	-1.082763	1.512760
H	2.752412	-2.635418	0.751350
N	-2.664852	3.684158	0.702360
N	1.218935	-1.518593	-0.162125
O	-5.713222	-0.800603	-0.324940
C	-7.111361	-0.799306	-0.091410
H	-7.618608	-0.046529	-0.705573
H	-7.460534	-1.790980	-0.378298
H	-7.338599	-0.628107	0.967188
O	0.116171	0.526871	-2.002160
H	-0.449954	1.044551	-2.590340
C	-2.074640	-3.051216	-0.224794
H	-2.824789	-2.935858	0.557412
C	-2.488479	-3.153741	-1.485684
H	-1.812844	-3.303016	-2.325345
H	-3.546370	-3.104385	-1.723924
C	2.267434	-1.118026	-1.205458
H	2.795804	-2.044949	-1.436594
H	1.712817	-0.789478	-2.079644
C	3.238581	-0.059053	-0.764308
C	4.466577	-0.419875	-0.208421
C	2.998092	1.303294	-0.975620
C	5.409189	0.525936	0.169393
C	3.926620	2.268313	-0.606540

H	2.071076	1.594597	-1.456541
C	5.125912	1.873783	-0.031237
H	3.747077	3.324090	-0.772831
F	4.771023	-1.710852	-0.024665
F	6.559293	0.145512	0.704452
F	6.030453	2.769965	0.332025
C	-0.650043	0.164904	-0.864829
H	-1.359300	-0.619627	-1.142802

1-c8

C	-2.525348	0.685293	-0.659592
C	-2.065437	1.965293	-0.209287
C	-3.880505	0.478581	-0.745665
C	-0.710329	2.354127	-0.133776
C	-3.066251	2.906925	0.175229
C	-4.785526	1.494288	-0.353126
H	-4.277864	-0.465235	-1.110773
C	-0.347118	3.604336	0.323014
H	0.083006	1.700653	-0.462930
C	-2.663625	4.179118	0.651389
H	-5.856717	1.319100	-0.420764
C	-1.341303	4.529102	0.731770
H	-3.445052	4.872090	0.943735
H	-1.070467	5.512873	1.096418
C	-0.678728	-3.325913	-0.571014
C	-1.524423	-2.767138	1.711954
C	-1.773267	-3.658916	0.479672
H	-1.094619	-3.098767	-1.554220
H	0.016765	-4.159382	-0.691897
H	-1.613735	-4.697254	0.789773
C	-0.733541	-0.926711	0.135025
H	-0.027190	-0.139625	0.397962
C	-1.635839	-1.284322	1.347790
H	-1.352293	-0.668710	2.206176
H	-2.671592	-1.027754	1.122089
H	-2.251804	-3.012409	2.489196
C	-0.102274	-3.029218	2.200755
H	0.077442	-2.524079	3.153421
H	0.059727	-4.098619	2.364614
C	0.874618	-2.493586	1.145684
H	1.370205	-1.577637	1.469957
H	1.644332	-3.219356	0.887378
N	-4.402508	2.658308	0.104555
N	0.162278	-2.143875	-0.150650

O	0.978499	3.865868	0.338083
C	1.421602	5.137265	0.782844
H	1.142559	5.314995	1.827605
H	2.508258	5.116611	0.701028
H	1.026890	5.940949	0.150933
O	-0.751593	-0.076814	-2.138933
H	-1.274875	0.441220	-2.765093
C	-3.172067	-3.571573	-0.071667
H	-3.574550	-2.579359	-0.268331
C	-3.937574	-4.633022	-0.308212
H	-3.590628	-5.645704	-0.115505
H	-4.944107	-4.529949	-0.700932
C	1.225619	-1.922255	-1.236263
H	1.666608	-2.908454	-1.393314
H	0.686580	-1.620464	-2.130574
C	2.295346	-0.922816	-0.894720
C	3.482460	-1.335534	-0.286913
C	2.178678	0.429705	-1.227882
C	4.490667	-0.439102	0.037218
C	3.167817	1.349320	-0.904414
H	1.293267	0.753589	-1.760205
C	4.317176	0.908678	-0.267257
H	3.054194	2.401776	-1.134482
F	3.678441	-2.628083	0.006849
F	5.597297	-0.864691	0.628473
F	5.280313	1.757879	0.060992
C	-1.592428	-0.448212	-1.061288
H	-2.232851	-1.282773	-1.376224

1-c9

C	2.570053	0.747129	-0.880671
C	1.842791	1.853906	-0.342092
C	3.830740	0.502360	-0.375705
C	0.639961	2.383541	-0.894122
C	2.383587	2.466552	0.825673
C	4.298941	1.225975	0.740035
H	4.466049	-0.254379	-0.822969
C	-0.037648	3.396250	-0.250774
H	0.295859	2.045098	-1.863612
C	1.647265	3.502359	1.470381
H	5.285479	1.016137	1.147042
C	0.464474	3.944603	0.962225
H	2.076005	3.931919	2.369125
H	-0.103399	4.736474	1.438148



C	0.447956	-1.311113	0.780025
C	1.816900	-3.330393	0.253946
C	1.254960	-2.469234	1.405596
H	0.986104	-0.362924	0.818446
H	-0.508960	-1.176037	1.281031
H	0.574792	-3.098899	1.991613
C	1.452108	-1.559578	-1.498769
H	1.167229	-2.039789	-2.440086
C	2.498088	-2.428682	-0.774228
H	3.036277	-3.015167	-1.521388
H	3.231855	-1.800620	-0.271562
H	2.529774	-4.056103	0.651516
C	0.649942	-4.039965	-0.434589
H	1.000239	-4.551708	-1.335838
H	0.205131	-4.795103	0.219083
C	-0.412044	-2.988233	-0.789489
H	-0.787377	-3.100057	-1.809292
H	-1.263768	-3.018077	-0.108770
N	3.584568	2.135019	1.361132
N	0.155362	-1.586429	-0.678904
O	-1.183051	3.953343	-0.682897
C	-1.767865	3.465280	-1.870602
H	-2.012794	2.397518	-1.781016
H	-2.686902	4.033325	-2.010349
H	-1.109966	3.620516	-2.734414
O	3.003830	-0.597094	-2.863518
H	3.478252	0.179499	-3.188394
C	2.303210	-1.925467	2.339490
H	3.000856	-1.198642	1.922252
C	2.405002	-2.272784	3.618608
H	1.718908	-2.981578	4.077073
H	3.179557	-1.860887	4.257326
C	-0.846759	-0.590662	-1.230308
H	-0.433784	0.391499	-1.013189
H	-0.858074	-0.747150	-2.312552
C	-2.243544	-0.675136	-0.682600
C	-2.610943	0.115928	0.406888
C	-3.242178	-1.439579	-1.296171
C	-3.908939	0.128056	0.899563
C	-4.546377	-1.445534	-0.820676
H	-2.998289	-2.032975	-2.172102
C	-4.871506	-0.662018	0.278153
H	-5.322617	-2.035490	-1.293616
F	-1.703352	0.889274	1.010161

F	-4.219910	0.885293	1.939194
F	-6.106120	-0.644303	0.753852
C	2.007761	-0.167293	-1.958962
H	1.216631	0.353485	-2.511601
1-c10			
C	2.126818	-0.641918	-1.578441
C	2.755063	0.408365	-0.841269
C	2.904677	-1.435217	-2.384850
C	2.077492	1.281537	0.040307
C	4.163874	0.548891	-0.998140
C	4.297549	-1.196631	-2.471081
H	2.463405	-2.243872	-2.959882
C	2.761145	2.244451	0.755169
H	1.003990	1.233946	0.187576
C	4.835684	1.562018	-0.269165
H	4.912862	-1.823860	-3.112080
C	4.163468	2.389003	0.591550
H	5.906958	1.653333	-0.412101
H	4.709685	3.146977	1.140274
C	-1.190368	-0.983712	1.251418
C	0.551931	-2.609109	1.965049
C	-0.399914	-1.507022	2.470146
H	-0.794819	-0.034991	0.883353
H	-2.239213	-0.840876	1.500242
H	-1.104361	-1.962509	3.176522
C	0.304896	-2.011041	-0.467561
H	0.328858	-2.943418	-1.039525
C	1.280075	-2.095227	0.725530
H	2.101041	-2.758975	0.442967
H	1.725045	-1.120855	0.933833
H	1.267419	-2.872427	2.746637
C	-0.287709	-3.824708	1.563257
H	0.336012	-4.563406	1.050776
H	-0.718776	-4.314273	2.440654
C	-1.422917	-3.344642	0.647348
H	-1.574964	-4.001116	-0.212313
H	-2.371855	-3.251092	1.181296
N	4.911207	-0.248163	-1.809081
N	-1.129757	-1.959524	0.097109
O	2.017517	2.997939	1.591555
C	2.644370	4.043919	2.315445
H	3.098860	4.777920	1.640607
H	1.849854	4.524012	2.886149

H	3.402077	3.655104	3.005607
O	0.113979	-1.340220	-2.730110
H	0.534403	-0.828807	-3.435336
C	0.289025	-0.366576	3.171735
H	0.973966	0.238420	2.576525
C	0.096559	-0.066358	4.452458
H	-0.585059	-0.635665	5.080419
H	0.617585	0.761048	4.923230
C	-2.213779	-1.675211	-0.961579
H	-1.804317	-2.017512	-1.910463
H	-3.049555	-2.317948	-0.683784
C	-2.712230	-0.258823	-1.071847
C	-3.756579	0.161316	-0.246849
C	-2.266428	0.635379	-2.049324
C	-4.306636	1.430615	-0.335756
C	-2.804146	1.911540	-2.163959
H	-1.504046	0.309287	-2.746354
C	-3.817677	2.304571	-1.303085
H	-2.461576	2.606349	-2.921724
F	-4.250727	-0.673696	0.680786
F	-5.283025	1.796119	0.480413
F	-4.346710	3.515501	-1.384810
C	0.633462	-0.897944	-1.485075
H	0.132342	0.031150	-1.186930

S-1-c11

C	-1.698862	-0.986596	1.012109
C	-3.062528	-0.887892	0.587843
C	-1.441440	-1.245293	2.334973
C	-3.471655	-0.656418	-0.745317
C	-4.056221	-1.018126	1.602399
C	-2.511697	-1.379676	3.252492
H	-0.420099	-1.341077	2.695104
C	-4.809757	-0.525602	-1.062986
H	-2.755379	-0.621190	-1.557325
C	-5.420092	-0.883912	1.244210
H	-2.304067	-1.584056	4.300314
C	-5.797065	-0.637656	-0.049561
H	-6.157038	-0.983562	2.033766
H	-6.849301	-0.538037	-0.288060
C	1.758415	1.561630	0.231818
C	-0.242298	3.037973	0.255893
C	1.203848	2.898348	0.770989
H	1.724470	0.769915	0.983310

H	2.788486	1.675787	-0.097254
H	1.798077	3.719364	0.352421
C	-0.453222	0.648207	-0.493088
H	-1.038850	0.663640	-1.414739
C	-0.973648	1.716601	0.485989
H	-2.049899	1.821135	0.326132
H	-0.845470	1.382437	1.519233
H	-0.749126	3.854927	0.773942
C	-0.186291	3.300499	-1.251897
H	-1.188103	3.238521	-1.687658
H	0.199762	4.301570	-1.462099
C	0.747164	2.258732	-1.886596
H	0.351691	1.857099	-2.822221
H	1.745535	2.660289	-2.077509
N	-3.769145	-1.259830	2.910833
N	0.953665	1.077548	-0.954211
O	-5.090092	-0.297725	-2.361386
C	-6.445194	-0.205805	-2.767666
H	-6.949770	0.641172	-2.288456
H	-6.418877	-0.045439	-3.845142
H	-6.989488	-1.132469	-2.553031
O	-0.593001	-1.672162	-1.049813
H	-1.102055	-2.455053	-0.800309
C	1.335874	2.951338	2.268645
H	0.775908	2.207265	2.836119
C	2.085798	3.837700	2.916283
H	2.664099	4.593198	2.389248
H	2.148151	3.844098	3.999712
C	1.699102	0.003072	-1.770678
H	0.929679	-0.631342	-2.207693
H	2.197666	0.554372	-2.568391
C	2.726268	-0.821782	-1.042995
C	4.033540	-0.342821	-0.947475
C	2.474511	-2.109378	-0.560448
C	5.050010	-1.074051	-0.353149
C	3.476982	-2.865697	0.035215
H	1.481328	-2.526888	-0.681342
C	4.757289	-2.342860	0.139657
H	3.288414	-3.865873	0.407555
F	4.333657	0.873779	-1.429827
F	6.273471	-0.575080	-0.266979
F	5.730768	-3.040211	0.704728
C	-0.533386	-0.790513	0.063244
H	0.383632	-0.991233	0.636910

## S-1-c12

C	2.398017	1.125183	-0.816501
C	1.429810	2.090410	-0.385598
C	3.618429	1.120958	-0.179921
C	0.226081	2.389540	-1.065791
C	1.724960	2.805915	0.813682
C	3.828592	1.929609	0.961398
H	4.426002	0.492559	-0.539154
C	-0.695978	3.270835	-0.537070
H	0.005979	1.987357	-2.049112
C	0.755586	3.698030	1.337870
H	4.788936	1.901352	1.471486
C	-0.434017	3.919436	0.697643
H	0.999631	4.211067	2.261859
H	-1.152814	4.608824	1.124208
C	0.710206	-1.323095	0.749256
C	2.416129	-3.068378	0.228452
C	1.686077	-2.341304	1.377948
H	1.077748	-0.298593	0.818572
H	-0.267531	-1.364871	1.225854
H	1.106866	-3.089988	1.931590
C	1.797542	-1.350877	-1.505558
H	1.624229	-1.856536	-2.460772
C	2.958960	-2.041817	-0.763972
H	3.609735	-2.510771	-1.504367
H	3.561634	-1.307291	-0.231958
H	3.231727	-3.670564	0.634462
C	1.404248	-3.951677	-0.503710
H	1.858296	-4.378714	-1.402886
H	1.078965	-4.784787	0.125204
C	0.187602	-3.088977	-0.870963
H	-0.135665	-3.240577	-1.903328
H	-0.664386	-3.277980	-0.216665
N	2.905683	2.701001	1.479895
N	0.504087	-1.613662	-0.721819
O	-1.816493	3.457638	-1.260696
C	-2.776252	4.399876	-0.810425
H	-2.340349	5.401293	-0.723443
H	-3.556686	4.411392	-1.570504
H	-3.209666	4.098497	0.150338
O	3.253336	-0.099626	-2.738340
H	3.572627	0.753879	-3.059467
C	2.602968	-1.650083	2.351309
H	3.167662	-0.799841	1.968812

C	2.741070	-2.009922	3.623505
H	2.184458	-2.841698	4.049530
H	3.418399	-1.484401	4.288799
C	-0.641694	-0.796339	-1.286259
H	-0.396371	0.243047	-1.083634
H	-0.625708	-0.965026	-2.366474
C	-2.005681	-1.093348	-0.730518
C	-2.487984	-0.340606	0.340503
C	-2.875233	-2.019000	-1.317216
C	-3.771704	-0.512149	0.839080
C	-4.162467	-2.212042	-0.833522
H	-2.545490	-2.590346	-2.179630
C	-4.602750	-1.456172	0.244168
H	-4.839773	-2.927233	-1.285242
F	-1.707127	0.573926	0.923672
F	-4.193753	0.218914	1.859885
F	-5.825999	-1.614030	0.725288
C	2.118860	0.124077	-1.927491
H	1.292055	0.486697	-2.549722

S-1-c13

C	2.651398	0.422487	-0.912060
C	2.118990	1.657948	-0.414816
C	3.856101	-0.000359	-0.398826
C	1.028176	2.356730	-0.985641
C	2.760778	2.223848	0.727102
C	4.442182	0.679098	0.695204
H	4.362374	-0.861867	-0.819747
C	0.531925	3.510085	-0.408947
H	0.586732	2.059813	-1.931207
C	2.214593	3.394031	1.313077
H	5.380477	0.319198	1.111661
C	1.119771	4.019866	0.778464
H	2.711129	3.787961	2.193355
H	0.734642	4.918333	1.245985
C	0.450801	-1.322018	0.889815
C	1.371558	-3.544594	0.234542
C	1.071119	-2.625704	1.438290
H	1.169803	-0.501469	0.877757
H	-0.415347	-1.014004	1.475441
H	0.331289	-3.132582	2.069179
C	1.181121	-1.699596	-1.469233
H	0.732932	-2.102624	-2.382591
C	2.113800	-2.756123	-0.844096

H	2.470608	-3.414130	-1.638592
H	2.991482	-2.281390	-0.408311
H	1.973204	-4.395085	0.562494
C	0.040641	-4.015958	-0.353100
H	0.211653	-4.554274	-1.290093
H	-0.473472	-4.699978	0.327359
C	-0.842842	-2.783540	-0.595575
H	-1.335098	-2.800337	-1.567759
H	-1.609540	-2.672886	0.173260
N	3.894936	1.715587	1.279853
N	-0.019746	-1.509093	-0.534876
O	-0.507337	4.087145	-1.041233
C	-1.010000	5.321804	-0.556650
H	-0.230829	6.091702	-0.543590
H	-1.793919	5.614395	-1.254255
H	-1.440375	5.211042	0.445627
O	2.842569	-1.004887	-2.873729
H	3.371565	-0.303829	-3.276386
C	2.272395	-2.312101	2.288939
H	3.065111	-1.730837	1.817778
C	2.405274	-2.694968	3.555036
H	1.632877	-3.264533	4.067128
H	3.295079	-2.454291	4.127852
C	-0.868035	-0.336014	-0.986840
H	-0.247962	0.546030	-0.856350
H	-1.054358	-0.492033	-2.052236
C	-2.149715	-0.118472	-0.236503
C	-3.342555	-0.694699	-0.669705
C	-2.204787	0.759239	0.852077
C	-4.547928	-0.453043	-0.025834
C	-3.398634	1.015805	1.513649
H	-1.297194	1.262821	1.173067
C	-4.563117	0.404486	1.071218
H	-3.448054	1.692964	2.358217
F	-3.348018	-1.503789	-1.735046
F	-5.661948	-1.024312	-0.455492
F	-5.717816	0.630147	1.678413
C	1.937711	-0.417806	-1.963008
H	1.222719	0.207347	-2.510532
S-1-c14			
C	0.874055	2.086210	0.558080
C	-0.463397	2.349087	0.117923
C	1.729773	3.149498	0.711081

C	-1.471151	1.368051	-0.028944
C	-0.783366	3.710476	-0.167421
C	1.301660	4.461532	0.399194
H	2.744182	2.999002	1.072486
C	-2.740031	1.712578	-0.449950
H	-1.287167	0.333262	0.227895
C	-2.091420	4.029207	-0.607139
H	1.989235	5.296381	0.513990
C	-3.051963	3.063674	-0.748756
H	-2.305777	5.071081	-0.819083
H	-4.044973	3.342145	-1.081036
C	3.194229	-1.692335	0.527563
C	3.765609	-0.445320	-1.561265
C	4.327755	-0.928601	-0.210421
H	3.012616	-1.299589	1.529184
H	3.425112	-2.755858	0.624290
H	5.114739	-1.657385	-0.432341
C	1.497894	-0.139618	-0.429589
H	0.515410	-0.182246	-0.902321
C	2.558615	0.482958	-1.376254
H	2.107127	0.695119	-2.349608
H	2.874787	1.447500	-0.974865
H	4.550709	0.072741	-2.116950
C	3.292801	-1.683375	-2.318065
H	3.035805	-1.437082	-3.351765
H	4.079417	-2.442723	-2.349283
C	2.047654	-2.219644	-1.602261
H	1.142346	-1.959258	-2.147550
H	2.077364	-3.303015	-1.474009
N	0.098368	4.738280	-0.033178
N	1.877938	-1.614588	-0.216807
O	-3.633154	0.703845	-0.547210
C	-4.988369	1.010156	-0.835052
H	-5.097537	1.437155	-1.838554
H	-5.516382	0.059909	-0.786403
H	-5.405539	1.698683	-0.091755
O	0.586134	-0.009787	1.785587
H	0.242924	0.602106	2.449198
C	4.959336	0.155787	0.622965
H	4.391392	1.071698	0.776554
C	6.173694	0.056786	1.156021
H	6.788948	-0.829951	1.021079
H	6.602294	0.861584	1.744587
C	0.877845	-2.477998	0.568944



H	1.255910	-3.496558	0.443913
H	0.988923	-2.192394	1.610531
C	-0.579836	-2.401163	0.194256
C	-1.502827	-2.096887	1.201174
C	-1.101666	-2.736122	-1.062155
C	-2.867294	-2.029522	0.951144
C	-2.462153	-2.675815	-1.332158
H	-0.448933	-3.084529	-1.851923
C	-3.336986	-2.310374	-0.323758
H	-2.857709	-2.925757	-2.309372
F	-1.109964	-1.889139	2.456821
F	-3.704629	-1.708501	1.925290
F	-4.643139	-2.245233	-0.550674
C	1.387917	0.690047	0.867707
H	2.396107	0.809897	1.285889

S-1-c15

C	-0.783597	-1.191312	0.156152
C	-2.161440	-1.530601	-0.004468
C	0.168164	-2.129565	-0.164534
C	-3.242097	-0.676871	0.317119
C	-2.441622	-2.827413	-0.530039
C	-0.227924	-3.391747	-0.662763
H	1.225554	-1.912005	-0.035534
C	-4.547188	-1.075989	0.113246
H	-3.090001	0.306301	0.747704
C	-3.792545	-3.206315	-0.730511
H	0.525560	-4.133781	-0.917018
C	-4.824804	-2.360077	-0.424381
H	-3.978184	-4.195031	-1.136017
H	-5.846354	-2.681562	-0.589389
C	0.266805	3.098159	0.714464
C	-1.033505	2.937420	-1.415993
C	-1.077373	3.456596	0.034657
H	0.133374	2.574587	1.661384
H	0.883468	3.981470	0.897059
H	-1.126309	4.551500	-0.032578
C	0.260554	0.943355	-0.530198
H	0.965626	0.294429	-1.052159
C	-0.884715	1.411726	-1.462941
H	-0.690693	1.093053	-2.491297
H	-1.816072	0.927754	-1.161099
H	-1.943861	3.239412	-1.940136
C	0.196007	3.551215	-2.079573

H	0.193979	3.367693	-3.157181
H	0.217699	4.635113	-1.932152
C	1.431763	2.891956	-1.457787
H	1.840187	2.128735	-2.118046
H	2.217785	3.614256	-1.232646
N	-1.478841	-3.731881	-0.852285
N	1.095472	2.178279	-0.156933
O	-5.499450	-0.181713	0.453523
C	-6.861670	-0.537392	0.292575
H	-7.120834	-1.413778	0.897835
H	-7.434505	0.321755	0.640984
H	-7.102376	-0.729839	-0.759467
O	0.658459	0.053952	1.664763
H	0.404064	-0.643292	2.282789
C	-2.324599	3.029243	0.776724
H	-3.214416	2.967477	0.150139
C	-2.454956	2.805478	2.081883
H	-1.629269	2.871760	2.787065
H	-3.421775	2.553710	2.505608
C	2.410002	1.892291	0.587701
H	2.979936	2.821024	0.501396
H	2.142770	1.744053	1.629155
C	3.221765	0.709116	0.125989
C	3.532833	-0.280434	1.063550
C	3.764484	0.562080	-1.157108
C	4.264858	-1.411437	0.721023
C	4.498233	-0.559981	-1.520344
H	3.640898	1.343666	-1.896593
C	4.733197	-1.551326	-0.579815
H	4.910548	-0.670750	-2.516308
F	3.173399	-0.160117	2.339221
F	4.525773	-2.332011	1.637236
F	5.428199	-2.634150	-0.893590
C	-0.327503	0.167100	0.665280
H	-1.180387	0.724456	1.059486

S-1-c16

C	1.337506	0.804990	-1.571222
C	2.532257	1.001214	-0.797431
C	0.496403	1.885739	-1.713680
C	3.616041	0.094313	-0.723883
C	2.624075	2.227579	-0.068083
C	0.713408	3.077256	-0.984460
H	-0.361790	1.842444	-2.379236

C	4.699506	0.341001	0.097151
H	3.635557	-0.800033	-1.333023
C	3.735054	2.439134	0.785300
H	0.015709	3.905613	-1.082762
C	4.746810	1.521656	0.883465
H	3.762900	3.369142	1.342762
H	5.587318	1.719571	1.538229
C	-0.574301	-0.560411	0.775293
C	0.689340	-2.706086	0.956119
C	0.215251	-1.468368	1.746197
H	-0.004985	0.318571	0.474053
H	-1.508699	-0.224236	1.222147
H	-0.463649	-1.811306	2.536150
C	0.336132	-1.634776	-1.298117
H	-0.000895	-2.400442	-2.004731
C	1.369494	-2.247868	-0.331763
H	1.862640	-3.080061	-0.838773
H	2.142084	-1.522493	-0.091840
H	1.386065	-3.286144	1.565120
C	-0.531507	-3.547868	0.583852
H	-0.237291	-4.357316	-0.090816
H	-0.982906	-4.005734	1.468133
C	-1.560174	-2.630252	-0.091823
H	-1.979879	-3.070530	-0.999236
H	-2.383670	-2.374899	0.576252
N	1.708460	3.231098	-0.149936
N	-0.931731	-1.308992	-0.493438
O	5.670154	-0.592875	0.088741
C	6.847815	-0.369236	0.844592
H	6.632117	-0.321090	1.918461
H	7.491922	-1.225300	0.645900
H	7.356951	0.548151	0.527764
O	1.945466	-1.205330	-2.879397
H	2.380068	-0.599993	-3.494650
C	1.332417	-0.693399	2.393783
H	2.086815	-0.272699	1.728680
C	1.434663	-0.498871	3.704719
H	0.700538	-0.891103	4.405078
H	2.261102	0.062794	4.128099
C	-1.924896	-0.532467	-1.339499
H	-1.441274	0.409782	-1.573272
H	-2.048084	-1.108232	-2.260617
C	-3.256940	-0.258007	-0.702012
C	-3.452316	0.951391	-0.034587

C	-4.354093	-1.115209	-0.832927
C	-4.677015	1.293813	0.521165
C	-5.589450	-0.795735	-0.285024
H	-4.245292	-2.045589	-1.381646
C	-5.742233	0.407198	0.390498
H	-6.443296	-1.455846	-0.382350
F	-2.438209	1.815291	0.086523
F	-4.824819	2.444924	1.156736
F	-6.907557	0.739471	0.922349
C	0.910669	-0.509029	-2.220009
H	0.129631	-0.255510	-2.951157

S-1-c17

C	0.027620	1.326058	-1.359911
C	-1.250864	0.692274	-1.435192
C	0.071621	2.680892	-1.145465
C	-1.443158	-0.684141	-1.684433
C	-2.391618	1.515987	-1.207126
C	-1.129955	3.405256	-0.961100
H	1.021228	3.205315	-1.106640
C	-2.706569	-1.243002	-1.662727
H	-0.618177	-1.354790	-1.898984
C	-3.676469	0.918968	-1.206986
H	-1.089219	4.479194	-0.790823
C	-3.840411	-0.424594	-1.416858
H	-4.528307	1.565712	-1.025738
H	-4.835783	-0.851452	-1.397627
C	3.503914	0.656122	0.769540
C	3.951748	-1.659469	-0.072558
C	4.619467	-0.349521	0.402193
H	3.395497	1.434211	0.016263
H	3.685146	1.120751	1.741203
H	5.196624	-0.584076	1.304620
C	1.735392	-0.522160	-0.538728
H	0.871571	-1.152956	-0.345506
C	2.897489	-1.356613	-1.133823
H	2.485566	-2.288368	-1.533404
H	3.345950	-0.811778	-1.967149
H	4.713546	-2.328838	-0.478314
C	3.240877	-2.303956	1.117451
H	2.626789	-3.144818	0.780916
H	3.957258	-2.692199	1.846791
C	2.368631	-1.238839	1.788135
H	1.396503	-1.621856	2.077133

H	2.853564	-0.816863	2.671685
N	-2.317455	2.854319	-0.973681
N	2.155088	-0.044528	0.863815
O	-2.772569	-2.567939	-1.884829
C	-4.028415	-3.218713	-1.783692
H	-4.729298	-2.856538	-2.544283
H	-3.827478	-4.275471	-1.956509
H	-4.460600	-3.088487	-0.785169
O	2.412138	1.379072	-1.848006
H	2.237621	1.872943	-2.660112
C	5.557025	0.252269	-0.610229
H	5.100157	0.636022	-1.521722
C	6.873169	0.333423	-0.441058
H	7.358689	-0.027381	0.463049
H	7.517743	0.760856	-1.202422
C	1.202562	0.909873	1.529895
H	1.619460	1.057418	2.531354
H	1.307024	1.853888	0.993219
C	-0.287392	0.624479	1.667315
C	-1.000851	-0.561466	1.529590
C	-1.034170	1.755749	2.030648
C	-2.378995	-0.620825	1.702354
C	-2.404866	1.719963	2.225135
H	-0.522679	2.706799	2.143873
C	-3.079741	0.523050	2.046572
H	-2.962448	2.613406	2.478450
F	-0.421444	-1.729125	1.182236
F	-3.008576	-1.774369	1.511372
F	-4.396833	0.449985	2.182515
C	1.307180	0.538484	-1.586239
H	1.126432	-0.103951	-2.463726

S-1-c18

C	1.516589	1.055528	-1.445792
C	2.766141	1.025160	-0.739052
C	0.830205	2.250013	-1.458623
C	3.716425	-0.020572	-0.809183
C	3.066051	2.161449	0.075913
C	1.253337	3.338338	-0.661731
H	-0.057974	2.375327	-2.073131
C	4.865511	0.006554	-0.042673
H	3.580938	-0.849996	-1.491066
C	4.238199	2.146746	0.872123
H	0.685724	4.266466	-0.665052

C	5.116267	1.096816	0.831643
H	4.425863	3.012826	1.497504
H	6.010360	1.122856	1.443417
C	-0.397895	-0.261967	0.930468
C	0.556309	-2.564351	0.836248
C	0.310976	-1.354943	1.762952
H	0.281600	0.545811	0.656324
H	-1.243912	0.162986	1.470495
H	-0.360769	-1.676389	2.567723
C	0.210244	-1.249469	-1.287346
H	-0.278425	-1.894209	-2.025171
C	1.208094	-2.083690	-0.458414
H	1.542630	-2.924552	-1.069713
H	2.091485	-1.497164	-0.220775
H	1.204304	-3.285977	1.338416
C	-0.792133	-3.195114	0.490054
H	-0.660065	-3.970873	-0.270232
H	-1.245279	-3.669410	1.364759
C	-1.724900	-2.090417	-0.025696
H	-2.266718	-2.379184	-0.926534
H	-2.452626	-1.787809	0.728627
N	2.298901	3.284216	0.123178
N	-0.942045	-0.832067	-0.362034
O	5.697016	-1.042150	-0.188690
C	6.924174	-1.053502	0.520604
H	6.759334	-1.070709	1.604324
H	7.429122	-1.970984	0.220214
H	7.547525	-0.192594	0.253144
O	1.762864	-0.896403	-2.943210
H	2.220572	-0.304783	-3.555019
C	1.561977	-0.797464	2.389205
H	2.327684	-0.426689	1.707453
C	1.766156	-0.731440	3.701096
H	1.026820	-1.082324	4.417651
H	2.685068	-0.322768	4.109066
C	-1.860943	0.161801	-1.051972
H	-1.283626	1.076468	-1.152337
H	-2.056093	-0.250030	-2.044610
C	-3.147199	0.469745	-0.340278
C	-4.308328	-0.239225	-0.646213
C	-3.250178	1.529185	0.567668
C	-5.525731	0.055709	-0.049449
C	-4.456745	1.842417	1.180414
H	-2.372536	2.130242	0.787945

C	-5.587310	1.100806	0.868880
H	-4.541812	2.660417	1.885995
F	-4.268134	-1.235763	-1.538023
F	-6.606894	-0.642955	-0.355715
F	-6.752239	1.375096	1.433442
C	0.874588	-0.132126	-2.157986
H	0.089902	0.283112	-2.806710

S-1-c19

C	-1.900337	-0.390763	1.614999
C	-2.644088	0.621428	0.929040
C	-2.606266	-1.377273	2.264569
C	-2.083736	1.779739	0.341527
C	-4.055483	0.433820	0.839250
C	-4.013776	-1.442148	2.143667
H	-2.088716	-2.128152	2.853321
C	-2.863757	2.686144	-0.349148
H	-1.037495	2.034951	0.460677
C	-4.829734	1.370671	0.109424
H	-4.560748	-2.240640	2.639637
C	-4.259783	2.466017	-0.481181
H	-5.897717	1.192055	0.046662
H	-4.881347	3.164853	-1.028116
C	-0.534877	-0.716666	-1.569676
C	-0.338645	-3.142030	-0.990175
C	-1.167891	-2.114410	-1.786949
H	-1.217896	-0.025883	-1.074513
H	-0.229207	-0.264067	-2.515629
H	-1.066624	-2.368085	-2.848210
C	0.377948	-1.360323	0.668831
H	1.357077	-1.463794	1.140652
C	-0.263692	-2.756083	0.488802
H	0.328131	-3.492297	1.038505
H	-1.262812	-2.770367	0.920285
H	-0.796788	-4.128698	-1.091001
C	1.079926	-3.152448	-1.555546
H	1.691034	-3.892936	-1.032502
H	1.072542	-3.424297	-2.614739
C	1.688863	-1.753468	-1.377473
H	2.577046	-1.769447	-0.745591
H	1.958637	-1.289185	-2.327276
N	-4.715645	-0.599255	1.427306
N	0.709935	-0.798244	-0.714139
O	-2.218736	3.751572	-0.861883

C	-2.971783	4.767844	-1.505192
H	-3.712880	5.202770	-0.825449
H	-2.250185	5.532576	-1.790307
H	-3.469132	4.386569	-2.404272
O	0.100521	-0.893239	2.896440
H	-0.414939	-0.486237	3.605878
C	-2.635449	-2.113527	-1.452350
H	-2.904853	-1.921737	-0.416236
C	-3.597267	-2.326105	-2.344953
H	-3.379529	-2.517936	-3.393397
H	-4.643455	-2.316763	-2.055976
C	1.358185	0.578698	-0.675021
H	1.455475	0.876488	-1.719744
H	0.643922	1.256553	-0.216147
C	2.702502	0.643674	-0.004701
C	3.845379	0.651858	-0.806774
C	2.880886	0.757079	1.378697
C	5.121228	0.757416	-0.272436
C	4.149140	0.858112	1.936514
H	2.026400	0.751408	2.046415
C	5.261961	0.861328	1.108219
H	4.291774	0.943589	3.007159
F	3.728565	0.545449	-2.135657
F	6.180199	0.757753	-1.066534
F	6.481209	0.959001	1.613469
C	-0.381202	-0.405725	1.657590
H	-0.021298	0.617553	1.512470

S-1-c20

C	0.839278	-0.774834	1.869599
C	1.820521	-1.338207	0.996887
C	1.001574	-0.923208	3.223176
C	1.770798	-1.262366	-0.414644
C	2.928000	-1.989718	1.609773
C	2.134495	-1.611932	3.721389
H	0.267685	-0.520110	3.913892
C	2.784781	-1.782085	-1.193374
H	0.931250	-0.816724	-0.937222
C	3.946953	-2.527321	0.784194
H	2.262447	-1.732645	4.794666
C	3.891554	-2.424899	-0.581047
H	4.779820	-3.019086	1.275269
H	4.692323	-2.840715	-1.181037
C	-0.173921	2.182367	-1.147068



C	1.484593	3.253597	0.353821
C	1.118365	3.025228	-1.126398
H	0.045639	1.130184	-1.328343
H	-0.863925	2.531711	-1.917498
H	0.916804	4.000887	-1.584697
C	-0.091167	1.509208	1.255804
H	-0.488450	1.903280	2.195797
C	1.386030	1.920291	1.092726
H	1.827681	1.985946	2.090123
H	1.946027	1.153346	0.554950
H	2.494445	3.661672	0.430164
C	0.460232	4.218485	0.955969
H	0.584409	4.276159	2.041456
H	0.589183	5.229176	0.559193
C	-0.943993	3.714795	0.595219
H	-1.644953	3.787368	1.428918
H	-1.365301	4.257753	-0.254338
N	3.068839	-2.119543	2.957151
N	-0.905578	2.251507	0.173499
O	2.644582	-1.627828	-2.528147
C	3.626810	-2.181516	-3.387415
H	3.707654	-3.266261	-3.255263
H	3.288201	-1.967178	-4.400859
H	4.606288	-1.715944	-3.226851
O	-1.483362	-0.123782	2.163277
H	-1.695986	-1.059300	2.282798
C	2.190264	2.342030	-1.933854
H	2.451275	1.323523	-1.644010
C	2.809835	2.909319	-2.964275
H	2.573672	3.918622	-3.294140
H	3.584962	2.385644	-3.514500
C	-2.369427	1.839099	0.031634
H	-2.786459	1.900692	1.036314
H	-2.811542	2.637184	-0.572327
C	-2.729842	0.496732	-0.560621
C	-3.598357	-0.310760	0.179472
C	-2.375054	0.045951	-1.838891
C	-4.026414	-1.549038	-0.283392
C	-2.788254	-1.190805	-2.317749
H	-1.773098	0.660720	-2.494738
C	-3.605510	-1.989144	-1.532300
H	-2.500845	-1.539777	-3.302567
F	-4.072535	0.093213	1.357021
F	-4.833407	-2.290208	0.461619

F	-4.015341	-3.172450	-1.962975
C	-0.354260	-0.010930	1.325276
H	-0.587557	-0.394014	0.324806
S-1-c21			
C	-2.048709	-0.364032	-0.993527
C	-3.327217	-0.698799	-0.434291
C	-1.493793	-1.255428	-1.876855
C	-4.102113	0.177303	0.364543
C	-3.847852	-1.992218	-0.725542
C	-2.122609	-2.499838	-2.129687
H	-0.565024	-1.051830	-2.400389
C	-5.314458	-0.224288	0.895809
H	-3.825399	1.214880	0.530415
C	-5.080632	-2.383845	-0.147965
H	-1.660977	-3.202398	-2.820072
C	-5.798715	-1.535429	0.651816
H	-5.442875	-3.380702	-0.375126
H	-6.740388	-1.865612	1.073549
C	1.549345	1.919273	0.585151
C	1.433828	3.372502	-1.419615
C	1.990891	3.282689	0.014880
H	0.658471	1.996748	1.207142
H	2.350850	1.459034	1.161595
H	3.085582	3.311750	-0.043969
C	-0.098038	1.387081	-1.238150
H	-0.034914	0.915507	-2.220560
C	-0.027558	2.917046	-1.411833
H	-0.527648	3.173984	-2.350411
H	-0.583513	3.407269	-0.605955
H	1.521813	4.393440	-1.797069
C	2.233922	2.397417	-2.291435
H	1.769315	2.295824	-3.277413
H	3.252038	2.762233	-2.450944
C	2.293004	1.036533	-1.576194
H	2.162887	0.195475	-2.257566
H	3.234026	0.896608	-1.041444
N	-3.234604	-2.877948	-1.556641
N	1.199565	0.948147	-0.529924
O	-5.972996	0.695417	1.623391
C	-7.243534	0.369806	2.163292
H	-7.170987	-0.449256	2.887877
H	-7.585760	1.270386	2.671951
H	-7.956576	0.106670	1.374051

O	-1.277763	1.097603	0.814386
H	-2.071149	0.754461	1.250177
C	1.548353	4.397229	0.922949
H	0.475396	4.500497	1.085475
C	2.384976	5.237855	1.523932
H	3.462342	5.163701	1.394061
H	2.024600	6.034255	2.167048
C	1.096228	-0.468533	0.024170
H	0.316889	-0.421493	0.782698
H	0.743787	-1.089569	-0.795985
C	2.365955	-1.034950	0.591896
C	3.227126	-1.773875	-0.218613
C	2.675367	-0.943640	1.953128
C	4.378163	-2.366862	0.280445
C	3.821022	-1.528055	2.477849
H	1.998512	-0.415258	2.617724
C	4.667588	-2.234521	1.635921
H	4.063368	-1.458884	3.531725
F	2.952434	-1.929868	-1.520226
F	5.178820	-3.051734	-0.521251
F	5.767306	-2.804112	2.104086
C	-1.435348	0.972284	-0.591199
H	-2.141531	1.741926	-0.943558

S-1-c22

C	-1.637584	-0.233071	1.378193
C	-2.910248	-0.610891	0.834186
C	-1.628960	0.621326	2.456378
C	-3.099870	-1.547387	-0.209973
C	-4.059835	0.018534	1.405065
C	-2.831119	1.183186	2.942205
H	-0.696138	0.880569	2.953218
C	-4.363486	-1.836740	-0.685808
H	-2.259869	-2.059079	-0.662250
C	-5.342007	-0.294820	0.888591
H	-2.806639	1.878940	3.777679
C	-5.501677	-1.196161	-0.128700
H	-6.194923	0.201498	1.338601
H	-6.496593	-1.415490	-0.497656
C	0.355887	2.361775	0.184144
C	-0.456429	1.691246	-2.081752
C	-0.591630	2.756723	-0.974804
H	-0.199745	2.103997	1.085368
H	1.050931	3.167824	0.428556

H	-0.244096	3.708747	-1.391912
C	0.302845	-0.067186	-0.416405
H	1.001631	-0.818089	-0.791621
C	-0.725880	0.299053	-1.512879
H	-0.678416	-0.451895	-2.305717
H	-1.736256	0.263034	-1.112371
H	-1.171988	1.908032	-2.878152
C	0.971750	1.729606	-2.619906
H	1.099416	0.975302	-3.401304
H	1.193709	2.702695	-3.066415
C	1.942269	1.454183	-1.460824
H	2.579725	0.591534	-1.654641
H	2.586163	2.307667	-1.240830
N	-4.004112	0.913090	2.428275
N	1.197890	1.156181	-0.170005
O	-4.426509	-2.739366	-1.682887
C	-5.692508	-3.099441	-2.209049
H	-6.195754	-2.237605	-2.662549
H	-5.490166	-3.843781	-2.978553
H	-6.335004	-3.541396	-1.438947
O	-0.274940	-2.105036	0.530909
H	-0.834755	-2.585353	1.156245
C	-1.999762	2.953701	-0.477689
H	-2.480434	2.099627	-0.002527
C	-2.664932	4.099703	-0.585133
H	-2.222169	4.981218	-1.043639
H	-3.680787	4.198418	-0.216139
C	2.233702	0.959941	0.929711
H	2.728176	1.927130	1.026807
H	1.693643	0.781787	1.857931
C	3.262670	-0.104920	0.667983
C	4.524057	0.291445	0.218259
C	3.055598	-1.469344	0.901293
C	5.547356	-0.618246	-0.004022
C	4.064416	-2.398393	0.679329
H	2.091858	-1.832340	1.241119
C	5.305102	-1.968115	0.232300
H	3.906800	-3.456138	0.853473
F	4.770697	1.584493	-0.022871
F	6.728338	-0.203623	-0.434542
F	6.283617	-2.832501	0.015936
C	-0.293390	-0.730746	0.867661
H	0.404946	-0.571635	1.697322

## S-1-c23

C	-1.157832	-0.485537	1.264951
C	-2.502240	-0.782422	0.874237
C	-0.887669	-0.312444	2.599060
C	-2.914777	-1.013273	-0.457535
C	-3.475053	-0.824051	1.916169
C	-1.931593	-0.399822	3.552103
H	0.123575	-0.101417	2.938778
C	-4.242445	-1.250168	-0.755762
H	-2.196006	-1.068454	-1.265636
C	-4.827638	-1.073246	1.578621
H	-1.713359	-0.261333	4.608649
C	-5.212815	-1.276049	0.279485
H	-5.549279	-1.098691	2.387906
H	-6.256295	-1.464697	0.056566
C	1.714591	2.437938	-0.231306
C	-0.541573	3.401137	-0.596802
C	0.880398	3.730336	-0.099278
H	1.779631	1.906260	0.719705
H	2.726857	2.657069	-0.575707
H	1.306749	4.497781	-0.756393
C	-0.214374	0.907373	-0.648075
H	-0.749230	0.556016	-1.533026
C	-0.979559	2.069388	0.011257
H	-2.046941	1.891879	-0.143291
H	-0.820729	2.065829	1.093289
H	-1.232766	4.199437	-0.319436
C	-0.479985	3.232210	-2.117512
H	-1.421232	2.820772	-2.494310
H	-0.320521	4.192270	-2.615843
C	0.692131	2.296894	-2.447844
H	0.450087	1.584020	-3.238173
H	1.584718	2.851468	-2.747763
N	-3.178617	-0.632327	3.231516
N	1.097981	1.481910	-1.225749
O	-4.529597	-1.453098	-2.057905
C	-5.859269	-1.774905	-2.426395
H	-6.550805	-0.957983	-2.188899
H	-5.837942	-1.925262	-3.505523
H	-6.196498	-2.697197	-1.939608
O	0.091792	-1.418129	-0.614445
H	0.033223	-2.239808	-0.109201
C	0.940231	4.243343	1.313673
H	0.529539	3.593118	2.086735

C	1.455106	5.420779	1.654310
H	1.875332	6.099139	0.915165
H	1.468576	5.755803	2.686467
C	2.113385	0.464727	-1.745388
H	1.551537	-0.186624	-2.414100
H	2.800886	1.065628	-2.348319
C	2.899134	-0.393548	-0.782226
C	2.888935	-1.772995	-1.009433
C	3.746419	0.078256	0.228298
C	3.609682	-2.654560	-0.213749
C	4.474765	-0.786632	1.035469
H	3.867264	1.139963	0.398028
C	4.394771	-2.153302	0.817022
H	5.123873	-0.415927	1.819984
F	2.206025	-2.294485	-2.026270
F	3.552230	-3.957060	-0.451244
F	5.077441	-3.002580	1.570089
C	-0.029631	-0.321982	0.264015
H	0.896818	-0.193857	0.845027

S-1-c24

C	-2.099603	0.018285	-1.172201
C	-3.326613	-0.410990	-0.563955
C	-1.717992	-0.608674	-2.331472
C	-3.936280	0.230643	0.541864
C	-3.971433	-1.547644	-1.131428
C	-2.462183	-1.703598	-2.834765
H	-0.842651	-0.300441	-2.893856
C	-5.103493	-0.261354	1.098101
H	-3.563312	1.164781	0.952740
C	-5.153989	-2.040829	-0.527377
H	-2.136542	-2.198663	-3.747074
C	-5.708155	-1.429427	0.565244
H	-5.612556	-2.917107	-0.972665
H	-6.615499	-1.830392	1.000783
C	1.820181	1.572138	0.505603
C	1.631539	3.526529	-1.011774
C	2.311428	3.015717	0.273494
H	1.015597	1.511297	1.235659
H	2.639143	0.932618	0.828845
H	3.394667	3.003799	0.102485
C	-0.046285	1.661749	-1.181942
H	-0.127930	1.475284	-2.254291
C	0.143279	3.174174	-0.954806

H	-0.419891	3.705571	-1.727946
H	-0.286692	3.460284	0.010227
H	1.772849	4.604598	-1.112536
C	2.257857	2.783123	-2.197816
H	1.699305	2.987984	-3.116738
H	3.286256	3.113949	-2.365157
C	2.258183	1.275976	-1.885372
H	1.974075	0.671308	-2.750426
H	3.229796	0.927355	-1.531669
N	-3.526349	-2.184420	-2.248409
N	1.272028	0.968428	-0.778983
O	-5.602066	0.434613	2.134911
C	-6.816267	0.009327	2.732823
H	-6.711707	-0.985238	3.181156
H	-7.028400	0.737012	3.515336
H	-7.637003	0.007417	2.006943
O	-1.024830	0.894392	0.848379
H	-1.777904	0.459101	1.272563
C	2.045287	3.858701	1.490606
H	1.003895	3.964820	1.794424
C	2.997311	4.458879	2.198357
H	4.049466	4.369159	1.937535
H	2.760374	5.063273	3.068016
C	1.101437	-0.538917	-0.631587
H	0.347350	-0.667765	0.142094
H	0.695689	-0.891032	-1.578637
C	2.352436	-1.300494	-0.299006
C	2.645505	-1.600062	1.031573
C	3.195787	-1.824589	-1.284047
C	3.751366	-2.360690	1.385706
C	4.309104	-2.586992	-0.955323
H	2.971115	-1.645438	-2.331131
C	4.580232	-2.849505	0.380099
H	4.965227	-2.995411	-1.714922
F	1.856997	-1.140095	2.006971
F	4.006083	-2.617216	2.659310
F	5.632658	-3.574552	0.726213
C	-1.341525	1.162411	-0.507694
H	-2.013637	2.035212	-0.556191
S-1-c25			
C	-1.720612	-0.168389	1.597753
C	-2.415058	0.829374	0.841881
C	-2.472928	-1.008937	2.385302

C	-1.790913	1.881521	0.131332
C	-3.838535	0.748406	0.817922
C	-3.885837	-0.965572	2.326528
H	-1.989858	-1.726919	3.039835
C	-2.525379	2.776727	-0.620748
H	-0.727682	2.072498	0.213717
C	-4.566255	1.666168	0.019441
H	-4.471738	-1.651195	2.934386
C	-3.937321	2.651332	-0.693783
H	-5.646391	1.567394	0.007890
H	-4.524760	3.340752	-1.288421
C	-0.710396	-1.031979	-1.566821
C	-0.513596	-3.358131	-0.660804
C	-1.387881	-2.424415	-1.523412
H	-1.317152	-0.257577	-1.097529
H	-0.509517	-0.722646	-2.594752
H	-1.387669	-2.833110	-2.540535
C	0.431136	-1.386128	0.631004
H	1.453439	-1.457912	1.009810
C	-0.270160	-2.762067	0.725176
H	0.347639	-3.436217	1.323139
H	-1.219814	-2.658947	1.247221
H	-1.008690	-4.327275	-0.565255
C	0.837954	-3.514530	-1.350983
H	1.484938	-4.177239	-0.769931
H	0.720883	-3.958709	-2.343440
C	1.486019	-2.126652	-1.470032
H	2.452701	-2.079861	-0.970651
H	1.627406	-1.828101	-2.511674
N	-4.552234	-0.156450	1.540550
N	0.623965	-1.040416	-0.849423
O	-1.822069	3.740568	-1.248097
C	-2.522528	4.764038	-1.936375
H	-3.206275	5.297953	-1.267172
H	-1.759447	5.454182	-2.295153
H	-3.077597	4.362575	-2.792024
O	0.284527	-0.777067	2.815472
H	-0.034613	-0.189660	3.513187
C	-2.819572	-2.322588	-1.071546
H	-2.994449	-1.919228	-0.077249
C	-3.857922	-2.689850	-1.816034
H	-3.735089	-3.094256	-2.818531
H	-4.873482	-2.599093	-1.444049
C	1.308743	0.303253	-1.098100



H	1.204774	0.472147	-2.171858
H	0.710232	1.058675	-0.597261
C	2.766202	0.397027	-0.732378
C	3.192483	0.850729	0.514956
C	3.757771	0.121298	-1.684063
C	4.539003	0.978879	0.832124
C	5.108695	0.242976	-1.393955
H	3.464474	-0.188710	-2.682440
C	5.493361	0.667104	-0.129556
H	5.871031	0.028241	-2.133370
F	2.310080	1.197839	1.455915
F	4.898011	1.405337	2.032343
F	6.772605	0.793740	0.182687
C	-0.206264	-0.305507	1.575355
H	0.237381	0.665516	1.355600

S-1-c26

C	-1.127358	1.361139	1.305899
C	-0.040359	2.072694	0.702409
C	-2.319990	2.029555	1.463705
C	1.287622	1.592855	0.628834
C	-0.331466	3.354378	0.147226
C	-2.484956	3.322250	0.912764
H	-3.140022	1.580251	2.012916
C	2.271299	2.301338	-0.028281
H	1.591165	0.665065	1.098193
C	0.698440	4.058429	-0.528159
H	-3.438263	3.834862	1.021097
C	1.965862	3.549189	-0.632108
H	0.446380	5.024061	-0.953020
H	2.730243	4.113182	-1.153624
C	-2.359029	-0.430026	-1.264724
C	-3.860993	-1.940133	-0.002866
C	-3.793720	-0.987825	-1.215477
H	-2.286222	0.554799	-0.800740
H	-1.988726	-0.354145	-2.288430
H	-3.985558	-1.572006	-2.123443
C	-1.679881	-1.208132	1.004564
H	-1.268555	-2.123356	1.430399
C	-3.208191	-1.252733	1.198413
H	-3.411275	-1.789413	2.126443
H	-3.616884	-0.249706	1.322014
H	-4.900654	-2.191875	0.216274
C	-3.054886	-3.199827	-0.342479

H	-2.924896	-3.819778	0.549897
H	-3.571502	-3.809527	-1.088573
C	-1.694867	-2.763711	-0.906749
H	-0.868879	-3.387196	-0.564210
H	-1.685378	-2.764719	-1.999622
N	-1.549566	3.950461	0.243172
N	-1.393635	-1.332022	-0.501317
O	3.492109	1.731710	-0.042349
C	4.540184	2.358563	-0.763828
H	4.781204	3.339831	-0.340899
H	5.399743	1.698037	-0.662884
H	4.284470	2.459907	-1.824546
O	-1.510347	-0.261381	3.080689
H	-1.107448	0.380120	3.680111
C	-4.787291	0.141844	-1.172755
H	-4.677989	0.860618	-0.360279
C	-5.763435	0.300563	-2.061158
H	-5.899399	-0.387710	-2.892333
H	-6.468246	1.122498	-1.989025
C	-0.018237	-0.955545	-0.974049
H	-0.023813	-1.163975	-2.047851
H	0.055400	0.128807	-0.869426
C	1.219032	-1.581866	-0.369079
C	2.400772	-1.099498	-0.938303
C	1.343577	-2.504171	0.670397
C	3.653654	-1.474044	-0.484218
C	2.593852	-2.907114	1.134544
H	0.474026	-2.932069	1.151908
C	3.741698	-2.387117	0.562027
H	2.687487	-3.624317	1.941387
F	2.325108	-0.223185	-1.944245
F	4.743540	-0.969629	-1.042268
F	4.941723	-2.746111	0.994864
C	-0.963547	-0.069785	1.791963
H	0.101859	-0.321250	1.802318

S-1-c27

C	-0.902668	-1.330772	0.372229
C	-2.323335	-1.298460	0.166575
C	-0.450077	-1.802720	1.585142
C	-2.963782	-1.037286	-1.068365
C	-3.139350	-1.568789	1.309559
C	-1.354052	-2.092728	2.632272
H	0.610547	-1.956757	1.758132

C	-4.340023	-0.964753	-1.158591
H	-2.390102	-0.914841	-1.977639
C	-4.547449	-1.462469	1.189902
H	-0.977234	-2.443536	3.590629
C	-5.143434	-1.157556	-0.004285
H	-5.136326	-1.651445	2.080985
H	-6.223450	-1.091518	-0.063384
C	-0.200040	1.727089	1.379233
C	-0.902817	2.820105	-0.749579
C	-1.221847	2.704451	0.754211
H	-0.655600	0.770860	1.633429
H	0.247276	2.142581	2.284505
H	-1.078669	3.693716	1.205007
C	0.419881	0.651795	-0.795967
H	1.254823	0.690909	-1.501623
C	-0.789753	1.428460	-1.367103
H	-0.676729	1.492868	-2.451531
H	-1.708838	0.878695	-1.182429
H	-1.692432	3.386849	-1.248173
C	0.442597	3.522196	-0.900559
H	0.731915	3.560285	-1.954679
H	0.393572	4.552244	-0.536700
C	1.490168	2.741431	-0.092364
H	2.361158	2.500452	-0.698747
H	1.820375	3.289601	0.794132
N	-2.648788	-1.938714	2.523109
N	0.943227	1.422440	0.423759
O	-4.838862	-0.708580	-2.383489
C	-6.244066	-0.682800	-2.562966
H	-6.706730	0.127578	-1.987275
H	-6.402110	-0.502555	-3.625838
H	-6.700059	-1.640507	-2.287200
O	-0.111311	-1.241200	-1.970691
H	-0.251960	-2.196633	-2.003715
C	-2.629532	2.258106	1.049317
H	-2.937961	1.299816	0.633421
C	-3.489107	2.961549	1.779606
H	-3.223961	3.920178	2.220009
H	-4.495813	2.600701	1.964355
C	2.035341	0.726198	1.235777
H	2.267978	1.434132	2.035214
H	1.562506	-0.139684	1.693829
C	3.311143	0.342704	0.528825
C	3.626742	-0.997958	0.304638

C	4.307251	1.281734	0.220760
C	4.818834	-1.393417	-0.288341
C	5.507995	0.914353	-0.369292
H	4.157440	2.326257	0.470480
C	5.754427	-0.425287	-0.633169
H	6.269618	1.647078	-0.608315
F	2.791583	-1.975859	0.683655
F	5.060966	-2.677643	-0.493959
F	6.888944	-0.809228	-1.193566
C	0.153208	-0.875531	-0.630883
H	1.090099	-1.338476	-0.316179

S-1-c28

C	0.086396	0.567316	-1.218061
C	-1.345405	0.664288	-1.201891
C	0.793535	1.739698	-1.122495
C	-2.212223	-0.430986	-1.421944
C	-1.912614	1.940274	-0.919978
C	0.124425	2.964346	-0.888045
H	1.871068	1.768372	-1.201140
C	-3.582304	-0.288091	-1.316804
H	-1.843661	-1.420248	-1.671798
C	-3.319450	2.052801	-0.795843
H	0.703394	3.880569	-0.791459
C	-4.140931	0.972596	-0.979017
H	-3.724221	3.030372	-0.557615
H	-5.212343	1.092415	-0.873655
C	3.018258	0.216936	0.923382
C	4.519673	-0.571156	-0.904083
C	4.395630	0.438782	0.255054
H	2.284182	0.959280	0.620463
H	3.105442	0.242404	2.011963
H	5.176495	0.206883	0.989231
C	2.095778	-1.210683	-0.934974
H	2.111604	-2.287589	-1.130203
C	3.239649	-0.567319	-1.743248
H	3.368481	-1.155524	-2.653683
H	2.981273	0.439266	-2.073409
H	5.386080	-0.324204	-1.521582
C	4.672460	-1.965906	-0.288460
H	4.598916	-2.735039	-1.062904
H	5.647630	-2.080469	0.192427
C	3.570500	-2.150188	0.765798
H	3.116550	-3.142200	0.727924

H	3.942887	-1.982048	1.779232
N	-1.172527	3.069237	-0.752705
N	2.448875	-1.135858	0.560313
O	-4.311193	-1.393974	-1.543824
C	-5.712665	-1.348962	-1.334172
H	-6.198065	-0.647476	-2.022104
H	-6.073004	-2.357005	-1.536535
H	-5.946304	-1.080494	-0.297643
O	0.701294	-1.226895	-2.738980
H	-0.089152	-0.889758	-3.180564
C	4.571240	1.876513	-0.152642
H	3.985719	2.226211	-1.002579
C	5.399197	2.721819	0.453922
H	6.013368	2.416660	1.298344
H	5.502312	3.750326	0.123392
C	1.346228	-1.555656	1.523742
H	1.030277	-2.545736	1.192054
H	1.861454	-1.677764	2.481034
C	0.127875	-0.688232	1.718277
C	-1.118977	-1.273864	1.496947
C	0.137974	0.603356	2.260488
C	-2.309046	-0.614827	1.771274
C	-1.037962	1.297986	2.501090
H	1.073778	1.088219	2.508377
C	-2.258559	0.685011	2.254344
H	-1.028091	2.307029	2.895291
F	-1.199553	-2.508668	0.984937
F	-3.470044	-1.216076	1.551890
F	-3.396184	1.321584	2.490124
C	0.666179	-0.828982	-1.377743
H	0.001571	-1.501941	-0.825749

S-1-c29

C	-0.766044	-0.945069	-0.454679
C	-2.142321	-1.201883	-0.134509
C	0.193867	-1.596442	0.286457
C	-3.253770	-0.681511	-0.841106
C	-2.389626	-2.052407	0.988604
C	-0.168196	-2.414848	1.379559
H	1.247584	-1.486682	0.048216
C	-4.546520	-0.971654	-0.452562
H	-3.118339	-0.043232	-1.704506
C	-3.728514	-2.327468	1.363067
H	0.604755	-2.901622	1.970359

C	-4.787070	-1.807654	0.669115
H	-3.881219	-2.974584	2.220024
H	-5.798239	-2.042015	0.979994
C	1.041253	1.712124	0.855085
C	-1.026215	3.090433	0.495440
C	-0.130355	2.433861	1.565963
H	0.963944	0.630362	0.953496
H	2.002609	2.026643	1.253640
H	0.285684	3.236184	2.186412
C	-0.226424	1.498387	-1.297569
H	-0.176042	1.940266	-2.297244
C	-1.450716	2.048872	-0.532922
H	-2.149295	2.479133	-1.255285
H	-1.979157	1.240633	-0.032476
H	-1.907128	3.521313	0.976320
C	-0.227927	4.171389	-0.228633
H	-0.822540	4.594876	-1.042805
H	0.032942	4.989773	0.447941
C	1.056626	3.537009	-0.776761
H	1.209976	3.743280	-1.838384
H	1.936835	3.882330	-0.230317
N	-1.409169	-2.628376	1.735049
N	1.057255	2.017907	-0.624139
O	-5.524546	-0.416048	-1.194170
C	-6.875725	-0.704129	-0.878745
H	-7.134999	-0.355407	0.127746
H	-7.471686	-0.160516	-1.611221
H	-7.085232	-1.776499	-0.965419
O	-1.080085	-0.076794	-2.747195
H	-1.353281	-0.991069	-2.900635
C	-0.866567	1.480082	2.470592
H	-1.279046	0.582877	2.009054
C	-1.025930	1.675871	3.775714
H	-0.619896	2.550618	4.278988
H	-1.570928	0.966900	4.390512
C	2.357055	1.581379	-1.319735
H	2.142605	1.646108	-2.389140
H	3.072600	2.368943	-1.076078
C	2.990224	0.251164	-1.006685
C	3.741486	0.064909	0.153738
C	2.993238	-0.791722	-1.942036
C	4.368979	-1.140783	0.439628
C	3.629318	-1.999417	-1.691747
H	2.490217	-0.655467	-2.894728

C	4.299073	-2.174723	-0.489127
H	3.624115	-2.804968	-2.416294
F	3.901688	1.063187	1.029953
F	5.046750	-1.285057	1.566354
F	4.904115	-3.317032	-0.210142
C	-0.285860	-0.031247	-1.577330
H	0.720596	-0.369176	-1.822017

S-1-c30

C	-0.988964	0.237621	-1.181228
C	-2.267988	-0.230977	-0.735150
C	-0.851693	1.571150	-1.463014
C	-2.607229	-1.590744	-0.541126
C	-3.264506	0.758950	-0.494201
C	-1.931784	2.458847	-1.235007
H	0.094210	1.971866	-1.812578
C	-3.854899	-1.957669	-0.073321
H	-1.935288	-2.399935	-0.807120
C	-4.528456	0.354570	0.000614
H	-1.810367	3.518700	-1.449416
C	-4.824134	-0.965032	0.219724
H	-5.261645	1.131842	0.187369
H	-5.803072	-1.239276	0.594486
C	2.955666	-1.037393	0.363770
C	2.341020	-3.437627	0.121084
C	3.532979	-2.464601	0.242565
H	2.946133	-0.539605	-0.603335
H	3.514007	-0.437549	1.085562
H	4.081888	-2.711799	1.159305
C	0.610835	-1.640446	-0.280154
H	-0.283239	-1.939248	0.268575
C	1.323955	-2.876478	-0.870266
H	0.561080	-3.625492	-1.105840
H	1.807468	-2.597842	-1.810964
H	2.691945	-4.421678	-0.196818
C	1.653884	-3.512257	1.485200
H	0.702922	-4.047976	1.407158
H	2.271084	-4.045835	2.213076
C	1.431864	-2.077545	1.976969
H	0.457178	-1.941080	2.449568
H	2.203485	-1.770021	2.686412
N	-3.083298	2.084844	-0.742472
N	1.513454	-1.070122	0.826990
O	-4.066262	-3.281600	0.070757

C	-5.349772	-3.731983	0.471051
H	-6.121901	-3.415268	-0.238968
H	-5.290799	-4.820062	0.478504
H	-5.602159	-3.376915	1.476947
O	1.296149	-0.139289	-2.005666
H	1.075534	0.202651	-2.881587
C	4.498114	-2.529416	-0.909605
H	4.087664	-2.325810	-1.898711
C	5.790772	-2.811021	-0.778592
H	6.238767	-3.012430	0.191863
H	6.451705	-2.854265	-1.638296
C	1.042370	0.228738	1.450451
H	-0.030691	0.094674	1.598297
H	1.506038	0.234410	2.442025
C	1.269320	1.588022	0.825865
C	0.273214	2.519613	1.129094
C	2.377436	2.055735	0.116495
C	0.338423	3.842819	0.721047
C	2.458022	3.375261	-0.315727
H	3.200775	1.404698	-0.132924
C	1.439192	4.264298	-0.014233
H	3.315446	3.729781	-0.875643
F	-0.813097	2.138502	1.807416
F	-0.654897	4.672796	1.001340
F	1.494129	5.525870	-0.418231
C	0.149467	-0.734736	-1.443608
H	-0.256226	-1.483194	-2.146201

S-1-c31

C	-1.365794	0.158891	1.645317
C	-1.738954	1.337511	0.926460
C	-2.304386	-0.394754	2.484045
C	-0.838086	2.125944	0.177651
C	-3.106418	1.731684	0.979231
C	-3.624324	0.118899	2.510151
H	-2.049727	-1.240820	3.113986
C	-1.270889	3.206794	-0.560616
H	0.228095	1.950133	0.229331
C	-3.527186	2.842061	0.204037
H	-4.365075	-0.338364	3.162308
C	-2.645417	3.559393	-0.562016
H	-4.576813	3.111947	0.250314
H	-3.002486	4.404347	-1.138788
C	-1.271748	-1.150036	-1.479502



C	-1.382929	-3.451761	-0.513564
C	-2.138799	-2.424555	-1.385704
H	-1.668591	-0.341829	-0.865685
H	-1.192177	-0.787065	-2.506878
H	-2.249116	-2.855544	-2.387840
C	0.122979	-1.699358	0.513517
H	1.118693	-2.092146	0.713707
C	-0.930867	-2.793948	0.787360
H	-0.492950	-3.531067	1.463931
H	-1.795353	-2.370170	1.296322
H	-2.038486	-4.298543	-0.298799
C	-0.133505	-3.907091	-1.266005
H	0.495945	-4.520138	-0.614192
H	-0.391138	-4.514060	-2.138610
C	0.625348	-2.659055	-1.728747
H	1.696968	-2.735162	-1.572978
H	0.439941	-2.448346	-2.784825
N	-4.034017	1.108151	1.755045
N	0.142587	-1.411016	-0.994152
O	-0.315610	3.870665	-1.250343
C	-0.670079	5.060977	-1.937880
H	-1.084985	5.805524	-1.249689
H	0.255557	5.443000	-2.367366
H	-1.385670	4.858527	-2.742806
O	0.433908	-1.095722	2.688687
H	0.377641	-0.446949	3.402413
C	-3.510804	-2.075727	-0.871984
H	-3.556759	-1.557645	0.086364
C	-4.638440	-2.355869	-1.517820
H	-4.639275	-2.860234	-2.481583
H	-5.606030	-2.092707	-1.102955
C	0.996671	-0.240327	-1.449261
H	1.202723	-0.441888	-2.504702
H	0.340359	0.629948	-1.414433
C	2.282166	0.138021	-0.738084
C	3.253310	-0.716321	-0.220892
C	2.574531	1.510951	-0.707173
C	4.431231	-0.243031	0.344613
C	3.752616	2.006470	-0.165214
H	1.864896	2.217786	-1.128375
C	4.678171	1.124046	0.367699
H	3.961279	3.069630	-0.147568
F	3.099857	-2.052596	-0.222134
F	5.307457	-1.100187	0.843776

F	5.806465	1.558406	0.906956
C	0.006253	-0.480765	1.490023
H	0.734228	0.277483	1.185176

S-1-c32

C	1.434857	-1.390121	-0.937875
C	2.722941	-0.989764	-0.446084
C	1.297124	-1.536956	-2.295861
C	3.074879	-0.952974	0.925204
C	3.701912	-0.617222	-1.412423
C	2.357970	-1.184678	-3.167228
H	0.382481	-1.906935	-2.748385
C	4.325059	-0.519570	1.329050
H	2.416153	-1.327676	1.702862
C	4.964451	-0.153264	-0.967229
H	2.224524	-1.288668	-4.241664
C	5.274860	-0.091677	0.365179
H	5.684445	0.137029	-1.724693
H	6.252707	0.260960	0.670905
C	-2.759038	-0.437862	0.490544
C	-3.257091	-2.876347	0.496669
C	-3.697234	-1.516688	1.073193
H	-1.967779	-0.153470	1.180691
H	-3.323112	0.446504	0.205282
H	-4.722214	-1.322102	0.734960
C	-1.059579	-2.064238	-0.430439
H	-0.946160	-2.604181	-1.372542
C	-1.737591	-2.988940	0.602932
H	-1.402278	-4.012095	0.407237
H	-1.397391	-2.725704	1.609212
H	-3.747222	-3.691486	1.033303
C	-3.626380	-2.900955	-0.990091
H	-3.183190	-3.773772	-1.479873
H	-4.709042	-2.969507	-1.125782
C	-3.123330	-1.599237	-1.631613
H	-2.679747	-1.760888	-2.617302
H	-3.921337	-0.859730	-1.731564
N	3.501962	-0.704674	-2.755878
N	-2.060855	-0.935605	-0.766231
O	4.557988	-0.542155	2.652236
C	5.836867	-0.164852	3.137753
H	6.056179	0.884233	2.908874
H	5.789172	-0.295175	4.218236
H	6.622928	-0.809185	2.728556

O	0.127694	-0.613926	1.002422
H	0.956583	-0.142406	1.159237
C	-3.688446	-1.451841	2.576442
H	-2.725366	-1.595872	3.066253
C	-4.770925	-1.223310	3.313760
H	-5.747828	-1.062126	2.863566
H	-4.721098	-1.189385	4.397349
C	-1.509191	0.230288	-1.609775
H	-0.697161	-0.183351	-2.201745
H	-2.325823	0.481872	-2.288106
C	-1.059423	1.493240	-0.927996
C	-1.992020	2.482992	-0.621283
C	0.290139	1.807001	-0.743754
C	-1.625039	3.703323	-0.072268
C	0.687344	3.024844	-0.209484
H	1.047679	1.094133	-1.044914
C	-0.274571	3.963418	0.135599
H	1.734378	3.266570	-0.069161
F	-3.296497	2.275784	-0.863163
F	-2.547141	4.606465	0.225531
F	0.072741	5.131499	0.655108
C	0.335056	-1.665863	0.082094
H	0.672774	-2.563210	0.629320

S-1-c33

C	0.698675	-1.372051	-0.229913
C	2.119239	-1.415766	-0.029575
C	0.203386	-1.953231	-1.375777
C	2.785650	-1.051125	1.164404
C	2.904300	-1.881091	-1.130925
C	1.073764	-2.432693	-2.380417
H	-0.868965	-2.041339	-1.525096
C	4.164274	-1.068513	1.246563
H	2.227943	-0.775622	2.049939
C	4.317385	-1.865639	-1.023076
H	0.666167	-2.868863	-3.290003
C	4.942411	-1.461634	0.125964
H	4.885148	-2.205416	-1.882517
H	6.024748	-1.471635	0.179204
C	0.349096	1.597843	-1.578097
C	0.988108	2.907135	0.444673
C	1.354871	2.634628	-1.030127
H	0.790865	0.604461	-1.648455
H	-0.023665	1.878357	-2.566015

H	1.241062	3.571791	-1.587711
C	-0.448228	0.838044	0.666390
H	-1.287698	1.051492	1.329308
C	0.809093	1.577401	1.172803
H	0.702648	1.729524	2.248903
H	1.694786	0.964553	1.027774
H	1.779992	3.491800	0.917800
C	-0.343775	3.655721	0.486125
H	-0.713609	3.714758	1.514199
H	-0.239753	4.679387	0.115540
C	-1.338142	2.902633	-0.402756
H	-2.330796	2.843663	0.031419
H	-1.416494	3.358777	-1.392828
N	2.377299	-2.359536	-2.290306
N	-0.865245	1.475553	-0.667944
O	4.689611	-0.698812	2.430019
C	6.095482	-0.738348	2.603546
H	6.602138	-0.041290	1.925663
H	6.273430	-0.430814	3.633502
H	6.489081	-1.750544	2.455709
O	-0.078811	-0.934106	2.077860
H	-0.004603	-1.885308	2.230222
C	2.762523	2.137002	-1.229376
H	3.028672	1.206444	-0.727370
C	3.668580	2.758574	-1.977596
H	3.445805	3.685143	-2.502035
H	4.672017	2.361403	-2.092524
C	-1.945324	0.754239	-1.450173
H	-2.360970	1.514486	-2.118751
H	-1.417672	0.034655	-2.076063
C	-3.068861	0.004229	-0.758820
C	-3.795154	0.395215	0.363918
C	-3.491192	-1.172157	-1.395751
C	-4.857721	-0.354108	0.856249
C	-4.560411	-1.928071	-0.936774
H	-2.976287	-1.501218	-2.293356
C	-5.240340	-1.516718	0.198170
H	-4.873398	-2.832914	-1.444068
F	-3.492628	1.507374	1.055482
F	-5.495524	0.052572	1.941637
F	-6.255379	-2.216168	0.678784
C	-0.314059	-0.717109	0.702792
H	-1.291376	-1.134975	0.434557

## S-1-c34

C	0.166830	-0.771684	1.032599
C	1.601462	-0.722514	1.044787
C	-0.498052	0.083239	1.875943
C	2.422951	-1.633120	0.347107
C	2.211431	0.330346	1.785425
C	0.214751	1.059160	2.615421
H	-1.572820	0.061669	1.987266
C	3.794780	-1.474818	0.327527
H	2.006691	-2.495973	-0.160262
C	3.618563	0.479331	1.731846
H	-0.331520	1.745810	3.258437
C	4.398509	-0.390962	1.016762
H	4.056887	1.304170	2.282898
H	5.472758	-0.250662	0.996475
C	-2.994425	0.642555	-0.340553
C	-4.347667	-1.360576	0.272433
C	-4.294530	0.176908	0.354666
H	-2.219731	0.924026	0.364372
H	-3.178690	1.501060	-0.985258
H	-5.148700	0.572094	-0.208057
C	-1.947490	-1.663909	-0.392463
H	-1.996628	-2.476013	-1.124282
C	-3.000870	-1.951824	0.694903
H	-3.072553	-3.036137	0.803707
H	-2.690637	-1.563814	1.667707
H	-5.151529	-1.741659	0.905895
C	-4.587740	-1.736126	-1.193750
H	-4.470477	-2.814422	-1.336851
H	-5.603047	-1.475405	-1.504244
C	-3.583260	-0.963211	-2.063406
H	-3.161787	-1.583023	-2.857044
H	-4.032790	-0.079256	-2.522034
N	1.511254	1.214045	2.548495
N	-2.419910	-0.448573	-1.219283
O	4.486611	-2.385899	-0.385909
C	5.902961	-2.344750	-0.367769
H	6.292984	-2.443314	0.651716
H	6.229791	-3.197647	-0.962045
H	6.284594	-1.422287	-0.821447
O	-0.368470	-3.096071	0.556286
H	-0.341865	-3.080352	1.521224
C	-4.383937	0.727764	1.752076
H	-3.681269	0.335335	2.487368

C	-5.265096	1.649093	2.129284
H	-5.989889	2.066600	1.433934
H	-5.299518	2.018461	3.149101
C	-1.410494	0.109814	-2.222101
H	-1.174941	-0.729602	-2.880434
H	-1.989710	0.831847	-2.805362
C	-0.108654	0.727610	-1.775909
C	-0.013584	1.955215	-1.118515
C	1.090394	0.145361	-2.203532
C	1.209759	2.528926	-0.806412
C	2.326103	0.719841	-1.941154
H	1.061047	-0.789322	-2.756012
C	2.380443	1.903079	-1.224788
H	3.246961	0.250559	-2.264472
F	-1.110631	2.636532	-0.766853
F	1.252854	3.674816	-0.146473
F	3.540870	2.470837	-0.933499
C	-0.471606	-1.763677	0.079460
H	0.134819	-1.741379	-0.827700

S-1-c35

C	1.95439200	0.94226100	-1.28870200
C	1.05612700	1.83380100	-0.62298700
C	3.24983100	1.36577900	-1.47601900
C	-0.32785300	1.60592200	-0.47188500
C	1.60897600	3.02523500	-0.06952300
C	3.68424300	2.59283100	-0.92138800
H	3.95402500	0.75184300	-2.02922200
C	-1.12608300	2.46386700	0.25331600
H	-0.81720900	0.78740600	-0.97545600
C	0.76693900	3.89119300	0.67362100
H	4.71636900	2.90812200	-1.05626300
C	-0.56515600	3.62182000	0.85014000
H	1.21791900	4.78420400	1.09307000
H	-1.18113800	4.30409600	1.42440300
C	0.59842000	-1.28781500	1.10956600
C	3.01494700	-1.93420800	1.34926800
C	1.88256000	-1.09502500	1.96639900
H	0.24393900	-0.35049600	0.68258000
H	-0.20896700	-1.69888800	1.71256400
H	1.67427600	-1.51103200	2.95874100
C	1.94307000	-1.68768300	-0.94057600
H	2.06090500	-2.46313700	-1.70144200
C	3.24555100	-1.56155900	-0.11702400

H	4.00634600	-2.21872700	-0.54715800
H	3.63541700	-0.54778600	-0.18405100
H	3.93566500	-1.78018900	1.91702200
C	2.59528500	-3.39990900	1.40346500
H	3.39173400	-4.04219000	1.01824900
H	2.39521400	-3.70811800	2.43347700
C	1.33329400	-3.56743300	0.54572700
H	1.50294200	-4.22750200	-0.30771600
H	0.49458100	-3.96477400	1.12163900
N	2.91394100	3.38031100	-0.21090100
N	0.83895200	-2.24755800	-0.03393600
O	-2.42881700	2.11946400	0.33840000
C	-3.35405700	3.01819500	0.92633700
H	-3.35074100	3.98506400	0.41129400
H	-4.32927800	2.54660300	0.80752800
H	-3.14831000	3.16462500	1.99288900
O	2.15609500	-0.73716700	-3.02666000
H	2.06623100	0.02611900	-3.61292800
C	2.22511800	0.36009400	2.15204700
H	2.73422100	0.86018800	1.33199900
C	1.93004500	1.05108400	3.24864500
H	1.42781200	0.59546000	4.09954000
H	2.18475800	2.10239300	3.33603400
C	-0.42525200	-2.60890600	-0.85942700
H	-0.21932100	-2.34033200	-1.89361800
H	-0.49253900	-3.69618700	-0.82252800
C	-1.72807900	-2.02132500	-0.40057900
C	-2.36698000	-1.05065500	-1.16628000
C	-2.38119000	-2.46213600	0.75640900
C	-3.55784000	-0.46015900	-0.76785300
C	-3.57289000	-1.89030900	1.17867500
H	-1.94947600	-3.26881400	1.34208800
C	-4.14368800	-0.87793500	0.41991900
H	-4.07430900	-2.21939500	2.08108500
F	-1.82250400	-0.63588600	-2.31882900
F	-4.11407800	0.48611400	-1.50342300
F	-5.26675200	-0.28961200	0.80937600
C	1.53108900	-0.43057300	-1.79337500
H	0.44556300	-0.43045400	-1.92550300

S-1-c36

C	-0.29499200	-1.18786500	-1.30309500
C	-1.62878100	-0.64678500	-1.31136100
C	-0.16955400	-2.54917700	-1.15615000

C	-1.96942900	0.70753300	-1.55136900
C	-2.68935400	-1.55937400	-1.01293400
C	-1.30414300	-3.36684000	-0.94557000
H	0.79318400	-3.04740800	-1.19270600
C	-3.26778600	1.15746800	-1.40678000
H	-1.23796400	1.42887800	-1.88720800
C	-4.01050000	-1.06770200	-0.88343000
H	-1.17697900	-4.44130900	-0.83311100
C	-4.30329400	0.25895100	-1.04966600
H	-4.78259500	-1.78793500	-0.63696700
H	-5.32327600	0.60336800	-0.92802900
C	3.11686700	0.82517900	0.72981500
C	4.71551600	-0.16107300	-0.88954500
C	4.53753300	0.96797000	0.14635000
H	2.42435300	1.47996500	0.20655000
H	3.09646300	1.03610300	1.80133100
H	5.27747000	0.82275900	0.94271600
C	2.28639300	-0.85051400	-0.95267200
H	2.32036500	-1.93700900	-1.02617400
C	3.45904300	-0.24947600	-1.75675900
H	3.62983900	-0.89170500	-2.62614200
H	3.17549600	0.73699500	-2.13556500
H	5.60022500	0.02647900	-1.50125000
C	4.84674400	-1.47939400	-0.12267900
H	4.79697100	-2.32962900	-0.80987000
H	5.80524800	-1.54029200	0.39978400
C	3.71303400	-1.54234100	0.90944400
H	3.27619200	-2.53934400	0.99422400
H	4.05170200	-1.23206700	1.90083300
N	-2.51745000	-2.89819300	-0.84206100
N	2.57950100	-0.58485700	0.54259000
O	-3.45893200	2.47484600	-1.62005600
C	-4.75792100	3.01417600	-1.44961500
H	-5.11594800	2.86967800	-0.42342000
H	-4.66210000	4.08070800	-1.65155400
H	-5.47091100	2.57596200	-2.15741900
O	0.83220700	1.04294000	-1.25736900
H	0.20703100	1.15225300	-0.52635200
C	4.72270200	2.35174000	-0.41517300
H	4.04269300	2.64812000	-1.21401200
C	5.65093600	3.20425100	0.00817800
H	6.34423800	2.94880900	0.80645500
H	5.75839200	4.18933800	-0.43419100
C	1.47441600	-0.91137800	1.53517300



H	1.18775800	-1.94053500	1.31848600
H	1.98061000	-0.90907100	2.50568600
C	0.21013200	-0.08626700	1.63653500
C	-0.96889900	-0.81274800	1.81929200
C	0.10722900	1.31055400	1.70802100
C	-2.20563200	-0.20135700	1.97919000
C	-1.12449400	1.94336200	1.83536200
H	0.98860500	1.93585500	1.65975300
C	-2.27873200	1.18410200	1.95224600
H	-1.20165700	3.02397900	1.85637000
F	-0.93926900	-2.14496700	1.84184300
F	-3.29089000	-0.93912100	2.13599000
F	-3.46526800	1.76540700	2.05500900
C	0.95244500	-0.33186400	-1.54603900
H	1.13599600	-0.38254500	-2.62871900

CPX-C1

C	-3.117238	-1.377052	0.203602
C	-4.482637	-1.284304	-0.211394
C	-2.765144	-2.419855	1.019855
C	-4.964469	-0.305658	-1.110057
C	-5.392768	-2.236909	0.329612
C	-3.747172	-3.336288	1.469057
H	-1.731773	-2.538010	1.333174
C	-6.304660	-0.239831	-1.426704
H	-4.276585	0.360070	-1.617256
C	-6.761786	-2.140706	-0.013400
H	-3.455982	-4.159169	2.120083
C	-7.218502	-1.164674	-0.862652
H	-7.438983	-2.872196	0.415179
H	-8.274306	-1.119245	-1.104302
C	-0.241316	1.593795	1.618832
C	-2.402099	2.065989	2.751176
C	-0.881699	1.924292	2.981697
H	-0.049233	0.525595	1.510161
H	0.703141	2.118091	1.477825
H	-0.502428	2.889754	3.340809
C	-2.361641	1.016469	0.457772
H	-3.090371	1.534600	-0.170959
C	-2.882853	0.889871	1.903263
H	-3.974861	0.840626	1.870784
H	-2.543715	-0.052614	2.342089
H	-2.924192	2.091239	3.710854
C	-2.644402	3.354463	1.962851

H	-3.688732	3.404566	1.638045
H	-2.450631	4.237386	2.579285
C	-1.700450	3.364012	0.751546
H	-2.191614	3.695843	-0.162641
H	-0.831189	4.001895	0.920535
N	-5.017334	-3.249012	1.165798
N	-1.157452	1.982466	0.486595
O	-6.667843	0.738863	-2.295240
C	-8.001633	0.776294	-2.749871
H	-8.705450	0.987819	-1.934213
H	-8.046424	1.587586	-3.477491
H	-8.287929	-0.162461	-3.240856
O	-1.981819	-0.241558	-1.588916
H	-1.056563	-0.563228	-1.801008
C	-0.527640	0.876156	4.001733
H	-0.659759	-0.161203	3.696952
C	-0.063870	1.149689	5.218275
H	0.107979	2.172123	5.548586
H	0.162916	0.361850	5.929899
C	-0.394519	1.961593	-0.831919
H	-0.008774	0.947637	-0.949256
H	-1.134689	2.151062	-1.609570
C	0.784012	2.890795	-0.915175
C	0.676170	4.217391	-1.324849
C	2.069842	2.373100	-0.721641
C	1.793852	5.024543	-1.484046
C	3.204716	3.158640	-0.880502
H	2.173416	1.319328	-0.479516
C	3.055028	4.483554	-1.255752
H	4.197404	2.745829	-0.736276
F	-0.524874	4.756490	-1.586834
F	1.656738	6.294053	-1.863313
F	4.116431	5.272884	-1.418192
C	-2.063596	-0.356747	-0.198987
H	-1.106086	-0.724698	0.194611
C	3.750207	-3.985898	0.329324
C	2.803425	-3.581875	-0.628063
C	2.413657	-4.526941	-1.605500
C	2.940007	-5.812080	-1.584913
C	3.871152	-6.201041	-0.621970
C	4.277987	-5.273477	0.330672
H	4.074971	-3.276506	1.086084
H	2.619922	-6.522943	-2.344569
H	4.275005	-7.209234	-0.622852

H	5.008421	-5.551074	1.086292
C	1.470851	-4.069879	-2.689806
H	2.056305	-3.565559	-3.474669
H	0.980729	-4.928114	-3.163708
C	0.440086	-3.081290	-2.154474
H	-0.147796	-2.650627	-2.970946
H	-0.265958	-3.594625	-1.483648
C	1.091480	-1.948817	-1.375258
C	2.216863	-2.239397	-0.629297
C	2.771102	-1.208009	0.283075
C	4.014785	-0.545915	0.000417
C	2.125248	-0.862465	1.454706
C	4.724727	-0.809420	-1.201956
C	4.553474	0.412028	0.907078
C	2.650029	0.093134	2.357008
C	5.903181	-0.166573	-1.482265
H	4.302555	-1.526840	-1.897603
C	5.782225	1.053753	0.595195
C	3.836370	0.720929	2.090614
H	2.088124	0.308923	3.261603
C	6.443947	0.773000	-0.572586
H	6.427366	-0.378186	-2.409470
H	6.186491	1.776224	1.300651
H	4.242604	1.452914	2.784180
H	7.382600	1.269089	-0.801898
O	0.907398	-1.417646	1.806578
C	1.010888	-2.722853	2.358837
H	1.361899	-3.440963	1.612195
H	1.693937	-2.724566	3.218242
H	0.009717	-3.000595	2.698683
O	0.523024	-0.799111	-1.426766

CPX-C2

C	0.593052	3.738877	-1.314637
C	1.935948	3.414523	-0.931653
C	0.293386	5.060739	-1.517416
C	2.398119	2.100250	-0.704452
C	2.848525	4.497911	-0.769327
C	1.281644	6.058736	-1.333808
H	-0.706085	5.357834	-1.825814
C	3.706739	1.860006	-0.339174
H	1.753408	1.241814	-0.840573
C	4.181418	4.219124	-0.383960
H	1.026540	7.104420	-1.499043

C	4.613070	2.934148	-0.170620
H	4.854389	5.062528	-0.269743
H	5.643098	2.750338	0.113483
C	-3.302461	2.163231	0.150603
C	-1.800483	2.464667	2.091189
C	-3.249531	2.663396	1.605914
H	-3.208782	2.986984	-0.562848
H	-4.235636	1.646998	-0.065127
H	-3.906868	2.037558	2.222221
C	-0.829989	1.989938	-0.177071
H	-0.101585	1.193417	-0.021305
C	-0.837547	2.965874	1.013856
H	0.182670	3.022959	1.403266
H	-1.104594	3.976751	0.687519
H	-1.640586	2.996370	3.032583
C	-1.556546	0.966381	2.262659
H	-0.493534	0.786010	2.432239
H	-2.093473	0.569074	3.128398
C	-2.025831	0.232387	0.997864
H	-1.310008	-0.521840	0.664150
H	-3.002234	-0.234994	1.131050
N	2.511568	5.806015	-0.968097
N	-2.170461	1.216661	-0.146861
O	4.040127	0.557983	-0.174010
C	5.352399	0.206365	0.213185
H	5.611158	0.648073	1.183990
H	5.354008	-0.881307	0.293209
H	6.086086	0.519645	-0.539543
O	-0.166946	1.814092	-2.558990
H	0.182902	0.956216	-2.193682
C	-3.738187	4.081797	1.695296
H	-3.161290	4.828014	1.147673
C	-4.805567	4.465163	2.389354
H	-5.411020	3.753292	2.946143
H	-5.112611	5.505683	2.431223
C	-2.459852	0.481963	-1.456079
H	-2.856953	1.229186	-2.144140
H	-1.502588	0.127759	-1.820640
C	-3.356160	-0.716433	-1.317173
C	-4.744441	-0.651555	-1.382323
C	-2.768935	-1.978615	-1.178052
C	-5.533367	-1.788328	-1.265771
C	-3.536312	-3.129174	-1.055075
H	-1.685221	-2.055721	-1.169277

C	-4.917337	-3.023869	-1.096138
H	-3.060921	-4.094759	-0.929529
F	-5.369828	0.525476	-1.557089
F	-6.860877	-1.691929	-1.320021
F	-5.691509	-4.102669	-0.978524
C	-0.498138	2.685183	-1.521031
H	-1.392420	3.245763	-1.839483
C	3.643125	-3.222096	0.839447
C	3.066257	-2.696700	-0.328307
C	3.829654	-2.740409	-1.518197
C	5.123377	-3.245172	-1.502692
C	5.694557	-3.738408	-0.328402
C	4.938833	-3.733048	0.839472
H	3.074950	-3.217348	1.764971
H	5.692007	-3.262009	-2.430604
H	6.706592	-4.132623	-0.332847
H	5.358175	-4.125194	1.762468
C	3.161288	-2.276075	-2.785918
H	2.504787	-3.082169	-3.149213
H	3.901948	-2.088648	-3.571437
C	2.308239	-1.038130	-2.532563
H	1.700725	-0.794311	-3.410477
H	2.951931	-0.170829	-2.333372
C	1.375953	-1.221377	-1.348999
C	1.731672	-2.090469	-0.345515
C	0.817070	-2.281976	0.813012
C	0.966659	-1.515557	2.016675
C	-0.205098	-3.212065	0.774272
C	1.946385	-0.488946	2.106974
C	0.126821	-1.752934	3.142634
C	-1.075409	-3.417359	1.872094
C	2.096809	0.241937	3.259120
H	2.574121	-0.299524	1.241781
C	0.327085	-0.999238	4.330181
C	-0.909679	-2.714776	3.034650
H	-1.864435	-4.155674	1.765300
C	1.289263	-0.024319	4.391368
H	2.848405	1.025154	3.304773
H	-0.306834	-1.203696	5.190043
H	-1.565450	-2.888846	3.884238
H	1.431078	0.546873	5.304321
O	-0.477143	-3.951801	-0.353426
C	0.430392	-5.012464	-0.613461
H	0.420341	-5.739809	0.209175

H	1.448984	-4.642347	-0.758940
H	0.081803	-5.495331	-1.528538
O	0.314462	-0.478648	-1.317908

CPX-C3

C	0.920742	3.700483	-1.073600
C	2.253541	3.310384	-0.715587
C	0.687834	5.033114	-1.293453
C	2.646553	1.979258	-0.460531
C	3.226494	4.346593	-0.596458
C	1.733094	5.979196	-1.157757
H	-0.302329	5.379167	-1.579875
C	3.942621	1.675590	-0.093446
H	1.960659	1.151288	-0.579023
C	4.549413	4.003739	-0.229363
H	1.529916	7.033816	-1.337936
C	4.910671	2.703510	0.020006
H	5.271348	4.810313	-0.154311
H	5.934231	2.472120	0.293061
C	-2.952830	2.268888	0.556070
C	-1.323732	2.409541	2.420916
C	-2.778446	2.723289	2.019632
H	-2.871288	3.101049	-0.147388
H	-3.925126	1.804447	0.407625
H	-3.445284	2.129193	2.657006
C	-0.515721	1.964613	0.084347
H	0.167476	1.117987	0.153141
C	-0.387239	2.884571	1.311171
H	0.654968	2.855318	1.640651
H	-0.598694	3.924363	1.040278
H	-1.083671	2.898120	3.368824
C	-1.171710	0.892044	2.530697
H	-0.112917	0.635965	2.619543
H	-1.682876	0.496699	3.412999
C	-1.760231	0.240840	1.270425
H	-1.115968	-0.545830	0.871991
H	-2.757163	-0.166397	1.444381
N	2.956690	5.666769	-0.817614
N	-1.897720	1.270657	0.169045
O	4.198296	0.369410	0.133012
C	5.523970	-0.059894	0.352532
H	5.942388	0.377443	1.269545
H	5.467253	-1.143623	0.457671
H	6.171958	0.191620	-0.496697

O	-0.043179	1.885886	-2.346693
H	0.304420	0.990341	-2.060839
C	-3.153647	4.170417	2.173985
H	-2.566010	4.886547	1.598764
C	-4.134839	4.611121	2.955578
H	-4.748511	3.930561	3.541819
H	-4.359511	5.669626	3.042860
C	-2.263119	0.566585	-1.133558
H	-2.341283	1.340645	-1.894876
H	-1.403890	-0.066868	-1.367303
C	-3.511802	-0.267582	-1.060293
C	-4.751757	0.258682	-1.415681
C	-3.454117	-1.627950	-0.738340
C	-5.906330	-0.512204	-1.413493
C	-4.595927	-2.419207	-0.726939
H	-2.494266	-2.080443	-0.507697
C	-5.815794	-1.854264	-1.062844
H	-4.541064	-3.470466	-0.471320
F	-4.863284	1.549113	-1.763308
F	-7.076557	0.027673	-1.745681
F	-6.929949	-2.584951	-1.061560
C	-0.237424	2.711409	-1.243833
H	-1.119760	3.338065	-1.458178
C	3.689713	-3.387693	0.748377
C	3.162456	-2.774401	-0.398525
C	3.966807	-2.751793	-1.561357
C	5.247191	-3.289472	-1.539300
C	5.766759	-3.876958	-0.384840
C	4.971856	-3.930646	0.755974
H	3.085147	-3.440631	1.649481
H	5.847108	-3.255896	-2.446986
H	6.768543	-4.296577	-0.383875
H	5.350789	-4.395579	1.662777
C	3.357145	-2.180440	-2.815328
H	2.701129	-2.943656	-3.263143
H	4.131161	-1.951837	-3.556636
C	2.518565	-0.945028	-2.504631
H	1.953371	-0.621458	-3.384962
H	3.171076	-0.110023	-2.215505
C	1.540416	-1.194125	-1.372619
C	1.845155	-2.136357	-0.422006
C	0.898646	-2.359146	0.700484
C	-0.202179	-3.260914	0.569428
C	1.071064	-1.717234	1.915639

C	-0.462130	-3.931007	-0.659283
C	-1.074753	-3.508582	1.669626
C	0.245274	-2.003069	3.031602
C	-1.523199	-4.789210	-0.786068
H	0.208946	-3.740186	-1.489863
C	-2.167990	-4.402499	1.507130
C	-0.808740	-2.871045	2.905460
H	0.432335	-1.519114	3.985047
C	-2.387833	-5.032930	0.309962
H	-1.701650	-5.292129	-1.732000
H	-2.821611	-4.587666	2.356494
H	-1.445910	-3.083470	3.760502
H	-3.215472	-5.728892	0.201427
O	2.040289	-0.761316	1.961462
C	2.666909	-0.483692	3.189548
H	2.979160	-1.404534	3.698333
H	2.022931	0.099661	3.864023
H	3.547699	0.110918	2.942017
O	0.486737	-0.442438	-1.319489

CPX-C4

C	-3.365171	0.595465	-1.295774
C	-4.585063	-0.138475	-1.166503
C	-3.353111	1.664025	-2.156793
C	-4.742072	-1.266984	-0.329562
C	-5.704169	0.311165	-1.927218
C	-4.521908	2.020808	-2.867068
H	-2.441506	2.233031	-2.314295
C	-5.950400	-1.921680	-0.237161
H	-3.920865	-1.648367	0.264100
C	-6.931192	-0.386107	-1.814367
H	-4.498778	2.871909	-3.545884
C	-7.063914	-1.475472	-0.991916
H	-7.766411	-0.024598	-2.405047
H	-8.018931	-1.984356	-0.929633
C	-0.441367	0.015104	2.112627
C	-2.526056	1.089966	2.946132
C	-1.683528	-0.200844	2.991507
H	-0.230561	-0.778277	1.391083
H	0.450425	0.139209	2.728106
H	-1.330343	-0.310146	4.026970
C	-1.854837	1.351985	0.507900
H	-1.789967	2.309334	-0.016000
C	-3.028599	1.348197	1.524556



H	-3.565330	2.301124	1.482286
H	-3.745791	0.572384	1.249497
H	-3.377208	1.002285	3.628490
C	-1.634206	2.260548	3.357749
H	-2.224851	3.175240	3.463658
H	-1.161188	2.061708	4.324742
C	-0.564548	2.457834	2.273471
H	-0.736899	3.356481	1.677357
H	0.438680	2.518949	2.694441
N	-5.663145	1.385683	-2.764337
N	-0.551207	1.296404	1.309781
O	-5.988106	-2.986445	0.605079
C	-7.186624	-3.721667	0.710333
H	-7.478883	-4.159983	-0.252298
H	-6.983123	-4.523762	1.420865
H	-8.009583	-3.104280	1.093086
O	-1.057184	0.121207	-1.500192
H	-0.495247	-0.668636	-1.199578
C	-2.485837	-1.444576	2.691048
H	-3.438055	-1.492262	3.222176
C	-2.135273	-2.473684	1.920957
H	-1.215208	-2.509882	1.338988
H	-2.804963	-3.324335	1.825561
C	0.723995	1.371326	0.482132
H	1.521625	1.288495	1.218860
H	0.746790	0.473160	-0.128955
C	0.929936	2.613547	-0.338104
C	1.675372	3.675934	0.172814
C	0.529472	2.690953	-1.676921
C	1.995635	4.786895	-0.596346
C	0.835892	3.795388	-2.463737
H	-0.017279	1.846874	-2.086602
C	1.567433	4.838116	-1.917407
H	0.530607	3.853765	-3.502263
F	2.120447	3.659574	1.436847
F	2.706427	5.783562	-0.072644
F	1.880538	5.909389	-2.644795
C	-2.074668	0.237108	-0.558058
H	-2.193603	-0.710619	-0.025694
C	4.898178	-3.135971	-0.664733
C	3.610335	-3.009799	-1.203162
C	3.297322	-3.755521	-2.358803
C	4.247497	-4.597441	-2.924501
C	5.523616	-4.717669	-2.375891

C	5.844032	-3.976544	-1.243102
H	5.156572	-2.573694	0.228803
H	3.985350	-5.165128	-3.815607
H	6.254631	-5.381945	-2.828011
H	6.832194	-4.058983	-0.797718
C	1.931483	-3.561270	-2.966357
H	1.946519	-2.646265	-3.578562
H	1.681598	-4.390896	-3.637662
C	0.869056	-3.395298	-1.883318
H	-0.096693	-3.118327	-2.318538
H	0.719613	-4.346261	-1.349881
C	1.260048	-2.325643	-0.876879
C	2.588689	-2.150450	-0.586710
C	3.016596	-1.109073	0.380404
C	2.729509	-1.206647	1.773162
C	3.700061	0.017192	-0.070411
C	1.997634	-2.309476	2.300807
C	3.127013	-0.173286	2.673798
C	4.137950	1.021647	0.825989
C	1.643486	-2.358084	3.622676
H	1.715208	-3.103285	1.618370
C	2.754588	-0.257703	4.045775
C	3.855607	0.926111	2.166895
H	4.682159	1.885368	0.460910
C	2.019505	-1.316382	4.510097
H	1.073905	-3.202850	3.998834
H	3.067027	0.536793	4.720132
H	4.177507	1.711388	2.845853
H	1.739911	-1.372451	5.558404
O	3.895481	0.105081	-1.410483
C	4.401329	1.302668	-1.944958
H	3.776919	2.165661	-1.670253
H	5.436489	1.490997	-1.630611
H	4.379325	1.176565	-3.028245
O	0.286012	-1.659332	-0.324830

S-CPX-C5

C	3.314005	-0.607436	-1.862300
C	4.122544	0.141740	-0.951695
C	3.867631	-0.985757	-3.057704
C	3.657256	0.620378	0.297505
C	5.470709	0.394247	-1.334948
C	5.215400	-0.663379	-3.342404
H	3.265440	-1.520699	-3.784186

C	4.511511	1.284601	1.151349
H	2.614498	0.523712	0.594288
C	6.311594	1.101893	-0.442442
H	5.651592	-0.972340	-4.291176
C	5.856011	1.533369	0.776918
H	7.333907	1.284943	-0.756524
H	6.527561	2.065477	1.441095
C	0.848371	-2.126018	1.426273
C	2.653502	-3.790875	1.046568
C	1.911960	-2.988646	2.134485
H	1.104666	-1.066539	1.343594
H	-0.104664	-2.178184	1.951030
H	1.414115	-3.706987	2.798698
C	1.827660	-2.397224	-0.869682
H	1.672287	-3.089139	-1.703327
C	3.067075	-2.828706	-0.066057
H	3.774852	-3.296756	-0.755866
H	3.574714	-1.963806	0.363864
H	3.529475	-4.282644	1.477037
C	1.679602	-4.824314	0.467986
H	2.122515	-5.304082	-0.411016
H	1.467406	-5.611916	1.197141
C	0.368883	-4.111981	0.089992
H	-0.021188	-4.427626	-0.878330
H	-0.412356	-4.268836	0.836681
N	6.003659	-0.011766	-2.522919
N	0.589015	-2.624491	0.021918
O	3.988957	1.658592	2.348313
C	4.731287	2.530675	3.170475
H	5.005082	3.449997	2.638025
H	4.075958	2.782635	4.005100
H	5.639042	2.050915	3.558943
O	1.108033	-1.098941	-2.707913
H	0.643813	-0.243272	-2.808646
C	2.809726	-2.124014	2.978772
H	3.263597	-1.260949	2.491491
C	3.053835	-2.348782	4.266409
H	2.603463	-3.185295	4.797146
H	3.709919	-1.701653	4.840213
C	-0.630354	-1.923200	-0.563580
H	-0.410730	-0.855715	-0.488537
H	-0.682708	-2.226528	-1.607502
C	-1.918027	-2.169736	0.164477
C	-2.808507	-3.150690	-0.259219

C	-2.328845	-1.311288	1.189963
C	-4.059218	-3.300901	0.321885
C	-3.566725	-1.457857	1.801246
H	-1.670094	-0.491503	1.465078
C	-4.427332	-2.446154	1.354537
H	-3.900961	-0.773871	2.571198
F	-2.476103	-3.980572	-1.260616
F	-4.895652	-4.244098	-0.111773
F	-5.635687	-2.593860	1.896727
C	1.881085	-0.998402	-1.531573
H	1.452381	-0.244341	-0.859256
C	-2.300102	4.510964	-0.788792
C	-1.408523	3.878032	0.094362
C	-0.752082	4.682612	1.053974
C	-0.980949	6.052154	1.094288
C	-1.866067	6.666081	0.208257
C	-2.528550	5.882135	-0.730166
H	-2.819553	3.914901	-1.534601
H	-0.459817	6.650494	1.839701
H	-2.035276	7.737876	0.255614
H	-3.225190	6.337852	-1.429243
C	0.149702	3.990895	2.044008
H	-0.468475	3.576726	2.856460
H	0.840337	4.706915	2.505276
C	0.910114	2.843549	1.387279
H	1.471961	2.263814	2.124680
H	1.645675	3.238226	0.668963
C	-0.018270	1.896530	0.639895
C	-1.138267	2.438651	0.029943
C	-2.007842	1.567102	-0.798883
C	-3.358204	1.266126	-0.406157
C	-1.553084	0.986851	-1.967642
C	-3.921275	1.825957	0.772597
C	-4.156597	0.368110	-1.170626
C	-2.335204	0.087062	-2.728700
C	-5.202248	1.521543	1.159162
H	-3.311984	2.500621	1.364167
C	-5.475992	0.067273	-0.741650
C	-3.606910	-0.226568	-2.334953
H	-1.897723	-0.343931	-3.624605
C	-5.992885	0.631690	0.395366
H	-5.615009	1.967533	2.059778
H	-6.072115	-0.621966	-1.335242
H	-4.211191	-0.919095	-2.915210

H	-7.003785	0.394898	0.713702
O	-0.272926	1.203260	-2.443549
C	0.014886	2.516652	-2.910587
H	-0.056316	3.244318	-2.099396
H	-0.673649	2.791228	-3.718631
H	1.036967	2.483339	-3.292775
O	0.322945	0.659859	0.599877

S-CPX-C6

C	2.908425	-1.427509	-1.095802
C	4.324828	-1.559139	-0.955537
C	2.147018	-2.567458	-1.042813
C	5.235621	-0.477361	-1.011857
C	4.838905	-2.868670	-0.727571
C	2.768098	-3.819480	-0.831718
H	1.067160	-2.506913	-1.151640
C	6.587164	-0.668301	-0.826325
H	4.904167	0.533243	-1.221953
C	6.233479	-3.034612	-0.548330
H	2.155238	-4.719034	-0.791354
C	7.095953	-1.969354	-0.588151
H	6.596632	-4.042335	-0.375392
H	8.157067	-2.134474	-0.442161
C	1.800622	2.742804	0.110298
C	2.302236	1.400610	2.153270
C	2.642994	2.704626	1.406644
H	2.419653	2.627217	-0.782057
H	1.261842	3.683024	0.008382
H	2.336911	3.542967	2.044418
C	1.493728	0.262482	0.036304
H	0.668701	-0.444142	0.155785
C	2.478157	0.199917	1.227876
H	2.295881	-0.729050	1.775807
H	3.510361	0.156637	0.872788
H	2.954222	1.300621	3.025366
C	0.839945	1.455623	2.581413
H	0.569552	0.520517	3.073249
H	0.671581	2.268984	3.294597
C	-0.039702	1.665137	1.340375
H	-0.802389	0.890917	1.227962
H	-0.537268	2.634430	1.359222
N	4.057905	-3.983760	-0.666235
N	0.785015	1.636819	0.071463
O	7.362193	0.445712	-0.887494

C	8.757329	0.301817	-0.739585
H	9.181663	-0.345578	-1.517328
H	9.175263	1.303932	-0.842981
H	9.020254	-0.097662	0.248287
O	1.377150	-0.114663	-2.423417
H	0.558615	-0.628577	-2.195192
C	4.108485	2.864254	1.107171
H	4.571086	2.091290	0.493025
C	4.854703	3.873030	1.546973
H	4.436863	4.668141	2.161081
H	5.912254	3.940800	1.311340
C	-0.143343	1.805729	-1.134549
H	0.493800	2.058811	-1.979627
H	-0.565394	0.812919	-1.302523
C	-1.281136	2.770049	-0.952581
C	-1.165865	4.140362	-1.167866
C	-2.549105	2.268344	-0.640061
C	-2.250294	4.996438	-1.029171
C	-3.648328	3.103596	-0.492677
H	-2.684789	1.197887	-0.519195
C	-3.489306	4.466124	-0.685504
H	-4.619167	2.697662	-0.236508
F	0.012764	4.682175	-1.516394
F	-2.102755	6.304612	-1.229514
F	-4.518779	5.302224	-0.552247
C	2.204917	-0.082888	-1.301448
H	2.958212	0.684539	-1.507637
C	-4.863661	-3.094149	0.381044
C	-4.118076	-2.491730	-0.643120
C	-4.605547	-2.593304	-1.962767
C	-5.801036	-3.254815	-2.218141
C	-6.542469	-3.831053	-1.187381
C	-6.062728	-3.749099	0.115861
H	-4.487945	-3.056896	1.400664
H	-6.160371	-3.318722	-3.243541
H	-7.475306	-4.343945	-1.402694
H	-6.614293	-4.209200	0.931896
C	-3.794614	-1.939280	-3.051670
H	-4.014398	-0.860300	-3.062977
H	-4.072182	-2.335161	-4.034990
C	-2.301627	-2.123919	-2.788501
H	-1.700489	-1.566268	-3.513678
H	-2.030128	-3.185094	-2.889448
C	-1.925610	-1.643043	-1.395387

C	-2.845152	-1.804303	-0.381341
C	-2.581147	-1.296522	0.986130
C	-1.495314	-1.769269	1.799208
C	-3.421547	-0.339249	1.538071
C	-0.593158	-2.762031	1.327657
C	-1.302427	-1.261945	3.116672
C	-3.224545	0.175645	2.840703
C	0.462156	-3.186368	2.094022
H	-0.762613	-3.178063	0.341961
C	-0.209864	-1.733232	3.895315
C	-2.191460	-0.277368	3.616381
H	-3.892978	0.947985	3.209513
C	0.664055	-2.661868	3.393488
H	1.146920	-3.935142	1.706871
H	-0.078454	-1.336291	4.899745
H	-2.037039	0.120579	4.616288
H	1.499090	-3.011239	3.993827
O	-4.425093	0.180447	0.758217
C	-5.740646	0.072284	1.270953
H	-5.887644	0.691734	2.165827
H	-5.983644	-0.970590	1.498210
H	-6.405462	0.425529	0.480551
O	-0.751652	-1.124932	-1.241412

S-CPX-C7

C	-3.108701	1.057196	-0.239447
C	-4.507060	1.290209	-0.422914
C	-2.310617	2.128260	0.083302
C	-5.448215	0.279526	-0.727381
C	-4.968438	2.630515	-0.267879
C	-2.878763	3.417996	0.206430
H	-1.242590	2.002256	0.246850
C	-6.785648	0.574569	-0.876558
H	-5.152095	-0.755341	-0.852824
C	-6.347473	2.902208	-0.434239
H	-2.236667	4.260217	0.459406
C	-7.243809	1.907730	-0.730593
H	-6.670559	3.930957	-0.313641
H	-8.293129	2.151208	-0.850304
C	-1.632132	-3.124639	0.560911
C	-2.793028	-2.261775	2.609797
C	-2.842291	-3.334265	1.498674
H	-1.915062	-3.003192	-0.484519
H	-0.923361	-3.952395	0.613249

H	-2.718846	-4.307291	1.994224
C	-1.794255	-0.656962	0.935058
H	-1.106165	0.141506	1.224866
C	-2.900331	-0.865608	1.998781
H	-2.810194	-0.105210	2.779927
H	-3.886815	-0.735322	1.542562
H	-3.616111	-2.430356	3.311489
C	-1.452381	-2.361883	3.332014
H	-1.426170	-1.663481	4.173366
H	-1.309574	-3.368894	3.738433
C	-0.331325	-2.017230	2.340440
H	0.157937	-1.060339	2.544652
H	0.426748	-2.797990	2.308738
N	-4.152052	3.677502	0.040573
N	-0.875437	-1.888004	0.934214
O	-7.600151	-0.474724	-1.162274
C	-8.974914	-0.226026	-1.353608
H	-9.149923	0.457834	-2.193845
H	-9.425789	-1.192941	-1.580199
H	-9.442497	0.184151	-0.449264
O	-1.678848	-0.370073	-1.570987
H	-1.018943	0.355346	-1.562818
C	-4.194693	-3.368370	0.824452
H	-5.027137	-3.338141	1.528288
C	-4.476288	-3.460040	-0.472850
H	-3.718207	-3.508277	-1.250281
H	-5.507037	-3.490044	-0.812655
C	0.287652	-1.639082	-0.028209
H	-0.116050	-1.770121	-1.027004
H	0.546468	-0.591646	0.147647
C	1.522548	-2.459218	0.192983
C	1.730033	-3.657542	-0.480105
C	2.574218	-1.948125	0.961213
C	2.934729	-4.342362	-0.396592
C	3.782878	-2.620718	1.069653
H	2.431020	-0.984005	1.441607
C	3.956960	-3.809785	0.380431
H	4.612456	-2.206257	1.629044
F	0.756523	-4.180837	-1.242650
F	3.108082	-5.486288	-1.059409
F	5.113710	-4.470134	0.441500
C	-2.472438	-0.319797	-0.417135
H	-3.249972	-1.065398	-0.585005
C	3.700457	3.881035	-0.882695



C	3.025818	3.465593	0.278411
C	3.006885	4.352226	1.380208
C	3.620291	5.595201	1.288521
C	4.279172	5.996027	0.126099
C	4.319580	5.124744	-0.957160
H	3.736361	3.214965	-1.740960
H	3.589188	6.262021	2.148569
H	4.754950	6.970768	0.072117
H	4.831298	5.413025	-1.871845
C	2.354998	3.872162	2.652176
H	3.074244	3.247204	3.204983
H	2.104206	4.717629	3.303427
C	1.121029	3.027393	2.351149
H	0.714762	2.575460	3.261287
H	0.328810	3.662705	1.924029
C	1.423533	1.908621	1.361321
C	2.350476	2.168525	0.364959
C	2.588785	1.154561	-0.693277
C	3.830747	0.437030	-0.780806
C	1.622520	0.845749	-1.628902
C	4.877916	0.671562	0.150435
C	4.025450	-0.561431	-1.777585
C	1.803009	-0.142903	-2.623202
C	6.050242	-0.038806	0.089925
H	4.724996	1.425724	0.915207
C	5.249238	-1.280137	-1.814729
C	2.978801	-0.838787	-2.693933
H	0.986731	-0.336184	-3.313467
C	6.241908	-1.027253	-0.904097
H	6.839468	0.159008	0.809875
H	5.382630	-2.042398	-2.578827
H	3.123024	-1.605577	-3.450691
H	7.173515	-1.584327	-0.940830
O	0.380357	1.458337	-1.602376
C	0.352793	2.785594	-2.116760
H	0.991765	3.442171	-1.519983
H	0.680386	2.795751	-3.163407
H	-0.685651	3.117605	-2.054376
O	0.764391	0.817404	1.497424

S-CPX-C8

C	-3.082146	1.138640	-0.233766
C	-4.466253	1.415075	-0.461033
C	-2.270698	2.174608	0.162899

C	-5.414459	0.451774	-0.876460
C	-4.905089	2.753689	-0.239751
C	-2.814830	3.469045	0.334517
H	-1.211007	2.017043	0.351849
C	-6.739614	0.785881	-1.055435
H	-5.130740	-0.572072	-1.091004
C	-6.271969	3.066164	-0.433066
H	-2.162331	4.282796	0.646600
C	-7.176606	2.114742	-0.827538
H	-6.577401	4.092191	-0.256652
H	-8.215868	2.389307	-0.965790
C	-1.699664	-3.095539	0.514344
C	-2.808110	-2.227010	2.596163
C	-2.845370	-3.344649	1.529544
H	-2.073227	-2.936365	-0.499683
H	-0.998493	-3.930291	0.476846
H	-2.647251	-4.291949	2.044878
C	-1.810356	-0.633696	0.903498
H	-1.111033	0.144712	1.218711
C	-2.930935	-0.846804	1.951435
H	-2.863784	-0.071509	2.719931
H	-3.913973	-0.731387	1.483587
H	-3.623766	-2.385658	3.307173
C	-1.457356	-2.286456	3.305430
H	-1.415431	-1.530188	4.094494
H	-1.315424	-3.263205	3.779467
C	-0.345463	-2.025689	2.277213
H	0.202924	-1.097019	2.459459
H	0.362738	-2.851964	2.233904
N	-4.078005	3.763391	0.151876
N	-0.912075	-1.877929	0.880571
O	-7.560517	-0.218735	-1.453312
C	-8.920375	0.074019	-1.687408
H	-9.042040	0.826198	-2.477114
H	-9.375772	-0.862018	-2.012620
H	-9.422722	0.420412	-0.775225
O	-1.678790	-0.280563	-1.597674
H	-1.007865	0.435032	-1.572042
C	-4.179075	-3.470351	0.844511
H	-4.515051	-2.613435	0.260470
C	-4.957301	-4.546067	0.914910
H	-4.663488	-5.427440	1.481240
H	-5.916933	-4.586742	0.409075
C	0.241427	-1.644049	-0.097458

H	-0.175976	-1.769940	-1.091445
H	0.516584	-0.600609	0.074254
C	1.468068	-2.481217	0.109222
C	1.653987	-3.679344	-0.570790
C	2.533516	-1.988412	0.870452
C	2.849783	-4.381184	-0.500358
C	3.733838	-2.677748	0.965281
H	2.409277	-1.024898	1.356918
C	3.885897	-3.866158	0.269874
H	4.573590	-2.276337	1.518992
F	0.667862	-4.186783	-1.327651
F	3.001397	-5.524483	-1.169412
F	5.034009	-4.542392	0.318280
C	-2.471178	-0.245297	-0.444967
H	-3.264579	-0.970890	-0.638490
C	3.776556	3.865556	-0.796980
C	3.094092	3.423672	0.349501
C	3.098994	4.267848	1.484075
C	3.745053	5.496748	1.438797
C	4.412645	5.923980	0.290987
C	4.427993	5.094575	-0.825326
H	3.793172	3.231980	-1.680159
H	3.732610	6.130332	2.324107
H	4.913743	6.887318	0.273586
H	4.945124	5.404844	-1.729667
C	2.435075	3.757126	2.737590
H	3.137476	3.092215	3.264868
H	2.207443	4.583026	3.421524
C	1.178581	2.958321	2.405728
H	0.760023	2.483304	3.298380
H	0.404357	3.631747	2.004412
C	1.451035	1.870281	1.373864
C	2.386139	2.141442	0.388735
C	2.606959	1.154595	-0.698087
C	3.838203	0.421360	-0.806316
C	1.632623	0.881437	-1.636620
C	4.892597	0.620138	0.125265
C	4.013577	-0.559513	-1.823619
C	1.793938	-0.090397	-2.650773
C	6.053585	-0.106734	0.045389
H	4.756762	1.360853	0.906032
C	5.225772	-1.296409	-1.880343
C	2.958461	-0.802947	-2.739917
H	0.972358	-0.256846	-3.341635

C	6.225903	-1.077822	-0.968963
H	6.848424	0.064070	0.766098
H	5.343778	-2.045639	-2.659685
H	3.087198	-1.557287	-3.511811
H	7.148442	-1.648613	-1.020801
O	0.399607	1.510912	-1.593389
C	0.391609	2.863523	-2.036937
H	1.034648	3.480651	-1.403537
H	0.724936	2.924604	-3.079936
H	-0.643160	3.204229	-1.961745
O	0.762014	0.792845	1.468154

S-CPX-C9

C	-3.461603	-1.314089	-0.649467
C	-4.723338	-0.750031	-1.020369
C	-3.414438	-2.655777	-0.372553
C	-4.901570	0.602083	-1.392989
C	-5.854465	-1.615573	-0.998003
C	-4.598980	-3.431202	-0.414735
H	-2.472748	-3.130302	-0.107319
C	-6.155297	1.093171	-1.688374
H	-4.045786	1.254743	-1.516097
C	-7.126904	-1.081279	-1.309006
H	-4.549860	-4.495862	-0.191280
C	-7.286406	0.240801	-1.638945
H	-7.973853	-1.759058	-1.282097
H	-8.275839	0.617029	-1.872582
C	-0.153941	0.226951	1.881656
C	-2.264965	0.238783	3.223875
C	-0.766444	-0.136517	3.254705
H	-0.008989	-0.633286	1.222742
H	0.817673	0.707296	1.995651
H	-0.283935	0.470152	4.031605
C	-2.342383	0.464689	0.711088
H	-3.017978	1.280547	0.439877
C	-2.879789	-0.302227	1.937455
H	-3.969843	-0.214818	1.950242
H	-2.656830	-1.367983	1.837523
H	-2.765430	-0.184700	4.098003
C	-2.386747	1.760413	3.206183
H	-3.425267	2.052040	3.018949
H	-2.092112	2.193868	4.166553
C	-1.466324	2.294122	2.102659
H	-1.936638	3.072441	1.502770

H	-0.537396	2.695952	2.511121
N	-5.781478	-2.944403	-0.693511
N	-1.055521	1.195471	1.149423
O	-6.219607	2.407243	-2.025278
C	-7.460350	2.940147	-2.429189
H	-8.204359	2.897986	-1.623010
H	-7.269299	3.984036	-2.681143
H	-7.855229	2.423068	-3.312995
O	-1.962980	0.233535	-1.705194
H	-1.041976	-0.033833	-1.969403
C	-0.556941	-1.584253	3.598384
H	-0.794237	-2.313399	2.824774
C	-0.129778	-2.007725	4.783657
H	0.141215	-1.315581	5.578193
H	-0.022930	-3.066702	4.998601
C	-0.333798	1.821255	-0.038445
H	0.003067	0.986369	-0.657709
H	-1.091072	2.387292	-0.581319
C	0.864917	2.659813	0.306275
C	0.771784	4.031063	0.536246
C	2.145051	2.096368	0.265371
C	1.894980	4.812502	0.767633
C	3.284255	2.857891	0.495519
H	2.263879	1.045284	0.019328
C	3.150197	4.212731	0.747502
H	4.265189	2.400723	0.460951
F	-0.422889	4.643049	0.537095
F	1.769044	6.118816	0.994860
F	4.217862	4.978480	0.969917
C	-2.199473	-0.471961	-0.521930
H	-1.366264	-1.160328	-0.333482
C	5.093465	-2.022556	-1.684078
C	4.066098	-1.135892	-2.038828
C	4.318764	-0.219208	-3.080804
C	5.557322	-0.197887	-3.711853
C	6.575189	-1.072105	-3.334658
C	6.332306	-1.988437	-2.315873
H	4.910535	-2.756179	-0.902728
H	5.729520	0.521500	-4.510383
H	7.538375	-1.042440	-3.835731
H	7.105727	-2.691755	-2.017355
C	3.214769	0.738930	-3.447147
H	3.216054	1.577520	-2.732555
H	3.383371	1.166073	-4.442200

C	1.858800	0.042464	-3.370630
H	1.040768	0.750749	-3.539208
H	1.787531	-0.729234	-4.150742
C	1.654943	-0.601503	-2.007336
C	2.753804	-1.147970	-1.373604
C	2.638187	-1.722622	-0.013258
C	1.726033	-2.781112	0.319772
C	3.453312	-1.241696	1.004586
C	0.868809	-3.363900	-0.656029
C	1.675364	-3.302075	1.645069
C	3.413063	-1.765389	2.316764
C	-0.011964	-4.361203	-0.324297
H	0.924449	-3.000479	-1.673454
C	0.753525	-4.338098	1.958587
C	2.543700	-2.774148	2.630722
H	4.067150	-1.350413	3.077575
C	-0.084404	-4.849876	1.003521
H	-0.652447	-4.790062	-1.090277
H	0.728858	-4.719842	2.977159
H	2.501614	-3.170506	3.641343
H	-0.785884	-5.640768	1.253910
O	4.283501	-0.190772	0.713900
C	5.618790	-0.280764	1.164940
H	5.714488	-0.014719	2.226675
H	6.023673	-1.285707	1.002659
H	6.194580	0.427576	0.565629
O	0.463912	-0.595939	-1.516630

S-CPX-C10

C	3.828730	1.309010	0.564419
C	4.547167	1.086415	-0.654173
C	4.428156	2.080308	1.525819
C	4.026393	0.373083	-1.758167
C	5.860815	1.630309	-0.745394
C	5.733158	2.591314	1.321507
H	3.912999	2.302085	2.456988
C	4.779978	0.176006	-2.894527
H	3.001962	0.024837	-1.751116
C	6.611124	1.407630	-1.924485
H	6.199258	3.197380	2.096623
C	6.095703	0.695823	-2.977746
H	7.608828	1.831563	-1.969459
H	6.695534	0.551213	-3.868986
C	0.711705	-1.183400	2.606371

C	2.991838	-2.058545	3.173914
C	1.718578	-1.412178	3.758638
H	0.376314	-0.145673	2.493598
H	-0.177716	-1.798811	2.742892
H	1.283276	-2.133209	4.461062
C	2.596632	-0.823601	0.993353
H	2.938761	-1.248030	0.046928
C	3.606714	-1.138342	2.125322
H	4.505639	-1.592651	1.697769
H	3.932053	-0.210639	2.598877
H	3.708288	-2.237702	3.980253
C	2.611376	-3.370509	2.492762
H	3.508121	-3.868210	2.111957
H	2.137333	-4.052748	3.205493
C	1.649461	-3.063683	1.334322
H	2.062355	-3.319436	0.356834
H	0.705764	-3.595143	1.449276
N	6.441323	2.369885	0.243765
N	1.296701	-1.596376	1.276573
O	4.180204	-0.520352	-3.894119
C	4.875191	-0.688923	-5.109526
H	5.805807	-1.254044	-4.970788
H	4.208079	-1.256635	-5.759171
H	5.103367	0.275271	-5.581249
O	1.623771	1.068600	-0.264506
H	0.736621	1.322901	0.123784
C	1.992484	-0.142790	4.520386
H	2.249129	0.737251	3.931605
C	1.930712	-0.040309	5.844466
H	1.658581	-0.887383	6.470998
H	2.141610	0.895549	6.352375
C	0.260981	-1.381707	0.164345
H	-0.086347	-0.353581	0.266649
H	0.795245	-1.508995	-0.777097
C	-0.934680	-2.281942	0.256662
C	-1.020492	-3.444122	-0.503170
C	-2.045618	-1.921345	1.025640
C	-2.151947	-4.245836	-0.486348
C	-3.174616	-2.727227	1.086931
H	-2.029470	-0.965903	1.541593
C	-3.222697	-3.879258	0.320985
H	-4.047751	-2.434513	1.656104
F	0.012851	-3.824162	-1.270008
F	-2.207886	-5.349047	-1.232028

F	-4.303163	-4.658413	0.328390
C	2.443168	0.717569	0.797036
H	2.046392	1.139655	1.731003
C	-4.117508	3.430076	-1.196677
C	-3.364934	3.234407	-0.029016
C	-3.535696	4.153681	1.028167
C	-4.415865	5.221088	0.893967
C	-5.154654	5.404552	-0.273826
C	-5.001272	4.497109	-1.317167
H	-4.001655	2.734075	-2.022583
H	-4.527595	5.919898	1.721238
H	-5.840397	6.242219	-0.363734
H	-5.565743	4.622525	-2.237600
C	-2.772237	3.897423	2.302307
H	-3.317382	3.148139	2.898551
H	-2.716053	4.807470	2.911110
C	-1.379946	3.351297	2.001345
H	-0.871343	3.037800	2.919162
H	-0.759363	4.133386	1.538423
C	-1.428710	2.158994	1.059499
C	-2.417924	2.116732	0.108346
C	-2.493766	0.997176	-0.866625
C	-3.604542	0.098956	-0.861653
C	-1.517082	0.821764	-1.840080
C	-4.655846	0.225278	0.091744
C	-3.692020	-0.959696	-1.811824
C	-1.582566	-0.251047	-2.764757
C	-5.726493	-0.630523	0.084446
H	-4.592588	1.020498	0.826580
C	-4.813539	-1.832423	-1.792465
C	-2.645692	-1.117968	-2.747255
H	-0.804794	-0.380726	-3.508879
C	-5.813124	-1.674065	-0.870091
H	-6.519691	-0.507360	0.817001
H	-4.861517	-2.633191	-2.527149
H	-2.695709	-1.929369	-3.469399
H	-6.665753	-2.346672	-0.863894
O	-0.509709	1.731159	-1.858691
C	0.456757	1.658127	-2.879113
H	0.002797	1.802852	-3.868858
H	1.002851	0.707204	-2.861636
H	1.165690	2.459730	-2.674024
O	-0.486052	1.274223	1.207274



## S-CPX-C11

C	-3.763389	-1.222245	1.026940
C	-4.407716	-1.369279	-0.243878
C	-4.414889	-1.703705	2.132901
C	-3.822956	-0.992176	-1.475729
C	-5.713027	-1.941362	-0.246595
C	-5.703480	-2.277346	2.011086
H	-3.953664	-1.643056	3.115456
C	-4.513158	-1.146419	-2.658937
H	-2.796784	-0.646606	-1.516392
C	-6.395786	-2.079395	-1.478160
H	-6.210809	-2.650266	2.899324
C	-5.821772	-1.690011	-2.660983
H	-7.388640	-2.516038	-1.452636
H	-6.369027	-1.817044	-3.587974
C	-0.705809	1.759197	2.334065
C	-3.001793	2.706219	2.701216
C	-1.712355	2.241370	3.409696
H	-0.344230	0.734469	2.471124
H	0.170386	2.406546	2.315927
H	-1.283735	3.121697	3.903415
C	-2.581574	0.971091	0.892311
H	-2.924200	1.092193	-0.137553
C	-3.608116	1.563829	1.891993
H	-4.494138	1.912305	1.352586
H	-3.954509	0.780780	2.568278
H	-3.718145	3.056081	3.449536
C	-2.642890	3.829336	1.733781
H	-3.547485	4.228326	1.265612
H	-2.157078	4.655846	2.262317
C	-1.703760	3.261142	0.660264
H	-2.149542	3.255983	-0.335979
H	-0.774541	3.825873	0.609784
N	-6.348628	-2.381688	0.877835
N	-1.307557	1.831433	0.951773
O	-3.863315	-0.759060	-3.787028
C	-4.469904	-1.000565	-5.036900
H	-5.404902	-0.437274	-5.151377
H	-3.754333	-0.658980	-5.785798
H	-4.667887	-2.068847	-5.190064
O	-1.515660	-1.204861	0.316963
H	-0.607207	-1.217411	0.752197
C	-1.950947	1.204119	4.473655
H	-2.260685	0.214679	4.140538

C	-1.802895	1.429293	5.775593
H	-1.480158	2.396606	6.155268
H	-1.991682	0.654433	6.512049
C	-0.281535	1.407424	-0.111630
H	0.035213	0.399814	0.140362
H	-0.809275	1.406386	-1.066857
C	0.946375	2.273374	-0.136887
C	1.083060	3.320879	-1.043215
C	2.028133	1.990520	0.703034
C	2.232859	4.095306	-1.095626
C	3.178948	2.768658	0.685435
H	1.963423	1.112902	1.340921
C	3.274793	3.811083	-0.220202
H	4.021405	2.538195	1.326754
F	0.084770	3.616560	-1.887652
F	2.335704	5.090053	-1.977143
F	4.381669	4.554133	-0.289384
C	-2.396202	-0.561051	1.163622
H	-2.078909	-0.674147	2.211070
C	4.373943	-3.349342	-0.643889
C	3.643418	-2.955896	0.486515
C	3.880303	-3.640604	1.696334
C	4.808215	-4.674618	1.746595
C	5.528074	-5.053924	0.615186
C	5.304790	-4.381037	-0.581932
H	4.200852	-2.841599	-1.588768
H	4.973431	-5.188314	2.692023
H	6.250800	-5.863119	0.669428
H	5.850846	-4.664441	-1.478256
C	3.130442	-3.180476	2.919956
H	3.651222	-2.310053	3.348470
H	3.125562	-3.961391	3.689210
C	1.710358	-2.759740	2.556313
H	1.202621	-2.301868	3.411305
H	1.119634	-3.640390	2.261047
C	1.698820	-1.754234	1.415224
C	2.646693	-1.872046	0.428862
C	2.696226	-0.928981	-0.720253
C	1.664381	-0.866540	-1.708074
C	3.778139	-0.071045	-0.860963
C	0.570111	-1.772616	-1.700873
C	1.701524	0.122882	-2.735347
C	3.862321	0.852277	-1.930823
C	-0.455186	-1.655979	-2.602020

H	0.558245	-2.555138	-0.950125
C	0.612389	0.237107	-3.640132
C	2.833431	0.964638	-2.827760
H	4.718759	1.511587	-2.018162
C	-0.453104	-0.622413	-3.568683
H	-1.289688	-2.349028	-2.559822
H	0.644731	1.018642	-4.396139
H	2.881953	1.705515	-3.622260
H	-1.293731	-0.524207	-4.248115
O	4.722844	-0.116916	0.120174
C	5.971329	0.482049	-0.122755
H	5.904671	1.579342	-0.158493
H	6.418405	0.120791	-1.057812
H	6.610499	0.192763	0.713121
O	0.750546	-0.856657	1.456869

S-CPX-C12

C	0.779644	3.666072	-1.318748
C	2.119358	3.271374	-0.998901
C	0.532833	5.006458	-1.466126
C	2.529097	1.930277	-0.849030
C	3.082113	4.308334	-0.819085
C	1.568410	5.954166	-1.278172
H	-0.462856	5.358481	-1.726030
C	3.837672	1.619216	-0.540386
H	1.838770	1.109793	-0.998022
C	4.410581	3.957082	-0.480309
H	1.353938	7.015123	-1.398213
C	4.791431	2.645851	-0.339577
H	5.121979	4.765018	-0.344297
H	5.819161	2.405364	-0.090956
C	-3.157469	2.326127	0.184224
C	-1.641019	2.574569	2.126484
C	-3.064333	2.876911	1.621093
H	-3.028515	3.114629	-0.562591
H	-4.123662	1.853356	0.012472
H	-3.774490	2.332384	2.255660
C	-0.701457	1.996051	-0.136222
H	-0.016649	1.157210	0.000221
C	-0.630917	2.973766	1.051586
H	0.387439	2.939078	1.448748
H	-0.803278	4.002413	0.719562
H	-1.449119	3.114722	3.057054
C	-1.514822	1.067490	2.338161

H	-0.470509	0.817716	2.525924
H	-2.089818	0.732216	3.206199
C	-2.012810	0.337560	1.083002
H	-1.338191	-0.462694	0.771802
H	-3.019408	-0.064620	1.215633
N	2.795729	5.636302	-0.956211
N	-2.090524	1.302692	-0.083810
O	4.120673	0.298386	-0.462691
C	5.391754	-0.133702	-0.023371
H	5.616177	0.253840	0.978627
H	5.335276	-1.222605	0.009342
H	6.179642	0.173608	-0.722176
O	-0.148225	1.781715	-2.538094
H	0.155817	0.894967	-2.181454
C	-3.433251	4.333495	1.651412
H	-2.801294	5.004448	1.068354
C	-4.459069	4.833643	2.333883
H	-5.114534	4.198578	2.925999
H	-4.677812	5.897068	2.333373
C	-2.402088	0.530144	-1.360669
H	-2.385514	1.254670	-2.173380
H	-1.557876	-0.154299	-1.494800
C	-3.712563	-0.210039	-1.349940
C	-3.771205	-1.538082	-0.928961
C	-4.884908	0.346085	-1.872685
C	-4.949140	-2.272550	-0.975638
C	-6.075662	-0.368112	-1.933244
H	-4.858153	1.362033	-2.255746
C	-6.099478	-1.677623	-1.478490
H	-6.981059	0.065990	-2.340742
F	-2.684423	-2.147415	-0.462789
F	-4.966284	-3.534066	-0.551914
F	-7.221213	-2.392617	-1.520761
C	-0.373222	2.672712	-1.491867
H	-1.242301	3.292576	-1.772352
C	3.509845	-3.437678	0.755719
C	2.898360	-2.919577	-0.396601
C	3.577360	-3.067774	-1.627412
C	4.826671	-3.672563	-1.670371
C	5.433926	-4.162983	-0.512925
C	4.759575	-4.049928	0.698511
H	3.005700	-3.345716	1.713264
H	5.331470	-3.770193	-2.629824
H	6.410928	-4.635063	-0.563163

H	5.208279	-4.435039	1.610822
C	2.868473	-2.591212	-2.867972
H	2.119655	-3.346067	-3.151845
H	3.568811	-2.500329	-3.706286
C	2.150086	-1.270854	-2.611120
H	1.503603	-1.006335	-3.454827
H	2.882466	-0.459728	-2.497073
C	1.293914	-1.321655	-1.359316
C	1.630753	-2.184998	-0.349526
C	0.797012	-2.260881	0.880746
C	1.045034	-1.416617	2.002671
C	-0.213823	-3.208276	0.984324
C	2.036157	-0.396195	1.940179
C	0.312378	-1.571844	3.215477
C	-0.982968	-3.330885	2.169522
C	2.283211	0.415262	3.017117
H	2.597369	-0.289873	1.018275
C	0.616082	-0.737311	4.326903
C	-0.715033	-2.540724	3.259388
H	-1.777846	-4.065746	2.230779
C	1.574488	0.237624	4.233249
H	3.039230	1.192498	2.942403
H	0.062981	-0.880258	5.252715
H	-1.292451	-2.662695	4.172862
H	1.794904	0.873596	5.085902
O	-0.416411	-4.000379	-0.098081
C	-1.393758	-5.009654	-0.032515
H	-2.401008	-4.595351	0.099451
H	-1.185945	-5.729851	0.770283
H	-1.347235	-5.526933	-0.992148
O	0.315643	-0.467894	-1.288297

S-CPX-C13

C	2.833103	-1.846819	-0.245204
C	4.237968	-1.873426	-0.502764
C	2.224480	-3.007631	0.161131
C	4.991911	-0.753865	-0.929870
C	4.911370	-3.112324	-0.299347
C	2.993708	-4.182627	0.324267
H	1.156103	-3.024721	0.361557
C	6.351760	-0.843509	-1.131298
H	4.525410	0.206390	-1.120793
C	6.308113	-3.175606	-0.525240
H	2.505941	-5.099601	0.649830

C	7.021743	-2.075634	-0.926079
H	6.795564	-4.131527	-0.364585
H	8.090422	-2.160851	-1.085605
C	1.949448	2.436950	0.836264
C	2.890703	1.271759	2.821428
C	2.934526	2.585492	2.015763
H	2.461141	2.207642	-0.101625
H	1.382150	3.353994	0.687590
H	2.587700	3.397857	2.666697
C	1.716025	-0.038529	1.022794
H	1.009740	-0.726335	1.495717
C	3.007280	0.097125	1.853257
H	3.161742	-0.840454	2.393529
H	3.880037	0.226688	1.207529
H	3.703961	1.255646	3.551445
C	1.531533	1.178794	3.518768
H	1.414740	0.192193	3.977682
H	1.449510	1.924205	4.315695
C	0.423910	1.417928	2.479548
H	-0.368146	0.667487	2.532945
H	-0.012376	2.413051	2.573938
N	4.285763	-4.250702	0.111697
N	0.974000	1.319812	1.075599
O	6.973724	0.297743	-1.524875
C	8.362359	0.258854	-1.770240
H	8.612866	-0.448716	-2.570462
H	8.637566	1.266240	-2.084922
H	8.925933	-0.001883	-0.865180
O	0.801805	-0.883783	-1.091273
H	0.116280	-1.225250	-0.449659
C	4.306113	2.945466	1.514288
H	4.788166	2.225739	0.851244
C	4.944052	4.069925	1.825042
H	4.499811	4.819054	2.477002
H	5.936302	4.282755	1.439596
C	-0.193717	1.395908	0.086301
H	0.226633	1.268679	-0.907731
H	-0.806824	0.515063	0.304935
C	-0.994735	2.661436	0.180937
C	-0.736310	3.722620	-0.683016
C	-2.085000	2.784829	1.045787
C	-1.499098	4.882206	-0.671860
C	-2.851734	3.940685	1.088761
H	-2.364418	1.939611	1.665265

C	-2.553538	4.982655	0.226947
H	-3.709673	4.025631	1.744517
F	0.283315	3.651912	-1.550044
F	-1.220459	5.879376	-1.508720
F	-3.282991	6.098061	0.228951
C	1.970840	-0.593293	-0.395548
H	2.515325	0.150303	-0.990648
C	-5.255913	-2.759809	-0.359837
C	-4.063418	-2.961901	0.353258
C	-4.008734	-4.059812	1.241756
C	-5.122688	-4.869687	1.425583
C	-6.309485	-4.638001	0.731768
C	-6.362076	-3.582643	-0.172189
H	-5.316724	-1.944609	-1.074437
H	-5.056238	-5.705212	2.120411
H	-7.172243	-5.279055	0.888482
H	-7.271643	-3.391446	-0.735942
C	-2.690752	-4.369467	1.907045
H	-2.080838	-4.960069	1.205838
H	-2.842864	-4.992183	2.796569
C	-1.922671	-3.099524	2.255451
H	-0.904264	-3.332888	2.584344
H	-2.417109	-2.575606	3.088344
C	-1.836555	-2.154957	1.067791
C	-2.894388	-2.088688	0.196590
C	-2.833843	-1.076150	-0.891847
C	-3.566234	0.147060	-0.819750
C	-2.011204	-1.287394	-1.990248
C	-4.470028	0.412142	0.251083
C	-3.433401	1.134372	-1.839819
C	-1.840786	-0.289556	-2.981938
C	-5.223712	1.556773	0.274691
H	-4.571081	-0.333192	1.033367
C	-4.211674	2.321363	-1.774289
C	-2.532240	0.891662	-2.901981
H	-1.157264	-0.451473	-3.807246
C	-5.100177	2.525164	-0.752290
H	-5.928467	1.722096	1.085506
H	-4.099587	3.061871	-2.563433
H	-2.403687	1.649064	-3.671690
H	-5.701429	3.429592	-0.720579
O	-1.369308	-2.481272	-2.039212
C	-0.520133	-2.757460	-3.128851
H	0.324286	-2.061070	-3.157375

H	-1.065066	-2.736250	-4.082349
H	-0.142983	-3.767171	-2.958171
O	-0.765187	-1.419733	0.992029

S-CPX-C14

C	-0.344009	-0.210963	2.452616
C	-1.114305	-1.416581	2.460828
C	0.505301	0.005548	3.506801
C	-1.981200	-1.802483	1.416738
C	-0.940378	-2.298257	3.566220
C	0.584075	-0.928018	4.568231
H	1.155182	0.876490	3.524892
C	-2.639408	-3.011058	1.447786
H	-2.090900	-1.191801	0.533920
C	-1.644206	-3.525497	3.580032
H	1.257386	-0.735180	5.402558
C	-2.474108	-3.886730	2.548333
H	-1.493466	-4.178869	4.433006
H	-2.989138	-4.839923	2.585652
C	-0.543334	3.633235	0.253352
C	-1.885272	3.857424	2.356222
C	-0.594834	4.313850	1.644130
H	0.391510	3.098800	0.039564
H	-0.683107	4.370319	-0.541546
H	-0.687372	5.394721	1.484410
C	-1.648155	1.594698	1.220186
H	-2.476931	0.926576	0.975994
C	-1.899661	2.342022	2.553322
H	-2.858952	2.033734	2.980878
H	-1.135846	2.049432	3.276408
H	-1.961040	4.362040	3.323076
C	-3.067003	4.223573	1.462481
H	-4.012422	4.031397	1.978065
H	-3.043846	5.288715	1.210450
C	-2.991504	3.371283	0.187793
H	-3.767894	2.605276	0.156736
H	-3.083820	3.976387	-0.712346
N	-0.103075	-2.040593	4.613073
N	-1.673007	2.637843	0.082233
O	-3.421434	-3.293227	0.371683
C	-4.034388	-4.560162	0.295665
H	-4.762383	-4.709849	1.103357
H	-4.557290	-4.582184	-0.661503
H	-3.293051	-5.369132	0.319783



O	-0.144302	0.061981	0.099714
H	0.649769	0.533879	-0.366150
C	0.656199	4.091341	2.450435
H	0.969247	3.062155	2.610300
C	1.387126	5.075211	2.965466
H	1.124695	6.121014	2.818945
H	2.282962	4.873031	3.544163
C	-1.547065	2.091541	-1.350898
H	-1.608849	2.989980	-1.970010
H	-0.541364	1.686960	-1.446998
C	-2.593661	1.103200	-1.793164
C	-3.790206	1.536861	-2.367678
C	-2.355860	-0.275774	-1.780621
C	-4.746358	0.649212	-2.839499
C	-3.298558	-1.183343	-2.246794
H	-1.412351	-0.634611	-1.386623
C	-4.493704	-0.715854	-2.763788
H	-3.105375	-2.247709	-2.197824
F	-4.055414	2.848339	-2.500101
F	-5.882838	1.105436	-3.364564
F	-5.425377	-1.557605	-3.211456
C	-0.345505	0.755311	1.271520
H	0.493822	1.444506	1.437091
C	5.286141	-1.371098	-1.664273
C	4.743043	-0.090119	-1.487954
C	5.572516	1.022017	-1.747898
C	6.878156	0.834108	-2.184712
C	7.403031	-0.445185	-2.363662
C	6.597573	-1.547208	-2.093889
H	4.663830	-2.239509	-1.465954
H	7.498659	1.706720	-2.382138
H	8.425367	-0.576600	-2.706764
H	6.988472	-2.553119	-2.225539
C	5.010349	2.393977	-1.472788
H	5.114210	2.602995	-0.396675
H	5.583373	3.162739	-2.004684
C	3.530076	2.467701	-1.833836
H	3.091331	3.413249	-1.497879
H	3.403517	2.423569	-2.926230
C	2.745205	1.329154	-1.206088
C	3.354784	0.110792	-1.056403
C	2.598220	-1.036122	-0.483352
C	1.636339	-1.760038	-1.250970
C	2.783570	-1.396766	0.842383

C	1.377508	-1.435680	-2.611816
C	0.869979	-2.801661	-0.653670
C	2.048139	-2.454441	1.430917
C	0.413341	-2.098358	-3.327453
H	1.966770	-0.646339	-3.067752
C	-0.128127	-3.463919	-1.415594
C	1.108729	-3.130626	0.698888
H	2.189603	-2.709382	2.475531
C	-0.353837	-3.125769	-2.724889
H	0.234929	-1.837318	-4.366931
H	-0.712640	-4.246567	-0.936563
H	0.517021	-3.912914	1.169095
H	-1.112449	-3.644919	-3.304961
O	3.676413	-0.655036	1.555590
C	4.105528	-1.141159	2.802113
H	3.302109	-1.128016	3.552005
H	4.503219	-2.161705	2.725322
H	4.903682	-0.470614	3.126070
O	1.507244	1.598798	-0.898097

S-CPX-C15

C	-2.890595	-1.835730	0.145844
C	-4.305805	-1.872689	0.337606
C	-2.257376	-2.988579	-0.245752
C	-5.086224	-0.759620	0.732971
C	-4.961434	-3.114703	0.097450
C	-3.011448	-4.166509	-0.451735
H	-1.181751	-2.994005	-0.409334
C	-6.452775	-0.860127	0.875146
H	-4.635371	0.202768	0.948410
C	-6.365944	-3.189175	0.262665
H	-2.504356	-5.077487	-0.764762
C	-7.104244	-2.096252	0.637624
H	-6.839141	-4.147834	0.077531
H	-8.177830	-2.190505	0.752718
C	-1.906345	2.431300	-0.914065
C	-2.740604	1.250694	-2.938766
C	-2.818868	2.574464	-2.151197
H	-2.473502	2.215750	-0.005447
H	-1.338497	3.343816	-0.740371
H	-2.426259	3.375980	-2.789509
C	-1.686399	-0.048562	-1.056339
H	-0.955092	-0.749518	-1.468828
C	-2.922666	0.085740	-1.968543

H	-3.049460	-0.855439	-2.509572
H	-3.832985	0.224839	-1.378140
H	-3.511101	1.233927	-3.713719
C	-1.344868	1.138960	-3.555395
H	-1.210037	0.146088	-3.995508
H	-1.209988	1.874250	-4.354612
C	-0.299283	1.382287	-2.455574
H	0.492422	0.630216	-2.458401
H	0.149267	2.373599	-2.532832
N	-4.310730	-4.245984	-0.294042
N	-0.931367	1.301861	-1.085897
O	-7.100270	0.275167	1.245446
C	-8.495883	0.221550	1.441299
H	-8.767573	-0.491780	2.229452
H	-8.792535	1.224784	1.749926
H	-9.024853	-0.040929	0.516064
O	-0.943839	-0.843585	1.157061
H	-0.220610	-1.236459	0.603724
C	-4.214953	2.951595	-1.737875
H	-4.745979	2.239701	-1.104568
C	-4.818858	4.081656	-2.093087
H	-4.324008	4.822578	-2.717423
H	-5.831743	4.307619	-1.774583
C	0.174812	1.373364	-0.035005
H	-0.303581	1.275677	0.936287
H	0.777045	0.474231	-0.195697
C	1.022756	2.610449	-0.106671
C	0.753113	3.695340	0.723876
C	2.190066	2.656791	-0.872671
C	1.586905	4.803448	0.778864
C	3.040363	3.754398	-0.837872
H	2.477305	1.789242	-1.456093
C	2.730621	4.822547	-0.011417
H	3.957975	3.775696	-1.413625
F	-0.339369	3.694856	1.499219
F	1.296398	5.826779	1.579079
F	3.526614	5.889507	0.052253
C	-2.045476	-0.577051	0.350649
H	-2.640787	0.173965	0.883402
C	5.323961	-2.581977	0.376139
C	4.299956	-2.471940	-0.576932
C	4.505694	-3.066832	-1.840000
C	5.695543	-3.729466	-2.115839
C	6.709736	-3.820871	-1.163116

C	6.514870	-3.241417	0.086735
H	5.173363	-2.152230	1.363276
H	5.833110	-4.180874	-3.096853
H	7.634432	-4.341971	-1.393710
H	7.287098	-3.312693	0.848502
C	3.411114	-2.914108	-2.865242
H	3.503422	-1.922424	-3.335939
H	3.518977	-3.658916	-3.662378
C	2.036628	-3.009261	-2.207362
H	1.238672	-2.781076	-2.921946
H	1.862196	-4.033596	-1.845002
C	1.912205	-2.044927	-1.036639
C	3.034489	-1.791837	-0.283418
C	2.956324	-0.847010	0.857431
C	2.170385	-1.138779	2.021777
C	3.622405	0.363397	0.815336
C	1.543520	-2.402149	2.189587
C	2.015808	-0.166123	3.049194
C	3.493701	1.324556	1.847742
C	0.777056	-2.668996	3.293735
H	1.689623	-3.152205	1.419424
C	1.203986	-0.466494	4.174190
C	2.691850	1.075463	2.928166
H	4.001948	2.279161	1.742983
C	0.592721	-1.686714	4.293479
H	0.303186	-3.640122	3.402400
H	1.083085	0.290114	4.946219
H	2.571222	1.823858	3.707728
H	-0.025943	-1.906619	5.158747
O	4.353719	0.685613	-0.306047
C	5.741291	0.857598	-0.093676
H	5.952711	1.697692	0.582533
H	6.190748	-0.056937	0.308485
H	6.179878	1.067757	-1.071504
O	0.734915	-1.544357	-0.821800

S-CPX-C16

C	2.774906	-2.347642	1.256871
C	3.888149	-1.575744	0.788254
C	3.040213	-3.491131	1.964998
C	3.769996	-0.368430	0.062374
C	5.190452	-2.083674	1.077351
C	4.375749	-3.896645	2.201558
H	2.226803	-4.098469	2.354972

C	4.896297	0.302655	-0.368263
H	2.807153	0.079730	-0.162766
C	6.321465	-1.368530	0.620565
H	4.569949	-4.809312	2.763003
C	6.189410	-0.202116	-0.088281
H	7.298795	-1.778537	0.852452
H	7.076256	0.323613	-0.423366
C	-1.053125	-3.562060	-0.601448
C	0.720612	-3.800992	-2.317694
C	-0.529928	-4.480552	-1.724867
H	-0.725529	-3.892094	0.387485
H	-2.141060	-3.535139	-0.599555
H	-1.291855	-4.546820	-2.511553
C	0.968595	-2.100603	-0.492611
H	1.273557	-1.178624	-0.990689
C	1.608571	-3.324096	-1.167330
H	2.597004	-3.026490	-1.528299
H	1.774408	-4.129513	-0.444321
H	1.259192	-4.499163	-2.963438
C	0.257544	-2.571036	-3.105766
H	1.120766	-1.964277	-3.397183
H	-0.259802	-2.867989	-4.023087
C	-0.698294	-1.748010	-2.225231
H	-0.471017	-0.679282	-2.249982
H	-1.743363	-1.914266	-2.490907
N	5.419543	-3.234907	1.774865
N	-0.554285	-2.154536	-0.775144
O	4.676954	1.447755	-1.059440
C	5.778415	2.217545	-1.483554
H	6.407605	1.667004	-2.195034
H	5.353139	3.091259	-1.978604
H	6.391225	2.547604	-0.635099
O	1.031935	-0.696826	1.515960
H	0.978085	-0.021798	0.786479
C	-0.286464	-5.867472	-1.199169
H	0.471139	-5.965652	-0.421075
C	-0.933000	-6.950862	-1.618936
H	-1.700074	-6.896278	-2.388275
H	-0.720771	-7.933536	-1.209393
C	-1.354268	-1.184661	0.098725
H	-1.155402	-1.448990	1.134508
H	-0.914333	-0.201211	-0.094913
C	-2.828515	-1.185399	-0.180214
C	-3.692028	-1.939079	0.610449

C	-3.396884	-0.360548	-1.153673
C	-5.067667	-1.910407	0.429459
C	-4.767935	-0.327771	-1.366431
H	-2.754391	0.300623	-1.724577
C	-5.594742	-1.102317	-0.570195
H	-5.209086	0.329625	-2.105513
F	-3.201077	-2.736496	1.569878
F	-5.864372	-2.647085	1.200838
F	-6.917001	-1.077648	-0.735526
C	1.320891	-1.958642	1.002311
H	0.718194	-2.690739	1.565557
C	-0.536192	5.338958	0.150070
C	0.311910	4.377549	-0.421788
C	1.362621	4.835106	-1.248846
C	1.507800	6.192370	-1.508671
C	0.641545	7.133556	-0.953682
C	-0.375439	6.695795	-0.112384
H	-1.333109	5.017384	0.813792
H	2.322296	6.520510	-2.152484
H	0.769530	8.190990	-1.166788
H	-1.054442	7.412145	0.343113
C	2.355018	3.820396	-1.759250
H	3.101605	3.636896	-0.971451
H	2.893018	4.212012	-2.631767
C	1.689235	2.488139	-2.081388
H	2.442852	1.723918	-2.290000
H	1.056766	2.585117	-2.977928
C	0.825282	2.012638	-0.926783
C	0.147005	2.939860	-0.178835
C	-0.797827	2.442126	0.856953
C	-2.206470	2.418084	0.630693
C	-0.313650	1.942536	2.058491
C	-2.778656	2.965966	-0.555109
C	-3.089407	1.865654	1.604195
C	-1.183109	1.351085	3.008879
C	-4.137008	3.003515	-0.733583
H	-2.109499	3.381185	-1.301923
C	-4.492028	1.900092	1.379326
C	-2.534780	1.311256	2.780794
H	-0.783565	0.924205	3.921426
C	-5.010059	2.469196	0.246426
H	-4.551052	3.452070	-1.632874
H	-5.151152	1.479566	2.135832
H	-3.197032	0.866013	3.519584

H	-6.084915	2.505634	0.092510
O	1.024751	2.033591	2.248106
C	1.581076	1.566832	3.455390
H	1.426872	0.489372	3.572054
H	1.175429	2.107096	4.321583
H	2.651135	1.765207	3.378275
O	0.739142	0.721929	-0.759053

S-CPX-C17

C	3.752169	-0.554943	1.376460
C	4.389785	0.644465	0.923551
C	4.504419	-1.447042	2.095525
C	3.735003	1.657534	0.186427
C	5.775576	0.792925	1.223859
C	5.871318	-1.186484	2.357326
H	4.058728	-2.363749	2.473918
C	4.433244	2.760017	-0.263009
H	2.670306	1.612087	-0.013671
C	6.456769	1.941950	0.759501
H	6.455386	-1.902110	2.933869
C	5.812189	2.905355	0.027762
H	7.510635	2.031722	1.001066
H	6.362463	3.772966	-0.317782
C	1.260097	-3.448448	-0.702978
C	2.773480	-2.470259	-2.406054
C	2.174786	-3.796884	-1.895231
H	1.757760	-3.600381	0.258085
H	0.359680	-4.059944	-0.712254
H	1.562820	-4.230644	-2.696007
C	2.054702	-1.098264	-0.434202
H	1.747829	-0.137240	-0.851135
C	3.260991	-1.661353	-1.203047
H	3.878987	-0.816639	-1.519420
H	3.889666	-2.277166	-0.552209
H	3.593267	-2.670228	-3.100729
C	1.653596	-1.681114	-3.092644
H	1.991297	-0.663849	-3.314179
H	1.373193	-2.148317	-4.041442
C	0.430790	-1.646584	-2.160647
H	-0.016859	-0.651778	-2.090384
H	-0.327925	-2.372435	-2.456640
N	6.499289	-0.119715	1.935930
N	0.841115	-2.005710	-0.749092
O	3.727776	3.665158	-0.983167

C	4.342153	4.879102	-1.350846
H	5.170943	4.719140	-2.052828
H	3.565386	5.465565	-1.842869
H	4.708010	5.427902	-0.474109
O	1.439691	0.063462	1.636071
H	0.940014	0.543484	0.922398
C	3.200411	-4.818777	-1.491652
H	3.913047	-4.515302	-0.724187
C	3.277933	-6.042882	-2.005073
H	2.581868	-6.387187	-2.766910
H	4.038645	-6.747463	-1.683756
C	-0.332365	-1.743306	0.193235
H	0.015600	-1.937065	1.205248
H	-0.540773	-0.673600	0.087398
C	-1.556286	-2.552342	-0.116126
C	-1.815852	-3.736175	0.569633
C	-2.527722	-2.092174	-1.007270
C	-2.978742	-4.463207	0.361963
C	-3.690773	-2.811671	-1.247615
H	-2.392303	-1.123680	-1.479060
C	-3.909072	-3.992306	-0.557837
H	-4.451934	-2.443637	-1.924674
F	-0.927105	-4.209041	1.453947
F	-3.196722	-5.593076	1.031712
F	-5.022666	-4.699484	-0.750825
C	2.293758	-0.888094	1.080468
H	2.115233	-1.853974	1.584823
C	-3.301816	4.291871	0.834542
C	-2.176737	3.943112	0.071678
C	-1.438254	4.984885	-0.526234
C	-1.833483	6.307570	-0.365595
C	-2.961779	6.638375	0.383575
C	-3.692850	5.619296	0.985572
H	-3.873158	3.507629	1.324030
H	-1.249001	7.094002	-0.839909
H	-3.257033	7.676989	0.501922
H	-4.567298	5.855766	1.586620
C	-0.243465	4.592222	-1.353656
H	-0.590213	4.278787	-2.350425
H	0.429258	5.445969	-1.499051
C	0.492708	3.421112	-0.710229
H	1.281236	3.053579	-1.371579
H	0.987459	3.743900	0.218012
C	-0.440828	2.261789	-0.405262



C	-1.743199	2.542590	-0.078604
C	-2.765729	1.487956	0.144321
C	-2.732931	0.592508	1.263619
C	-3.842148	1.392804	-0.724568
C	-1.668199	0.622646	2.203132
C	-3.774048	-0.360740	1.460997
C	-4.901860	0.478772	-0.503812
C	-1.593229	-0.293209	3.221145
H	-0.902657	1.381027	2.089564
C	-3.675049	-1.292572	2.527641
C	-4.872487	-0.373387	0.566470
H	-5.723665	0.445646	-1.213648
C	-2.600065	-1.275178	3.378981
H	-0.750855	-0.264226	3.905299
H	-4.466237	-2.028943	2.651207
H	-5.673335	-1.092384	0.721525
H	-2.527378	-2.002105	4.182982
O	-3.853000	2.167647	-1.854383
C	-4.935567	3.069736	-1.983953
H	-5.902730	2.551770	-2.045463
H	-4.953646	3.781230	-1.151200
H	-4.767856	3.612515	-2.916108
O	0.093496	1.072179	-0.452915

S-CPX-C18

C	-2.943745	-1.597197	0.047319
C	-4.351031	-1.627252	0.292476
C	-2.354195	-2.712279	-0.494173
C	-5.087112	-0.556421	0.854702
C	-5.047237	-2.817722	-0.065912
C	-3.145595	-3.842064	-0.804683
H	-1.284122	-2.725722	-0.688434
C	-6.449465	-0.644262	1.038834
H	-4.604243	0.362446	1.168713
C	-6.446375	-2.881273	0.144289
H	-2.673117	-4.722077	-1.237268
C	-7.141920	-1.826884	0.677639
H	-6.950454	-3.800201	-0.136326
H	-8.212709	-1.911630	0.822195
C	-1.843893	2.749728	-0.438096
C	-2.871968	1.933244	-2.550978
C	-2.830549	3.120226	-1.566627
H	-2.363852	2.409054	0.461350
H	-1.222321	3.602351	-0.164751

H	-2.443262	3.996906	-2.100481
C	-1.751971	0.319622	-0.969858
H	-1.083680	-0.340987	-1.528578
C	-3.037477	0.637198	-1.761348
H	-3.240927	-0.201301	-2.432611
H	-3.899853	0.710649	-1.092883
H	-3.695654	2.064413	-3.257576
C	-1.531031	1.865690	-3.282775
H	-1.475235	0.944880	-3.871493
H	-1.416541	2.705237	-3.975206
C	-0.401215	1.901280	-2.242883
H	0.359644	1.141232	-2.419544
H	0.073063	2.882840	-2.200750
N	-4.440672	-3.909568	-0.610236
N	-0.934402	1.630540	-0.853961
O	-7.051507	0.450091	1.573206
C	-8.443745	0.411413	1.796824
H	-8.719642	-0.383836	2.500598
H	-8.702687	1.377418	2.231942
H	-8.999868	0.277433	0.860231
O	-0.917739	-0.790573	1.059332
H	-0.233912	-1.100119	0.392094
C	-4.174384	3.478765	-0.994273
H	-4.700468	2.689363	-0.455388
C	-4.740030	4.676838	-1.106855
H	-4.249969	5.494571	-1.631091
H	-5.716102	4.884387	-0.679477
C	0.254974	1.509569	0.107385
H	-0.157803	1.280295	1.087528
H	0.802522	0.623062	-0.230820
C	1.131826	2.728147	0.176812
C	2.222839	2.878235	-0.676679
C	0.966563	3.689172	1.180197
C	3.087793	3.958987	-0.575533
C	1.819714	4.778114	1.303326
H	0.158351	3.565983	1.895070
C	2.878325	4.904241	0.418325
H	1.693514	5.517755	2.085175
F	2.471748	1.980643	-1.630479
F	4.124776	4.063179	-1.401163
F	3.727362	5.926507	0.515051
C	-2.056041	-0.393096	0.367853
H	-2.603799	0.290407	1.028604
C	4.956337	-2.960326	0.353262

C	3.828000	-2.972230	-0.481582
C	3.850469	-3.828262	-1.605994
C	4.976436	-4.593967	-1.881621
C	6.098903	-4.554077	-1.055505
C	6.075102	-3.737921	0.070276
H	4.956430	-2.329628	1.237447
H	4.970409	-5.243697	-2.755268
H	6.972517	-5.157354	-1.285565
H	6.933377	-3.700527	0.736471
C	2.595754	-3.937236	-2.435779
H	1.915784	-4.649352	-1.942684
H	2.820446	-4.347058	-3.427575
C	1.882049	-2.594850	-2.545703
H	0.901241	-2.707618	-3.019976
H	2.468461	-1.905751	-3.172978
C	1.683393	-1.962630	-1.178939
C	2.646949	-2.141526	-0.220493
C	2.488228	-1.425745	1.074477
C	3.184097	-0.207528	1.339217
C	1.599642	-1.898350	2.029534
C	4.122998	0.328266	0.410471
C	2.955631	0.511088	2.548678
C	1.368819	-1.186267	3.232573
C	4.801856	1.487948	0.679094
H	4.292254	-0.207565	-0.517096
C	3.658947	1.722671	2.788331
C	2.027006	-0.010038	3.478927
H	0.655936	-1.558338	3.959009
C	4.567592	2.200126	1.881796
H	5.514586	1.875541	-0.043388
H	3.469485	2.259300	3.715536
H	1.844508	0.529450	4.405490
H	5.106401	3.123290	2.077308
O	0.949945	-3.053043	1.732441
C	-0.104940	-3.472620	2.566344
H	-0.881487	-2.702454	2.634405
H	0.250454	-3.743718	3.570039
H	-0.521885	-4.361707	2.089695
O	0.612651	-1.236305	-1.031107
S-CPX-C19			
C	3.257641	-1.705925	1.225970
C	4.140101	-0.725514	0.664207
C	3.812059	-2.713894	1.971807

C	3.713930	0.377421	-0.109898
C	5.535620	-0.898332	0.910717
C	5.213779	-2.784959	2.156611
H	3.179482	-3.468345	2.433843
C	4.632750	1.266565	-0.628747
H	2.665031	0.577136	-0.308324
C	6.447643	0.035909	0.367730
H	5.638356	-3.593563	2.749826
C	6.017802	1.097126	-0.387416
H	7.502042	-0.118758	0.571284
H	6.741947	1.797843	-0.787411
C	-0.322971	-3.820105	-0.297133
C	1.382468	-3.841230	-2.097894
C	0.324003	-4.705699	-1.381781
H	0.124913	-3.990128	0.685946
H	-1.391920	-4.013538	-0.216034
H	-0.443310	-4.986991	-2.113503
C	1.353071	-1.977337	-0.416306
H	1.437659	-1.050503	-0.985969
C	2.201724	-3.096130	-1.043859
H	3.088395	-2.634041	-1.486707
H	2.566198	-3.787696	-0.277034
H	2.024350	-4.471045	-2.719163
C	0.644155	-2.802061	-2.945909
H	1.350784	-2.059065	-3.328675
H	0.162135	-3.271434	-3.808831
C	-0.423885	-2.121766	-2.074323
H	-0.440702	-1.038238	-2.196654
H	-1.417957	-2.528534	-2.264292
N	6.055589	-1.923379	1.647961
N	-0.138585	-2.361455	-0.607215
O	4.122108	2.282404	-1.366631
C	4.989642	3.275907	-1.862053
H	5.718955	2.862979	-2.571495
H	4.351029	3.992342	-2.380084
H	5.521144	3.788545	-1.050117
O	1.200333	-0.480800	1.523563
H	0.969384	0.130415	0.765533
C	0.870294	-5.967720	-0.775331
H	1.665170	-5.847761	-0.038336
C	0.444045	-7.189928	-1.079796
H	-0.349115	-7.353446	-1.806160
H	0.875066	-8.073491	-0.619341
C	-1.087310	-1.500327	0.233162

H	-0.761973	-1.588265	1.268165
H	-0.890075	-0.470925	-0.084603
C	-2.539536	-1.870211	0.126913
C	-3.359715	-1.345412	-0.869414
C	-3.149773	-2.655477	1.111273
C	-4.720126	-1.618761	-0.914549
C	-4.508319	-2.940628	1.089513
H	-2.540760	-3.038068	1.924911
C	-5.286066	-2.415287	0.070466
H	-4.978624	-3.542407	1.858178
F	-2.859754	-0.558896	-1.822833
F	-5.474262	-1.092544	-1.874426
F	-6.596800	-2.650244	0.024433
C	1.741170	-1.669104	1.045207
H	1.353260	-2.487474	1.675888
C	-1.705181	4.936679	0.195767
C	-0.707410	4.187593	-0.446331
C	0.087412	4.840278	-1.415127
C	-0.152305	6.171016	-1.735267
C	-1.162386	6.896690	-1.104369
C	-1.930462	6.270756	-0.128613
H	-2.315313	4.465483	0.960497
H	0.471188	6.652230	-2.487132
H	-1.337525	7.936474	-1.365560
H	-2.716087	6.819934	0.384214
C	1.237140	4.069715	-2.014302
H	2.083673	4.108800	-1.311564
H	1.568936	4.533939	-2.951454
C	0.883583	2.601527	-2.223961
H	1.771464	2.029599	-2.508406
H	0.145108	2.498072	-3.034313
C	0.307690	1.994534	-0.957090
C	-0.468207	2.772945	-0.139991
C	-1.103156	2.137752	1.046445
C	-2.468049	1.721769	1.026641
C	-0.355966	1.897841	2.190956
C	-3.300370	1.962859	-0.104790
C	-3.041999	1.058371	2.150102
C	-0.914765	1.215608	3.300239
C	-4.620949	1.598003	-0.103105
H	-2.862046	2.452360	-0.967891
C	-4.410649	0.676489	2.115175
C	-2.222619	0.805089	3.274426
H	-0.308041	1.007602	4.173944

C	-5.188759	0.948169	1.021273
H	-5.237411	1.796646	-0.974918
H	-4.833058	0.173208	2.982164
H	-2.646931	0.291170	4.133988
H	-6.236659	0.660733	1.006435
O	0.928665	2.330420	2.169605
C	1.776786	2.017547	3.249418
H	1.872444	0.933662	3.373965
H	1.431761	2.480546	4.184306
H	2.750410	2.434170	2.986258
O	0.555658	0.729067	-0.754682

S-CPX-C20

C	-2.978521	-1.768745	0.152335
C	-4.396494	-1.751189	0.326859
C	-2.383233	-2.948835	-0.217278
C	-5.140420	-0.606811	0.702640
C	-5.094712	-2.970415	0.089698
C	-3.178267	-4.100133	-0.420781
H	-1.306400	-2.997225	-0.366398
C	-6.511396	-0.655884	0.828970
H	-4.657472	0.340248	0.916750
C	-6.503053	-2.991412	0.236803
H	-2.701071	-5.032778	-0.716476
C	-7.205223	-1.868931	0.592912
H	-7.008285	-3.934000	0.053679
H	-8.282998	-1.922076	0.694975
C	-1.800370	2.440977	-0.932468
C	-2.675248	1.282092	-2.954719
C	-2.706147	2.610742	-2.171675
H	-2.375571	2.259890	-0.021634
H	-1.192387	3.329225	-0.767717
H	-2.284330	3.394902	-2.812920
C	-1.686983	-0.047422	-1.055210
H	-0.979655	-0.784253	-1.446988
C	-2.906920	0.127165	-1.983580
H	-3.060457	-0.810498	-2.523825
H	-3.818417	0.299727	-1.404014
H	-3.442503	1.293296	-3.732997
C	-1.282773	1.113451	-3.564807
H	-1.185859	0.115535	-4.003365
H	-1.114248	1.841903	-4.363890
C	-0.234308	1.315429	-2.459741
H	0.525786	0.531548	-2.456288

H	0.255963	2.286628	-2.538440
N	-4.481647	-4.129210	-0.281366
N	-0.875191	1.269020	-1.092536
O	-7.120781	0.505540	1.182538
C	-8.519174	0.504421	1.365690
H	-8.823841	-0.192946	2.156077
H	-8.781235	1.520184	1.664448
H	-9.049065	0.255028	0.437357
O	-1.016516	-0.830902	1.187365
H	-0.303600	-1.272218	0.658920
C	-4.088387	3.039465	-1.761791
H	-4.644891	2.350739	-1.124762
C	-4.651715	4.187625	-2.125498
H	-4.130055	4.906154	-2.754147
H	-5.656277	4.451453	-1.809690
C	0.229771	1.297855	-0.038645
H	-0.255255	1.223458	0.931345
H	0.791383	0.371706	-0.191844
C	1.130598	2.496800	-0.110143
C	0.906596	3.588665	0.724691
C	2.296816	2.499106	-0.879656
C	1.785680	4.661085	0.784169
C	3.189002	3.563176	-0.844301
H	2.546254	1.622657	-1.467269
C	2.926391	4.638010	-0.009689
H	4.100129	3.556824	-1.431052
F	-0.184172	3.630628	1.500264
F	1.539049	5.691697	1.589517
F	3.765160	5.671525	0.054913
C	-2.090899	-0.539035	0.353496
H	-2.667923	0.242929	0.861096
C	5.335830	-2.507296	0.291370
C	4.261664	-2.464542	-0.610211
C	4.445544	-3.047344	-1.881636
C	5.656246	-3.646785	-2.209848
C	6.715194	-3.680072	-1.304237
C	6.545935	-3.101483	-0.049875
H	5.209879	-2.075316	1.280846
H	5.773844	-4.092850	-3.195973
H	7.654614	-4.153872	-1.574164
H	7.355489	-3.122483	0.675419
C	3.309995	-2.945097	-2.867824
H	3.349031	-1.954596	-3.349099
H	3.418621	-3.690743	-3.664173

C	1.963084	-3.086782	-2.165074
H	1.133966	-2.888056	-2.852506
H	1.837065	-4.115926	-1.796594
C	1.841377	-2.128910	-0.988647
C	2.975437	-1.848915	-0.258694
C	2.899323	-0.933373	0.904598
C	2.085114	-1.225275	2.046953
C	3.618358	0.250468	0.909739
C	1.430270	-2.479040	2.188090
C	1.936278	-0.267475	3.089833
C	3.500769	1.192428	1.959149
C	0.637844	-2.743810	3.273539
H	1.578824	-3.224430	1.414312
C	1.093323	-0.564274	4.193717
C	2.656937	0.949777	3.010810
H	4.048080	2.128716	1.903943
C	0.451467	-1.770313	4.282794
H	0.145501	-3.707865	3.361663
H	0.975801	0.183967	4.974411
H	2.545659	1.685761	3.803418
H	-0.191037	-1.988228	5.130959
O	4.397820	0.517419	-0.186287
C	5.664888	1.084243	0.056072
H	5.602439	2.160635	0.273412
H	6.173166	0.578611	0.885756
H	6.244034	0.939649	-0.858188
O	0.655966	-1.661386	-0.750202

S-CPX-C21

C	3.797070	-0.471295	1.363207
C	4.393040	0.755804	0.928289
C	4.585164	-1.356155	2.052057
C	3.697845	1.766005	0.225076
C	5.778599	0.937551	1.210824
C	5.947751	-1.061791	2.300125
H	4.171381	-2.293330	2.416426
C	4.357088	2.897982	-0.209522
H	2.631643	1.694520	0.040913
C	6.419579	2.115227	0.761080
H	6.560280	-1.772145	2.853167
C	5.736143	3.075786	0.061535
H	7.474405	2.229511	0.987593
H	6.255783	3.965968	-0.273990
C	1.370238	-3.392777	-0.750309



C	2.828569	-2.328028	-2.449579
C	2.280942	-3.684545	-1.960449
H	1.883720	-3.550563	0.201438
H	0.489901	-4.032883	-0.763671
H	1.673580	-4.121167	-2.763165
C	2.092583	-1.024483	-0.438037
H	1.747333	-0.064912	-0.827940
C	3.306041	-1.529344	-1.235811
H	3.890656	-0.657414	-1.541610
H	3.963592	-2.137740	-0.606980
H	3.644691	-2.485421	-3.159378
C	1.673901	-1.562065	-3.104097
H	1.974501	-0.529729	-3.308613
H	1.395702	-2.018680	-4.058690
C	0.463513	-1.586541	-2.155383
H	-0.013009	-0.607775	-2.056256
H	-0.276609	-2.328802	-2.457633
N	6.538816	0.031120	1.892280
N	0.904853	-1.963951	-0.758075
O	3.614081	3.799001	-0.896212
C	4.183274	5.042588	-1.236521
H	5.002627	4.931376	-1.958747
H	3.378992	5.618907	-1.695202
H	4.548843	5.575111	-0.349720
O	1.470239	0.070757	1.667060
H	0.950615	0.555814	0.971486
C	3.345322	-4.679849	-1.592590
H	4.056897	-4.369701	-0.826786
C	3.457671	-5.888625	-2.135069
H	2.764075	-6.238921	-2.896446
H	4.245610	-6.574132	-1.839021
C	-0.262431	-1.760249	0.205730
H	0.106721	-1.965304	1.207951
H	-0.505827	-0.695691	0.127963
C	-1.465010	-2.600636	-0.104123
C	-1.677770	-3.805701	0.560327
C	-2.464150	-2.152412	-0.970354
C	-2.821847	-4.563085	0.356631
C	-3.609201	-2.901364	-1.206772
H	-2.364564	-1.171774	-1.425654
C	-3.781145	-4.101463	-0.537726
H	-4.392024	-2.542233	-1.863549
F	-0.760429	-4.269517	1.420049
F	-2.994979	-5.712305	1.006231

F	-4.876658	-4.837279	-0.727112
C	2.345283	-0.841146	1.078215
H	2.202370	-1.822762	1.563128
C	-3.478319	4.194581	0.779295
C	-2.315779	3.875179	0.061515
C	-1.608969	4.931615	-0.548217
C	-2.069302	6.238899	-0.441141
C	-3.233926	6.539272	0.263454
C	-3.935483	5.505414	0.875220
H	-4.027170	3.400070	1.278014
H	-1.507953	7.036968	-0.924030
H	-3.581863	7.565576	0.338831
H	-4.839020	5.718111	1.441171
C	-0.378271	4.572013	-1.337344
H	-0.686888	4.227287	-2.336406
H	0.262195	5.450190	-1.483281
C	0.389385	3.444066	-0.655047
H	1.207274	3.097427	-1.291386
H	0.849095	3.804748	0.277184
C	-0.503950	2.253837	-0.348421
C	-1.819772	2.489904	-0.039864
C	-2.807272	1.403534	0.183274
C	-2.743523	0.493953	1.288176
C	-3.894188	1.301642	-0.674382
C	-1.674364	0.535848	2.223168
C	-3.763262	-0.483617	1.481664
C	-4.934725	0.366858	-0.454215
C	-1.572573	-0.392013	3.227659
H	-0.927634	1.313648	2.117732
C	-3.635935	-1.428368	2.534216
C	-4.871953	-0.502822	0.601596
H	-5.773020	0.330750	-1.143704
C	-2.555649	-1.399609	3.377853
H	-0.727479	-0.352357	3.907984
H	-4.410911	-2.182526	2.653338
H	-5.659203	-1.236504	0.757526
H	-2.460958	-2.135608	4.171265
O	-3.922439	2.116907	-1.771427
C	-5.110802	2.849436	-1.988786
H	-5.928487	2.216705	-2.361290
H	-5.430069	3.361046	-1.073768
H	-4.871382	3.597354	-2.746801
O	0.072859	1.083914	-0.383158

## S-CPX-C22

C	-2.791791	-1.828135	0.080384
C	-4.203535	-1.894104	0.289567
C	-2.145589	-2.960224	-0.348355
C	-4.996714	-0.805787	0.726535
C	-4.842793	-3.138779	0.020293
C	-2.882859	-4.144358	-0.577372
H	-1.072251	-2.942953	-0.523582
C	-6.360441	-0.930556	0.876106
H	-4.557479	0.155717	0.968619
C	-6.244543	-3.239060	0.194894
H	-2.365077	-5.038432	-0.920249
C	-6.995849	-2.168576	0.606853
H	-6.705236	-4.198909	-0.014031
H	-8.066971	-2.282251	0.726811
C	-1.891359	2.485262	-0.864370
C	-2.787966	1.365016	-2.897563
C	-2.857601	2.655736	-2.056815
H	-2.416965	2.235867	0.060389
H	-1.326589	3.399294	-0.687395
H	-2.507477	3.488709	-2.679425
C	-1.650298	0.013779	-1.100018
H	-0.923858	-0.665857	-1.554417
C	-2.915578	0.159692	-1.969888
H	-3.041743	-0.761794	-2.544004
H	-3.809336	0.257207	-1.347461
H	-3.586317	1.365416	-3.644031
C	-1.415328	1.298802	-3.570184
H	-1.285879	0.326625	-4.055484
H	-1.319169	2.067950	-4.342658
C	-0.332053	1.508887	-2.500403
H	0.463310	0.762467	-2.558691
H	0.106683	2.505886	-2.558386
N	-4.179125	-4.248477	-0.409410
N	-0.911364	1.374433	-1.111642
O	-7.021278	0.183763	1.285086
C	-8.415082	0.104843	1.485137
H	-8.673369	-0.635890	2.252214
H	-8.724443	1.093668	1.826141
H	-8.944618	-0.136388	0.554461
O	-0.836699	-0.827867	1.069345
H	-0.122659	-1.190572	0.480997
C	-4.241320	2.989538	-1.570627
H	-4.732433	2.243456	-0.944529

C	-4.878753	4.121817	-1.852723
H	-4.424861	4.896647	-2.466945
H	-5.879536	4.316196	-1.479800
C	0.234882	1.424201	-0.102317
H	-0.201665	1.276330	0.882172
H	0.845881	0.543108	-0.323172
C	1.052060	2.683705	-0.151439
C	0.794288	3.716697	0.746258
C	2.173698	2.809674	-0.975933
C	1.594655	4.849103	0.816058
C	2.983714	3.937764	-0.934088
H	2.451001	1.983351	-1.620096
C	2.688816	4.950670	-0.034577
H	3.855162	4.033916	-1.571150
F	-0.253873	3.641695	1.575154
F	1.315066	5.818791	1.683261
F	3.450005	6.041693	0.036520
C	-1.963513	-0.560170	0.301230
H	-2.559325	0.164519	0.868972
C	5.499808	-2.158122	0.117012
C	4.320553	-2.503065	-0.561429
C	4.405112	-3.510458	-1.547942
C	5.630640	-4.087255	-1.860119
C	6.798538	-3.708499	-1.200411
C	6.719385	-2.747488	-0.197726
H	5.455347	-1.424302	0.916224
H	5.668190	-4.858043	-2.627905
H	7.748718	-4.168984	-1.455090
H	7.612833	-2.452499	0.347183
C	3.121881	-3.995056	-2.174880
H	2.668095	-4.738792	-1.500744
H	3.321988	-4.508977	-3.122400
C	2.125567	-2.858101	-2.371159
H	1.144242	-3.241465	-2.670628
H	2.469157	-2.189494	-3.175866
C	1.953337	-2.028353	-1.109946
C	3.028511	-1.873736	-0.267540
C	2.892804	-0.926729	0.869987
C	2.118694	-1.258206	2.027156
C	3.474881	0.327107	0.815760
C	1.534159	-2.544601	2.180296
C	1.917066	-0.298457	3.058980
C	3.303615	1.276736	1.852124
C	0.773180	-2.847534	3.278290

H	1.706757	-3.278397	1.399683
C	1.117700	-0.639770	4.181501
C	2.528306	0.973895	2.940065
H	3.758694	2.258825	1.763022
C	0.553111	-1.882644	4.289122
H	0.330529	-3.834694	3.375092
H	0.964519	0.106347	4.958063
H	2.379642	1.709965	3.726577
H	-0.058671	-2.133661	5.150900
O	4.176696	0.648367	-0.319428
C	5.368306	1.380298	-0.147923
H	5.973164	0.971821	0.670800
H	5.178113	2.445603	0.046300
H	5.923271	1.283267	-1.083280
O	0.799715	-1.452200	-0.954680

S-CPX-C23

C	-2.952617	-1.452101	-0.313647
C	-4.365434	-1.399243	-0.107638
C	-2.430942	-2.539368	-0.967334
C	-5.035253	-0.343909	0.557230
C	-5.138926	-2.479131	-0.621489
C	-3.296238	-3.559388	-1.426235
H	-1.359578	-2.619490	-1.134000
C	-6.405878	-0.337861	0.691193
H	-4.493554	0.488848	0.992331
C	-6.545316	-2.451562	-0.456223
H	-2.877076	-4.420563	-1.943461
C	-7.175470	-1.411153	0.177289
H	-7.109245	-3.288236	-0.855314
H	-8.254152	-1.423242	0.283195
C	-1.634910	2.832095	-0.162499
C	-2.616314	2.378757	-2.405999
C	-2.592050	3.388907	-1.240359
H	-2.178592	2.389115	0.675979
H	-0.990558	3.617253	0.233074
H	-2.185376	4.335512	-1.618050
C	-1.611310	0.503287	-1.049496
H	-0.939328	-0.099964	-1.665852
C	-2.844544	0.977585	-1.845826
H	-3.024385	0.261839	-2.652376
H	-3.742394	0.968101	-1.223099
H	-3.408450	2.647168	-3.109760
C	-1.250114	2.399206	-3.092675

H	-1.196266	1.597914	-3.835720
H	-1.089149	3.345822	-3.617483
C	-0.158452	2.210957	-2.028156
H	0.572174	1.450633	-2.304336
H	0.362526	3.146426	-1.816904
N	-4.598623	-3.546076	-1.274403
N	-0.753805	1.751463	-0.717239
O	-6.938653	0.738548	1.327927
C	-8.335043	0.782987	1.520414
H	-8.686628	-0.058373	2.130777
H	-8.534045	1.715892	2.049408
H	-8.875473	0.789617	0.565181
O	-0.903162	-0.928619	0.825276
H	-0.220407	-1.190731	0.144786
C	-3.947552	3.665921	-0.649283
H	-4.484065	2.811973	-0.233622
C	-4.510984	4.869546	-0.606263
H	-4.011834	5.750141	-1.005113
H	-5.494942	5.018948	-0.172725
C	0.387637	1.425187	0.246991
H	-0.067108	1.025905	1.151011
H	0.927210	0.601144	-0.225323
C	1.289860	2.578043	0.580586
C	2.438834	2.835203	-0.166420
C	1.091759	3.334621	1.738915
C	3.330605	3.837371	0.192557
C	1.968398	4.344808	2.118370
H	0.234395	3.112473	2.367317
C	3.084150	4.590548	1.334679
H	1.812055	4.930065	3.016839
F	2.716083	2.121384	-1.254410
F	4.421788	4.054236	-0.535326
F	3.951805	5.545122	1.665762
C	-1.992640	-0.366344	0.173405
H	-2.511017	0.257207	0.912852
C	5.212746	-2.076003	0.221597
C	4.219077	-2.059396	-0.769469
C	4.613133	-2.344424	-2.095992
C	5.949219	-2.583077	-2.396207
C	6.927952	-2.568485	-1.404420
C	6.545195	-2.324710	-0.089154
H	4.933227	-1.900399	1.256109
H	6.225563	-2.795168	-3.427697
H	7.968371	-2.756005	-1.653925

H	7.288536	-2.326379	0.704186
C	3.536000	-2.460772	-3.145336
H	3.102679	-3.471972	-3.090547
H	3.960960	-2.351431	-4.150098
C	2.418734	-1.451354	-2.909268
H	1.571408	-1.633553	-3.578613
H	2.783963	-0.432005	-3.111644
C	1.916514	-1.494898	-1.476866
C	2.809888	-1.779756	-0.471557
C	2.336862	-1.671677	0.933782
C	1.454060	-2.644107	1.496912
C	2.689066	-0.582871	1.714400
C	1.035674	-3.780374	0.751244
C	0.940133	-2.476472	2.813457
C	2.202387	-0.421614	3.033490
C	0.143266	-4.678285	1.274776
H	1.442857	-3.912936	-0.245607
C	0.020681	-3.427065	3.330714
C	1.342895	-1.348559	3.564605
H	2.494566	0.443764	3.620042
C	-0.378082	-4.499570	2.579036
H	-0.167189	-5.538296	0.687616
H	-0.371400	-3.280316	4.334610
H	0.955387	-1.217728	4.572135
H	-1.090577	-5.215628	2.978420
O	3.491778	0.360266	1.128561
C	4.331912	1.117927	1.963789
H	4.877032	0.478844	2.669997
H	3.777869	1.883810	2.526361
H	5.046815	1.613985	1.303807
O	0.671745	-1.174058	-1.296418

S-CPX-C24

C	-2.383373	-1.352793	-1.416972
C	-3.812211	-1.383844	-1.546441
C	-1.656384	-0.890338	-2.482711
C	-4.691552	-1.952951	-0.593233
C	-4.372754	-0.820648	-2.728729
C	-2.323719	-0.374936	-3.620279
H	-0.574136	-0.846144	-2.437164
C	-6.058880	-1.928144	-0.772503
H	-4.324824	-2.468607	0.287674
C	-5.779787	-0.797159	-2.878070
H	-1.733337	0.016680	-4.446724

C	-6.614713	-1.327296	-1.927905
H	-6.175501	-0.349922	-3.783939
H	-7.687484	-1.293989	-2.078492
C	-0.097713	0.192230	1.933110
C	-1.317155	-1.239145	3.574086
C	0.007768	-0.496789	3.307727
H	0.469228	-0.308345	1.148885
H	0.254915	1.221451	1.985991
H	0.115426	0.269189	4.086860
C	-2.086175	-1.152624	1.178670
H	-3.166039	-0.988099	1.171963
C	-1.683916	-2.069876	2.348470
H	-2.524018	-2.738050	2.567654
H	-0.838181	-2.688403	2.035092
H	-1.212840	-1.873560	4.457803
C	-2.416826	-0.193672	3.780238
H	-3.396529	-0.680597	3.826484
H	-2.274906	0.344820	4.721897
C	-2.366062	0.802934	2.611126
H	-3.353613	1.034430	2.210326
H	-1.886903	1.740617	2.898190
N	-3.625059	-0.309675	-3.748355
N	-1.539704	0.252537	1.470789
O	-6.799078	-2.506785	0.207227
C	-8.198257	-2.579121	0.040731
H	-8.468765	-3.140677	-0.862303
H	-8.576590	-3.106308	0.917259
H	-8.654464	-1.581968	-0.001782
O	-0.342547	-2.113788	-0.261604
H	0.169336	-1.312815	-0.588478
C	1.226107	-1.378237	3.355854
H	1.369341	-2.070767	2.525974
C	2.120447	-1.325633	4.337683
H	2.020791	-0.620262	5.161044
H	2.997750	-1.962558	4.337228
C	-1.691096	1.144129	0.249868
H	-0.983196	0.764602	-0.492066
H	-2.720403	1.015520	-0.089736
C	-1.373243	2.593837	0.490407
C	-2.370761	3.513623	0.802844
C	-0.073019	3.080285	0.311983
C	-2.097198	4.865105	0.964535
C	0.224900	4.428069	0.469196
H	0.703762	2.377700	0.028448



C	-0.791270	5.312405	0.795932
H	1.230915	4.805570	0.326621
F	-3.639206	3.109341	0.962231
F	-3.072650	5.716189	1.272143
F	-0.542147	6.610574	0.953806
C	-1.702332	-1.873010	-0.154125
H	-2.156458	-2.861102	0.024940
C	5.523831	-0.230247	-1.884149
C	4.330838	0.505457	-1.810353
C	4.328227	1.809596	-2.352577
C	5.475734	2.328857	-2.940909
C	6.653424	1.586799	-3.002725
C	6.668062	0.302463	-2.467530
H	5.550278	-1.237021	-1.478209
H	5.445826	3.334280	-3.357333
H	7.543035	2.006113	-3.463727
H	7.575316	-0.294856	-2.508047
C	3.057491	2.614004	-2.242111
H	3.010122	3.078084	-1.241702
H	3.050549	3.431078	-2.972525
C	1.842180	1.710380	-2.414598
H	0.907033	2.258864	-2.260135
H	1.815686	1.316246	-3.441584
C	1.893221	0.531683	-1.454439
C	3.112882	-0.036993	-1.187635
C	3.195774	-1.287875	-0.393528
C	3.944336	-1.351358	0.822315
C	2.601133	-2.455058	-0.860056
C	4.559266	-0.194044	1.378659
C	4.113915	-2.589647	1.506745
C	2.705233	-3.670823	-0.140168
C	5.329046	-0.273074	2.509353
H	4.411084	0.757646	0.879496
C	4.933590	-2.644313	2.666412
C	3.457591	-3.736600	1.003839
H	2.212324	-4.564602	-0.504240
C	5.536866	-1.515864	3.155787
H	5.793007	0.623505	2.910732
H	5.074161	-3.604681	3.158349
H	3.562283	-4.682242	1.530361
H	6.166581	-1.568222	4.039532
O	1.940682	-2.369802	-2.044084
C	1.280127	-3.509014	-2.540427
H	1.982588	-4.327109	-2.750284

H	0.500286	-3.846388	-1.848747
H	0.814048	-3.194413	-3.476090
O	0.753485	0.133619	-0.977360

S-CPX-C25

C	-3.799597	-1.347699	0.566918
C	-4.626209	-1.007770	-0.551858
C	-4.318313	-2.200152	1.506547
C	-4.197607	-0.206458	-1.635937
C	-5.954956	-1.521526	-0.559678
C	-5.645679	-2.678035	1.383696
H	-3.718652	-2.513342	2.357181
C	-5.057549	0.108994	-2.665711
H	-3.166531	0.117582	-1.703886
C	-6.814385	-1.175196	-1.629126
H	-6.044631	-3.353174	2.139027
C	-6.389546	-0.374592	-2.658520
H	-7.822606	-1.575650	-1.608783
H	-7.074238	-0.131939	-3.463103
C	-0.560088	1.048336	2.605921
C	-2.804567	1.923030	3.298788
C	-1.440015	1.423672	3.819206
H	-0.357720	-0.023044	2.497142
H	0.408548	1.539321	2.657344
H	-0.969166	2.258084	4.354010
C	-2.519553	0.725250	1.087636
H	-2.966162	1.242534	0.234460
C	-3.398585	0.891275	2.348948
H	-4.409976	1.176645	2.045076
H	-3.494931	-0.069359	2.860962
H	-3.477105	2.094077	4.143569
C	-2.590558	3.213616	2.510741
H	-3.537345	3.540071	2.069119
H	-2.240442	4.017956	3.164865
C	-1.547817	2.952798	1.412724
H	-1.890676	3.265001	0.423566
H	-0.611335	3.471318	1.616012
N	-6.451957	-2.345446	0.408195
N	-1.200245	1.488314	1.310663
O	-4.545333	0.884954	-3.656130
C	-5.346779	1.151201	-4.785439
H	-6.240812	1.731567	-4.522502
H	-4.725424	1.741497	-5.460019
H	-5.651249	0.226627	-5.291973

O	-1.655959	-1.038204	-0.416518
H	-0.767674	-1.370252	-0.089533
C	-1.551801	0.267538	4.775827
H	-1.871575	-0.684579	4.351920
C	-1.274715	0.344394	6.073821
H	-0.930142	1.270115	6.529900
H	-1.372602	-0.515862	6.728606
C	-0.210640	1.273482	0.152061
H	0.260734	0.302574	0.346395
H	-0.814277	1.184239	-0.749746
C	0.810698	2.360427	-0.024908
C	2.010809	2.364466	0.684974
C	0.638354	3.348449	-0.998584
C	2.971863	3.346299	0.489326
C	1.597067	4.324976	-1.233484
H	-0.265337	3.336246	-1.600570
C	2.760823	4.314660	-0.482407
H	1.468626	5.080871	-1.999320
F	2.267950	1.427848	1.600572
F	4.087655	3.347407	1.209276
F	3.706731	5.230696	-0.682148
C	-2.392887	-0.785542	0.731421
H	-1.923708	-1.290311	1.586130
C	4.276696	-3.188531	-1.259498
C	3.542321	-2.981945	-0.081670
C	3.934249	-3.694045	1.072842
C	5.007020	-4.576268	1.022893
C	5.725867	-4.772544	-0.155390
C	5.353591	-4.067982	-1.295965
H	3.991339	-2.653806	-2.161126
H	5.288708	-5.114755	1.926231
H	6.561816	-5.465864	-0.179363
H	5.897923	-4.207851	-2.226508
C	3.178310	-3.418307	2.346986
H	3.570872	-2.493894	2.800192
H	3.336329	-4.222031	3.075803
C	1.693628	-3.218900	2.059957
H	1.155871	-2.898664	2.958634
H	1.241750	-4.166882	1.731693
C	1.464301	-2.175495	0.977695
C	2.397464	-2.061767	-0.027305
C	2.218087	-1.068685	-1.116554
C	3.154297	-0.002411	-1.297870
C	1.166953	-1.172864	-2.020919

C	4.279451	0.150852	-0.437627
C	2.996160	0.935407	-2.359283
C	0.968868	-0.203352	-3.036744
C	5.202521	1.141324	-0.646678
H	4.392419	-0.539785	0.389946
C	3.967714	1.955584	-2.547182
C	1.866497	0.821223	-3.200591
H	0.121368	-0.281213	-3.708738
C	5.055163	2.053500	-1.720226
H	6.052626	1.234600	0.022417
H	3.831328	2.659031	-3.365891
H	1.721970	1.548958	-3.995771
H	5.793834	2.835003	-1.872643
O	0.353808	-2.251157	-1.880316
C	-0.659048	-2.473230	-2.833451
H	-0.241321	-2.572152	-3.844444
H	-1.416578	-1.681953	-2.812613
H	-1.132397	-3.412513	-2.545172
O	0.374443	-1.482272	1.079495

S-CPX-C26

C	0.781109	3.658605	-1.347662
C	2.102697	3.302346	-0.920038
C	0.528018	4.982361	-1.595851
C	2.519146	1.981337	-0.636591
C	3.035630	4.366498	-0.743667
C	1.540419	5.955423	-1.414809
H	-0.454837	5.300214	-1.934967
C	3.789273	1.728898	-0.158492
H	1.868836	1.131509	-0.803786
C	4.336678	4.069399	-0.273212
H	1.323669	7.002587	-1.620305
C	4.713784	2.785046	0.023829
H	5.025384	4.898978	-0.152343
H	5.715512	2.586971	0.387974
C	-3.132588	2.343862	0.241005
C	-1.539592	2.448472	2.125351
C	-2.982971	2.789008	1.707059
H	-2.991251	3.179860	-0.450414
H	-4.113899	1.915774	0.045687
H	-3.668975	2.202589	2.330649
C	-0.696547	1.959693	-0.189342
H	-0.041910	1.095740	-0.073313
C	-0.578955	2.899705	1.023763

H	0.455590	2.859179	1.375137
H	-0.771062	3.938302	0.734362
H	-1.296830	2.934288	3.073731
C	-1.423408	0.929558	2.244471
H	-0.375109	0.651478	2.369311
H	-1.962086	0.553798	3.118510
C	-2.002472	0.280013	0.978000
H	-1.368369	-0.522197	0.594713
H	-3.010696	-0.104592	1.136620
N	2.747197	5.677063	-0.995420
N	-2.100609	1.311367	-0.130230
O	4.074635	0.432880	0.108947
C	5.367975	0.060815	0.537286
H	5.623739	0.534500	1.493555
H	5.331903	-1.022477	0.659178
H	6.124419	0.316372	-0.214670
O	-0.044137	1.757839	-2.570856
H	0.170107	0.849944	-2.210732
C	-3.337685	4.241405	1.859239
H	-2.724939	4.949917	1.300604
C	-4.327268	4.696108	2.622064
H	-4.964038	4.023594	3.192652
H	-4.535078	5.758016	2.710233
C	-2.509053	0.662206	-1.454041
H	-2.907036	1.465921	-2.075148
H	-1.600628	0.279436	-1.901253
C	-3.463126	-0.490622	-1.320619
C	-4.846594	-0.345907	-1.292834
C	-2.940215	-1.787021	-1.279059
C	-5.691190	-1.442399	-1.183516
C	-3.764664	-2.898551	-1.165698
H	-1.862589	-1.919008	-1.338333
C	-5.137151	-2.716866	-1.115067
H	-3.339597	-3.894065	-1.116295
F	-5.411810	0.872035	-1.367179
F	-7.011846	-1.271827	-1.148148
F	-5.963678	-3.756910	-1.003130
C	-0.345958	2.642850	-1.536188
H	-1.223659	3.235343	-1.846729
C	3.308240	-3.714540	0.554909
C	2.945389	-2.779937	-0.430254
C	3.890699	-2.487871	-1.440678
C	5.126428	-3.125610	-1.440924
C	5.474279	-4.047304	-0.453669

C	4.553563	-4.334545	0.548534
H	2.597275	-3.956906	1.340007
H	5.837914	-2.886104	-2.229500
H	6.445409	-4.533136	-0.472621
H	4.799222	-5.050851	1.328173
C	3.578329	-1.413515	-2.454025
H	3.962826	-0.461786	-2.066262
H	4.108141	-1.609349	-3.393539
C	2.082855	-1.256658	-2.713908
H	1.888324	-0.316657	-3.240682
H	1.720009	-2.064811	-3.366418
C	1.244950	-1.298871	-1.446834
C	1.643473	-2.108892	-0.412299
C	0.703036	-2.347698	0.715696
C	0.883970	-1.713390	1.989337
C	-0.385816	-3.190608	0.574303
C	1.937471	-0.781117	2.192171
C	-0.009873	-1.970136	3.068659
C	-1.297699	-3.421145	1.632641
C	2.101398	-0.154398	3.402276
H	2.601962	-0.564701	1.362481
C	0.201445	-1.324701	4.316313
C	-1.114234	-2.833076	2.854457
H	-2.136308	-4.084837	1.445009
C	1.231742	-0.435660	4.483313
H	2.907088	0.563143	3.531907
H	-0.480294	-1.540777	5.135822
H	-1.808424	-3.023668	3.669277
H	1.380085	0.056492	5.440229
O	-0.691788	-3.811317	-0.614184
C	0.172415	-4.871661	-0.995621
H	1.185225	-4.513578	-1.196615
H	0.206717	-5.641421	-0.213631
H	-0.253929	-5.298519	-1.905711
O	0.157284	-0.595486	-1.434602

S-CPX-C27

C	2.637938	-1.525539	-1.051823
C	4.027284	-1.761305	-0.815853
C	1.789932	-2.603285	-1.029088
C	5.014407	-0.747214	-0.788797
C	4.426216	-3.107379	-0.570179
C	2.296464	-3.898811	-0.781590
H	0.725942	-2.469343	-1.194120

C	6.334045	-1.041180	-0.523621
H	4.770327	0.291047	-0.984370
C	5.791700	-3.379345	-0.311863
H	1.612520	-4.745948	-0.767091
C	6.730439	-2.380778	-0.282776
H	6.066606	-4.413278	-0.131309
H	7.766240	-2.625309	-0.077765
C	1.906663	2.649037	0.368495
C	1.819280	1.091286	2.298434
C	2.364345	2.453080	1.827869
H	2.710544	2.431291	-0.339721
H	1.575725	3.668636	0.182892
H	1.910480	3.234849	2.449561
C	1.280791	0.267206	-0.025763
H	0.354198	-0.312966	-0.009350
C	2.124949	0.029076	1.245633
H	1.886894	-0.965814	1.630366
H	3.192512	0.025603	1.007090
H	2.269898	0.820899	3.256761
C	0.301164	1.185539	2.419077
H	-0.109949	0.191947	2.601914
H	0.001786	1.820069	3.258353
C	-0.269063	1.764865	1.116685
H	-1.128047	1.199570	0.749203
H	-0.559241	2.810504	1.226497
N	3.561013	-4.159903	-0.557366
N	0.772777	1.725288	0.017682
O	7.189595	0.013023	-0.509749
C	8.560392	-0.233895	-0.286348
H	8.982339	-0.894726	-1.053940
H	9.051718	0.738109	-0.342694
H	8.737113	-0.669785	0.705302
O	1.294094	-0.121453	-2.478981
H	0.369219	-0.441639	-2.277380
C	3.859111	2.581286	1.934266
H	4.452141	1.858013	1.372432
C	4.478658	3.508381	2.658611
H	3.924783	4.251454	3.228442
H	5.561803	3.558606	2.712160
C	0.143143	2.146872	-1.308402
H	0.966685	2.359615	-1.989236
H	-0.394366	1.272402	-1.662523
C	-0.847966	3.274373	-1.220688
C	-0.500881	4.621398	-1.259701

C	-2.209885	2.957480	-1.193922
C	-1.460728	5.624202	-1.218803
C	-3.188750	3.941061	-1.154258
H	-2.508988	1.913891	-1.218484
C	-2.805327	5.272677	-1.161540
H	-4.240189	3.679244	-1.130012
F	0.786348	4.997613	-1.338127
F	-1.093971	6.904093	-1.244296
F	-3.712147	6.247942	-1.122856
C	2.050664	-0.135930	-1.309959
H	2.871539	0.573326	-1.465456
C	-4.563629	-3.359351	0.385772
C	-3.426909	-3.188303	-0.420282
C	-3.010785	-4.279900	-1.214401
C	-3.729189	-5.469024	-1.201553
C	-4.861901	-5.620917	-0.402435
C	-5.269805	-4.558511	0.396470
H	-4.895626	-2.538366	1.015678
H	-3.391619	-6.295056	-1.824801
H	-5.411585	-6.557547	-0.403259
H	-6.146389	-4.657358	1.031307
C	-1.742850	-4.120059	-2.013601
H	-0.883269	-4.316774	-1.350901
H	-1.693018	-4.861200	-2.818998
C	-1.616984	-2.703546	-2.564805
H	-0.648604	-2.552196	-3.053747
H	-2.387335	-2.532415	-3.332564
C	-1.792401	-1.657209	-1.472817
C	-2.682904	-1.924098	-0.458497
C	-2.954358	-0.899999	0.585814
C	-2.411842	-1.097110	1.906556
C	-3.728535	0.232401	0.383172
C	-1.547896	-2.192560	2.184098
C	-2.686886	-0.186715	2.965723
C	-3.955391	1.170528	1.428590
C	-1.015415	-2.381476	3.436080
H	-1.312190	-2.878658	1.377596
C	-2.145600	-0.420696	4.256024
C	-3.464741	0.966209	2.684488
H	-4.560482	2.040544	1.193634
C	-1.325981	-1.494599	4.492711
H	-0.356602	-3.225625	3.619092
H	-2.382639	0.280220	5.053211
H	-3.671150	1.678881	3.479102



H	-0.910126	-1.661965	5.481849
O	-4.317528	0.629783	-0.780841
C	-4.728857	-0.297373	-1.774999
H	-3.905397	-0.550522	-2.446020
H	-5.132009	-1.210806	-1.329322
H	-5.515766	0.215481	-2.334238
O	-1.132135	-0.554668	-1.593811

S-CPX-C28

C	2.753369	-1.912517	-0.978195
C	4.143852	-2.120270	-0.724950
C	1.934128	-3.011096	-1.023984
C	5.103165	-1.082492	-0.643132
C	4.574517	-3.463920	-0.525862
C	2.471182	-4.301486	-0.815636
H	0.872085	-2.891192	-1.213752
C	6.425656	-1.352249	-0.367294
H	4.834053	-0.044493	-0.805533
C	5.942220	-3.709981	-0.253874
H	1.811303	-5.166697	-0.849114
C	6.853639	-2.689215	-0.170311
H	6.241962	-4.742546	-0.108108
H	7.892234	-2.914421	0.042574
C	2.046750	2.192106	0.636989
C	1.911272	0.551847	2.498788
C	2.458008	1.937713	2.102561
H	2.864157	1.995061	-0.061009
H	1.732796	3.224388	0.496836
H	1.977530	2.690485	2.740000
C	1.406062	-0.165044	0.142999
H	0.475373	-0.739717	0.155862
C	2.257314	-0.446002	1.396460
H	2.052638	-1.469596	1.720146
H	3.325861	-0.400722	1.167939
H	2.344241	0.240047	3.452879
C	0.386894	0.639710	2.589186
H	-0.038628	-0.363667	2.682596
H	0.069081	1.216324	3.462832
C	-0.147459	1.311796	1.316530
H	-1.010412	0.786284	0.903636
H	-0.408873	2.358071	1.482098
N	3.737342	-4.538152	-0.571675
N	0.908769	1.298130	0.233104
O	7.253386	-0.277419	-0.299056

C	8.627882	-0.500036	-0.074042
H	9.071255	-1.120744	-0.862768
H	9.096778	0.484508	-0.088962
H	8.808028	-0.969197	0.901748
O	1.295089	-0.518744	-2.295432
H	0.380858	-0.820148	-2.019016
C	3.947315	2.075278	2.261865
H	4.566561	1.389839	1.681429
C	4.531785	2.971936	3.050832
H	3.950742	3.677872	3.640519
H	5.611966	3.033279	3.139837
C	0.272931	1.764537	-1.072268
H	1.040735	1.690820	-1.838639
H	-0.498392	1.020160	-1.288952
C	-0.317304	3.145983	-1.021925
C	0.433571	4.253748	-1.411191
C	-1.662554	3.356696	-0.704622
C	-0.105008	5.532568	-1.447430
C	-2.223818	4.627269	-0.731068
H	-2.286699	2.507467	-0.445305
C	-1.439685	5.707925	-1.101241
H	-3.266659	4.780424	-0.481681
F	1.720839	4.108281	-1.755761
F	0.646113	6.568980	-1.812211
F	-1.947622	6.939086	-1.137694
C	2.127904	-0.531853	-1.178256
H	2.925488	0.196648	-1.370906
C	-4.851922	-3.259676	0.696203
C	-3.967258	-3.001980	-0.361993
C	-4.019619	-3.854986	-1.487268
C	-4.901576	-4.928085	-1.512605
C	-5.763928	-5.180931	-0.446484
C	-5.737728	-4.331851	0.654844
H	-4.847735	-2.606101	1.564279
H	-4.920841	-5.573530	-2.389013
H	-6.449979	-6.022266	-0.481520
H	-6.409530	-4.504017	1.492133
C	-3.142316	-3.515358	-2.665783
H	-3.638210	-2.731711	-3.260268
H	-3.020902	-4.383266	-3.323814
C	-1.788403	-2.983532	-2.207522
H	-1.199337	-2.618889	-3.055631
H	-1.213507	-3.796848	-1.736813
C	-1.940468	-1.857012	-1.198928

C	-3.009168	-1.891675	-0.338067
C	-3.138362	-0.842996	0.707239
C	-3.815467	0.386292	0.437013
C	-2.643927	-1.044723	1.986765
C	-4.346807	0.663389	-0.854668
C	-3.984790	1.366638	1.458384
C	-2.827981	-0.083948	3.013151
C	-5.011520	1.834340	-1.109585
H	-4.213542	-0.085850	-1.627626
C	-4.676814	2.573275	1.163209
C	-3.474592	1.096212	2.749890
H	-2.447974	-0.272080	4.011822
C	-5.186145	2.801597	-0.088597
H	-5.415658	2.022259	-2.099881
H	-4.805476	3.308150	1.954732
H	-3.612827	1.830048	3.540179
H	-5.727828	3.719513	-0.300681
O	-1.940544	-2.193761	2.198500
C	-1.841683	-2.685475	3.514349
H	-2.823760	-2.731395	4.001567
H	-1.161135	-2.083324	4.133669
H	-1.435190	-3.694147	3.427361
O	-1.013939	-0.953432	-1.170206

S-CPX-C29

C	3.584124	-0.851520	-1.628743
C	4.397727	-0.078118	-0.744672
C	4.187162	-1.429514	-2.716331
C	3.899082	0.597605	0.394728
C	5.791306	-0.010766	-1.030360
C	5.579435	-1.281771	-2.913710
H	3.590800	-1.980379	-3.436041
C	4.748938	1.275855	1.240333
H	2.837653	0.611286	0.623083
C	6.633509	0.714010	-0.152345
H	6.050574	-1.747395	-3.777839
C	6.137224	1.338224	0.962886
H	7.691063	0.752501	-0.391767
H	6.810534	1.879099	1.617813
C	0.250880	-1.884791	1.069783
C	2.154353	-3.413726	1.587394
C	1.098370	-2.477515	2.216330
H	0.517963	-0.851501	0.840067
H	-0.812203	-1.899325	1.308550

H	0.453796	-3.088467	2.861179
C	1.871025	-2.433284	-0.730987
H	1.992001	-3.193653	-1.510073
C	2.848194	-2.683846	0.442137
H	3.700728	-3.258770	0.070151
H	3.250451	-1.739518	0.810946
H	2.882330	-3.708511	2.347277
C	1.444401	-4.635762	1.009674
H	2.153148	-5.243077	0.437540
H	1.035920	-5.269886	1.802286
C	0.304576	-4.145150	0.108589
H	0.264984	-4.666207	-0.847496
H	-0.666101	-4.255827	0.594294
N	6.368330	-0.614056	-2.107628
N	0.441437	-2.674476	-0.201078
O	4.173359	1.856869	2.325787
C	4.969302	2.653460	3.175596
H	5.432699	3.486436	2.632571
H	4.289645	3.051629	3.929866
H	5.749881	2.061849	3.670555
O	1.432757	-1.009207	-2.650328
H	0.767997	-0.270630	-2.537472
C	1.707744	-1.390983	3.063503
H	2.190807	-0.565939	2.541875
C	1.686756	-1.393430	4.393738
H	1.195546	-2.183044	4.959071
H	2.158879	-0.600705	4.965771
C	-0.614419	-2.280002	-1.228146
H	-0.545988	-1.196652	-1.338040
H	-0.314230	-2.754514	-2.161984
C	-2.031578	-2.606584	-0.850446
C	-2.636650	-3.817245	-1.179731
C	-2.834094	-1.615903	-0.275668
C	-3.974204	-4.063514	-0.905253
C	-4.177286	-1.834659	0.004142
H	-2.394900	-0.642557	-0.079106
C	-4.735488	-3.062673	-0.309439
H	-4.794408	-1.058994	0.444377
F	-1.933412	-4.789895	-1.781538
F	-4.519404	-5.237639	-1.219384
F	-6.019427	-3.315103	-0.057027
C	2.087726	-1.056825	-1.418424
H	1.691821	-0.263064	-0.774647
C	-1.915066	4.774177	0.285653

C	-1.521760	3.987659	-0.810209
C	-1.340724	4.635374	-2.053031
C	-1.538974	6.005836	-2.164897
C	-1.929603	6.773069	-1.067734
C	-2.119681	6.144493	0.158125
H	-2.058894	4.301585	1.253663
H	-1.390803	6.481524	-3.132704
H	-2.083485	7.842977	-1.173322
H	-2.424202	6.722425	1.027085
C	-0.975145	3.779799	-3.238758
H	-1.891083	3.320665	-3.642807
H	-0.545886	4.391006	-4.040875
C	-0.018249	2.663865	-2.831323
H	0.155713	1.972699	-3.662162
H	0.958014	3.088365	-2.552550
C	-0.549617	1.868992	-1.647624
C	-1.283466	2.544405	-0.690892
C	-1.734518	1.837570	0.531204
C	-3.136141	1.668749	0.812370
C	-0.839242	1.331952	1.457611
C	-4.126466	2.111891	-0.106084
C	-3.569090	1.021732	2.005577
C	-1.265177	0.664579	2.631337
C	-5.462612	1.949937	0.157798
H	-3.798225	2.577266	-1.028821
C	-4.959995	0.879664	2.258709
C	-2.597448	0.509010	2.902066
H	-0.502803	0.295004	3.310957
C	-5.889182	1.336783	1.359540
H	-6.200576	2.295178	-0.560151
H	-5.274712	0.394740	3.179906
H	-2.923413	0.008402	3.810400
H	-6.950120	1.221740	1.561741
O	0.525431	1.438054	1.294506
C	1.026673	2.757159	1.487334
H	0.630650	3.444353	0.734764
H	0.761903	3.119228	2.489599
H	2.111768	2.693204	1.406573
O	-0.252696	0.621697	-1.598676
S-CPX-C30			
C	-3.379413	0.665328	-1.260813
C	-4.641209	0.002329	-1.151949
C	-3.285289	1.716140	-2.138635

C	-4.882834	-1.101297	-0.302103
C	-5.714395	0.502346	-1.946825
C	-4.413829	2.124219	-2.885498
H	-2.340023	2.231876	-2.280073
C	-6.129353	-1.682180	-0.226312
H	-4.098739	-1.519285	0.316422
C	-6.982344	-0.120238	-1.850883
H	-4.325403	2.959371	-3.578533
C	-7.197708	-1.184509	-1.013424
H	-7.781097	0.278119	-2.467779
H	-8.181592	-1.636739	-0.964932
C	-0.582733	-0.014135	2.246399
C	-2.646714	1.165799	2.998487
C	-1.868680	-0.163657	3.079246
H	-0.375482	-0.830569	1.547755
H	0.295049	0.081845	2.888310
H	-1.567280	-0.282832	4.129638
C	-1.888608	1.365938	0.581074
H	-1.759323	2.311501	0.047940
C	-3.091039	1.436041	1.560096
H	-3.574464	2.415683	1.492692
H	-3.840560	0.697276	1.270594
H	-3.522158	1.123157	3.653889
C	-1.712081	2.294418	3.430510
H	-2.260435	3.236861	3.519058
H	-1.274183	2.077843	4.410255
C	-0.608497	2.436110	2.372602
H	-0.732577	3.330898	1.759372
H	0.385656	2.469276	2.816973
N	-5.591711	1.556792	-2.801036
N	-0.613410	1.260732	1.424395
O	-6.248336	-2.728233	0.631740
C	-7.498703	-3.370427	0.742417
H	-7.814396	-3.811350	-0.211650
H	-7.362144	-4.166305	1.475632
H	-8.276522	-2.683196	1.099747
O	-1.092565	0.078775	-1.391895
H	-0.582072	-0.729211	-1.066229
C	-2.722024	-1.366603	2.751400
H	-3.704194	-1.350549	3.226896
C	-2.385810	-2.427305	2.019132
H	-1.435858	-2.526454	1.496073
H	-3.096679	-3.240579	1.898347
C	0.686406	1.280226	0.630919

H	1.458775	1.168435	1.390417
H	0.687129	0.379061	0.025565
C	0.964229	2.507317	-0.190528
C	1.729960	3.545681	0.335939
C	0.619476	2.582455	-1.544624
C	2.129013	4.629003	-0.433588
C	0.999855	3.662610	-2.331476
H	0.056386	1.756265	-1.967312
C	1.755913	4.679314	-1.769836
H	0.739442	3.719033	-3.382205
F	2.126338	3.527360	1.616639
F	2.872907	5.594591	0.103416
F	2.147728	5.723565	-2.500046
C	-2.131183	0.251715	-0.480511
H	-2.310127	-0.685311	0.053757
C	4.693451	-3.358741	-0.371940
C	3.404030	-3.234884	-0.911292
C	3.077048	-4.024620	-2.035212
C	4.011871	-4.905700	-2.564876
C	5.287381	-5.023992	-2.013880
C	5.623364	-4.239659	-0.915754
H	4.967091	-2.758281	0.491678
H	3.737896	-5.507268	-3.429696
H	6.006274	-5.718580	-2.438710
H	6.612342	-4.316088	-0.471523
C	1.713825	-3.835102	-2.650198
H	1.741956	-2.954490	-3.311411
H	1.448333	-4.693305	-3.278160
C	0.657529	-3.595590	-1.575668
H	-0.306234	-3.330290	-2.021531
H	0.499882	-4.513576	-0.989473
C	1.066469	-2.480590	-0.626192
C	2.399996	-2.328092	-0.333930
C	2.849780	-1.285860	0.625101
C	3.554309	-0.125781	0.150381
C	2.601052	-1.371731	1.983087
C	3.740973	0.098288	-1.241162
C	4.018218	0.870378	1.056950
C	3.067313	-0.383966	2.888337
C	4.345927	1.240339	-1.700378
H	3.373317	-0.649495	-1.935525
C	4.661786	2.031659	0.553599
C	3.766624	0.705732	2.443840
H	2.856800	-0.530439	3.944018

C	4.819188	2.218303	-0.795001
H	4.464734	1.396616	-2.768463
H	5.005092	2.783605	1.259633
H	4.123000	1.458787	3.141955
H	5.298715	3.117453	-1.171019
O	1.844299	-2.366179	2.546636
C	2.407177	-3.668738	2.517596
H	2.530258	-4.034934	1.494889
H	3.380086	-3.680614	3.026868
H	1.709665	-4.312360	3.057531
O	0.111411	-1.755977	-0.133108

S-CPX-C31

C	-3.379413	0.665328	-1.260813
C	-4.641209	0.002329	-1.151949
C	-3.285289	1.716140	-2.138635
C	-4.882834	-1.101297	-0.302103
C	-5.714395	0.502346	-1.946825
C	-4.413829	2.124219	-2.885498
H	-2.340023	2.231876	-2.280073
C	-6.129353	-1.682180	-0.226312
H	-4.098739	-1.519285	0.316422
C	-6.982344	-0.120238	-1.850883
H	-4.325403	2.959371	-3.578533
C	-7.197708	-1.184509	-1.013424
H	-7.781097	0.278119	-2.467779
H	-8.181592	-1.636739	-0.964932
C	-0.582733	-0.014135	2.246399
C	-2.646714	1.165799	2.998487
C	-1.868680	-0.163657	3.079246
H	-0.375482	-0.830569	1.547755
H	0.295049	0.081845	2.888310
H	-1.567280	-0.282832	4.129638
C	-1.888608	1.365938	0.581074
H	-1.759323	2.311501	0.047940
C	-3.091039	1.436041	1.560096
H	-3.574464	2.415683	1.492692
H	-3.840560	0.697276	1.270594
H	-3.522158	1.123157	3.653889
C	-1.712081	2.294418	3.430510
H	-2.260435	3.236861	3.519058
H	-1.274183	2.077843	4.410255
C	-0.608497	2.436110	2.372602
H	-0.732577	3.330898	1.759372



H	0.385656	2.469276	2.816973
N	-5.591711	1.556792	-2.801036
N	-0.613410	1.260732	1.424395
O	-6.248336	-2.728233	0.631740
C	-7.498703	-3.370427	0.742417
H	-7.814396	-3.811350	-0.211650
H	-7.362144	-4.166305	1.475632
H	-8.276522	-2.683196	1.099747
O	-1.092565	0.078775	-1.391895
H	-0.582072	-0.729211	-1.066229
C	-2.722024	-1.366603	2.751400
H	-3.704194	-1.350549	3.226896
C	-2.385810	-2.427305	2.019132
H	-1.435858	-2.526454	1.496073
H	-3.096679	-3.240579	1.898347
C	0.686406	1.280226	0.630919
H	1.458775	1.168435	1.390417
H	0.687129	0.379061	0.025565
C	0.964229	2.507317	-0.190528
C	1.729960	3.545681	0.335939
C	0.619476	2.582455	-1.544624
C	2.129013	4.629003	-0.433588
C	0.999855	3.662610	-2.331476
H	0.056386	1.756265	-1.967312
C	1.755913	4.679314	-1.769836
H	0.739442	3.719033	-3.382205
F	2.126338	3.527360	1.616639
F	2.872907	5.594591	0.103416
F	2.147728	5.723565	-2.500046
C	-2.131183	0.251715	-0.480511
H	-2.310127	-0.685311	0.053757
C	4.693451	-3.358741	-0.371940
C	3.404030	-3.234884	-0.911292
C	3.077048	-4.024620	-2.035212
C	4.011871	-4.905700	-2.564876
C	5.287381	-5.023992	-2.013880
C	5.623364	-4.239659	-0.915754
H	4.967091	-2.758281	0.491678
H	3.737896	-5.507268	-3.429696
H	6.006274	-5.718580	-2.438710
H	6.612342	-4.316088	-0.471523
C	1.713825	-3.835102	-2.650198
H	1.741956	-2.954490	-3.311411
H	1.448333	-4.693305	-3.278160

C	0.657529	-3.595590	-1.575668
H	-0.306234	-3.330290	-2.021531
H	0.499882	-4.513576	-0.989473
C	1.066469	-2.480590	-0.626192
C	2.399996	-2.328092	-0.333930
C	2.849780	-1.285860	0.625101
C	3.554309	-0.125781	0.150381
C	2.601052	-1.371731	1.983087
C	3.740973	0.098288	-1.241162
C	4.018218	0.870378	1.056950
C	3.067313	-0.383966	2.888337
C	4.345927	1.240339	-1.700378
H	3.373317	-0.649495	-1.935525
C	4.661786	2.031659	0.553599
C	3.766624	0.705732	2.443840
H	2.856800	-0.530439	3.944018
C	4.819188	2.218303	-0.795001
H	4.464734	1.396616	-2.768463
H	5.005092	2.783605	1.259633
H	4.123000	1.458787	3.141955
H	5.298715	3.117453	-1.171019
O	1.844299	-2.366179	2.546636
C	2.407177	-3.668738	2.517596
H	2.530258	-4.034934	1.494889
H	3.380086	-3.680614	3.026868
H	1.709665	-4.312360	3.057531
O	0.111411	-1.755977	-0.133108

S-CPX-C32

C	-3.007659	-1.990294	-1.240501
C	-4.237580	-1.256464	-1.256997
C	-3.043471	-3.291254	-1.673108
C	-4.349003	0.108155	-0.911620
C	-5.413764	-1.957481	-1.651965
C	-4.266593	-3.884003	-2.070025
H	-2.134416	-3.885744	-1.707655
C	-5.566427	0.752024	-0.923948
H	-3.473168	0.691247	-0.670011
C	-6.652372	-1.273225	-1.644516
H	-4.276328	-4.920221	-2.404206
C	-6.740771	0.048162	-1.286113
H	-7.533025	-1.832642	-1.942312
H	-7.705467	0.542331	-1.297198
C	0.631892	-1.632277	1.261860

C	-1.174258	-2.752945	2.572007
C	0.187049	-2.974745	1.882667
H	0.903929	-1.684349	0.202404
H	1.490887	-1.227657	1.796835
H	0.913289	-3.232049	2.662836
C	-1.757688	-1.065789	0.750934
H	-2.446538	-0.232531	0.897310
C	-2.226196	-2.309657	1.555267
H	-3.169901	-2.087002	2.063334
H	-2.438114	-3.129289	0.866951
H	-1.493690	-3.680124	3.055528
C	-1.008999	-1.637690	3.600817
H	-1.922448	-1.524935	4.192308
H	-0.195149	-1.872245	4.294102
C	-0.712241	-0.330746	2.852257
H	-1.546121	0.371829	2.902560
H	0.175275	0.168780	3.239041
N	-5.417950	-3.263386	-2.047722
N	-0.448715	-0.576236	1.384674
O	-5.548911	2.067828	-0.583730
C	-6.764548	2.782668	-0.588775
H	-7.481250	2.368703	0.132141
H	-6.513225	3.802649	-0.294899
H	-7.221482	2.798617	-1.586265
O	-1.353354	-0.303038	-1.579726
H	-0.379593	-0.458276	-1.838016
C	0.186234	-4.105921	0.891050
H	-0.367516	-3.958735	-0.033744
C	0.829604	-5.253102	1.079663
H	1.420927	-5.434565	1.973963
H	0.810323	-6.044489	0.336982
C	0.128875	0.708664	0.788980
H	1.074012	0.860278	1.307759
H	0.361638	0.482523	-0.246065
C	-0.731075	1.934036	0.921764
C	-0.586001	2.791791	2.011543
C	-1.629842	2.315485	-0.078034
C	-1.341675	3.948531	2.142567
C	-2.405757	3.462981	0.033927
H	-1.706178	1.677836	-0.952429
C	-2.260796	4.269611	1.149839
H	-3.128495	3.729969	-0.727550
F	0.301672	2.522837	2.983010
F	-1.185535	4.735049	3.205867

F	-2.991816	5.374570	1.297061
C	-1.682814	-1.390550	-0.775776
H	-0.923502	-2.171637	-0.903820
C	5.398029	1.400056	-1.483768
C	4.070809	1.318504	-1.929725
C	3.648486	2.234663	-2.915671
C	4.535704	3.178093	-3.421333
C	5.850625	3.250162	-2.964961
C	6.275325	2.353744	-1.989084
H	5.748439	0.695546	-0.734063
H	4.187648	3.875315	-4.181384
H	6.532390	3.993428	-3.368455
H	7.298644	2.388462	-1.623610
C	2.207393	2.174984	-3.352473
H	1.589906	2.716479	-2.618071
H	2.071588	2.676948	-4.317273
C	1.725813	0.728996	-3.415245
H	0.654655	0.679458	-3.637673
H	2.245696	0.194704	-4.223942
C	1.982916	0.006701	-2.100228
C	3.128515	0.318295	-1.401832
C	3.434798	-0.322198	-0.100082
C	3.661781	-1.727210	0.042876
C	3.520562	0.466461	1.043197
C	3.606913	-2.605987	-1.075556
C	3.947810	-2.290323	1.322289
C	3.825054	-0.082474	2.311010
C	3.808467	-3.952238	-0.927314
H	3.403584	-2.181108	-2.050787
C	4.149939	-3.692774	1.443626
C	4.029554	-1.434092	2.445054
H	3.888313	0.559859	3.183301
C	4.080084	-4.508033	0.346717
H	3.764492	-4.602715	-1.796143
H	4.368537	-4.104593	2.426610
H	4.261657	-1.856783	3.419612
H	4.237278	-5.578057	0.448456
O	3.221263	1.788763	0.889138
C	3.683584	2.704543	1.853969
H	3.112883	2.639303	2.790123
H	4.750157	2.558874	2.064274
H	3.536211	3.694290	1.419300
O	1.098916	-0.865735	-1.726136

## S-CPX-C33

C	-3.539258	1.666311	-1.343247
C	-4.571571	0.698043	-1.134673
C	-3.887416	2.857058	-1.929098
C	-4.352699	-0.596023	-0.607356
C	-5.900598	1.077681	-1.489767
C	-5.236111	3.120383	-2.259693
H	-3.132414	3.602716	-2.159366
C	-5.402775	-1.464319	-0.406990
H	-3.360158	-0.952987	-0.361053
C	-6.955868	0.160721	-1.271888
H	-5.499824	4.072397	-2.717728
C	-6.725386	-1.080987	-0.738172
H	-7.956706	0.476589	-1.547170
H	-7.556453	-1.759643	-0.583853
C	-0.033940	1.011156	1.309555
C	-1.845752	2.199912	2.554896
C	-1.127559	0.847410	2.390871
H	-0.040112	0.219989	0.549985
H	0.965291	1.040971	1.748800
H	-0.610763	0.620826	3.332535
C	-1.634216	2.484913	0.043944
H	-1.603587	3.446413	-0.476204
C	-2.587715	2.546370	1.263763
H	-3.033720	3.543045	1.339577
H	-3.406583	1.840747	1.118550
H	-2.552747	2.154175	3.387061
C	-0.801015	3.282229	2.815874
H	-1.284645	4.232095	3.061873
H	-0.167763	3.006802	3.665554
C	0.050065	3.451958	1.549371
H	-0.162979	4.379109	1.013526
H	1.113385	3.432015	1.782156
N	-6.219282	2.283739	-2.039517
N	-0.196513	2.325967	0.574949
O	-5.084652	-2.676428	0.123243
C	-6.105483	-3.635687	0.279568
H	-6.583825	-3.877368	-0.677874
H	-5.617916	-4.529775	0.670730
H	-6.869573	-3.302737	0.993760
O	-1.332237	1.437926	-2.165068
H	-0.744148	0.631033	-2.115448
C	-2.058169	-0.309254	2.097848
H	-1.671949	-1.062309	1.415074

C	-3.267227	-0.488824	2.622106
H	-3.725093	0.216219	3.313061
H	-3.847891	-1.368450	2.361890
C	0.808688	2.415329	-0.571093
H	0.676217	1.498940	-1.138684
H	0.496843	3.264427	-1.179590
C	2.247991	2.533808	-0.159600
C	2.856883	3.782151	-0.042618
C	3.049398	1.399898	-0.001446
C	4.206108	3.915578	0.248677
C	4.403730	1.509575	0.291259
H	2.622629	0.408844	-0.131396
C	4.972814	2.765632	0.413138
H	5.013118	0.622949	0.409934
F	2.132379	4.901030	-0.201141
F	4.755522	5.123140	0.363322
F	6.268591	2.906775	0.690486
C	-2.079294	1.408064	-0.986708
H	-1.986596	0.431637	-0.503809
C	3.708397	-3.760497	-0.878889
C	3.161079	-2.601581	-1.449348
C	3.807167	-2.057717	-2.579216
C	4.955015	-2.654994	-3.087679
C	5.497209	-3.795439	-2.498599
C	4.862371	-4.346069	-1.389370
H	3.212811	-4.212087	-0.023123
H	5.435270	-2.215619	-3.960001
H	6.395089	-4.250479	-2.906549
H	5.259009	-5.244762	-0.923598
C	3.226468	-0.805069	-3.182847
H	3.576541	0.068661	-2.610439
H	3.577978	-0.671510	-4.212178
C	1.702479	-0.846119	-3.126662
H	1.269761	0.097723	-3.475693
H	1.324536	-1.637976	-3.789297
C	1.213525	-1.105537	-1.708837
C	1.950418	-1.958047	-0.911025
C	1.554735	-2.233456	0.492639
C	0.279317	-2.787686	0.850049
C	2.449943	-1.978855	1.523805
C	-0.701885	-3.099617	-0.132987
C	-0.038535	-3.052024	2.214669
C	2.133852	-2.230418	2.878707
C	-1.926587	-3.605003	0.220830

H	-0.468667	-2.917082	-1.173533
C	-1.308853	-3.595619	2.548586
C	0.915221	-2.754606	3.217560
H	2.862880	-1.994902	3.648107
C	-2.238655	-3.855675	1.578699
H	-2.671114	-3.808354	-0.542206
H	-1.533754	-3.780668	3.596175
H	0.670424	-2.948840	4.258758
H	-3.216243	-4.247616	1.843450
O	3.662097	-1.428064	1.198658
C	4.805302	-2.000062	1.799582
H	4.977256	-1.606112	2.810605
H	4.724813	-3.091855	1.841523
H	5.654313	-1.736840	1.164571
O	0.133488	-0.501783	-1.338034

S-CPX-C34

C	-0.492998	1.987562	0.773016
C	0.585665	2.907168	0.592567
C	-1.311081	2.171071	1.857619
C	1.530536	2.818830	-0.453230
C	0.736639	3.937948	1.564990
C	-1.082221	3.242025	2.750587
H	-2.112597	1.469802	2.063603
C	2.582058	3.702760	-0.540344
H	1.490960	2.024459	-1.185737
C	1.828223	4.831196	1.449869
H	-1.742055	3.376165	3.606446
C	2.737994	4.725482	0.427282
H	1.922963	5.602844	2.206772
H	3.563485	5.426136	0.371928
C	-1.333271	-0.546682	-2.851857
C	-1.654575	1.855102	-3.458386
C	-0.766914	0.615506	-3.694156
H	-0.605910	-1.064917	-2.215412
H	-1.803502	-1.299539	-3.489890
H	-0.895749	0.346708	-4.752326
C	-1.935395	1.097067	-1.049479
H	-2.794658	1.322853	-0.412317
C	-1.609314	2.284045	-1.991252
H	-2.316747	3.102290	-1.822757
H	-0.618809	2.674497	-1.754385
H	-1.313547	2.676182	-4.096033
C	-3.095092	1.481160	-3.797043

H	-3.739438	2.364904	-3.773847
H	-3.157681	1.056604	-4.804236
C	-3.580696	0.461625	-2.757929
H	-4.293604	0.894924	-2.054006
H	-4.053757	-0.402160	-3.223157
N	-0.101729	4.101839	2.627154
N	-2.433225	-0.067652	-1.926241
O	3.431011	3.517228	-1.586672
C	4.607796	4.289910	-1.641661
H	5.218554	4.159967	-0.738601
H	5.165488	3.924809	-2.505066
H	4.390446	5.356855	-1.781114
O	-0.997729	-0.326103	0.695480
H	-0.444598	-1.099854	0.326005
C	0.702690	0.915283	-3.511561
H	1.022356	1.826568	-4.019526
C	1.615155	0.202540	-2.855588
H	1.393573	-0.705692	-2.303407
H	2.646422	0.537016	-2.804466
C	-2.932208	-1.298932	-1.164671
H	-3.248584	-1.986886	-1.951777
H	-2.070530	-1.732836	-0.665832
C	-4.074352	-1.058248	-0.212030
C	-5.392754	-1.218499	-0.638943
C	-3.866085	-0.784125	1.145249
C	-6.471005	-1.066897	0.221909
C	-4.931051	-0.632316	2.025340
H	-2.840420	-0.696722	1.490523
C	-6.228284	-0.768462	1.557147
H	-4.767414	-0.424187	3.076472
F	-5.666312	-1.537535	-1.914190
F	-7.714878	-1.216940	-0.227975
F	-7.270144	-0.625347	2.373766
C	-0.738123	0.767060	-0.115460
H	0.147243	0.575762	-0.729516
C	4.671177	-2.625561	0.900052
C	3.679128	-2.745586	-0.085037
C	4.008031	-3.440020	-1.268446
C	5.275929	-3.986039	-1.432633
C	6.252231	-3.855786	-0.446456
C	5.939673	-3.168010	0.721966
H	4.436654	-2.106657	1.825475
H	5.504807	-4.517765	-2.354663
H	7.237976	-4.289343	-0.588890



H	6.683432	-3.061392	1.507775
C	2.961794	-3.517975	-2.351443
H	2.995992	-2.589173	-2.943223
H	3.179484	-4.340953	-3.042201
C	1.565858	-3.660475	-1.752554
H	0.793850	-3.586621	-2.526080
H	1.456673	-4.649221	-1.282973
C	1.297392	-2.586424	-0.708931
C	2.335529	-2.173874	0.088852
C	2.128066	-1.157309	1.151570
C	1.287922	-1.400452	2.285908
C	2.776868	0.063389	1.074820
C	0.594102	-2.630096	2.447722
C	1.106715	-0.392998	3.274986
C	2.651355	1.041412	2.090244
C	-0.266538	-2.824516	3.496916
H	0.755418	-3.411339	1.713547
C	0.206583	-0.620917	4.348416
C	1.824330	0.821507	3.157914
H	3.163449	1.993188	1.990570
C	-0.476107	-1.804292	4.455180
H	-0.788320	-3.772150	3.599172
H	0.070056	0.165801	5.087361
H	1.692162	1.593678	3.911757
H	-1.165192	-1.968582	5.279236
O	3.507923	0.315652	-0.055860
C	4.755736	0.945576	0.115489
H	4.654083	2.000819	0.403837
H	5.361352	0.419635	0.863723
H	5.257072	0.894914	-0.852881
O	0.075443	-2.145114	-0.655420

S-CPX-C35

C	1.758973	1.836464	0.734983
C	2.957775	2.451494	0.240636
C	0.583076	2.125365	0.094493
C	4.226987	2.339511	0.859525
C	2.850518	3.230979	-0.945459
C	0.591858	2.933654	-1.070601
H	-0.357435	1.693874	0.420392
C	5.345252	2.935870	0.316156
H	4.361294	1.821202	1.803003
C	4.018166	3.819642	-1.486616
H	-0.345067	3.128310	-1.585149

C	5.242925	3.677652	-0.885315
H	3.905229	4.396238	-2.398801
H	6.115236	4.144564	-1.327748
C	1.099859	-2.357426	1.606503
C	3.110046	-2.454136	3.093457
C	1.667274	-2.965874	2.906463
H	0.225166	-1.722183	1.759432
H	0.805331	-3.135399	0.900885
H	1.716956	-4.056568	2.798972
C	2.698084	-0.375022	1.730174
H	3.584627	-0.081881	1.163269
C	3.107237	-0.929393	3.108265
H	4.101584	-0.543861	3.358301
H	2.410386	-0.557678	3.863320
H	3.515242	-2.845946	4.030325
C	3.962503	-2.916236	1.907600
H	4.971884	-2.502202	1.996289
H	4.057342	-4.006205	1.898494
C	3.309251	-2.443577	0.595661
H	3.997016	-1.894263	-0.048194
H	2.904051	-3.278792	0.023320
N	1.673138	3.453521	-1.596562
N	2.141441	-1.531657	0.882450
O	6.505715	2.763279	1.000662
C	7.667984	3.406971	0.526962
H	7.538695	4.495793	0.486350
H	8.455020	3.166096	1.242526
H	7.959411	3.038969	-0.465168
O	0.620344	0.633594	2.571816
H	-0.060805	0.242122	1.940320
C	0.765689	-2.644549	4.069576
H	0.473279	-1.599921	4.170220
C	0.310664	-3.550298	4.929868
H	0.562215	-4.605196	4.838074
H	-0.339862	-3.272322	5.753382
C	1.564566	-0.981589	-0.412951
H	0.678265	-0.416276	-0.127717
H	2.322846	-0.308641	-0.817964
C	1.145070	-2.014104	-1.417367
C	2.018824	-2.484171	-2.395000
C	-0.184571	-2.440337	-1.460299
C	1.605975	-3.384771	-3.365518
C	-0.620540	-3.338583	-2.427000
H	-0.890006	-2.036286	-0.737221

C	0.279313	-3.806384	-3.370019
H	-1.660411	-3.639872	-2.465200
F	3.296352	-2.072240	-2.418391
F	2.464802	-3.827544	-4.282671
F	-0.102738	-4.666438	-4.314195
C	1.823880	0.903823	1.941530
H	2.428412	1.440991	2.688520
C	-5.800488	0.742052	0.361808
C	-4.671570	0.579180	1.179233
C	-4.841644	0.701018	2.575302
C	-6.102313	0.945350	3.106506
C	-7.218037	1.090576	2.282808
C	-7.056216	0.994677	0.904834
H	-5.687254	0.664769	-0.716137
H	-6.212071	1.033744	4.185746
H	-8.196368	1.280811	2.714372
H	-7.911082	1.112799	0.244105
C	-3.610014	0.623937	3.441279
H	-3.122421	1.611222	3.449630
H	-3.877608	0.395033	4.479307
C	-2.611925	-0.393513	2.897920
H	-1.670584	-0.339783	3.454095
H	-3.002949	-1.414890	3.022743
C	-2.326339	-0.166862	1.420647
C	-3.342542	0.288927	0.621450
C	-3.108761	0.452226	-0.837107
C	-2.944622	1.763933	-1.396778
C	-3.036438	-0.626186	-1.697051
C	-3.027293	2.927233	-0.582893
C	-2.684732	1.933104	-2.786188
C	-2.760914	-0.462663	-3.076843
C	-2.876484	4.180459	-1.120602
H	-3.211538	2.801533	0.478654
C	-2.528316	3.242155	-3.313218
C	-2.583652	0.782904	-3.610358
H	-2.700867	-1.354772	-3.692628
C	-2.626414	4.344307	-2.502912
H	-2.943664	5.054690	-0.479685
H	-2.327934	3.355917	-4.375810
H	-2.377300	0.906442	-4.670370
H	-2.503398	5.340454	-2.917350
O	-3.170223	-1.932158	-1.280673
C	-4.430293	-2.302977	-0.744415
H	-4.600746	-1.857206	0.238420

H	-5.241313	-2.005726	-1.420968
H	-4.413068	-3.391956	-0.656437
O	-1.127002	-0.452673	1.000869

S-CPX-C36

C	-2.098177	-1.826098	-0.792499
C	-3.360600	-2.444513	-0.525342
C	-1.772045	-1.568521	-2.098291
C	-3.784073	-2.858086	0.760070
C	-4.226393	-2.667028	-1.633572
C	-2.705132	-1.851211	-3.124311
H	-0.802085	-1.144300	-2.334007
C	-5.023481	-3.430678	0.953177
H	-3.135940	-2.774402	1.625769
C	-5.494672	-3.251273	-1.403099
H	-2.443258	-1.631623	-4.158180
C	-5.897568	-3.622060	-0.145237
H	-6.136790	-3.404306	-2.264237
H	-6.873855	-4.071817	-0.006856
C	-0.168651	1.448650	1.686644
C	-1.350665	0.498785	3.640824
C	-0.226510	1.471208	3.225903
H	0.578954	0.741813	1.324270
H	0.047717	2.436125	1.284516
H	-0.501666	2.477441	3.570348
C	-1.735424	-0.486125	1.367397
H	-2.823628	-0.576956	1.322167
C	-1.244496	-0.776535	2.795717
H	-1.870670	-1.572745	3.212879
H	-0.211866	-1.142547	2.761930
H	-1.280953	0.272210	4.707465
C	-2.682702	1.183655	3.310513
H	-3.512021	0.475162	3.406937
H	-2.878868	2.013216	3.996353
C	-2.598316	1.727660	1.873960
H	-3.526362	1.588729	1.318129
H	-2.341608	2.788654	1.853563
N	-3.895638	-2.358878	-2.920419
N	-1.504696	1.013611	1.113180
O	-5.325962	-3.784749	2.228211
C	-6.560225	-4.420993	2.476476
H	-6.644903	-5.367898	1.928655
H	-6.580994	-4.624676	3.547755
H	-7.408661	-3.774450	2.217936

O	0.059485	-1.024710	-0.233438
H	0.824202	-1.104388	0.438537
C	1.119042	1.128754	3.801127
H	1.529216	0.169170	3.491173
C	1.804226	1.935763	4.606719
H	1.426172	2.913056	4.902778
H	2.773670	1.646852	5.002277
C	-1.580428	1.339338	-0.367487
H	-0.683571	0.899364	-0.805774
H	-2.449757	0.801401	-0.747756
C	-1.691565	2.805407	-0.685664
C	-2.943044	3.382402	-0.894259
C	-0.565810	3.617682	-0.862975
C	-3.090055	4.718489	-1.240392
C	-0.689729	4.958913	-1.208036
H	0.424534	3.186261	-0.736928
C	-1.951248	5.501159	-1.394197
H	0.181153	5.588766	-1.347790
F	-4.057151	2.649612	-0.758553
F	-4.301062	5.235862	-1.424700
F	-2.101908	6.781141	-1.726817
C	-1.119397	-1.478782	0.320332
H	-0.951439	-2.401494	0.902907
C	5.813801	0.110524	-0.827974
C	5.154514	-0.508261	0.246899
C	5.947588	-1.013223	1.301691
C	7.328574	-0.863827	1.273059
C	7.967383	-0.232601	0.206081
C	7.198805	0.245808	-0.849181
H	5.227398	0.487095	-1.661747
H	7.917320	-1.257367	2.099765
H	9.048022	-0.123771	0.199340
H	7.675631	0.730398	-1.697269
C	5.250581	-1.764313	2.407602
H	5.096763	-2.805936	2.085072
H	5.876335	-1.801035	3.306976
C	3.888843	-1.152377	2.715508
H	3.323020	-1.776561	3.414142
H	4.021118	-0.166772	3.191911
C	3.049158	-0.964032	1.461912
C	3.692046	-0.625532	0.294219
C	2.910854	-0.343359	-0.944306
C	2.787327	-1.385108	-1.932813
C	2.278323	0.857785	-1.210439

C	3.388159	-2.656457	-1.732335
C	2.041249	-1.188081	-3.126714
C	1.551710	1.062362	-2.415293
C	3.256259	-3.659645	-2.659358
H	3.948780	-2.822409	-0.819238
C	1.920276	-2.240595	-4.068641
C	1.429917	0.072490	-3.344464
H	1.111803	2.040222	-2.585705
C	2.515512	-3.454890	-3.844762
H	3.726019	-4.622664	-2.480421
H	1.346413	-2.064853	-4.975922
H	0.879873	0.246763	-4.266455
H	2.419474	-4.256296	-4.571469
O	2.209584	1.958463	-0.393011
C	3.196714	2.248276	0.584667
H	3.014837	1.703237	1.514773
H	4.202104	2.022479	0.220382
H	3.107035	3.322818	0.770354
O	1.768397	-1.065262	1.624342

S-CPX-C37

C	2.573912	-1.422952	-1.104761
C	3.963100	-1.717925	-0.940999
C	1.689330	-2.470156	-1.090579
C	4.993590	-0.749853	-0.985821
C	4.317547	-3.077222	-0.701450
C	2.156667	-3.786544	-0.872998
H	0.628644	-2.283392	-1.227476
C	6.309664	-1.092356	-0.765034
H	4.787227	0.286956	-1.224049
C	5.678834	-3.399867	-0.483670
H	1.442570	-4.608593	-0.855400
C	6.658694	-2.440393	-0.503882
H	5.918550	-4.441860	-0.298845
H	7.689961	-2.724471	-0.329135
C	1.911893	2.796269	0.161467
C	2.233199	1.369754	2.187307
C	2.791670	2.583739	1.419356
H	2.478043	2.669653	-0.763853
H	1.478698	3.797113	0.150631
H	2.680501	3.464160	2.063677
C	1.298979	0.372444	0.043813
H	0.383433	-0.224263	0.078913
C	2.192706	0.137634	1.285502

H	1.801260	-0.719252	1.840853
H	3.208081	-0.124941	0.980794
H	2.863282	1.171986	3.058902
C	0.808735	1.695527	2.622879
H	0.396436	0.861373	3.191816
H	0.795356	2.580928	3.267300
C	-0.050967	1.936815	1.374100
H	-0.861082	1.212995	1.271134
H	-0.479873	2.938476	1.374127
N	3.413019	-4.096181	-0.664826
N	0.769554	1.826126	0.107233
O	7.208208	-0.074540	-0.818112
C	8.574522	-0.372985	-0.635709
H	8.941606	-1.071304	-1.398389
H	9.102879	0.575918	-0.735875
H	8.768236	-0.789852	0.360935
O	1.247970	0.100878	-2.429351
H	0.355706	-0.310201	-2.237094
C	4.247794	2.457624	1.064736
H	4.540335	1.582033	0.487278
C	5.182110	3.334516	1.420129
H	4.943374	4.223779	2.000250
H	6.222743	3.190918	1.146031
C	-0.139669	2.128415	-1.082120
H	0.476289	1.992468	-1.968899
H	-0.882017	1.322054	-1.088763
C	-0.762980	3.496799	-1.082813
C	-2.026077	3.714408	-0.531915
C	-0.156755	4.569540	-1.745641
C	-2.648496	4.955444	-0.599883
C	-0.758436	5.819232	-1.826560
H	0.806421	4.413643	-2.222256
C	-2.005113	6.002263	-1.248621
H	-0.287336	6.648886	-2.340501
F	-2.671508	2.731833	0.089891
F	-3.846447	5.134717	-0.053225
F	-2.613631	7.185130	-1.306220
C	2.030400	-0.002412	-1.278070
H	2.872433	0.683111	-1.419673
C	-4.457532	-3.475647	0.515550
C	-3.862879	-2.846639	-0.590114
C	-4.277144	-3.245860	-1.880593
C	-5.239862	-4.236085	-2.029708
C	-5.824711	-4.850799	-0.922412

C	-5.428009	-4.460090	0.352175
H	-4.148599	-3.190154	1.518019
H	-5.543990	-4.527215	-3.033588
H	-6.577635	-5.622064	-1.056338
H	-5.867660	-4.928770	1.228923
C	-3.677317	-2.521937	-3.059577
H	-4.214368	-1.570911	-3.197727
H	-3.809674	-3.100970	-3.980643
C	-2.203405	-2.203397	-2.820824
H	-1.807630	-1.559767	-3.612920
H	-1.607965	-3.129743	-2.831012
C	-1.995815	-1.503840	-1.488150
C	-2.828188	-1.820764	-0.443194
C	-2.614452	-1.179123	0.879998
C	-1.586833	-1.634219	1.773027
C	-3.413644	-0.132912	1.300321
C	-0.709827	-2.689678	1.404869
C	-1.424504	-1.041997	3.057974
C	-3.250313	0.465822	2.575703
C	0.286782	-3.115144	2.246270
H	-0.858921	-3.154159	0.435935
C	-0.394714	-1.513706	3.916672
C	-2.285501	0.020701	3.438449
H	-3.903851	1.292384	2.840107
C	0.448776	-2.520244	3.520293
H	0.954925	-3.913551	1.936867
H	-0.287008	-1.059127	4.899473
H	-2.162817	0.479751	4.416762
H	1.233170	-2.870598	4.184963
O	-4.368240	0.391882	0.471009
C	-5.684376	-0.067148	0.724682
H	-5.990728	0.150225	1.758337
H	-5.769692	-1.144114	0.542356
H	-6.337623	0.473643	0.037184
O	-1.002153	-0.681752	-1.391179

S-CPX-C38

C	2.995202	-0.594181	-0.978275
C	4.415613	-0.453268	-0.852077
C	2.479969	-1.862146	-1.074799
C	5.086070	0.786359	-0.731628
C	5.191764	-1.647878	-0.826786
C	3.352539	-2.977320	-1.052748
H	1.409000	-2.024093	-1.179842



C	6.453598	0.850471	-0.581775
H	4.549917	1.726291	-0.746965
C	6.596082	-1.549451	-0.682064
H	2.928174	-3.974745	-1.133267
C	7.225009	-0.336289	-0.557822
H	7.159500	-2.476796	-0.668697
H	8.302377	-0.301059	-0.443331
C	0.975708	3.089076	0.494025
C	1.803799	1.752131	2.452714
C	1.940648	3.093867	1.702712
H	1.495945	3.203850	-0.456617
H	0.227114	3.878432	0.555906
H	1.612643	3.882236	2.394526
C	1.208110	0.602841	0.278277
H	0.549957	-0.270763	0.252802
C	2.136881	0.595750	1.515330
H	2.031893	-0.360459	2.035807
H	3.180310	0.675328	1.200084
H	2.486637	1.747487	3.308146
C	0.364537	1.580319	2.922228
H	0.256973	0.620194	3.435543
H	0.084068	2.369603	3.627348
C	-0.555660	1.616872	1.695583
H	-1.148988	0.710564	1.581638
H	-1.246610	2.458645	1.741423
N	4.654380	-2.896682	-0.929924
N	0.225004	1.792431	0.415954
O	6.982637	2.099877	-0.458555
C	8.383556	2.228777	-0.373858
H	8.881919	1.816721	-1.260463
H	8.583217	3.299779	-0.317026
H	8.784222	1.742270	0.524992
O	1.319428	0.662007	-2.212369
H	0.656670	-0.076586	-2.208430
C	3.380330	3.386238	1.342578
H	4.109861	3.009183	2.059418
C	3.828491	4.063189	0.288491
H	3.173673	4.488574	-0.468594
H	4.893602	4.206847	0.137222
C	-0.757010	1.797001	-0.759844
H	-0.240042	2.278554	-1.586896
H	-0.877002	0.747346	-1.023602
C	-2.113883	2.393612	-0.504589
C	-2.365814	3.753538	-0.655338

C	-3.203112	1.557774	-0.229395
C	-3.641767	4.281854	-0.510991
C	-4.490838	2.059653	-0.091228
H	-3.037323	0.489972	-0.117866
C	-4.700090	3.422714	-0.231994
H	-5.328586	1.397208	0.098434
F	-1.365600	4.602562	-0.944028
F	-3.846825	5.590191	-0.651514
F	-5.919071	3.945618	-0.106898
C	2.052374	0.614209	-1.026312
H	2.657626	1.524441	-1.018340
C	-4.598366	-2.388791	0.641828
C	-3.876566	-2.039333	-0.512030
C	-4.623686	-1.683704	-1.659470
C	-6.008951	-1.581735	-1.593373
C	-6.703396	-1.864503	-0.418157
C	-5.984901	-2.297145	0.692343
H	-4.062040	-2.745494	1.515445
H	-6.555766	-1.291109	-2.488563
H	-7.785302	-1.776687	-0.381907
H	-6.504629	-2.566687	1.608493
C	-3.886572	-1.520157	-2.964152
H	-3.714134	-2.523111	-3.383810
H	-4.499368	-0.976584	-3.692256
C	-2.535841	-0.840849	-2.778287
H	-1.921203	-0.928487	-3.679669
H	-2.676595	0.237555	-2.601735
C	-1.741643	-1.401919	-1.610808
C	-2.409958	-2.001361	-0.553938
C	-1.584329	-2.419695	0.610196
C	-0.621168	-3.476738	0.501190
C	-1.674585	-1.768646	1.829055
C	-0.497267	-4.243293	-0.689661
C	0.226967	-3.802264	1.598170
C	-0.848609	-2.095072	2.930577
C	0.411762	-5.264721	-0.783107
H	-1.152002	-4.006855	-1.520341
C	1.172063	-4.855221	1.466368
C	0.092151	-3.084160	2.810983
H	-0.961137	-1.563283	3.870805
C	1.262301	-5.575537	0.305563
H	0.481573	-5.842313	-1.700394
H	1.818032	-5.085448	2.310123
H	0.731458	-3.338051	3.652676

H	1.985706	-6.380632	0.215661
O	-2.560784	-0.720123	1.904824
C	-3.173809	-0.442057	3.141369
H	-3.516131	-1.360698	3.632351
H	-2.501987	0.101422	3.821850
H	-4.035645	0.188944	2.915619
O	-0.474533	-1.191754	-1.622448

S-CPX-C39

C	1.485055	3.701211	-1.004477
C	2.722161	3.098694	-0.603125
C	1.474874	5.058513	-1.198565
C	2.890815	1.715676	-0.381537
C	3.843038	3.964675	-0.430063
C	2.646526	5.825731	-0.989418
H	0.566714	5.561487	-1.522253
C	4.123869	1.198104	-0.036763
H	2.074348	1.016531	-0.510305
C	5.085931	3.406549	-0.049360
H	2.616955	6.903515	-1.143473
C	5.236862	2.055929	0.139796
H	5.920505	4.088588	0.076073
H	6.205898	1.654818	0.414993
C	-2.699429	3.024191	0.220552
C	-1.292471	3.003552	2.264737
C	-2.606125	3.548454	1.669008
H	-2.389217	3.779607	-0.506159
H	-3.719048	2.723151	-0.018635
H	-3.441598	3.136199	2.248314
C	-0.321269	2.273754	0.058207
H	0.199917	1.328957	0.226039
C	-0.160458	3.220800	1.261847
H	0.810750	3.013690	1.719305
H	-0.133155	4.264319	0.931703
H	-1.074116	3.507112	3.210081
C	-1.445455	1.496600	2.468663
H	-0.472568	1.058019	2.702495
H	-2.130747	1.271484	3.291434
C	-1.987906	0.875554	1.173305
H	-1.463918	-0.039813	0.897899
H	-3.058837	0.671697	1.236865
N	3.791506	5.316280	-0.615994
N	-1.808462	1.833118	0.014301
O	4.181141	-0.146145	0.097168

C	5.406658	-0.771957	0.405946
H	5.791627	-0.440643	1.379939
H	5.192196	-1.841229	0.440592
H	6.160993	-0.579091	-0.367411
O	0.333837	2.025576	-2.320503
H	0.490192	1.093414	-1.979784
C	-2.717510	5.047099	1.695016
H	-1.929679	5.600275	1.182312
C	-3.699091	5.714731	2.294211
H	-4.505580	5.200488	2.812674
H	-3.732567	6.799933	2.293271
C	-2.155409	1.112964	-1.284642
H	-2.002807	1.832641	-2.087888
H	-1.404627	0.322885	-1.384198
C	-3.549009	0.546926	-1.338674
C	-3.789093	-0.770237	-0.942750
C	-4.620479	1.257783	-1.889564
C	-5.051158	-1.344366	-1.038384
C	-5.890422	0.703888	-2.000099
H	-4.450052	2.265869	-2.256125
C	-6.096461	-0.596612	-1.567122
H	-6.719386	1.255070	-2.428275
F	-2.807313	-1.520911	-0.453813
F	-5.249621	-2.594257	-0.637240
F	-7.300274	-1.158454	-1.655477
C	0.196250	2.910993	-1.257090
H	-0.542584	3.671478	-1.562511
C	2.972794	-3.853057	0.830675
C	2.583907	-3.113772	-0.298282
C	3.383863	-3.215544	-1.459933
C	4.542194	-3.981337	-1.447286
C	4.935022	-4.684208	-0.306436
C	4.132446	-4.624785	0.828163
H	2.359572	-3.814362	1.727279
H	5.144961	-4.037906	-2.351974
H	5.844246	-5.278411	-0.313095
H	4.408040	-5.178368	1.722260
C	2.891913	-2.518411	-2.701089
H	2.108442	-3.141618	-3.160486
H	3.694912	-2.423573	-3.440988
C	2.292987	-1.156133	-2.369127
H	1.782521	-0.732284	-3.240140
H	3.088317	-0.454304	-2.088205
C	1.294260	-1.229312	-1.226984

C	1.420489	-2.224654	-0.288339
C	0.415639	-2.355588	0.798785
C	-0.558625	-3.410716	0.742822
C	0.373225	-1.508212	1.886979
C	-0.614839	-4.297698	-0.365412
C	-1.516061	-3.574409	1.783300
C	-0.547765	-1.695225	2.948598
C	-1.566371	-5.282120	-0.437148
H	0.109319	-4.169072	-1.162179
C	-2.490499	-4.601677	1.681573
C	-1.476662	-2.697816	2.897354
H	-0.500413	-1.019028	3.797741
C	-2.518591	-5.438053	0.596487
H	-1.592515	-5.947521	-1.295357
H	-3.218747	-4.710912	2.481968
H	-2.189787	-2.834349	3.706723
H	-3.270439	-6.218827	0.527090
O	1.196843	-0.404118	1.966266
C	2.444016	-0.656131	2.592262
H	3.008953	-1.413226	2.040995
H	2.298498	-0.984151	3.631548
H	2.993838	0.286992	2.577340
O	0.395980	-0.299659	-1.178752

S-CPX-C40

C	2.826980	-0.910938	1.732363
C	4.214149	-0.550198	1.658787
C	2.077183	-0.357299	2.736050
C	5.143338	-1.119585	0.754450
C	4.680878	0.439084	2.571383
C	2.656036	0.600379	3.603523
H	1.022620	-0.589700	2.833022
C	6.458632	-0.705649	0.720870
H	4.870620	-1.927602	0.084371
C	6.033284	0.850888	2.506049
H	2.040322	1.049446	4.381152
C	6.909703	0.306334	1.602724
H	6.354394	1.612485	3.208879
H	7.939026	0.645167	1.583248
C	-0.099823	-0.982560	-1.452004
C	1.315692	-2.503766	-2.849157
C	-0.121368	-2.232909	-2.357053
H	-0.498193	-1.155663	-0.451253
H	-0.675723	-0.162985	-1.886511

H	-0.742079	-2.014984	-3.234529
C	2.298919	-1.496096	-0.758539
H	3.261076	-1.004131	-0.916489
C	2.202264	-2.760458	-1.636020
H	3.211483	-3.053780	-1.945631
H	1.783448	-3.579368	-1.045716
H	1.309506	-3.379450	-3.503699
C	1.848135	-1.281169	-3.596816
H	2.875757	-1.463596	-3.926752
H	1.248343	-1.086504	-4.491078
C	1.802440	-0.057684	-2.664858
H	2.776082	0.417235	-2.533761
H	1.103456	0.696542	-3.026796
N	3.896238	1.012870	3.527734
N	1.312341	-0.448165	-1.291345
O	7.254799	-1.325296	-0.186791
C	8.623740	-0.986216	-0.226454
H	9.117343	-1.186882	0.732663
H	9.065616	-1.619933	-0.996213
H	8.773204	0.066517	-0.497963
O	1.020783	-2.479651	1.113685
H	0.333649	-1.799242	1.313122
C	-0.696117	-3.440861	-1.655057
H	-0.577122	-3.481174	-0.573967
C	-1.289962	-4.440428	-2.298669
H	-1.438760	-4.420638	-3.377342
H	-1.677659	-5.302498	-1.765234
C	1.319750	0.759175	-0.365403
H	0.748217	0.449511	0.515690
H	2.364362	0.921749	-0.096465
C	0.731151	2.016948	-0.938853
C	1.556791	2.969846	-1.534581
C	-0.625853	2.319686	-0.811588
C	1.061945	4.176100	-2.006959
C	-1.143698	3.524449	-1.275105
H	-1.301092	1.610001	-0.343008
C	-0.296349	4.445114	-1.867772
H	-2.195774	3.757772	-1.158040
F	2.870413	2.733117	-1.674189
F	1.876312	5.061967	-2.577504
F	-0.757888	5.610214	-2.320269
C	2.235898	-1.915718	0.747182
H	2.945174	-2.757292	0.745685
C	-5.318298	0.961828	1.131638

C	-3.968745	1.189393	1.447768
C	-3.649051	2.372343	2.149943
C	-4.648102	3.276575	2.491319
C	-5.980916	3.045037	2.155296
C	-6.308905	1.877288	1.474404
H	-5.594099	0.046934	0.614710
H	-4.376064	4.182303	3.030402
H	-6.748746	3.762050	2.430344
H	-7.344141	1.667349	1.218094
C	-2.200284	2.631645	2.477892
H	-1.715507	3.112261	1.614995
H	-2.115522	3.336301	3.313012
C	-1.464503	1.331780	2.790365
H	-0.386418	1.507839	2.873095
H	-1.800325	0.931900	3.758724
C	-1.693410	0.265959	1.725478
C	-2.910480	0.234964	1.083442
C	-3.240356	-0.830929	0.098333
C	-3.482900	-2.185291	0.512032
C	-3.413166	-0.534568	-1.240010
C	-3.288627	-2.593356	1.858804
C	-3.936092	-3.155297	-0.425463
C	-3.856190	-1.497384	-2.178766
C	-3.511464	-3.890448	2.243819
H	-2.954190	-1.854938	2.577908
C	-4.163825	-4.488827	0.003196
C	-4.129530	-2.774443	-1.777302
H	-3.963442	-1.204432	-3.219669
C	-3.951872	-4.853681	1.307038
H	-3.349256	-4.181462	3.277549
H	-4.506568	-5.218668	-0.726794
H	-4.466635	-3.518713	-2.494083
H	-4.124261	-5.878094	1.624407
O	-3.086367	0.719251	-1.711663
C	-4.174247	1.508684	-2.159598
H	-4.753757	0.995856	-2.938629
H	-4.836355	1.768463	-1.326406
H	-3.741234	2.417317	-2.584524
O	-0.716343	-0.546846	1.506477

S-CPX-C41

C	0.470938	1.846976	0.846426
C	1.494437	2.716083	0.347507
C	-0.545456	2.418102	1.564796

C	2.602171	2.280949	-0.411621
C	1.377715	4.105039	0.642073
C	-0.561648	3.813558	1.802919
H	-1.362531	1.812585	1.942088
C	3.556169	3.166638	-0.861237
H	2.710726	1.240624	-0.673915
C	2.371083	4.991930	0.165194
H	-1.386484	4.242456	2.368909
C	3.441404	4.546692	-0.569841
H	2.253276	6.044398	0.401312
H	4.181498	5.256503	-0.921172
C	0.181844	-2.465174	1.817086
C	0.898726	-1.178923	3.819801
C	-0.307674	-1.866961	3.152230
H	-0.489829	-2.282121	0.967906
H	0.342816	-3.543521	1.900738
H	-0.591319	-2.715965	3.789386
C	1.521637	-0.356646	1.493886
H	2.510260	-0.074691	1.124561
C	1.362707	0.020337	2.989719
H	2.311021	0.398693	3.385925
H	0.642886	0.832285	3.075673
H	0.643929	-0.857691	4.832952
C	2.048997	-2.185385	3.858922
H	2.866785	-1.814747	4.483570
H	1.718324	-3.138492	4.284897
C	2.554908	-2.382121	2.423965
H	3.470544	-1.820993	2.226336
H	2.748572	-3.429879	2.200235
N	0.353334	4.640976	1.368889
N	1.529667	-1.898539	1.421189
O	4.575741	2.630085	-1.588453
C	5.601273	3.484780	-2.041839
H	6.113162	3.980644	-1.207206
H	6.312713	2.846466	-2.567846
H	5.219868	4.244239	-2.736331
O	0.621473	0.058325	-0.754283
H	-0.141038	-0.580258	-0.981129
C	-1.548776	-1.013586	2.989536
H	-2.180186	-1.255613	2.132323
C	-1.938186	-0.046240	3.815543
H	-1.358553	0.252104	4.686715
H	-2.862267	0.493865	3.632545
C	1.862269	-2.500045	0.054664



H	1.799593	-3.578610	0.216832
H	1.053182	-2.218495	-0.615728
C	3.212813	-2.140633	-0.501004
C	4.338004	-2.918632	-0.229215
C	3.372200	-1.068135	-1.382678
C	5.585813	-2.613598	-0.755069
C	4.611845	-0.735886	-1.914975
H	2.488124	-0.490819	-1.630216
C	5.713824	-1.509114	-1.590253
H	4.731606	0.127835	-2.557831
F	4.248588	-4.006702	0.552466
F	6.640207	-3.371549	-0.462569
F	6.920520	-1.219016	-2.074454
C	0.451503	0.340895	0.598756
H	-0.537507	-0.008863	0.916851
C	-5.580908	-0.475192	-1.873864
C	-4.648748	-1.397074	-1.373391
C	-5.090268	-2.717726	-1.142704
C	-6.405498	-3.077793	-1.413299
C	-7.319768	-2.149496	-1.906899
C	-6.896381	-0.843624	-2.133974
H	-5.265547	0.546134	-2.065227
H	-6.719452	-4.103893	-1.229822
H	-8.345450	-2.442957	-2.111193
H	-7.592256	-0.104085	-2.521697
C	-4.093662	-3.691905	-0.570728
H	-4.024921	-3.539962	0.519340
H	-4.423567	-4.725128	-0.729372
C	-2.716379	-3.451752	-1.178544
H	-1.955729	-4.086440	-0.710914
H	-2.730738	-3.700441	-2.249860
C	-2.286505	-2.000961	-1.021612
C	-3.251238	-1.023210	-1.086369
C	-2.916364	0.421163	-0.997564
C	-3.507458	1.241327	0.016545
C	-2.089282	1.038530	-1.928946
C	-4.305442	0.680814	1.055261
C	-3.307216	2.651689	0.023303
C	-1.854298	2.436436	-1.895969
C	-4.862419	1.469111	2.030090
H	-4.469203	-0.391629	1.060428
C	-3.907188	3.443734	1.038168
C	-2.468442	3.223772	-0.960600
H	-1.198779	2.895998	-2.626301

C	-4.664864	2.871545	2.025872
H	-5.469800	1.014485	2.808409
H	-3.743810	4.519092	1.019162
H	-2.288355	4.295610	-0.947624
H	-5.118440	3.486161	2.798085
O	-1.547439	0.245867	-2.888195
C	-0.507268	0.764787	-3.681400
H	-0.865050	1.538019	-4.375284
H	0.300451	1.169248	-3.059164
H	-0.129993	-0.079165	-4.261966
O	-1.017155	-1.817414	-0.838681

S-CPX-C42

C	0.571088	1.946322	-0.956683
C	-0.452165	2.902502	-0.674579
C	1.283220	2.100721	-2.118876
C	-1.279070	2.862057	0.469702
C	-0.642387	3.954765	-1.616556
C	0.998873	3.173471	-2.992283
H	2.043290	1.377641	-2.393989
C	-2.220462	3.837131	0.704469
H	-1.216393	2.050932	1.181621
C	-1.632160	4.933651	-1.357052
H	1.563475	3.276389	-3.917821
C	-2.400027	4.893822	-0.222070
H	-1.755331	5.723336	-2.091093
H	-3.146672	5.661435	-0.053478
C	1.655068	-0.515561	2.667459
C	2.028321	1.897453	3.184638
C	1.147167	0.673845	3.507656
H	0.882351	-1.050567	2.102872
H	2.172265	-1.245743	3.295471
H	1.334921	0.434306	4.564169
C	2.138946	1.079863	0.778711
H	2.956049	1.281784	0.080748
C	1.894309	2.291945	1.713256
H	2.603383	3.092704	1.479928
H	0.898630	2.697064	1.533632
H	1.736233	2.738064	3.821255
C	3.483515	1.514365	3.440510
H	4.133728	2.390420	3.361679
H	3.604982	1.105376	4.448871
C	3.892639	0.473758	2.388938
H	4.554434	0.893039	1.628926

H	4.397049	-0.382438	2.835272
N	0.078420	4.078225	-2.765943
N	2.687647	-0.068070	1.651818
O	-2.933885	3.710919	1.852949
C	-4.002664	4.599481	2.079789
H	-4.739674	4.557603	1.268713
H	-4.473821	4.270951	3.007209
H	-3.653588	5.633528	2.201818
O	1.104158	-0.364771	-0.887490
H	0.554901	-1.119097	-0.485914
C	-0.329905	0.972547	3.400054
H	-0.616841	1.919820	3.859112
C	-1.285125	0.216899	2.862615
H	-1.100184	-0.728757	2.359350
H	-2.314991	0.562021	2.866486
C	3.123311	-1.323148	0.893300
H	3.459404	-2.004823	1.677541
H	2.230179	-1.744111	0.440350
C	4.228183	-1.122581	-0.110172
C	5.558098	-1.326253	0.258302
C	3.969472	-0.834078	-1.455064
C	6.601471	-1.208148	-0.649316
C	4.998746	-0.713240	-2.381195
H	2.931737	-0.714541	-1.750453
C	6.310052	-0.896509	-1.971888
H	4.798185	-0.493466	-3.423480
F	5.876232	-1.654562	1.520670
F	7.858306	-1.400395	-0.255261
F	7.318460	-0.785993	-2.834054
C	0.883377	0.737271	-0.073109
H	0.039859	0.540923	0.596053
C	-4.440747	-3.079921	-0.991815
C	-3.432287	-3.161725	-0.018410
C	-3.602049	-4.093373	1.028598
C	-4.729213	-4.905591	1.069493
C	-5.720223	-4.815110	0.093113
C	-5.568754	-3.891869	-0.936052
H	-4.335280	-2.367929	-1.805382
H	-4.834480	-5.620489	1.883683
H	-6.595736	-5.456441	0.138516
H	-6.329859	-3.803836	-1.706965
C	-2.543819	-4.133781	2.100813
H	-2.732894	-3.320510	2.820328
H	-2.595589	-5.073635	2.662593

C	-1.158627	-3.930447	1.496169
H	-0.394414	-3.840434	2.275435
H	-0.886435	-4.799037	0.877773
C	-1.099217	-2.682916	0.627730
C	-2.224993	-2.320007	-0.074668
C	-2.217570	-1.160391	-1.005844
C	-3.084174	-0.035863	-0.782333
C	-1.439295	-1.148294	-2.148252
C	-3.907429	0.045894	0.373257
C	-3.154682	1.023540	-1.730913
C	-1.460313	-0.065175	-3.059630
C	-4.777552	1.091129	0.553656
H	-3.844189	-0.749156	1.108965
C	-4.070530	2.086604	-1.523188
C	-2.301738	0.993199	-2.864405
H	-0.788757	-0.108136	-3.911129
C	-4.876415	2.115528	-0.414841
H	-5.403186	1.127071	1.441273
H	-4.114760	2.884220	-2.260505
H	-2.319869	1.823421	-3.565915
H	-5.589883	2.924127	-0.278434
O	-0.575083	-2.174378	-2.444522
C	-1.204585	-3.346412	-2.929455
H	-1.926597	-3.747097	-2.210289
H	-1.715546	-3.149629	-3.882616
H	-0.411008	-4.079419	-3.092012
O	0.036734	-2.060974	0.619692

S-CPX-C43

C	-2.718748	-1.886651	-0.799544
C	-4.147767	-1.865012	-0.918658
C	-1.984271	-1.915264	-1.954310
C	-5.040744	-1.925462	0.178650
C	-4.692804	-1.784115	-2.232246
C	-2.634629	-1.855534	-3.209603
H	-0.901206	-1.921135	-1.913776
C	-6.406352	-1.871498	-0.005741
H	-4.689119	-2.051873	1.197019
C	-6.097834	-1.720117	-2.388942
H	-2.035669	-1.860084	-4.118785
C	-6.944506	-1.754602	-1.310648
H	-6.483033	-1.647257	-3.400641
H	-8.015386	-1.703234	-1.469157
C	-0.111536	0.597686	1.639759

C	-1.487047	0.138489	3.681943
C	-0.046711	0.223565	3.135500
H	0.439030	-0.079390	0.983783
H	0.288394	1.598174	1.461877
H	0.473078	1.029244	3.667862
C	-2.346881	-0.632647	1.441994
H	-3.371800	-0.322918	1.225152
C	-2.212345	-0.977379	2.938446
H	-3.212119	-1.138866	3.356599
H	-1.651602	-1.909082	3.049560
H	-1.448881	-0.085370	4.751219
C	-2.218739	1.457122	3.437780
H	-3.241888	1.394841	3.821604
H	-1.720293	2.274370	3.968111
C	-2.239233	1.752591	1.928253
H	-3.248778	1.844959	1.525842
H	-1.696563	2.668005	1.693113
N	-3.932201	-1.772946	-3.364209
N	-1.553834	0.650360	1.155893
O	-7.163494	-1.938047	1.118415
C	-8.567976	-1.953733	0.985100
H	-8.907049	-2.808360	0.386324
H	-8.963821	-2.047579	1.996999
H	-8.943664	-1.024731	0.537683
O	-0.728280	-2.305468	0.601154
H	-0.136192	-1.780447	-0.012630
C	0.691041	-1.071651	3.386122
H	0.736848	-1.779041	2.561206
C	1.207369	-1.383085	4.570130
H	1.183532	-0.688426	5.408360
H	1.701398	-2.333561	4.739493
C	-1.615962	0.940072	-0.336075
H	-0.968744	0.202097	-0.810172
H	-2.654138	0.773701	-0.628712
C	-1.155243	2.307338	-0.742807
C	-2.044320	3.376026	-0.839446
C	0.170524	2.517958	-1.121602
C	-1.627869	4.631803	-1.254424
C	0.611573	3.769662	-1.535897
H	0.858780	1.678125	-1.112904
C	-0.291124	4.817670	-1.595797
H	1.648585	3.918400	-1.810167
F	-3.338445	3.213399	-0.521631
F	-2.495306	5.640418	-1.325232

F	0.093469	6.032490	-1.987557
C	-2.054041	-1.901597	0.574370
H	-2.597419	-2.670898	1.143289
C	5.717816	-1.315488	-0.899407
C	4.454396	-1.472702	-1.492867
C	4.379115	-2.224938	-2.685695
C	5.519293	-2.815981	-3.216477
C	6.762432	-2.670200	-2.602825
C	6.853379	-1.906417	-1.444409
H	5.812369	-0.725460	0.007037
H	5.433181	-3.391552	-4.136273
H	7.644328	-3.138446	-3.029998
H	7.813684	-1.769093	-0.954299
C	3.050340	-2.285064	-3.392928
H	2.939992	-1.372278	-3.999495
H	3.016346	-3.132080	-4.087631
C	1.888372	-2.341107	-2.407270
H	0.941030	-2.216241	-2.941437
H	1.848805	-3.321564	-1.909783
C	1.988879	-1.261325	-1.339521
C	3.239078	-0.866201	-0.928252
C	3.361163	0.135528	0.166828
C	3.616766	-0.269440	1.520158
C	3.266731	1.489793	-0.085860
C	3.833800	-1.636324	1.848654
C	3.733932	0.699511	2.557535
C	3.303699	2.452367	0.951492
C	4.215147	-2.006111	3.112089
H	3.726013	-2.376560	1.062761
C	4.104094	0.281898	3.863069
C	3.521582	2.067443	2.246940
H	3.177024	3.497374	0.684370
C	4.362593	-1.036484	4.131237
H	4.405502	-3.052414	3.333651
H	4.203225	1.034413	4.642141
H	3.580742	2.808463	3.040509
H	4.668663	-1.342039	5.127849
O	3.087381	1.985364	-1.357883
C	4.225089	1.907142	-2.203644
H	5.082845	2.415978	-1.744884
H	4.494679	0.870806	-2.422435
H	3.952159	2.418221	-3.129559
O	0.870993	-0.816982	-0.846634

## S-CPX-C44

C	-2.177744	-1.945955	0.216351
C	-3.316578	-2.269637	-0.596519
C	-0.972593	-2.461350	-0.172098
C	-4.652755	-1.945114	-0.258628
C	-3.081826	-2.982706	-1.806952
C	-0.855977	-3.197871	-1.374953
H	-0.099667	-2.282133	0.440266
C	-5.702052	-2.257617	-1.096752
H	-4.899802	-1.480988	0.689455
C	-4.175971	-3.275231	-2.654731
H	0.117234	-3.587413	-1.672559
C	-5.459334	-2.919585	-2.324139
H	-3.963101	-3.806865	-3.576467
H	-6.272905	-3.167260	-2.996098
C	-1.382017	1.882139	2.251469
C	-3.810736	2.160131	2.709448
C	-2.401330	2.595862	3.162064
H	-1.005139	0.958253	2.696459
H	-0.558429	2.543629	1.991356
H	-2.321989	3.682513	3.026523
C	-2.984375	0.264567	1.263416
H	-3.617465	0.225433	0.373466
C	-3.815665	0.646861	2.501146
H	-4.836967	0.276706	2.361230
H	-3.400132	0.133721	3.374402
H	-4.554540	2.461241	3.451704
C	-4.091210	2.819400	1.355626
H	-5.001345	2.399518	0.914920
H	-4.246397	3.896997	1.465585
C	-2.884085	2.571898	0.438142
H	-3.176299	2.317203	-0.581361
H	-2.224894	3.441344	0.395353
N	-1.851215	-3.430697	-2.193509
N	-2.040949	1.435756	0.962667
O	-6.939791	-1.897196	-0.664843
C	-8.053176	-2.234788	-1.460567
H	-8.140555	-3.320187	-1.597439
H	-8.928685	-1.871406	-0.920828
H	-8.011307	-1.748564	-2.443826
O	-1.175582	-1.041220	2.269458
H	0.231573	-0.667085	1.938435
C	-2.106014	2.284141	4.603383
H	-2.048810	1.227854	4.865428

C	-1.905808	3.207503	5.539035
H	-1.937184	4.270703	5.309126
H	-1.701548	2.937409	6.570545
C	-1.013559	1.037913	-0.088546
H	-0.405399	0.254606	0.353302
H	-1.578735	0.620856	-0.923651
C	-0.132537	2.173245	-0.526448
C	-0.438600	2.919280	-1.658930
C	1.037391	2.494969	0.171851
C	0.355676	3.979727	-2.072615
C	1.828306	3.570763	-0.206302
H	1.345545	1.853034	0.991870
C	1.483799	4.302479	-1.330541
H	2.742954	3.811233	0.320918
F	-1.525699	2.630696	-2.388825
F	0.041721	4.667610	-3.169625
F	2.245794	5.317690	-1.742684
C	-2.290228	-1.132663	1.517333
H	-3.100481	-1.662904	2.073161
C	5.210821	-2.475146	-0.026053
C	3.960269	-2.543345	0.599087
C	3.563744	-3.771455	1.165588
C	4.422178	-4.865268	1.127246
C	5.672619	-4.777996	0.520375
C	6.058482	-3.577358	-0.065261
H	5.524448	-1.548289	-0.495082
H	4.100020	-5.803649	1.573772
H	6.332745	-5.640332	0.499503
H	7.024925	-3.492711	-0.554619
C	2.173127	-3.884197	1.738914
H	1.472225	-4.110893	0.920044
H	2.111023	-4.721484	2.442174
C	1.733615	-2.588458	2.410444
H	0.667803	-2.618300	2.662250
H	2.283142	-2.436857	3.351010
C	1.999736	-1.401613	1.516438
C	3.047635	-1.378654	0.662731
C	3.343753	-0.184042	-0.179362
C	2.639635	0.067680	-1.393335
C	4.369456	0.676818	0.181667
C	1.552126	-0.747812	-1.804797
C	3.002370	1.165726	-2.224200
C	4.756591	1.750130	-0.659313
C	0.836276	-0.467194	-2.939259



H	1.300936	-1.601316	-1.189903
C	2.251006	1.429184	-3.401192
C	4.090194	1.979476	-1.835911
H	5.577922	2.399856	-0.377954
C	1.184850	0.641658	-3.748996
H	0.004046	-1.106808	-3.222018
H	2.533599	2.278618	-4.019312
H	4.381931	2.813031	-2.470172
H	0.612027	0.859217	-4.645530
O	4.982808	0.415914	1.365902
C	6.170877	1.099152	1.680128
H	6.932069	0.971776	0.898928
H	5.997504	2.171819	1.842535
H	6.534269	0.654901	2.607700
O	1.176376	-0.349910	1.661808

S-CPX-C45

C	2.956418	-2.168508	1.048715
C	3.952139	-1.236592	0.606215
C	3.383604	-3.319225	1.659136
C	3.665756	-0.004613	-0.025046
C	5.315803	-1.598042	0.824541
C	4.765781	-3.574987	1.825685
H	2.663748	-4.045505	2.028910
C	4.685813	0.832975	-0.425576
H	2.650154	0.334408	-0.205388
C	6.335058	-0.714761	0.399919
H	5.088379	-4.494863	2.311143
C	6.039218	0.476288	-0.212392
H	7.362413	-1.013477	0.579931
H	6.843725	1.133549	-0.522111
C	-0.844019	-3.640349	-0.738909
C	0.883186	-3.633114	-2.519219
C	-0.289097	-4.445594	-1.931745
H	-0.452032	-3.996867	0.216954
H	-1.929728	-3.706684	-0.697349
H	-1.069631	-4.526289	-2.698687
C	1.056172	-2.023305	-0.605700
H	1.264160	-1.053623	-1.060586
C	1.768890	-3.150557	-1.369281
H	2.716852	-2.752614	-1.742034
H	2.024106	-3.979316	-0.700428
H	1.453306	-4.248603	-3.219677
C	0.296130	-2.403234	-3.219616

H	1.095801	-1.709429	-3.497142
H	-0.224601	-2.689119	-4.138569
C	-0.694517	-1.715808	-2.264824
H	-0.555241	-0.632655	-2.232269
H	-1.731665	-1.951614	-2.509111
N	5.706791	-2.760353	1.425196
N	-0.467984	-2.189420	-0.846047
O	4.303256	1.992477	-1.018813
C	5.292192	2.903221	-1.440174
H	5.951723	2.464498	-2.200391
H	4.753500	3.745273	-1.876525
H	5.897580	3.261191	-0.597609
O	1.044076	-0.760664	1.503749
H	0.928667	-0.038713	0.839007
C	0.083089	-5.837204	-1.503075
H	0.863685	-5.919380	-0.746248
C	-0.476987	-6.943231	-1.983670
H	-1.262875	-6.905768	-2.734834
H	-0.169779	-7.928339	-1.646355
C	-1.310428	-1.337799	0.102882
H	-1.074045	-1.656665	1.115286
H	-0.940776	-0.316916	-0.031931
C	-2.789150	-1.403076	-0.151637
C	-3.594902	-2.255787	0.598291
C	-3.422626	-0.522722	-1.033152
C	-4.977479	-2.264665	0.470830
C	-4.803313	-0.520126	-1.187963
H	-2.828986	0.212817	-1.564187
C	-5.572382	-1.391132	-0.431590
H	-5.295210	0.163471	-1.870062
F	-3.042217	-3.109171	1.470253
F	-5.716205	-3.097055	1.200483
F	-6.899266	-1.407327	-0.551096
C	1.454911	-1.936641	0.881890
H	0.968598	-2.771570	1.413301
C	-1.431101	5.155921	-0.152870
C	-0.430627	4.314912	-0.662270
C	0.486853	4.868579	-1.583292
C	0.354393	6.188376	-1.997297
C	-0.664336	7.002668	-1.505246
C	-1.549039	6.478185	-0.568384
H	-2.120709	4.767584	0.590993
H	1.070664	6.589544	-2.712504
H	-0.756331	8.032023	-1.839782

H	-2.338941	7.100922	-0.155695
C	1.642328	4.008114	-2.028134
H	2.418089	4.035280	-1.246797
H	2.092727	4.406706	-2.945503
C	1.222288	2.554707	-2.207354
H	2.095207	1.918835	-2.379353
H	0.557671	2.455479	-3.080037
C	0.487602	2.042751	-0.981995
C	-0.298171	2.909914	-0.264589
C	-1.102645	2.343209	0.848707
C	-0.484314	1.957736	2.080515
C	-2.456204	2.105142	0.696802
C	0.891886	2.214382	2.327572
C	-1.240474	1.300085	3.091302
C	-3.219894	1.468858	1.705897
C	1.482840	1.820342	3.498668
H	1.464349	2.722090	1.558089
C	-0.598244	0.900322	4.292715
C	-2.619752	1.064572	2.869049
H	-4.275054	1.272584	1.541223
C	0.733430	1.149208	4.492868
H	2.538219	2.016373	3.663755
H	-1.186067	0.391965	5.053841
H	-3.201738	0.560803	3.637185
H	1.216715	0.835422	5.413590
O	-3.023848	2.446104	-0.506155
C	-4.322853	2.989672	-0.468254
H	-4.415873	3.746051	0.320971
H	-5.092564	2.219595	-0.315167
H	-4.484028	3.464732	-1.438163
O	0.603267	0.772434	-0.724301

S-CPX-C46

C	-3.400245	1.412867	0.764593
C	-4.023658	0.300899	0.106900
C	-4.212594	2.308251	1.411016
C	-3.322773	-0.702859	-0.595496
C	-5.445545	0.209397	0.198320
C	-5.617547	2.133248	1.415449
H	-3.785295	3.153438	1.945712
C	-3.991650	-1.767343	-1.160077
H	-2.242743	-0.699168	-0.704206
C	-6.100520	-0.892356	-0.398755
H	-6.247755	2.857126	1.930347

C	-5.399475	-1.870014	-1.059730
H	-7.180590	-0.940360	-0.307203
H	-5.930947	-2.706967	-1.498678
C	0.177724	3.982201	-0.090289
C	-1.284039	4.006732	-2.094682
C	-0.403268	4.894231	-1.191051
H	-0.394208	4.050694	0.839209
H	1.212634	4.244284	0.129456
H	0.422545	5.288571	-1.796089
C	-1.322421	2.035028	-0.539461
H	-1.253477	1.145981	-1.167197
C	-2.170223	3.127740	-1.211496
H	-2.947598	2.633679	-1.800927
H	-2.692204	3.733127	-0.462376
H	-1.889636	4.630868	-2.756912
C	-0.356946	3.090811	-2.899230
H	-0.943091	2.330729	-3.424979
H	0.195689	3.659170	-3.653504
C	0.636962	2.422178	-1.934867
H	0.745783	1.352874	-2.116596
H	1.616880	2.902507	-1.965498
N	-6.225222	1.128404	0.840657
N	0.147673	2.540694	-0.508086
O	-3.212137	-2.683158	-1.792971
C	-3.811345	-3.862221	-2.277514
H	-4.536009	-3.653144	-3.075591
H	-2.997874	-4.465433	-2.682354
H	-4.308594	-4.421604	-1.474313
O	-1.251981	0.497108	1.382987
H	-0.904612	-0.087360	0.662079
C	-1.128217	6.060436	-0.580092
H	-2.002578	5.823977	0.027399
C	-0.767183	7.330674	-0.735960
H	0.100659	7.608575	-1.330359
H	-1.325729	8.141430	-0.278550
C	1.043466	1.697742	0.401567
H	0.626944	1.769549	1.404610
H	0.903101	0.670911	0.051483
C	2.496290	2.078931	0.406724
C	3.392126	1.485852	-0.484078
C	3.028932	2.910450	1.396668
C	4.755870	1.741913	-0.421346
C	4.389806	3.183044	1.477988
H	2.357606	3.340617	2.134156

C	5.245465	2.594395	0.560767
H	4.798794	3.829005	2.245943
F	2.966754	0.655019	-1.430038
F	5.586252	1.152907	-1.276517
F	6.556398	2.824382	0.608178
C	-1.883159	1.607333	0.833342
H	-1.727846	2.443485	1.535237
C	2.692435	-4.264358	0.148188
C	1.781993	-3.620913	-0.702464
C	1.608630	-4.145588	-2.002647
C	2.353259	-5.242580	-2.419454
C	3.269788	-5.859589	-1.569068
C	3.426204	-5.366479	-0.277609
H	2.822104	-3.895627	1.161384
H	2.204549	-5.629156	-3.426395
H	3.844169	-6.716472	-1.909461
H	4.126438	-5.840063	0.406090
C	0.545566	-3.524918	-2.874981
H	-0.430816	-3.948699	-2.590247
H	0.709978	-3.778898	-3.928764
C	0.470837	-2.013956	-2.679715
H	-0.407941	-1.598135	-3.183231
H	1.360984	-1.529101	-3.110100
C	0.386976	-1.650473	-1.210261
C	1.011926	-2.444921	-0.287173
C	0.951081	-2.041731	1.142688
C	-0.231695	-2.269479	1.911639
C	2.013694	-1.393147	1.749032
C	-1.383396	-2.874793	1.336279
C	-0.301666	-1.844111	3.268423
C	1.957436	-0.982736	3.103136
C	-2.533947	-3.030799	2.062440
H	-1.338757	-3.183820	0.297418
C	-1.502930	-2.037803	4.000405
C	0.823889	-1.209152	3.841020
H	2.804783	-0.481916	3.559870
C	-2.598667	-2.610663	3.412420
H	-3.410889	-3.470014	1.594779
H	-1.541831	-1.705732	5.035547
H	0.778333	-0.887499	4.878822
H	-3.519545	-2.738821	3.974026
O	3.106371	-1.139279	0.963085
C	4.342094	-0.925047	1.597205
H	4.557659	-1.706798	2.336991

H	4.391663	0.057606	2.089902
H	5.095795	-0.959479	0.807715
O	-0.244049	-0.549213	-0.920540
S-CPX-C47			
C	-3.490198	0.172425	1.375809
C	-4.794366	0.605090	0.987708
C	-3.261172	-0.050078	2.710830
C	-5.156279	0.932860	-0.338737
C	-5.779944	0.711645	2.012796
C	-4.308892	0.103106	3.646477
H	-2.267547	-0.323045	3.054652
C	-6.440968	1.317351	-0.652100
H	-4.431567	0.897646	-1.141466
C	-7.091915	1.109820	1.658869
H	-4.116914	-0.082519	4.701915
C	-7.427419	1.402853	0.361779
H	-7.824934	1.177787	2.455817
H	-8.442204	1.703727	0.127775
C	-0.856034	-1.583728	-1.824002
C	-2.965908	-2.921772	-1.644778
C	-2.171200	-1.963336	-2.549688
H	-0.657306	-0.507167	-1.784994
H	0.004597	-2.055165	-2.299372
H	-1.883493	-2.532963	-3.444446
C	-2.113035	-1.582670	0.333601
H	-1.965911	-1.946111	1.353697
C	-3.349240	-2.243185	-0.327768
H	-3.793181	-2.978749	0.350502
H	-4.111344	-1.484374	-0.509758
H	-3.862455	-3.274146	-2.161595
C	-2.059608	-4.103356	-1.306073
H	-2.621672	-4.878202	-0.776660
H	-1.657151	-4.557034	-2.217644
C	-0.919221	-3.593695	-0.413936
H	-1.023485	-3.901845	0.628279
H	0.047881	-3.939798	-0.773383
N	-5.531025	0.452816	3.326889
N	-0.858967	-2.083176	-0.401648
O	-6.679163	1.596790	-1.960905
C	-7.960380	2.056878	-2.330129
H	-8.218759	2.989670	-1.813545
H	-7.911889	2.244396	-3.403453
H	-8.734471	1.304408	-2.131784

O	-1.254191	0.676888	0.925210
H	-0.618823	0.926715	0.186481
C	-2.918585	-0.747188	-3.047428
H	-2.283969	0.080724	-3.364697
C	-4.237317	-0.629648	-3.179013
H	-4.931191	-1.409801	-2.876100
H	-4.686063	0.274846	-3.576586
C	0.423319	-1.658507	0.326611
H	0.475233	-0.575759	0.262830
H	0.302016	-1.965286	1.366688
C	1.676335	-2.218559	-0.284379
C	2.284355	-3.357298	0.236347
C	2.313850	-1.560814	-1.340856
C	3.465686	-3.859998	-0.288545
C	3.485277	-2.060360	-1.897474
H	1.893208	-0.618786	-1.683855
C	4.055360	-3.202892	-1.362291
H	3.986031	-1.544796	-2.708675
F	1.722076	-4.010538	1.263328
F	4.026232	-4.950845	0.233795
F	5.196764	-3.689819	-1.853861
C	-2.320806	-0.033599	0.410412
H	-2.587899	0.314755	-0.596330
C	4.037937	3.874133	0.747182
C	3.047157	3.575759	-0.199088
C	2.694637	4.579374	-1.125474
C	3.314709	5.822776	-1.080029
C	4.297243	6.105711	-0.132721
C	4.656703	5.119433	0.780039
H	4.319597	3.118313	1.474954
H	3.025150	6.582322	-1.804036
H	4.772015	7.082433	-0.108900
H	5.417390	5.320457	1.530136
C	1.671904	4.233997	-2.177796
H	2.177367	3.702416	-2.999183
H	1.233926	5.142649	-2.607162
C	0.590261	3.321852	-1.607475
H	-0.072971	2.954311	-2.397367
H	-0.036913	3.878704	-0.894597
C	1.183521	2.115932	-0.896648
C	2.371081	2.267988	-0.227900
C	2.997283	1.138199	0.510727
C	2.442579	0.611942	1.718573
C	4.174414	0.575730	0.038658

C	1.286676	1.181921	2.316404
C	3.036194	-0.516269	2.359080
C	4.809480	-0.495229	0.713862
C	0.720452	0.630917	3.436244
H	0.848286	2.059676	1.855479
C	2.417930	-1.078458	3.507423
C	4.237948	-1.042375	1.831831
H	5.728953	-0.919581	0.326324
C	1.277991	-0.525336	4.032399
H	-0.170921	1.083196	3.860740
H	2.873320	-1.951935	3.968672
H	4.709569	-1.889143	2.324844
H	0.816051	-0.957687	4.915876
O	4.654856	1.068421	-1.136651
C	5.975003	0.757661	-1.506078
H	6.095634	-0.304594	-1.763911
H	6.689518	1.015057	-0.713613
H	6.189253	1.361754	-2.389276
O	0.477941	1.017130	-0.946260

S-CPX-C48

C	0.187417	1.791847	0.857823
C	1.291852	2.633654	0.508089
C	0.375805	0.897445	1.877770
C	1.263641	3.543478	-0.573260
C	2.476297	2.524438	1.288132
C	1.595475	0.879001	2.595528
H	-0.386176	0.181193	2.164358
C	2.365531	4.312819	-0.876203
H	0.400452	3.599784	-1.225680
C	3.586478	3.338212	0.959966
H	1.721518	0.168721	3.409681
C	3.544334	4.212331	-0.096364
H	4.479851	3.233515	1.566637
H	4.417884	4.810509	-0.329174
C	-3.935150	2.786090	-0.315181
C	-3.861690	2.750385	2.180141
C	-3.964361	3.675284	0.949518
H	-3.187058	3.086041	-1.049557
H	-4.908812	2.772848	-0.809934
H	-4.960995	4.135939	0.998137
C	-2.302161	1.283719	0.811838
H	-2.108281	0.211917	0.903703
C	-2.542370	1.973313	2.179626



H	-2.549200	1.235869	2.988442
H	-1.708614	2.649797	2.381665
H	-3.942154	3.348199	3.092906
C	-5.003907	1.741241	2.100765
H	-5.065642	1.156094	3.022546
H	-5.964795	2.250128	1.971814
C	-4.723827	0.806685	0.917731
H	-4.384017	-0.177777	1.241535
H	-5.597848	0.667861	0.282093
N	2.607736	1.666916	2.339288
N	-3.626353	1.350807	0.032016
O	2.241621	5.146468	-1.943730
C	3.389941	5.824385	-2.398532
H	4.197776	5.125087	-2.649502
H	3.086021	6.358538	-3.300013
H	3.755620	6.550171	-1.660108
O	-0.996447	1.637141	-1.260400
H	-0.455262	0.720193	-1.277148
C	-2.980891	4.822667	0.993693
H	-2.880724	5.269019	1.983316
C	-2.297780	5.360275	-0.012448
H	-2.340052	4.985938	-1.032431
H	-1.641010	6.207920	0.152446
C	-3.616337	0.550645	-1.280845
H	-4.468433	0.938411	-1.842244
H	-2.684588	0.835106	-1.767848
C	-3.739256	-0.938201	-1.133841
C	-5.000222	-1.532125	-1.225631
C	-2.627529	-1.779599	-1.011039
C	-5.177500	-2.903585	-1.158780
C	-2.787273	-3.161823	-0.950090
H	-1.610901	-1.377354	-0.987307
C	-4.053828	-3.712551	-1.018979
H	-1.910654	-3.797091	-0.886518
F	-6.100839	-0.769733	-1.383135
F	-6.398356	-3.431085	-1.240186
F	-4.233297	-5.032044	-0.964613
C	-1.118155	1.973315	0.081941
H	-1.321710	3.048743	0.132588
C	4.446582	-2.748446	-1.034761
C	3.675816	-1.590686	-1.221616
C	4.253366	-0.519023	-1.936283
C	5.543502	-0.629434	-2.441090
C	6.297435	-1.786594	-2.248675

C	5.739631	-2.844906	-1.538429
H	4.020586	-3.584370	-0.486230
H	5.968158	0.209570	-2.989519
H	7.304368	-1.858809	-2.649873
H	6.309394	-3.756625	-1.378176
C	3.424199	0.728574	-2.086191
H	3.475051	1.310943	-1.153304
H	3.817398	1.368608	-2.884815
C	1.965752	0.367097	-2.343810
H	1.346294	1.268735	-2.361005
H	1.862246	-0.115873	-3.327710
C	1.426943	-0.582268	-1.281874
C	2.300375	-1.483164	-0.712721
C	1.838855	-2.402919	0.355862
C	2.431591	-2.348318	1.667605
C	0.823830	-3.320685	0.158079
C	3.520415	-1.481715	1.957122
C	1.927899	-3.157388	2.726349
C	0.312392	-4.115594	1.213087
C	4.081068	-1.431735	3.207724
H	3.891863	-0.829229	1.176846
C	2.517788	-3.074314	4.015065
C	0.839040	-4.029940	2.470562
H	-0.494384	-4.806600	0.985808
C	3.576203	-2.235910	4.254154
H	4.900301	-0.745697	3.399366
H	2.117267	-3.699329	4.810342
H	0.450333	-4.646429	3.277516
H	4.024253	-2.184447	5.242507
O	0.215012	-3.520493	-1.057664
C	1.048166	-3.963786	-2.115406
H	1.764589	-3.195565	-2.416535
H	1.591574	-4.872122	-1.824022
H	0.380725	-4.192603	-2.949424
O	0.164597	-0.501481	-1.007032

S-CPX-C49

C	2.116536	-1.901905	-1.172971
C	3.327676	-1.192641	-1.473181
C	1.670062	-2.808956	-2.096622
C	3.893001	-0.228192	-0.609588
C	3.973110	-1.480841	-2.707097
C	2.395330	-3.018017	-3.297741
H	0.762891	-3.385866	-1.949596

C	5.050185	0.432876	-0.957934
H	3.383668	0.070186	0.298583
C	5.163523	-0.790412	-3.032085
H	2.025204	-3.741787	-4.022522
C	5.697891	0.147134	-2.184074
H	5.637148	-1.024306	-3.979695
H	6.608674	0.662880	-2.466193
C	-0.048035	-1.469008	2.685815
C	0.641774	-3.883701	2.672352
C	0.882921	-2.512843	3.347452
H	0.459107	-0.573050	2.330341
H	-0.845299	-1.153202	3.360757
H	0.541034	-2.634131	4.384885
C	0.318721	-2.616927	0.511556
H	-0.266362	-2.889082	-0.366328
C	0.962018	-3.858896	1.169650
H	0.595284	-4.782233	0.708268
H	2.041907	-3.828329	0.999131
H	1.241764	-4.649769	3.172442
C	-0.848004	-4.193198	2.811716
H	-1.065220	-5.218866	2.499617
H	-1.166484	-4.093097	3.854147
C	-1.613223	-3.211088	1.916368
H	-1.972747	-3.687636	1.003190
H	-2.470244	-2.765368	2.421081
N	3.501002	-2.394191	-3.606355
N	-0.730234	-2.066679	1.473832
O	5.493893	1.368661	-0.075535
C	6.585269	2.179863	-0.448537
H	6.384771	2.720784	-1.382281
H	6.713427	2.899951	0.360683
H	7.508535	1.596509	-0.558458
O	1.087287	-0.256787	0.269609
H	0.723405	0.158897	-0.615558
C	2.346853	-2.155812	3.451791
H	2.947755	-2.953224	3.891555
C	2.943914	-1.011865	3.129386
H	2.422909	-0.167953	2.684364
H	4.010396	-0.884624	3.288838
C	-1.624721	-1.001512	0.837297
H	-2.222614	-0.608212	1.659364
H	-0.962463	-0.215929	0.487867
C	-2.499262	-1.507064	-0.273782
C	-3.819284	-1.875130	-0.018953

C	-2.053972	-1.549733	-1.599030
C	-4.671918	-2.298389	-1.028071
C	-2.889593	-1.980017	-2.623317
H	-1.068202	-1.149072	-1.837471
C	-4.191803	-2.351765	-2.332260
H	-2.553085	-1.995567	-3.653649
F	-4.307261	-1.832086	1.230698
F	-5.924993	-2.648103	-0.748441
F	-5.017421	-2.761453	-3.293344
C	1.440920	-1.589349	0.156314
H	2.212860	-1.755135	0.915993
C	-2.165953	4.489595	0.263469
C	-2.175012	3.338372	-0.540434
C	-3.330117	3.084413	-1.313453
C	-4.411755	3.955604	-1.266564
C	-4.390160	5.090791	-0.457943
C	-3.256828	5.350993	0.306587
H	-1.282812	4.712481	0.855768
H	-5.288866	3.739824	-1.874293
H	-5.242464	5.763734	-0.432273
H	-3.215155	6.235701	0.936911
C	-3.339205	1.840107	-2.164777
H	-3.620113	0.972395	-1.544203
H	-4.090642	1.920143	-2.958817
C	-1.949992	1.595248	-2.743142
H	-1.911383	0.669615	-3.324049
H	-1.681927	2.416772	-3.422884
C	-0.905838	1.527184	-1.639077
C	-1.043514	2.403283	-0.578557
C	0.044356	2.503844	0.425792
C	-0.170745	2.204838	1.811799
C	1.330836	2.834345	0.026459
C	-1.467473	1.916391	2.322776
C	0.924028	2.166670	2.722660
C	2.421840	2.788811	0.929589
C	-1.664130	1.603535	3.645314
H	-2.310672	1.962059	1.641471
C	0.693965	1.824036	4.081648
C	2.226649	2.453312	2.240682
H	3.420174	3.018299	0.571623
C	-0.569365	1.548154	4.540330
H	-2.669561	1.410446	4.010831
H	1.544065	1.792213	4.759732
H	3.066699	2.421265	2.930865

H	-0.733209	1.305712	5.586646
O	1.522700	3.267453	-1.250375
C	2.517683	2.618167	-2.017920
H	3.524940	2.765115	-1.604244
H	2.300558	1.550062	-2.101196
H	2.474537	3.075719	-3.008131
O	0.036691	0.652512	-1.801680

S-CPX-C50

C	2.405196	1.615520	0.308213
C	3.559306	1.988061	-0.461811
C	1.224943	2.224115	-0.012860
C	4.868252	1.511229	-0.209863
C	3.369966	2.905331	-1.535731
C	1.151349	3.149258	-1.080092
H	0.324682	1.988115	0.531067
C	5.934117	1.885278	-1.000709
H	5.083904	0.864963	0.633368
C	4.481608	3.267496	-2.332010
H	0.190780	3.607709	-1.311262
C	5.737433	2.771542	-2.086465
H	4.304994	3.965205	-3.144256
H	6.565276	3.075058	-2.717026
C	1.291840	-2.324247	1.937047
C	3.693087	-2.923184	2.169801
C	2.274065	-3.252908	2.677850
H	1.056163	-1.425454	2.512489
H	0.380251	-2.852720	1.664804
H	2.058057	-4.299945	2.427166
C	3.011163	-0.778876	1.025736
H	3.586988	-0.691147	0.100054
C	3.868252	-1.405584	2.139918
H	4.916291	-1.141301	1.963646
H	3.577196	-0.962207	3.097590
H	4.441727	-3.395284	2.811509
C	3.806670	-3.434852	0.730690
H	4.731541	-3.067558	0.274194
H	3.837559	-4.528297	0.699954
C	2.583659	-2.939795	-0.057193
H	2.842776	-2.588883	-1.056770
H	1.823993	-3.718087	-0.155721
N	2.167192	3.477704	-1.839515
N	1.917626	-1.794427	0.662943
O	7.142044	1.358398	-0.665149

C	8.276915	1.765692	-1.395035
H	8.435376	2.849382	-1.324561
H	9.125525	1.250912	-0.942456
H	8.205112	1.478690	-2.452198
O	1.419827	0.565883	2.308026
H	-0.035717	0.426314	2.054755
C	2.109816	-3.087926	4.163496
H	2.219809	-2.075273	4.550845
C	1.831070	-4.085089	4.997853
H	1.695222	-5.105091	4.643798
H	1.722409	-3.919582	6.065234
C	0.878572	-1.153112	-0.242937
H	0.397945	-0.372747	0.338949
H	1.436721	-0.694824	-1.061154
C	-0.164583	-2.109576	-0.746361
C	-0.026122	-2.737084	-1.979532
C	-1.331791	-2.362012	-0.014417
C	-0.979287	-3.622660	-2.463764
C	-2.285674	-3.263239	-0.466558
H	-1.505927	-1.796221	0.896113
C	-2.101645	-3.886875	-1.689851
H	-3.201331	-3.440531	0.085010
F	1.048308	-2.492663	-2.748821
F	-0.816892	-4.202224	-3.652558
F	-3.017443	-4.728938	-2.169372
C	2.492609	0.639381	1.495291
H	3.383970	1.007912	2.055532
C	-4.461348	3.183151	-0.044647
C	-3.262993	3.004522	0.656687
C	-2.704223	4.113639	1.323167
C	-3.352901	5.342961	1.287121
C	-4.550770	5.506239	0.594691
C	-5.099644	4.419385	-0.076006
H	-4.904770	2.342840	-0.569106
H	-2.907170	6.189515	1.805270
H	-5.045160	6.473125	0.577811
H	-6.032344	4.527571	-0.622563
C	-1.368522	3.947092	2.003823
H	-0.574225	4.092951	1.256972
H	-1.224459	4.721469	2.765021
C	-1.211179	2.560043	2.619463
H	-0.171563	2.383493	2.916063
H	-1.827066	2.466836	3.526132
C	-1.628048	1.479264	1.650590

C	-2.578679	1.691581	0.716010
C	-3.031738	0.620314	-0.217214
C	-4.184063	-0.160745	0.096052
C	-2.407870	0.419918	-1.439478
C	-4.835323	-0.048893	1.357125
C	-4.715932	-1.078057	-0.854600
C	-2.945587	-0.479402	-2.394018
C	-5.930243	-0.815959	1.656228
H	-4.441758	0.656255	2.081654
C	-5.853548	-1.859231	-0.515710
C	-4.077966	-1.195969	-2.109857
H	-2.464666	-0.611585	-3.355861
C	-6.447490	-1.737038	0.712441
H	-6.408607	-0.717637	2.626356
H	-6.241764	-2.559474	-1.251878
H	-4.478495	-1.888903	-2.845754
H	-7.316033	-2.338482	0.964377
O	-1.262767	1.117749	-1.673522
C	-0.627915	0.967987	-2.924176
H	-0.294697	-0.065401	-3.089892
H	-1.283162	1.272348	-3.749916
H	0.243419	1.623040	-2.900986
O	-1.031243	0.283509	1.804147

S-CPX-C51

C	-3.598608	-0.447221	1.644323
C	-4.724756	0.196071	1.045105
C	-3.770289	-1.029790	2.874258
C	-4.675371	0.886854	-0.188797
C	-5.966132	0.117292	1.740498
C	-5.043347	-1.024714	3.488558
H	-2.927723	-1.486806	3.384461
C	-5.810676	1.444786	-0.735017
H	-3.740102	1.036528	-0.717259
C	-7.114389	0.701667	1.153198
H	-5.172226	-1.494862	4.462215
C	-7.051828	1.343677	-0.056581
H	-8.049628	0.622522	1.697502
H	-7.950940	1.777712	-0.478516
C	-0.832297	-1.590220	-1.675484
C	-2.764353	-3.183722	-1.609981
C	-1.964339	-2.224751	-2.515508
H	-0.943450	-0.515128	-1.497870
H	0.135880	-1.725238	-2.152222

H	-1.516633	-2.824988	-3.317503
C	-2.023806	-1.972837	0.488949
H	-1.902317	-2.601749	1.377266
C	-3.228342	-2.441573	-0.362934
H	-3.872278	-3.078676	0.250010
H	-3.836104	-1.582840	-0.655321
H	-3.625153	-3.572345	-2.160495
C	-1.851190	-4.324280	-1.165268
H	-2.388019	-4.978903	-0.471606
H	-1.543544	-4.935662	-2.019165
C	-0.608760	-3.725918	-0.486271
H	-0.427736	-4.146013	0.505828
H	0.290988	-3.886810	-1.079370
N	-6.113844	-0.494700	2.949285
N	-0.732614	-2.233691	-0.311674
O	-5.653130	2.073510	-1.925991
C	-6.763612	2.731195	-2.495672
H	-7.158134	3.507884	-1.828699
H	-6.395775	3.197739	-3.410061
H	-7.565449	2.025781	-2.748917
O	-1.258865	-0.099629	1.877570
H	-0.712695	0.558445	1.369326
C	-2.818509	-1.163691	-3.156150
H	-3.263340	-0.424378	-2.490634
C	-3.049904	-1.079729	-4.462534
H	-2.616379	-1.785559	-5.168153
H	-3.678920	-0.297130	-4.875104
C	0.506042	-1.690475	0.421428
H	0.529830	-0.616826	0.194493
H	0.299350	-1.801765	1.484491
C	1.800684	-2.371418	0.083867
C	2.574373	-1.993003	-1.012380
C	2.330040	-3.343981	0.936746
C	3.792350	-2.598134	-1.289442
C	3.558245	-3.945062	0.697004
H	1.770371	-3.618967	1.825657
C	4.281480	-3.564346	-0.420983
H	3.973081	-4.686778	1.369322
F	2.155904	-1.040930	-1.849582
F	4.490229	-2.242575	-2.361940
F	5.467047	-4.111489	-0.683363
C	-2.232893	-0.514701	0.973124
H	-2.206823	0.142454	0.101623
C	3.522486	4.035857	0.583073



C	2.472983	3.576823	-0.228250
C	2.111310	4.363032	-1.344204
C	2.774499	5.555934	-1.606524
C	3.814070	5.999626	-0.790372
C	4.185027	5.226846	0.305534
H	3.816104	3.450727	1.450096
H	2.474822	6.146036	-2.471147
H	4.322931	6.934369	-1.008009
H	4.990756	5.554880	0.957491
C	1.024518	3.833849	-2.244294
H	1.460385	3.090239	-2.930700
H	0.610280	4.636143	-2.866178
C	-0.068346	3.150517	-1.428261
H	-0.796461	2.652985	-2.077822
H	-0.619558	3.895639	-0.835414
C	0.502593	2.109661	-0.477544
C	1.754131	2.327989	0.056423
C	2.337544	1.357003	1.015342
C	3.553764	0.662635	0.720139
C	1.740628	1.123468	2.249374
C	4.249323	0.871429	-0.505618
C	4.115020	-0.254628	1.655628
C	2.261059	0.165070	3.154240
C	5.440774	0.244281	-0.760410
H	3.815903	1.545018	-1.235821
C	5.348260	-0.895479	1.359123
C	3.423030	-0.502922	2.862434
H	1.758379	-0.027161	4.095534
C	6.007301	-0.645590	0.184923
H	5.952497	0.422490	-1.701357
H	5.761828	-1.588425	2.088783
H	3.830508	-1.220802	3.570497
H	6.950957	-1.137833	-0.031421
O	0.635547	1.861942	2.537170
C	0.079087	1.784176	3.828907
H	0.820510	2.029025	4.600847
H	-0.355463	0.796532	4.020709
H	-0.719767	2.526562	3.848811
O	-0.256975	1.095462	-0.220975

S-CPX-C52

C	-3.273490	-1.471282	-0.277762
C	-4.554766	-1.136268	-0.821606
C	-3.155769	-2.653057	0.405365

C	-4.808298	0.026525	-1.585070
C	-5.629285	-2.031457	-0.551127
C	-4.286804	-3.486660	0.584214
H	-2.198725	-2.952018	0.823781
C	-6.080945	0.316653	-2.028274
H	-3.992437	0.671199	-1.887797
C	-6.921842	-1.708616	-1.026628
H	-4.179273	-4.425091	1.126073
C	-7.155594	-0.560879	-1.740995
H	-7.723495	-2.405926	-0.806569
H	-8.158809	-0.345635	-2.090931
C	-0.288106	0.929488	1.925194
C	-2.524217	1.379734	2.911614
C	-1.040763	1.123859	3.257096
H	-0.153256	-0.123377	1.663975
H	0.701262	1.376916	1.949628
H	-0.649002	2.015284	3.763979
C	-2.313167	0.708238	0.493223
H	-2.954309	1.384180	-0.079178
C	-2.962880	0.372880	1.849678
H	-4.048544	0.380564	1.718774
H	-2.696323	-0.643456	2.154508
H	-3.138179	1.289325	3.810967
C	-2.637204	2.781338	2.310706
H	-3.635841	2.932237	1.888057
H	-2.482436	3.552159	3.071790
C	-1.561471	2.919419	1.224758
H	-1.932465	3.425322	0.331362
H	-0.688466	3.467940	1.582077
N	-5.485566	-3.195907	0.147303
N	-1.060348	1.564678	0.788557
O	-6.218749	1.465422	-2.741597
C	-7.478417	1.766010	-3.297627
H	-8.242712	1.909806	-2.522526
H	-7.348004	2.700777	-3.844561
H	-7.811299	0.985604	-3.993693
O	-1.840608	-0.190146	-1.723314
H	-0.909625	-0.518990	-1.915936
C	-0.852675	-0.051047	4.173445
H	-1.087274	-1.031151	3.760810
C	-0.431216	0.046891	5.430611
H	-0.164436	1.003558	5.874745
H	-0.332917	-0.830007	6.063710
C	-0.174361	1.710286	-0.446007

H	0.419224	0.787235	-0.526288
H	-0.861349	1.691355	-1.290506
C	0.655505	2.965248	-0.525241
C	1.877708	3.126471	0.123665
C	0.260524	3.995541	-1.386680
C	2.663797	4.258053	-0.050416
C	1.027105	5.137615	-1.581430
H	-0.671152	3.887094	-1.933691
C	2.231930	5.261203	-0.908565
H	0.714575	5.925127	-2.256970
F	2.337428	2.198686	0.965935
F	3.819108	4.370370	0.599589
F	2.996035	6.339094	-1.067043
C	-2.069694	-0.545896	-0.390869
H	-1.197381	-1.088868	-0.002371
C	4.982114	-2.777699	-0.870681
C	4.015628	-2.126468	-1.651896
C	4.273575	-1.978791	-3.032321
C	5.445825	-2.481873	-3.583787
C	6.395856	-3.129746	-2.795326
C	6.155590	-3.269884	-1.431889
H	4.800690	-2.909496	0.192836
H	5.621346	-2.357273	-4.651026
H	7.306552	-3.519532	-3.241209
H	6.881048	-3.775460	-0.799119
C	3.264578	-1.217437	-3.854810
H	3.446492	-0.139158	-3.723332
H	3.389985	-1.434818	-4.922001
C	1.840070	-1.520677	-3.397249
H	1.116324	-0.876158	-3.906892
H	1.578109	-2.560754	-3.642781
C	1.691028	-1.318831	-1.897458
C	2.761654	-1.621963	-1.085749
C	2.620136	-1.469264	0.381225
C	1.712877	-2.268902	1.142461
C	3.399305	-0.542275	1.064958
C	0.926748	-3.285710	0.526798
C	1.595095	-2.097741	2.552916
C	3.277727	-0.361023	2.463781
C	0.078990	-4.071285	1.262500
H	1.036704	-3.437539	-0.540341
C	0.701227	-2.925398	3.288872
C	2.389023	-1.115686	3.188104
H	3.880213	0.384436	2.971618

C	-0.047475	-3.886110	2.663400
H	-0.492756	-4.854200	0.771077
H	0.636486	-2.788022	4.366112
H	2.291822	-0.966931	4.260088
H	-0.716861	-4.521321	3.236862
O	4.258620	0.190117	0.310016
C	5.250890	0.951870	0.950637
H	4.827820	1.819438	1.473333
H	5.834671	0.347270	1.656952
H	5.911630	1.306199	0.157782
O	0.556267	-0.901012	-1.453240

S-CPX-C53

C	0.313269	2.088205	1.063741
C	1.605165	2.689880	0.894715
C	0.138335	1.280425	2.153585
C	1.937742	3.511771	-0.204065
C	2.592051	2.431195	1.884713
C	1.193432	1.087904	3.080707
H	-0.789990	0.753596	2.343650
C	3.198655	4.054508	-0.325495
H	1.227021	3.677502	-1.004882
C	3.872190	3.013514	1.741131
H	1.031677	0.432536	3.932555
C	4.180177	3.807001	0.664373
H	4.608612	2.799221	2.508502
H	5.174687	4.229588	0.579444
C	-3.207024	3.208240	-1.358180
C	-3.705522	4.051925	0.951359
C	-3.364788	4.483113	-0.494464
H	-2.257682	3.147366	-1.890212
H	-4.020966	3.112873	-2.080955
H	-4.257358	5.010736	-0.859067
C	-2.182709	2.069079	0.585132
H	-2.203058	1.080732	1.043042
C	-2.608175	3.177480	1.575507
H	-2.978966	2.747289	2.511885
H	-1.727914	3.773909	1.831118
H	-3.876235	4.940948	1.565585
C	-4.972179	3.201278	0.875325
H	-5.359353	2.989487	1.875989
H	-5.759859	3.726384	0.325183
C	-4.609075	1.884453	0.177244
H	-4.539335	1.056026	0.882964

H	-5.328187	1.607765	-0.593557
N	2.371334	1.642234	2.977672
N	-3.258988	1.971498	-0.497005
O	3.419412	4.816075	-1.429937
C	4.727208	5.281051	-1.671508
H	5.446208	4.453985	-1.732859
H	4.689720	5.794436	-2.633337
H	5.057200	5.990082	-0.900764
O	-0.483799	1.928817	-1.237368
H	-0.052346	0.933874	-1.140581
C	-2.246372	5.496594	-0.570103
H	-2.371973	6.322233	0.131126
C	-1.202781	5.518912	-1.394215
H	-0.993630	4.735182	-2.118226
H	-0.484340	6.331338	-1.355961
C	-3.087929	0.736916	-1.395778
H	-3.785769	0.896507	-2.220394
H	-2.064506	0.792863	-1.760206
C	-3.361788	-0.573079	-0.713924
C	-4.627809	-1.154300	-0.793156
C	-2.359076	-1.276415	-0.036423
C	-4.914744	-2.370622	-0.194110
C	-2.633151	-2.490067	0.584346
H	-1.329343	-0.911029	-0.050539
C	-3.904525	-3.029308	0.500298
H	-1.856512	-3.034930	1.108072
F	-5.620875	-0.536240	-1.460273
F	-6.136943	-2.894086	-0.285121
F	-4.194600	-4.195299	1.075616
C	-0.765416	2.414120	0.028995
H	-0.758977	3.506952	-0.045764
C	4.117668	-3.297437	-0.459693
C	3.577663	-2.013905	-0.640833
C	4.451880	-0.980976	-1.049178
C	5.795935	-1.250498	-1.273411
C	6.317652	-2.531385	-1.094321
C	5.467678	-3.552023	-0.681585
H	3.466001	-4.106939	-0.142962
H	6.449893	-0.438957	-1.588018
H	7.371467	-2.725042	-1.272753
H	5.853486	-4.557740	-0.535409
C	3.875315	0.404734	-1.179545
H	3.820577	0.866051	-0.181930
H	4.523417	1.042646	-1.792187

C	2.466374	0.345163	-1.755679
H	2.013558	1.339662	-1.771737
H	2.498023	-0.013476	-2.795844
C	1.588156	-0.598310	-0.951054
C	2.157296	-1.720100	-0.409554
C	1.321690	-2.723563	0.306801
C	0.668108	-3.780421	-0.410936
C	1.183225	-2.700311	1.681748
C	0.720866	-3.844662	-1.829591
C	-0.054135	-4.793758	0.282665
C	0.469630	-3.708935	2.376368
C	0.081055	-4.843963	-2.516410
H	1.279477	-3.076394	-2.353821
C	-0.708840	-5.814657	-0.455661
C	-0.125407	-4.739027	1.698823
H	0.409419	-3.633592	3.458313
C	-0.645957	-5.841188	-1.824425
H	0.132612	-4.873488	-3.601196
H	-1.264886	-6.575424	0.087401
H	-0.671063	-5.512886	2.233508
H	-1.150687	-6.626581	-2.379937
O	1.694209	-1.679956	2.441283
C	3.064986	-1.799251	2.786973
H	3.222526	-2.650846	3.464481
H	3.693267	-1.923231	1.900433
H	3.333574	-0.868888	3.291970
O	0.318911	-0.325391	-0.883516

S-CPX-C54

C	-0.353708	0.725824	2.339710
C	-0.768291	-0.479311	2.993113
C	0.309401	1.653516	3.102059
C	-1.395359	-1.554347	2.327361
C	-0.524387	-0.591614	4.391730
C	0.522251	1.431362	4.483843
H	0.684637	2.565832	2.645850
C	-1.792108	-2.682247	3.007874
H	-1.516745	-1.528052	1.255796
C	-0.952270	-1.758398	5.067650
H	1.047178	2.182899	5.072594
C	-1.577136	-2.784432	4.403625
H	-0.759699	-1.817943	6.133879
H	-1.884546	-3.667189	4.952816
C	-1.965436	2.966337	-1.108528

C	-3.482083	3.352850	0.841641
C	-2.530277	4.046099	-0.154219
H	-0.880023	2.879440	-1.047356
H	-2.226128	3.182153	-2.147240
H	-3.129921	4.748934	-0.745431
C	-2.143430	1.200044	0.640938
H	-2.628819	0.230482	0.767952
C	-2.743271	2.253466	1.600373
H	-3.420454	1.763650	2.306767
H	-1.940926	2.689491	2.199887
H	-3.875042	4.097072	1.539867
C	-4.618423	2.710249	0.049219
H	-5.331670	2.240236	0.732589
H	-5.165266	3.464839	-0.525253
C	-4.025543	1.653999	-0.897629
H	-4.380746	0.649892	-0.663565
H	-4.259513	1.857167	-1.943499
N	0.112456	0.367274	5.126264
N	-2.521854	1.600281	-0.801537
O	-2.377125	-3.659424	2.259511
C	-2.723508	-4.869102	2.892159
H	-3.489401	-4.720964	3.665105
H	-3.129593	-5.512619	2.110086
H	-1.848417	-5.357104	3.340330
O	-0.094596	0.065663	0.022019
H	1.021826	-0.811616	0.517348
C	-1.427898	4.823510	0.511002
H	-0.677890	4.244937	1.047386
C	-1.317681	6.147736	0.459485
H	-2.031393	6.763315	-0.084575
H	-0.505168	6.666591	0.959252
C	-1.981383	0.656603	-1.882824
H	-2.188785	1.170782	-2.824058
H	-0.909541	0.591241	-1.684331
C	-2.572826	-0.726491	-1.907434
C	-3.701884	-1.016144	-2.672925
C	-1.950550	-1.789797	-1.244703
C	-4.236297	-2.294969	-2.737139
C	-2.472345	-3.077079	-1.287930
H	-1.047886	-1.555024	-0.685393
C	-3.616636	-3.319845	-2.029064
H	-2.005786	-3.887891	-0.741203
F	-4.313666	-0.051232	-3.381644
F	-5.325098	-2.532855	-3.467683

F	-4.150278	-4.539898	-2.089268
C	-0.598720	1.003639	0.845767
H	-0.143635	2.009635	0.683543
C	5.593989	0.151986	-1.366060
C	4.888598	-0.861718	-0.704661
C	5.596646	-2.011847	-0.300130
C	6.961211	-2.112237	-0.543996
C	7.653704	-1.093076	-1.195750
C	6.959697	0.038590	-1.609098
H	5.067080	1.044714	-1.689573
H	7.489806	-3.007559	-0.222458
H	8.720508	-1.186217	-1.377636
H	7.481160	0.844198	-2.119349
C	4.815727	-3.128470	0.345785
H	4.350651	-3.735458	-0.445613
H	5.480645	-3.791336	0.910555
C	3.712975	-2.577672	1.243651
H	3.049796	-3.374029	1.593195
H	4.147383	-2.105803	2.137014
C	2.877450	-1.554729	0.513263
C	3.445028	-0.747121	-0.419949
C	2.664799	0.293889	-1.142530
C	2.529712	1.609792	-0.618843
C	2.067071	-0.004796	-2.356447
C	3.087749	1.966095	0.639958
C	1.816609	2.607613	-1.344386
C	1.374877	0.987606	-3.092202
C	2.941169	3.231099	1.146860
H	3.630223	1.207085	1.193744
C	1.680109	3.910305	-0.793155
C	1.259059	2.261637	-2.596078
H	0.937056	0.752013	-4.056028
C	2.224778	4.218196	0.426596
H	3.377040	3.479142	2.110492
H	1.129671	4.662651	-1.354450
H	0.738165	3.023182	-3.173450
H	2.115008	5.217794	0.838412
O	2.188427	-1.283852	-2.794865
C	1.414039	-1.695893	-3.892499
H	0.342935	-1.517262	-3.721223
H	1.719344	-1.201009	-4.824579
H	1.584503	-2.768765	-3.993371
O	1.618090	-1.542986	0.922905



## S-CPX-C55

C	-3.562228	-0.618276	1.686850
C	-4.632692	0.081142	1.048660
C	-3.818539	-1.231509	2.886214
C	-4.494580	0.798819	-0.163025
C	-5.910350	0.030791	1.675837
C	-5.122279	-1.195852	3.432876
H	-3.018751	-1.729209	3.425951
C	-5.577789	1.412518	-0.752875
H	-3.530135	0.919744	-0.644003
C	-7.003558	0.675324	1.047119
H	-5.318547	-1.687612	4.384256
C	-6.854917	1.344231	-0.140676
H	-7.967915	0.618531	1.541051
H	-7.714827	1.822409	-0.595392
C	-0.782218	-1.608046	-1.641844
C	-2.698964	-3.216220	-1.677005
C	-1.871388	-2.240109	-2.538045
H	-0.944842	-0.552614	-1.403811
H	0.195657	-1.668249	-2.112387
H	-1.382452	-2.825370	-3.327294
C	-1.975040	-2.117237	0.489700
H	-1.870512	-2.814466	1.328013
C	-3.169821	-2.506702	-0.413699
H	-3.851629	-3.142137	0.158360
H	-3.737799	-1.615694	-0.687101
H	-3.555960	-3.577252	-2.251751
C	-1.805634	-4.379502	-1.251999
H	-2.350400	-5.031434	-0.561888
H	-1.512296	-4.987356	-2.113446
C	-0.549005	-3.808824	-0.577001
H	-0.337473	-4.279869	0.385484
H	0.333557	-3.930613	-1.204684
N	-6.142910	-0.609181	2.856622
N	-0.675248	-2.328084	-0.318246
O	-5.333783	2.057877	-1.920721
C	-6.382911	2.780399	-2.527035
H	-6.774337	3.558416	-1.859909
H	-5.948728	3.250901	-3.409781
H	-7.202753	2.120087	-2.837977
O	-1.218715	-0.405805	2.064040
H	-0.627956	0.251438	1.615513
C	-2.701111	-1.175371	-3.203308
H	-3.238643	-0.488932	-2.549311

C	-2.802933	-1.026827	-4.520508
H	-2.273450	-1.678255	-5.212734
H	-3.414050	-0.241999	-4.955104
C	0.569695	-1.828470	0.435269
H	0.607483	-0.741979	0.266914
H	0.370326	-1.993364	1.493568
C	1.859991	-2.498305	0.051495
C	2.629899	-2.080384	-1.031988
C	2.399796	-3.499021	0.866084
C	3.858200	-2.658386	-1.323195
C	3.630876	-4.083624	0.604045
H	1.848785	-3.802298	1.750683
C	4.354413	-3.656836	-0.498341
H	4.047881	-4.849099	1.247883
F	2.219240	-1.095955	-1.836121
F	4.570840	-2.218464	-2.358748
F	5.546011	-4.184185	-0.778244
C	-2.167513	-0.699824	1.084578
H	-2.064340	0.030797	0.280029
C	3.317944	4.331191	0.712476
C	2.107311	3.897383	0.152608
C	1.282953	4.864107	-0.461574
C	1.667786	6.199402	-0.489299
C	2.872894	6.615861	0.073793
C	3.697946	5.668626	0.672026
H	3.966636	3.605361	1.195409
H	1.012488	6.926326	-0.966314
H	3.159566	7.663363	0.044887
H	4.640818	5.971223	1.120787
C	0.012178	4.384917	-1.114364
H	0.256110	3.981827	-2.109521
H	-0.685895	5.216591	-1.266567
C	-0.630506	3.273137	-0.292486
H	-1.481186	2.830911	-0.822519
H	-1.017755	3.678132	0.654886
C	0.359850	2.159705	0.016014
C	1.679143	2.490699	0.213158
C	2.694344	1.449828	0.514860
C	2.669569	0.675606	1.713464
C	3.728345	1.214886	-0.387769
C	1.652792	0.855457	2.694973
C	3.662708	-0.317856	1.962650
C	4.752360	0.277680	-0.112416
C	1.581129	0.052511	3.801712

H	0.931787	1.651588	2.542175
C	3.568347	-1.130662	3.125424
C	4.715061	-0.472704	1.036124
H	5.561424	0.125469	-0.817705
C	2.543103	-0.967295	4.017443
H	0.781902	0.199506	4.521857
H	4.328999	-1.891581	3.287662
H	5.492822	-1.207343	1.231488
H	2.476776	-1.595706	4.901395
O	3.699553	1.935017	-1.537588
C	4.623583	1.625721	-2.549642
H	4.561279	0.568664	-2.841210
H	5.655430	1.858370	-2.252892
H	4.353267	2.252402	-3.401057
O	-0.137995	0.966167	0.110685

S-CPX-C56

C	1.106352	-1.923649	1.592061
C	2.014824	-1.276336	2.490641
C	0.618845	-3.148617	1.975990
C	2.568872	0.000274	2.254744
C	2.372169	-1.967677	3.684574
C	1.028416	-3.742360	3.194125
H	-0.097894	-3.671199	1.348259
C	3.457024	0.566818	3.140533
H	2.256901	0.566501	1.391639
C	3.287695	-1.360855	4.576263
H	0.629916	-4.716430	3.476487
C	3.827712	-0.125541	4.319164
H	3.545538	-1.907455	5.477511
H	4.523922	0.310073	5.027016
C	0.377566	-1.774676	-2.747446
C	2.340528	-3.269906	-2.357702
C	0.873239	-3.238294	-2.832611
H	-0.511715	-1.665554	-2.128508
H	0.135668	-1.379984	-3.735801
H	0.865439	-3.541296	-3.886545
C	1.828547	-1.356875	-0.760849
H	2.580399	-0.633134	-0.438742
C	2.443437	-2.767221	-0.919039
H	3.491351	-2.753973	-0.602705
H	1.930187	-3.459356	-0.248018
H	2.718313	-4.293639	-2.428743
C	3.150564	-2.337523	-3.255022

H	4.214066	-2.402098	-3.007220
H	3.042246	-2.625143	-4.305850
C	2.651948	-0.899522	-3.044180
H	3.397699	-0.275140	-2.550163
H	2.378537	-0.416188	-3.982072
N	1.877479	-3.193929	4.025673
N	1.426669	-0.860309	-2.166917
O	3.925540	1.801495	2.810653
C	4.776152	2.463482	3.717893
H	5.719133	1.920499	3.864077
H	4.992358	3.434711	3.270412
H	4.291454	2.615822	4.690766
O	0.181064	-0.040716	0.389901
H	-0.555888	0.656869	1.486424
C	-0.009267	-4.194287	-2.076139
H	-0.273471	-3.916026	-1.057813
C	-0.461978	-5.339845	-2.577309
H	-0.238384	-5.648618	-3.596565
H	-1.078314	-6.011523	-1.987109
C	0.831248	0.553840	-2.204808
H	0.457600	0.667341	-3.224652
H	0.017050	0.530501	-1.478598
C	1.778471	1.671877	-1.863960
C	2.539155	2.303600	-2.847172
C	1.849062	2.185003	-0.564696
C	3.388534	3.360296	-2.551339
C	2.697140	3.237624	-0.243128
H	1.209775	1.723427	0.182513
C	3.468023	3.813710	-1.238986
H	2.770380	3.605698	0.773360
F	2.470111	1.905810	-4.129557
F	4.113111	3.929742	-3.514270
F	4.298499	4.821294	-0.968639
C	0.641795	-1.295540	0.265641
H	-0.128308	-2.005319	-0.110379
C	-5.414777	1.079100	0.190057
C	-4.287679	1.824734	0.562092
C	-4.416663	3.227036	0.633137
C	-5.631994	3.834664	0.338674
C	-6.742458	3.081033	-0.035311
C	-6.624915	1.697240	-0.106999
H	-5.343936	-0.003006	0.139246
H	-5.710017	4.918061	0.405878
H	-7.686012	3.569412	-0.260838

H	-7.480569	1.089698	-0.389605
C	-3.197684	4.025944	1.018517
H	-2.563452	4.172414	0.130384
H	-3.483820	5.021479	1.375306
C	-2.391404	3.281468	2.076815
H	-1.447224	3.790049	2.289890
H	-2.959078	3.231832	3.017007
C	-2.080888	1.877210	1.618567
C	-2.993870	1.180488	0.885790
C	-2.830553	-0.253160	0.528268
C	-2.853250	-0.676313	-0.834525
C	-2.754070	-1.225502	1.516530
C	-2.835640	0.264730	-1.903224
C	-2.897052	-2.061484	-1.167480
C	-2.758445	-2.605136	1.187074
C	-2.895991	-0.142871	-3.211271
H	-2.773477	1.319823	-1.658004
C	-2.984274	-2.453824	-2.531594
C	-2.849807	-3.010808	-0.119215
H	-2.722224	-3.349214	1.974823
C	-2.989749	-1.519209	-3.534147
H	-2.887028	0.596874	-4.007017
H	-3.033470	-3.514471	-2.763639
H	-2.891426	-4.070599	-0.359851
H	-3.063997	-1.828774	-4.572883
O	-2.718128	-0.789102	2.797041
C	-2.395290	-1.697584	3.822864
H	-3.185592	-2.446223	3.972317
H	-1.442148	-2.203842	3.627278
H	-2.300653	-1.098781	4.729408
O	-0.899986	1.449648	2.035036

S-CPX-C57

C	3.242208	-2.040887	-1.309131
C	4.280509	-1.089336	-1.060491
C	3.598617	-3.246967	-1.857168
C	4.055243	0.216434	-0.566622
C	5.620008	-1.500045	-1.328806
C	4.958231	-3.539166	-2.110721
H	2.843506	-3.984035	-2.113808
C	5.109557	1.059790	-0.299867
H	3.055071	0.596864	-0.398799
C	6.679311	-0.603296	-1.053159
H	5.228456	-4.501850	-2.542062

C	6.442110	0.646927	-0.541964
H	7.688485	-0.942342	-1.262213
H	7.276104	1.308278	-0.336474
C	-0.374177	-1.261493	1.170909
C	1.324710	-2.510006	2.500136
C	0.679591	-1.127683	2.290148
H	-0.310299	-0.466365	0.417980
H	-1.386864	-1.268257	1.575949
H	0.135393	-0.849841	3.202759
C	1.243676	-2.796756	-0.017487
H	1.202833	-3.759567	-0.535605
C	2.123056	-2.895159	1.253571
H	2.518963	-3.910791	1.355618
H	2.979290	-2.227515	1.151668
H	1.983248	-2.494859	3.372285
C	0.217105	-3.543440	2.699272
H	0.639062	-4.510041	2.990066
H	-0.461625	-3.227013	3.497758
C	-0.554387	-3.697293	1.379514
H	-0.321222	-4.631371	0.860264
H	-1.630050	-3.663672	1.542670
N	5.944590	-2.719462	-1.845070
N	-0.216912	-2.577535	0.427916
O	4.782292	2.280485	0.209773
C	5.805221	3.231284	0.403676
H	6.331607	3.454541	-0.532792
H	5.308900	4.134967	0.760387
H	6.529352	2.899353	1.158332
O	1.077329	-1.750514	-2.233916
H	0.542529	-0.903453	-2.210509
C	1.673947	-0.022163	2.011718
H	1.348683	0.725017	1.290538
C	2.860729	0.123077	2.593844
H	3.250038	-0.579410	3.328136
H	3.490526	0.971471	2.344043
C	-1.147461	-2.601135	-0.785603
H	-1.056643	-1.607971	-1.229110
H	-0.721979	-3.322160	-1.482727
C	-2.583935	-2.948566	-0.509588
C	-3.511821	-1.958202	-0.197919
C	-3.066342	-4.251883	-0.671232
C	-4.861564	-2.240123	-0.025802
C	-4.409168	-4.562214	-0.500722
H	-2.370249	-5.038780	-0.945967

C	-5.300169	-3.549776	-0.176182
H	-4.783300	-5.571317	-0.628145
F	-3.122082	-0.692967	-0.063697
F	-5.713875	-1.267041	0.270257
F	-6.593473	-3.812898	-0.008122
C	1.775437	-1.742209	-1.025063
H	1.683418	-0.763088	-0.551994
C	-2.722475	4.353104	-0.558262
C	-2.569247	3.096870	-1.165806
C	-3.526818	2.711142	-2.130468
C	-4.563912	3.570303	-2.471176
C	-4.698190	4.819009	-1.865726
C	-3.770932	5.200526	-0.901462
H	-2.000323	4.669509	0.189172
H	-5.286465	3.251954	-3.220753
H	-5.514317	5.480004	-2.143202
H	-3.858045	6.168389	-0.414060
C	-3.419193	1.326791	-2.719758
H	-3.911936	0.619094	-2.036631
H	-3.956179	1.270609	-3.673962
C	-1.963372	0.902929	-2.892791
H	-1.896890	-0.156312	-3.169403
H	-1.497264	1.472855	-3.709807
C	-1.144483	1.131861	-1.632367
C	-1.464930	2.195599	-0.825090
C	-0.581044	2.526036	0.324756
C	-0.958222	2.229750	1.667919
C	0.647018	3.142124	0.108738
C	-2.184276	1.565165	1.959678
C	-0.102136	2.561612	2.758252
C	1.495384	3.486997	1.192170
C	-2.509941	1.210221	3.242827
H	-2.850328	1.342349	1.134792
C	-0.469763	2.185848	4.078407
C	1.121278	3.211401	2.482332
H	2.453124	3.959329	1.007943
C	-1.639839	1.515516	4.320479
H	-3.451517	0.704100	3.439841
H	0.203911	2.435378	4.895045
H	1.785211	3.464461	3.305030
H	-1.910773	1.232786	5.333935
O	0.973075	3.406008	-1.179489
C	2.225952	3.980878	-1.460753
H	2.321608	4.985015	-1.023262

H	3.051763	3.351441	-1.106402
H	2.275466	4.064750	-2.547562
O	-0.165915	0.315552	-1.404843

S-CPX-C58

C	-0.129133	0.596473	2.001842
C	-0.617972	-0.525424	2.746961
C	0.776208	1.414067	2.627147
C	-1.512344	-1.483815	2.224452
C	-0.169877	-0.672096	4.091137
C	1.175182	1.162873	3.961648
H	1.207314	2.263154	2.104275
C	-1.970650	-2.528315	2.994202
H	-1.807602	-1.438126	1.188228
C	-0.660066	-1.753325	4.859919
H	1.900565	1.825124	4.432663
C	-1.544613	-2.663890	4.337308
H	-0.303917	-1.841998	5.881151
H	-1.894927	-3.483144	4.954984
C	-1.756653	3.036200	-1.284355
C	-2.874240	3.741682	0.835183
C	-1.902831	4.198652	-0.272227
H	-0.719328	2.727522	-1.421467
H	-2.158602	3.314556	-2.261610
H	-2.375183	5.042597	-0.789583
C	-2.039611	1.356774	0.544000
H	-2.661840	0.485055	0.754520
C	-2.330945	2.501766	1.542261
H	-3.044655	2.161249	2.298888
H	-1.411992	2.749425	2.077889
H	-3.010162	4.556323	1.551790
C	-4.203946	3.379020	0.177303
H	-4.947816	3.132047	0.940137
H	-4.594051	4.226027	-0.396407
C	-3.983609	2.167570	-0.742876
H	-4.484069	1.273576	-0.368741
H	-4.336807	2.348464	-1.758436
N	0.720814	0.174394	4.688117
N	-2.521866	1.812609	-0.850018
O	-2.827096	-3.393748	2.381505
C	-3.284500	-4.509379	3.108976
H	-2.455659	-5.155944	3.425337
H	-3.865445	-4.210209	3.991544
H	-3.932269	-5.066888	2.430622



O	-0.329014	-0.121665	-0.306462
H	0.702334	-1.101834	0.017438
C	-0.575774	4.675337	0.254882
H	0.085116	3.926110	0.687494
C	-0.184441	5.946159	0.222054
H	-0.804938	6.727682	-0.212289
H	0.770736	6.254499	0.636396
C	-2.338362	0.765835	-1.957667
H	-2.579508	1.297533	-2.881148
H	-1.283197	0.485366	-1.908317
C	-3.190614	-0.466690	-1.827137
C	-4.454795	-0.540506	-2.410000
C	-2.704030	-1.611687	-1.188777
C	-5.238568	-1.681772	-2.317434
C	-3.474515	-2.762388	-1.074481
H	-1.697765	-1.551473	-0.780740
C	-4.740459	-2.787223	-1.635500
H	-3.104739	-3.631902	-0.544214
F	-4.959239	0.505501	-3.087950
F	-6.449236	-1.712844	-2.873950
F	-5.512028	-3.870501	-1.541849
C	-0.540554	0.898730	0.550589
H	0.051564	1.802806	0.289677
C	5.570855	-0.446425	-1.384012
C	4.641978	-1.445436	-1.056272
C	5.081026	-2.786993	-1.082526
C	6.403289	-3.085603	-1.389892
C	7.319870	-2.080725	-1.692365
C	6.891068	-0.758338	-1.694895
H	5.259972	0.593290	-1.391926
H	6.718130	-4.127333	-1.398969
H	8.350841	-2.329348	-1.926468
H	7.586211	0.041227	-1.936470
C	4.062207	-3.868887	-0.831440
H	3.524888	-4.072344	-1.770701
H	4.552887	-4.802898	-0.536204
C	3.052163	-3.430553	0.220414
H	2.233799	-4.149847	0.310791
H	3.535341	-3.362650	1.205817
C	2.462074	-2.081943	-0.119309
C	3.236275	-1.133134	-0.717928
C	2.740432	0.247869	-0.978581
C	3.066518	1.318530	-0.082521
C	1.989006	0.545409	-2.096400

C	3.798283	1.083108	1.112919
C	2.667751	2.654448	-0.374441
C	1.592309	1.872287	-2.389869
C	4.118933	2.110655	1.962867
H	4.092950	0.064814	1.342650
C	3.011987	3.698207	0.524967
C	1.927999	2.906428	-1.558051
H	1.023880	2.038824	-3.301119
C	3.723208	3.436407	1.668837
H	4.674236	1.904911	2.873132
H	2.709210	4.714301	0.281346
H	1.629453	3.926907	-1.787551
H	3.985970	4.242365	2.347954
O	1.556460	-0.424255	-2.960817
C	2.537360	-0.889481	-3.871955
H	2.880719	-0.077044	-4.528021
H	3.400618	-1.320009	-3.354181
H	2.054385	-1.660458	-4.475889
O	1.211895	-1.969519	0.278152

S-CPX-C59

C	-3.842943	-1.465427	-0.609719
C	-4.926822	-0.570689	-0.880212
C	-4.100919	-2.811614	-0.644913
C	-4.791121	0.835478	-0.931968
C	-6.209858	-1.148471	-1.098015
C	-5.412752	-3.278905	-0.904339
H	-3.304224	-3.527955	-0.461540
C	-5.886271	1.643605	-1.149418
H	-3.814290	1.296393	-0.861159
C	-7.313898	-0.292039	-1.321973
H	-5.605060	-4.350313	-0.929332
C	-7.168815	1.071863	-1.340557
H	-8.281922	-0.755339	-1.481741
H	-8.036516	1.697752	-1.515169
C	-0.060011	-0.355861	1.419569
C	-1.400748	-1.724002	3.034762
C	-0.199328	-1.761211	2.072487
H	0.133261	-0.432606	0.342813
H	0.742373	0.223429	1.882122
H	0.711764	-1.907870	2.666346
C	-2.542705	-0.395989	1.216261
H	-3.382483	0.302145	1.270549
C	-2.707523	-1.532453	2.251171

H	-3.525893	-1.305079	2.942758
H	-2.978159	-2.452479	1.732137
H	-1.447885	-2.642289	3.624958
C	-1.223489	-0.517672	3.955144
H	-1.948198	-0.537301	4.774603
H	-0.221353	-0.515326	4.395303
C	-1.442558	0.744372	3.114167
H	-2.434522	1.179791	3.266208
H	-0.690455	1.502504	3.329455
N	-6.440093	-2.493683	-1.106235
N	-1.332744	0.440398	1.640180
O	-5.647844	2.980652	-1.170995
C	-6.715133	3.851594	-1.471441
H	-7.505309	3.803274	-0.710902
H	-6.287786	4.855072	-1.478568
H	-7.147575	3.638834	-2.457209
O	-1.951229	-0.092110	-1.204953
H	-1.038859	-0.455304	-1.480043
C	-0.241091	-2.901439	1.073500
H	0.188721	-2.677967	0.096315
C	-0.734008	-4.114892	1.321049
H	-1.176053	-4.399549	2.273963
H	-0.701203	-4.888930	0.559335
C	-1.383245	1.759385	0.882040
H	-1.513236	1.476030	-0.162075
H	-2.295935	2.250412	1.231905
C	-0.205895	2.674670	1.047883
C	0.773012	2.683404	0.057286
C	-0.094690	3.616756	2.075680
C	1.846702	3.560899	0.095426
C	0.979713	4.494437	2.145251
H	-0.874963	3.680416	2.827972
C	1.949864	4.450187	1.155874
H	1.075611	5.218115	2.946008
F	0.685645	1.847520	-0.969710
F	2.777825	3.521921	-0.849949
F	3.008905	5.254944	1.209355
C	-2.450417	-0.972436	-0.245365
H	-1.804115	-1.851684	-0.198337
C	5.187097	-0.818837	-1.799748
C	3.892273	-0.426664	-2.174172
C	3.760111	0.415294	-3.300416
C	4.884023	0.814453	-4.013091
C	6.163714	0.412330	-3.632170

C	6.305856	-0.404379	-2.515272
H	5.314822	-1.465881	-0.936322
H	4.755230	1.461338	-4.879290
H	7.032877	0.734746	-4.198427
H	7.293826	-0.729760	-2.198762
C	2.378020	0.905200	-3.648826
H	2.149873	1.779701	-3.022522
H	2.338159	1.242823	-4.691216
C	1.325039	-0.167934	-3.385957
H	0.316020	0.242156	-3.501609
H	1.424875	-0.983726	-4.116790
C	1.447700	-0.761592	-1.991143
C	2.701536	-0.855008	-1.429927
C	2.891111	-1.473305	-0.090910
C	3.228607	-0.675420	1.045019
C	2.785946	-2.846669	0.090822
C	3.399086	0.733697	0.929643
C	3.398286	-1.263863	2.332551
C	2.984986	-3.441482	1.362075
C	3.690018	1.505430	2.024705
H	3.305334	1.175090	-0.056316
C	3.678546	-0.434944	3.452842
C	3.275420	-2.667188	2.455402
H	2.891534	-4.514026	1.484963
C	3.818429	0.920093	3.308284
H	3.846182	2.573881	1.906666
H	3.795818	-0.901780	4.428584
H	3.418664	-3.132008	3.427963
H	4.046755	1.544302	4.167574
O	2.466159	-3.577808	-1.006258
C	2.394422	-4.976327	-0.893986
H	3.355174	-5.413039	-0.588446
H	1.616333	-5.290277	-0.185529
H	2.139174	-5.341685	-1.889806
O	0.354216	-1.169622	-1.429593

S-CPX-C60

C	2.194408	-1.947226	-0.982823
C	3.308064	-1.219322	-1.528435
C	1.698319	-2.983423	-1.732091
C	3.957217	-0.158559	-0.856096
C	3.791488	-1.619994	-2.807294
C	2.251188	-3.284938	-3.001281
H	0.876515	-3.605920	-1.396872

C	5.049134	0.466418	-1.421144
H	3.581130	0.213317	0.089241
C	4.897467	-0.942525	-3.368082
H	1.828592	-4.103930	-3.582051
C	5.522448	0.076759	-2.697146
H	5.238475	-1.265365	-4.346151
H	6.373497	0.571776	-3.150906
C	0.053988	-1.124080	2.911920
C	0.843935	-3.474879	3.277258
C	1.010117	-2.009621	3.743396
H	0.528600	-0.250399	2.471998
H	-0.802117	-0.789681	3.502303
H	0.649916	-1.986473	4.781529
C	0.591375	-2.551552	0.939528
H	0.041580	-2.990206	0.110271
C	1.244432	-3.653653	1.805778
H	0.937610	-4.649366	1.466537
H	2.330290	-3.601548	1.690162
H	1.442815	-4.133861	3.912982
C	-0.640625	-3.819549	3.390010
H	-0.806695	-4.888775	3.229519
H	-1.019156	-3.575768	4.387893
C	-1.388209	-3.018603	2.316566
H	-1.674152	-3.640891	1.466908
H	-2.290535	-2.543314	2.700799
N	3.253624	-2.642193	-3.535313
N	-0.524155	-1.910879	1.758862
O	5.625926	1.452822	-0.684698
C	6.617503	2.251177	-1.286224
H	6.250032	2.730619	-2.202838
H	6.865842	3.021799	-0.554658
H	7.523829	1.676027	-1.517337
O	1.369369	-0.211882	0.513600
H	0.938587	0.167464	-0.349768
C	2.455539	-1.572787	3.804471
H	3.073387	-2.239198	4.408713
C	3.019584	-0.493190	3.268291
H	2.488376	0.219303	2.642243
H	4.076181	-0.296946	3.425409
C	-1.414238	-0.988808	0.926743
H	-2.067388	-0.476390	1.633739
H	-0.756115	-0.251565	0.484894
C	-2.211016	-1.677277	-0.144058
C	-3.528596	-2.065560	0.090157

C	-1.698880	-1.856953	-1.433249
C	-4.311325	-2.639658	-0.901552
C	-2.462389	-2.437691	-2.439134
H	-0.716748	-1.449224	-1.664377
C	-3.763935	-2.825517	-2.166409
H	-2.070148	-2.562266	-3.441934
F	-4.083855	-1.895179	1.299525
F	-5.564619	-3.006507	-0.642331
F	-4.525026	-3.379517	-3.109153
C	1.689081	-1.555231	0.407426
H	2.545332	-1.701803	1.076735
C	-2.619035	4.284614	-0.250023
C	-2.423596	3.057611	-0.902643
C	-3.383582	2.664874	-1.859424
C	-4.493137	3.462426	-2.112240
C	-4.685748	4.666838	-1.437544
C	-3.734950	5.075788	-0.507790
H	-1.875466	4.626122	0.465599
H	-5.220126	3.134297	-2.852796
H	-5.557383	5.280364	-1.646544
H	-3.852158	6.023464	0.012116
C	-3.143539	1.365261	-2.581105
H	-3.455538	0.525366	-1.939521
H	-3.741461	1.312403	-3.498251
C	-1.655482	1.223122	-2.882530
H	-1.430229	0.269485	-3.367918
H	-1.338982	2.019834	-3.570999
C	-0.833466	1.307541	-1.602468
C	-1.251654	2.206048	-0.636256
C	-0.559763	2.358053	0.667037
C	0.828885	2.708997	0.771503
C	-1.254169	2.150012	1.851597
C	1.616588	2.967679	-0.382824
C	1.460836	2.789890	2.045267
C	-0.638908	2.269993	3.117990
C	2.955608	3.236987	-0.278936
H	1.137697	2.928790	-1.353075
C	2.851182	3.072364	2.121009
C	0.692822	2.573947	3.215561
H	-1.226350	2.080840	4.012641
C	3.587673	3.278062	0.985395
H	3.541495	3.410327	-1.176389
H	3.320513	3.117858	3.101349
H	1.174461	2.643522	4.187790

H	4.653732	3.470823	1.050499
O	-2.552878	1.693822	1.787721
C	-3.534816	2.470189	2.447456
H	-3.375694	2.503233	3.533960
H	-3.557774	3.488587	2.047514
H	-4.491727	1.986219	2.243527
O	0.184552	0.515118	-1.548505

S-CPX-C61

C	-1.521605	-1.716462	0.088325
C	-2.771226	-2.329732	-0.263869
C	-0.508727	-1.760183	-0.829773
C	-3.881579	-2.445842	0.607861
C	-2.887076	-2.861756	-1.579909
C	-0.730269	-2.337076	-2.105148
H	0.452186	-1.305398	-0.618964
C	-5.061123	-3.029306	0.194384
H	-3.833330	-2.123942	1.642722
C	-4.112103	-3.447776	-1.976786
H	0.085494	-2.347982	-2.824886
C	-5.183667	-3.530319	-1.123325
H	-4.169660	-3.841508	-2.986359
H	-6.104446	-3.990931	-1.462123
C	-0.805321	2.261727	1.630536
C	-2.296710	1.870530	3.595902
C	-0.951773	2.477685	3.149421
H	0.091975	1.705379	1.339820
H	-0.781537	3.212067	1.096421
H	-0.996772	3.554934	3.351835
C	-2.262021	0.157656	1.744647
H	-3.256929	-0.088380	1.366132
C	-2.312434	0.383075	3.268688
H	-3.218505	-0.088746	3.664368
H	-1.452880	-0.110229	3.728152
H	-2.424774	2.025459	4.670541
C	-3.434478	2.544096	2.822207
H	-4.393129	2.107012	3.118127
H	-3.478291	3.612876	3.052820
C	-3.213353	2.351993	1.308065
H	-4.056304	1.856703	0.819525
H	-3.045206	3.302157	0.801452
N	-1.871075	-2.852134	-2.491257
N	-1.988718	1.510237	1.053309
O	-6.056325	-3.083827	1.118558

C	-7.252806	-3.747913	0.777656
H	-7.071557	-4.798212	0.516888
H	-7.883376	-3.704104	1.666702
H	-7.770146	-3.252066	-0.053915
O	-0.035138	-0.864316	1.871431
H	0.521891	-0.361985	1.188002
C	0.239765	1.906534	3.876876
H	0.568329	0.919316	3.552822
C	0.895309	2.551251	4.837348
H	0.608187	3.551069	5.158623
H	1.754170	2.107403	5.331372
C	-1.763684	1.288835	-0.439467
H	-0.719795	0.966092	-0.533856
H	-2.426928	0.471581	-0.724336
C	-2.055858	2.471926	-1.322797
C	-1.082179	3.424633	-1.619355
C	-3.296479	2.599487	-1.957518
C	-1.338980	4.485117	-2.481420
C	-3.575044	3.648001	-2.824373
H	-4.058322	1.847381	-1.774966
C	-2.589089	4.589401	-3.077891
H	-4.535661	3.742792	-3.316689
F	0.130684	3.353578	-1.077629
F	-0.393455	5.382975	-2.733704
F	-2.819006	5.609356	-3.900716
C	-1.337919	-1.068969	1.457144
H	-1.760118	-1.794073	2.172028
C	5.811382	-0.760791	-0.381106
C	4.845869	0.184149	-0.002957
C	5.281926	1.496179	0.284098
C	6.624842	1.830440	0.159976
C	7.571216	0.885335	-0.234034
C	7.154539	-0.415715	-0.495542
H	5.503086	-1.780390	-0.592445
H	6.936899	2.849425	0.382943
H	8.617451	1.161706	-0.329618
H	7.876771	-1.170050	-0.796919
C	4.258456	2.478933	0.793154
H	4.121653	2.310860	1.872835
H	4.615629	3.508591	0.672284
C	2.908788	2.286094	0.109367
H	2.143070	2.898117	0.597363
H	2.958392	2.616771	-0.938796
C	2.467245	0.831865	0.146237



C	3.419437	-0.148840	0.092312
C	2.982355	-1.570477	0.063112
C	2.836183	-2.276235	-1.168063
C	2.658844	-2.223237	1.242537
C	3.111531	-1.651084	-2.417794
C	2.377490	-3.625297	-1.180726
C	2.181131	-3.557271	1.233075
C	2.957068	-2.331316	-3.597948
H	3.449549	-0.619850	-2.410960
C	2.232430	-4.305429	-2.419630
C	2.050220	-4.237314	0.050524
H	1.912818	-4.050021	2.160453
C	2.516853	-3.678451	-3.603951
H	3.175001	-1.835211	-4.539632
H	1.879759	-5.334217	-2.409987
H	1.681565	-5.260213	0.051579
H	2.398871	-4.204582	-4.546708
O	2.816490	-1.513319	2.390286
C	2.335458	-2.062485	3.591024
H	1.261974	-2.274932	3.524941
H	2.882415	-2.972026	3.876084
H	2.504178	-1.299698	4.354299
O	1.179208	0.617358	0.179419

S-CPX-C62

C	-2.396237	-1.343372	-1.526358
C	-3.823430	-1.245417	-1.649635
C	-1.634945	-0.869566	-2.562165
C	-4.749609	-1.834414	-0.754091
C	-4.334310	-0.520871	-2.764585
C	-2.257371	-0.194846	-3.640627
H	-0.555647	-0.952003	-2.538099
C	-6.109825	-1.672103	-0.915716
H	-4.428737	-2.484638	0.052392
C	-5.733676	-0.355803	-2.894021
H	-1.636228	0.208913	-4.438165
C	-6.611789	-0.903599	-1.993333
H	-6.088909	0.212592	-3.747359
H	-7.677618	-0.761355	-2.129278
C	-0.184196	-0.068523	1.966562
C	-1.367943	-1.677484	3.463561
C	-0.063187	-0.878668	3.271558
H	0.388413	-0.486205	1.139086
H	0.151610	0.956722	2.100551

H	0.026188	-0.186412	4.119173
C	-2.136204	-1.392751	1.084941
H	-3.218542	-1.253166	1.099015
C	-1.706932	-2.401675	2.165309
H	-2.526566	-3.112754	2.316781
H	-0.842985	-2.960555	1.795786
H	-1.247137	-2.387478	4.285561
C	-2.497873	-0.687934	3.759056
H	-3.463049	-1.205089	3.756678
H	-2.373221	-0.230913	4.745341
C	-2.473385	0.412818	2.686088
H	-3.469474	0.644991	2.302230
H	-2.034092	1.337372	3.063638
N	-3.545932	0.014715	-3.740484
N	-1.627415	-0.001690	1.505804
O	-6.897362	-2.287196	0.004357
C	-8.296047	-2.249478	-0.174716
H	-8.591886	-2.687787	-1.135981
H	-8.717106	-2.845876	0.635603
H	-8.687943	-1.226416	-0.106407
O	-0.390772	-2.241315	-0.419219
H	0.116327	-1.418171	-0.680240
C	1.172950	-1.736689	3.240764
H	1.341338	-2.325104	2.338693
C	2.050628	-1.786358	4.237558
H	1.925775	-1.186652	5.137720
H	2.936537	-2.408439	4.177167
C	-1.795534	0.992794	0.365540
H	-0.962542	0.796604	-0.328313
H	-2.743417	0.735009	-0.108898
C	-1.850985	2.444315	0.766489
C	-0.705453	3.219780	0.948142
C	-3.083790	3.100258	0.861681
C	-0.777357	4.576800	1.240668
C	-3.182523	4.455323	1.150363
H	-3.992809	2.532530	0.686098
C	-2.021157	5.186896	1.341184
H	-4.141119	4.955988	1.218302
F	0.513552	2.685675	0.858381
F	0.336418	5.279009	1.415071
F	-2.072867	6.486919	1.620933
C	-1.745999	-1.992529	-0.307350
H	-2.220808	-2.984495	-0.220220
C	5.408163	0.124078	-1.851874

C	4.188886	0.786466	-1.636484
C	4.126900	2.165652	-1.937320
C	5.243303	2.825258	-2.436461
C	6.447571	2.154144	-2.643410
C	6.521338	0.797617	-2.344316
H	5.480169	-0.937317	-1.631073
H	5.168605	3.887495	-2.662499
H	7.312124	2.683584	-3.033205
H	7.450241	0.254844	-2.499253
C	2.829008	2.882300	-1.665495
H	2.774483	3.140298	-0.596728
H	2.781888	3.824136	-2.224463
C	1.643499	1.984093	-2.000202
H	0.696440	2.453708	-1.718421
H	1.602386	1.804411	-3.085479
C	1.749103	0.639655	-1.297748
C	2.999031	0.088376	-1.128998
C	3.129322	-1.276957	-0.564449
C	3.861094	-1.515040	0.649160
C	2.566029	-2.370975	-1.197510
C	4.463413	-0.449146	1.370936
C	4.014136	-2.837596	1.155402
C	2.657775	-3.676305	-0.658641
C	5.213216	-0.686019	2.494660
H	4.324403	0.562743	1.006023
C	4.804005	-3.053773	2.315646
C	3.369513	-3.909930	0.485225
H	2.157113	-4.477959	-1.191882
C	5.402813	-2.005354	2.966463
H	5.672464	0.145140	3.022189
H	4.930756	-4.072347	2.676497
H	3.462392	-4.916925	0.884809
H	6.012431	-2.183814	3.847987
O	1.864872	-2.255311	-2.373121
C	2.659468	-1.971714	-3.511308
H	3.181216	-1.014289	-3.414094
H	3.395551	-2.769683	-3.681195
H	1.972924	-1.929394	-4.360082
O	0.634405	0.094092	-0.944960

S-CPX-C63

C	-1.207590	-1.826208	-0.795794
C	-2.427916	-2.379696	-1.311845
C	-0.239319	-1.477098	-1.699140

C	-3.463240	-2.920297	-0.510384
C	-2.589246	-2.402246	-2.727226
C	-0.497642	-1.575065	-3.087924
H	0.719030	-1.095018	-1.377440
C	-4.622569	-3.414297	-1.070920
H	-3.360210	-3.017769	0.564780
C	-3.796564	-2.900313	-3.272117
H	0.279032	-1.271133	-3.787289
C	-4.800685	-3.388880	-2.475085
H	-3.893939	-2.892488	-4.352855
H	-5.708709	-3.768574	-2.928996
C	-0.857835	1.336529	2.158360
C	-2.198148	0.052234	3.835937
C	-1.043825	1.059746	3.664523
H	0.079333	0.952876	1.756647
H	-0.881417	2.402897	1.942834
H	-1.342620	1.988245	4.167732
C	-2.024230	-0.812465	1.478934
H	-3.019703	-1.044498	1.094804
C	-1.925230	-1.172999	2.972714
H	-2.650532	-1.966349	3.184944
H	-0.926899	-1.569325	3.174750
H	-2.282232	-0.226689	4.889414
C	-3.497352	0.695634	3.344053
H	-4.305647	-0.042640	3.357585
H	-3.797602	1.521140	3.996432
C	-3.282997	1.226325	1.915720
H	-4.077272	0.919512	1.231326
H	-3.222792	2.315104	1.891456
N	-1.629071	-1.986799	-3.603106
N	-1.980648	0.721497	1.344371
O	-5.541835	-3.909391	-0.202280
C	-6.697517	-4.526861	-0.725039
H	-6.443539	-5.373508	-1.375095
H	-7.256574	-4.892340	0.137146
H	-7.321874	-3.816789	-1.282414
O	0.313742	-1.416343	1.098967
H	0.701527	-0.614893	0.620015
C	0.249479	0.585990	4.277191
H	0.818227	-0.154548	3.714404
C	0.714444	1.032353	5.439823
H	0.188387	1.790567	6.017563
H	1.646070	0.656332	5.850130
C	-1.850374	1.110844	-0.124775

H	-0.776497	1.029843	-0.360421
H	-2.406625	0.353471	-0.677854
C	-2.405404	2.460527	-0.495941
C	-1.668387	3.637821	-0.370496
C	-3.670262	2.561128	-1.086797
C	-2.173391	4.865497	-0.783222
C	-4.195446	3.774896	-1.510750
H	-4.250628	1.654876	-1.233271
C	-3.439423	4.925433	-1.351883
H	-5.173023	3.844281	-1.972988
F	-0.445579	3.633310	0.162292
F	-1.445435	5.967111	-0.637175
F	-3.908265	6.108040	-1.742373
C	-0.981224	-1.685108	0.707629
H	-1.217336	-2.679308	1.123204
C	5.422516	-0.479725	-1.836098
C	4.399755	0.454819	-1.615676
C	4.502117	1.706000	-2.262225
C	5.567343	1.970417	-3.115646
C	6.564607	1.023529	-3.340963
C	6.487806	-0.201129	-2.685447
H	5.380919	-1.440280	-1.332732
H	5.622019	2.941487	-3.604744
H	7.390122	1.244196	-4.011779
H	7.260570	-0.950789	-2.836805
C	3.471934	2.757845	-1.936151
H	3.770676	3.261935	-1.003268
H	3.443406	3.527959	-2.715782
C	2.093328	2.143215	-1.724239
H	1.389776	2.884010	-1.334503
H	1.686647	1.781338	-2.681634
C	2.140221	0.972778	-0.759537
C	3.256342	0.175762	-0.735585
C	3.254581	-1.027520	0.139862
C	3.416557	-0.909821	1.552693
C	3.035397	-2.289562	-0.391440
C	3.624024	0.353738	2.173950
C	3.357156	-2.063980	2.385533
C	2.999119	-3.442819	0.428252
C	3.772899	0.459949	3.531775
H	3.667594	1.231829	1.538573
C	3.511423	-1.922527	3.790748
C	3.152928	-3.326075	1.784415
H	2.838332	-4.422479	-0.007352

C	3.719622	-0.691830	4.355489
H	3.932172	1.434747	3.984179
H	3.470638	-2.815395	4.411048
H	3.117769	-4.213007	2.412668
H	3.853344	-0.596247	5.429883
O	2.844555	-2.349096	-1.741121
C	2.492927	-3.579430	-2.321014
H	3.292173	-4.326029	-2.219602
H	1.564937	-3.980648	-1.890724
H	2.333469	-3.375959	-3.381341
O	1.061888	0.765912	-0.060769

S-CPX-C64

C	-2.610753	-1.071858	-1.213011
C	-4.043589	-1.004146	-1.296138
C	-1.895903	-0.865484	-2.363590
C	-4.921859	-1.305200	-0.226196
C	-4.610561	-0.624551	-2.545883
C	-2.572909	-0.515698	-3.558089
H	-0.810853	-0.898875	-2.361374
C	-6.289676	-1.200234	-0.367920
H	-4.556512	-1.671192	0.727305
C	-6.016722	-0.512562	-2.657466
H	-1.990526	-0.330121	-4.458855
C	-6.847958	-0.783665	-1.600343
H	-6.416177	-0.212029	-3.620564
H	-7.920619	-0.690526	-1.724352
C	-0.053624	0.629623	1.962137
C	-1.717182	-0.027813	3.690448
C	-0.249959	0.404005	3.475265
H	0.340654	-0.251489	1.454716
H	0.615321	1.459727	1.758517
H	-0.092996	1.351323	4.007831
C	-2.230062	-0.359489	1.250440
H	-3.247537	0.014188	1.111543
C	-2.094743	-1.050585	2.618024
H	-3.050725	-1.530931	2.853391
H	-1.338979	-1.839371	2.542890
H	-1.843403	-0.443871	4.692914
C	-2.596852	1.208504	3.493162
H	-3.653829	0.925127	3.450878
H	-2.479080	1.914104	4.321038
C	-2.163634	1.889121	2.187098
H	-3.014337	2.247830	1.603802

H	-1.497674	2.734806	2.366381
N	-3.870017	-0.371368	-3.663149
N	-1.395668	0.929344	1.308664
O	-7.029273	-1.517373	0.726444
C	-8.434634	-1.528086	0.607760
H	-8.768948	-2.227556	-0.168603
H	-8.814438	-1.860101	1.574872
H	-8.832635	-0.528321	0.391178
O	-0.616693	-1.804029	0.071915
H	-0.018947	-1.209335	-0.481492
C	0.728559	-0.599111	4.012058
H	0.774546	-1.551174	3.487230
C	1.503519	-0.388142	5.070674
H	1.502341	0.559977	5.604533
H	2.183925	-1.152224	5.435023
C	-1.235596	1.527733	-0.077736
H	-0.464451	0.939849	-0.604902
H	-2.198362	1.378551	-0.569496
C	-0.899741	2.995505	-0.127347
C	0.410974	3.462315	-0.030837
C	-1.890994	3.943061	-0.406700
C	0.726302	4.807061	-0.180979
C	-1.602877	5.293326	-0.561094
H	-2.916496	3.606778	-0.528021
C	-0.288638	5.717797	-0.445486
H	-2.375300	6.019818	-0.784195
F	1.421509	2.629381	0.219785
F	1.988293	5.208394	-0.078065
F	0.027344	7.002719	-0.587891
C	-1.938005	-1.402606	0.117807
H	-2.489360	-2.276089	0.500790
C	5.475607	-1.233883	-0.784269
C	4.456506	-0.317512	-1.089823
C	4.828929	0.911840	-1.677247
C	6.166302	1.185516	-1.937028
C	7.168678	0.268432	-1.622482
C	6.812409	-0.944002	-1.041161
H	5.210986	-2.192722	-0.346768
H	6.428950	2.139374	-2.391254
H	8.209561	0.498102	-1.831439
H	7.575811	-1.677770	-0.795195
C	3.741012	1.919583	-1.953027
H	3.542708	2.485527	-1.031909
H	4.070640	2.644869	-2.706252

C	2.448202	1.234586	-2.389389
H	1.621232	1.951038	-2.440546
H	2.565895	0.814573	-3.399721
C	2.053822	0.108521	-1.447645
C	3.042833	-0.613821	-0.836604
C	2.692485	-1.771689	0.024348
C	2.223397	-3.007014	-0.531789
C	2.839932	-1.691677	1.393484
C	2.026267	-3.160013	-1.929536
C	1.935652	-4.113710	0.314945
C	2.603783	-2.806651	2.236197
C	1.552045	-4.335785	-2.451411
H	2.263349	-2.321081	-2.574792
C	1.445785	-5.318015	-0.253316
C	2.155511	-3.987194	1.710010
H	2.770663	-2.703670	3.305137
C	1.251611	-5.428630	-1.605320
H	1.405476	-4.432554	-3.523437
H	1.224738	-6.153775	0.406902
H	1.960372	-4.839678	2.356380
H	0.871953	-6.353261	-2.030792
O	3.154604	-0.480734	1.961754
C	4.418454	-0.411381	2.589639
H	4.513555	-1.145382	3.402540
H	5.221961	-0.569203	1.860682
H	4.501678	0.592653	3.011098
O	0.782451	-0.128379	-1.338175

S-CPX-C65

C	1.649747	-2.539980	-0.120258
C	0.923603	-2.293901	1.093121
C	1.654387	-3.830984	-0.586324
C	0.811005	-1.032414	1.711463
C	0.265858	-3.398444	1.709801
C	0.975741	-4.858998	0.110372
H	2.168407	-4.075144	-1.513032
C	0.106711	-0.850850	2.878105
H	1.235212	-0.151274	1.263159
C	-0.479372	-3.180843	2.894441
H	0.997529	-5.875557	-0.280521
C	-0.566498	-1.941356	3.476292
H	-0.983812	-4.038650	3.326515
H	-1.147656	-1.808466	4.382068
C	4.842653	-0.134931	-2.091767



C	5.913043	-1.400137	-0.214218
C	5.900164	-1.214353	-1.746931
H	4.048840	-0.513415	-2.738170
H	5.302059	0.723229	-2.588055
H	6.885428	-0.826479	-2.032235
C	3.456686	-0.762116	-0.126573
H	3.024552	-0.271673	0.742849
C	4.528224	-1.790378	0.302448
H	4.549962	-1.875285	1.393275
H	4.244377	-2.776705	-0.075991
H	6.646941	-2.167322	0.046578
C	6.294560	-0.061126	0.414577
H	6.382674	-0.165282	1.499742
H	7.265347	0.278804	0.039514
C	5.205036	0.968894	0.074966
H	4.663487	1.299321	0.961947
H	5.609531	1.853802	-0.418292
N	0.304299	-4.670229	1.217253
N	4.167056	0.393993	-0.856045
O	0.136130	0.405820	3.393416
C	-0.763584	0.741745	4.423056
H	-1.798224	0.550379	4.121248
H	-0.538200	0.205076	5.354413
H	-0.633326	1.812771	4.589109
O	1.458951	-0.596426	-1.558498
H	-0.022637	-0.692015	-1.182007
C	5.680774	-2.493005	-2.508818
H	4.712205	-2.976526	-2.389803
C	6.596882	-3.047998	-3.296880
H	7.573297	-2.591946	-3.447968
H	6.406997	-3.980261	-3.819646
C	3.235349	1.525588	-1.308137
H	3.884498	2.213495	-1.855907
H	2.514284	1.030521	-1.961029
C	2.490144	2.247367	-0.220018
C	3.004904	3.368958	0.427926
C	1.186312	1.865178	0.099876
C	2.274409	4.048562	1.394034
C	0.434767	2.521304	1.063110
H	0.788172	0.995783	-0.407396
C	0.991767	3.607399	1.712022
H	-0.550390	2.148453	1.321556
F	4.234066	3.827978	0.132659
F	2.801464	5.108231	2.008092

F	0.315022	4.258819	2.661022
C	2.327483	-1.448914	-0.981736
H	2.892879	-2.041174	-1.740685
C	-5.023341	1.964300	-1.306362
C	-3.795453	1.509339	-1.805712
C	-3.333761	2.040435	-3.028622
C	-4.069063	3.022064	-3.681950
C	-5.275802	3.486615	-3.160741
C	-5.754317	2.943074	-1.973585
H	-5.410463	1.538019	-0.384774
H	-3.694656	3.424713	-4.621175
H	-5.837815	4.255338	-3.683043
H	-6.700901	3.280331	-1.560033
C	-2.080273	1.453511	-3.629342
H	-2.352824	0.540530	-4.180924
H	-1.640697	2.144019	-4.357836
C	-1.058726	1.080697	-2.559489
H	-0.226551	0.514865	-2.989070
H	-0.630879	1.991580	-2.114271
C	-1.707483	0.269585	-1.460926
C	-2.995402	0.496395	-1.100780
C	-3.592092	-0.294527	0.008889
C	-4.443358	-1.410579	-0.282216
C	-3.338095	0.002495	1.330293
C	-4.747699	-1.780319	-1.619695
C	-5.006489	-2.178726	0.774924
C	-3.896022	-0.760063	2.384040
C	-5.567162	-2.846129	-1.889161
H	-4.312416	-1.203889	-2.428902
C	-5.848322	-3.278917	0.465015
C	-4.707023	-1.827110	2.115605
H	-3.662541	-0.481070	3.407236
C	-6.126994	-3.606163	-0.836234
H	-5.786832	-3.111050	-2.919424
H	-6.268942	-3.859155	1.282892
H	-5.130653	-2.415927	2.925240
H	-6.773352	-4.449242	-1.062774
O	-2.518808	1.055397	1.686673
C	-3.208650	2.282216	1.853008
H	-3.624019	2.635893	0.902312
H	-4.019240	2.183277	2.588346
H	-2.478626	3.007668	2.222713
O	-0.978380	-0.639382	-0.827540

## TS-C1

C	1.431847	3.295197	-1.950627
C	2.754313	2.911388	-1.557640
C	1.312448	4.336201	-2.835960
C	3.041744	1.836702	-0.690290
C	3.838156	3.683736	-2.068129
C	2.461699	5.016648	-3.307548
H	0.333426	4.650794	-3.188759
C	4.337521	1.553034	-0.310428
H	2.266259	1.167121	-0.341995
C	5.157141	3.364224	-1.666519
H	2.347692	5.838679	-4.012024
C	5.413577	2.329563	-0.803398
H	5.961225	3.969950	-2.070933
H	6.434672	2.106523	-0.516021
C	-2.281198	3.498400	0.247157
C	-0.463351	4.518614	1.615167
C	-1.678517	4.843568	0.724806
H	-2.455478	3.472611	-0.827771
H	-3.236421	3.295060	0.733017
H	-2.427595	5.337676	1.354052
C	0.048058	2.553854	0.087484
H	0.554319	1.652540	0.436615
C	0.619769	3.801085	0.806209
H	1.429917	3.484513	1.470212
H	1.059689	4.485412	0.079828
H	-0.060908	5.445997	2.031338
C	-0.934951	3.585357	2.728146
H	-0.145436	3.430703	3.466542
H	-1.796196	4.016620	3.249187
C	-1.302930	2.233411	2.104621
H	-0.556856	1.464786	2.310881
H	-2.270331	1.869205	2.447631
N	3.680884	4.725696	-2.934879
N	-1.387507	2.341080	0.597618
O	4.487687	0.505093	0.530960
C	5.785822	0.054447	0.865964
H	6.348732	0.827798	1.403717
H	5.639111	-0.810849	1.511982
H	6.338968	-0.253171	-0.028992
O	-0.028207	1.375022	-2.105124
H	0.428020	0.628922	-1.632803
C	-1.358914	5.774282	-0.413640
H	-0.608454	5.444411	-1.130562

C	-1.929288	6.964054	-0.578801
H	-2.682812	7.337536	0.111469
H	-1.664264	7.610801	-1.409501
C	-1.936355	1.034149	0.037548
H	-1.982104	1.167636	-1.041918
H	-1.162364	0.291818	0.250653
C	-3.255420	0.589781	0.589568
C	-4.448167	0.971023	-0.016995
C	-3.318011	-0.353913	1.616614
C	-5.670714	0.467808	0.399542
C	-4.528365	-0.872466	2.051794
H	-2.395166	-0.710607	2.062072
C	-5.698097	-0.457985	1.435695
H	-4.577257	-1.621701	2.832663
F	-4.437590	1.844722	-1.032251
F	-6.794898	0.860910	-0.189271
F	-6.876777	-0.934587	1.826455
C	0.154507	2.604698	-1.469377
H	-0.660191	3.241923	-1.833867
C	3.721371	-2.733567	2.419537
C	3.267919	-2.545982	1.106507
C	4.105187	-2.945620	0.043068
C	5.354584	-3.491870	0.312895
C	5.800860	-3.663472	1.623260
C	4.974118	-3.285901	2.676413
H	3.087569	-2.440085	3.251237
H	5.987220	-3.796377	-0.518222
H	6.778212	-4.096015	1.815658
H	5.300770	-3.419497	3.703989
C	3.570883	-2.819422	-1.359272
H	2.930763	-3.687751	-1.569096
H	4.386188	-2.842835	-2.090395
C	2.732490	-1.557191	-1.529505
H	2.212651	-1.571327	-2.490358
H	3.378161	-0.669073	-1.526890
C	1.711106	-1.413199	-0.422771
C	1.962370	-1.931747	0.809268
C	0.959118	-1.789961	1.899978
C	1.007566	-0.687832	2.812801
C	-0.020683	-2.744249	2.085728
C	1.986506	0.336041	2.676537
C	0.084692	-0.607517	3.895660
C	-0.949122	-2.662364	3.152945
C	2.047198	1.376085	3.571497

H	2.711896	0.262153	1.872044
C	0.173581	0.482380	4.803325
C	-0.896819	-1.622407	4.041573
H	-1.701409	-3.441144	3.232096
C	1.136381	1.448311	4.653022
H	2.816153	2.136012	3.461256
H	-0.529656	0.528743	5.631332
H	-1.606030	-1.562303	4.863208
H	1.206437	2.263903	5.367519
O	-0.159836	-3.794441	1.218481
C	0.648751	-4.922362	1.517319
H	0.430956	-5.303222	2.523885
H	1.714532	-4.679288	1.443884
H	0.393242	-5.686425	0.781099
O	0.611745	-0.723285	-0.686008
C	-0.916393	-1.760943	-1.409492
H	-1.084910	-2.218234	-0.448025
H	-1.382410	-0.821951	-1.641733
C	-0.304886	-2.520622	-2.488129
C	0.185381	-3.808843	-2.254672
C	-0.130334	-1.928554	-3.745372
C	0.842629	-4.496972	-3.268243
H	0.034741	-4.255751	-1.277615
C	0.531970	-2.615107	-4.752681
H	-0.510902	-0.925443	-3.915946
C	1.022071	-3.900059	-4.514244
H	1.217325	-5.500213	-3.087385
H	0.665883	-2.153288	-5.726109
H	1.537027	-4.438443	-5.304667
I	-3.693602	-2.505176	-1.751038

TS-C2

C	-2.189536	2.468656	-0.270804
C	-3.503600	2.671715	0.261878
C	-1.478780	3.576303	-0.658699
C	-4.323808	1.640986	0.770234
C	-3.996999	4.007731	0.287500
C	-2.060255	4.865659	-0.562798
H	-0.467674	3.493536	-1.049305
C	-5.582556	1.902744	1.263490
H	-3.968236	0.623363	0.827416
C	-5.300004	4.245174	0.785591
H	-1.477797	5.731849	-0.869846
C	-6.086058	3.225862	1.261450

H	-5.652806	5.271237	0.787008
H	-7.076399	3.446845	1.642662
C	-0.157110	-0.948224	-2.145478
C	-1.616694	0.165640	-3.818349
C	-0.158550	0.010139	-3.354773
H	0.462629	-0.607913	-1.310329
H	0.185435	-1.939225	-2.437961
H	0.387196	-0.514282	-4.151685
C	-2.275445	0.161496	-1.360290
H	-3.236914	-0.130099	-0.936653
C	-2.467867	0.844240	-2.738808
H	-3.523979	0.810078	-3.025517
H	-2.200433	1.896853	-2.649902
H	-1.662504	0.740753	-4.746728
C	-2.182797	-1.238514	-4.040007
H	-3.157543	-1.190322	-4.533834
H	-1.516214	-1.826361	-4.679303
C	-2.337809	-1.915910	-2.671234
H	-3.375959	-1.936722	-2.333534
H	-1.958518	-2.937290	-2.676054
N	-3.274446	5.088228	-0.128780
N	-1.556586	-1.171338	-1.610773
O	-6.270562	0.830801	1.742749
C	-7.554038	1.045119	2.287278
H	-8.252111	1.438585	1.537413
H	-7.905594	0.067953	2.621493
H	-7.520702	1.728286	3.145315
O	-1.408207	0.556358	0.921832
H	-0.447669	0.306464	1.042184
C	0.602144	1.287113	-3.087496
H	1.502385	1.169194	-2.481764
C	0.318107	2.494000	-3.570198
H	-0.551552	2.687803	-4.194678
H	0.960402	3.338626	-3.337377
C	-1.411840	-2.074572	-0.389015
H	-0.818813	-2.918835	-0.743339
H	-0.814684	-1.521856	0.328197
C	-2.704732	-2.544318	0.214976
C	-3.276093	-3.752403	-0.181509
C	-3.344802	-1.830149	1.232107
C	-4.467683	-4.212401	0.361223
C	-4.544627	-2.263778	1.783324
H	-2.874837	-0.916702	1.581098
C	-5.101452	-3.451636	1.338045

H	-5.056465	-1.682811	2.541210
F	-2.682672	-4.516620	-1.110981
F	-4.991960	-5.363619	-0.050380
F	-6.251969	-3.897233	1.838522
C	-1.532864	1.096984	-0.367215
H	-0.545663	1.269239	-0.805016
C	5.045723	-2.827144	1.422749
C	3.744609	-2.460428	1.783969
C	3.234251	-2.907749	3.018561
C	4.028692	-3.683108	3.855592
C	5.326989	-4.034944	3.490646
C	5.830626	-3.605932	2.266821
H	5.448236	-2.490061	0.472094
H	3.621685	-4.023124	4.805671
H	5.936225	-4.640472	4.155209
H	6.840713	-3.872418	1.968213
C	1.800892	-2.575482	3.354145
H	1.145328	-3.312388	2.862312
H	1.624463	-2.668722	4.431156
C	1.422203	-1.180811	2.861966
H	0.343667	-1.014672	2.963501
H	1.914987	-0.409879	3.469831
C	1.811013	-0.985373	1.411539
C	2.904655	-1.623239	0.909714
C	3.226001	-1.511269	-0.541143
C	2.634624	-2.425549	-1.461739
C	4.075832	-0.533003	-1.036576
C	1.828159	-3.513755	-1.019117
C	2.820545	-2.260291	-2.865235
C	4.263023	-0.363146	-2.431875
C	1.219789	-4.358167	-1.913210
H	1.702847	-3.660646	0.048561
C	2.166927	-3.142755	-3.768277
C	3.636684	-1.198394	-3.319462
H	4.886218	0.441085	-2.804096
C	1.375363	-4.164612	-3.309529
H	0.614318	-5.184703	-1.550747
H	2.313565	-2.994970	-4.835767
H	3.772701	-1.050874	-4.387552
H	0.887857	-4.838949	-4.007472
O	4.687546	0.259345	-0.121527
C	5.611343	1.242368	-0.562251
H	6.442068	0.782178	-1.111241
H	5.120869	2.011185	-1.169049

H	5.993039	1.710419	0.345239
O	1.068453	-0.152679	0.696496
C	1.885189	1.724029	0.505933
H	0.981164	1.992254	-0.007328
H	2.689758	1.280694	-0.050469
C	2.052042	2.053452	1.908466
C	0.981459	2.586132	2.637722
C	3.254633	1.749964	2.558177
C	1.115930	2.817214	3.999075
H	0.045340	2.803524	2.130484
C	3.385797	1.985704	3.921083
H	4.064951	1.307167	1.988642
C	2.318531	2.520067	4.641322
H	0.285038	3.231022	4.562073
H	4.318574	1.748729	4.423403
H	2.423482	2.704533	5.706533
I	2.756454	4.076805	-0.811911

TS-C3

C	3.523707	0.614688	0.180746
C	4.918596	0.652505	0.495700
C	2.936527	1.771491	-0.266480
C	5.662212	-0.464220	0.940800
C	5.593528	1.896509	0.319713
C	3.702030	2.954414	-0.391965
H	1.885566	1.800637	-0.536603
C	7.012171	-0.365706	1.197300
H	5.198843	-1.430455	1.093855
C	6.978780	1.968440	0.601259
H	3.218387	3.865844	-0.740937
C	7.682216	0.870987	1.027219
H	7.466208	2.927706	0.462487
H	8.743323	0.962159	1.228932
C	1.879562	-3.436060	-0.772197
C	3.108149	-2.524594	-2.758098
C	3.105104	-3.639555	-1.690560
H	2.142950	-3.345628	0.281082
H	1.161038	-4.250453	-0.857172
H	2.971280	-4.591691	-2.222304
C	2.080384	-0.958420	-1.060033
H	1.438881	-0.131894	-1.368986
C	3.226816	-1.161943	-2.080677
H	3.190995	-0.362568	-2.826311
H	4.194204	-1.086574	-1.575886



H	3.949824	-2.678729	-3.440367
C	1.791676	-2.563786	-3.528450
H	1.797125	-1.805039	-4.316269
H	1.653192	-3.537600	-4.008979
C	0.642873	-2.285518	-2.549386
H	0.126068	-1.348427	-2.758823
H	-0.098845	-3.082755	-2.552125
N	4.980154	3.032455	-0.117895
N	1.145510	-2.177003	-1.130667
O	7.625073	-1.506571	1.606819
C	8.998518	-1.457228	1.925722
H	9.199350	-0.750850	2.740870
H	9.265555	-2.463399	2.250975
H	9.607624	-1.187844	1.053166
O	1.772453	-0.536726	1.394872
H	1.115902	0.181742	1.202853
C	4.436197	-3.723409	-0.978147
H	5.293846	-3.609802	-1.641837
C	4.668934	-3.948300	0.312294
H	3.881908	-4.093167	1.048485
H	5.685521	-3.994562	0.690483
C	-0.049643	-1.952586	-0.203691
H	0.325749	-2.125059	0.802529
H	-0.276767	-0.887668	-0.294383
C	-1.285444	-2.747069	-0.494668
C	-1.484863	-4.019718	0.029849
C	-2.348884	-2.149515	-1.174876
C	-2.679722	-4.700155	-0.146311
C	-3.554996	-2.806130	-1.362781
H	-2.232341	-1.134603	-1.537476
C	-3.711193	-4.080373	-0.842929
H	-4.389356	-2.321998	-1.856197
F	-0.506935	-4.624227	0.722467
F	-2.835498	-5.922509	0.352297
F	-4.853058	-4.743865	-1.000118
C	2.677797	-0.651526	0.338084
H	3.331175	-1.485366	0.601090
C	-1.496540	4.689041	-2.252392
C	-1.130467	4.189038	-0.994703
C	-0.867146	5.108614	0.041192
C	-0.940992	6.474125	-0.211095
C	-1.288812	6.959026	-1.470324
C	-1.575103	6.057646	-2.489512
H	-1.724148	3.995051	-3.056831

H	-0.730960	7.171049	0.597365
H	-1.344173	8.028899	-1.647870
H	-1.860558	6.416956	-3.474246
C	-0.591762	4.570897	1.421746
H	-1.553057	4.385200	1.921236
H	-0.061179	5.312549	2.028510
C	0.186813	3.260765	1.379478
H	0.215092	2.799192	2.368725
H	1.231296	3.451283	1.091015
C	-0.413339	2.277927	0.393783
C	-1.018536	2.738875	-0.735110
C	-1.559851	1.805234	-1.762232
C	-2.965942	1.526885	-1.815486
C	-0.756218	1.241897	-2.732969
C	-3.850102	2.018477	-0.817924
C	-3.504872	0.716918	-2.856023
C	-1.292919	0.472162	-3.794110
C	-5.179352	1.684164	-0.825400
H	-3.444000	2.653025	-0.037220
C	-4.890684	0.405960	-2.849576
C	-2.635624	0.216384	-3.858798
H	-0.608215	0.095775	-4.549792
C	-5.708162	0.866060	-1.850523
H	-5.833203	2.043971	-0.037547
H	-5.289575	-0.214086	-3.649083
H	-3.045947	-0.382775	-4.667300
H	-6.762303	0.607578	-1.842163
O	0.618794	1.353690	-2.698450
C	1.158624	2.552760	-3.237705
H	0.839134	3.426554	-2.661913
H	0.856983	2.677278	-4.285684
H	2.244560	2.451760	-3.178157
O	-0.276278	0.988461	0.655363
C	-1.746220	0.174511	1.704518
H	-2.440785	0.336238	0.895052
H	-1.176487	-0.737072	1.721078
C	-1.759441	1.022759	2.890239
C	-0.787408	0.846881	3.882220
C	-2.685241	2.062901	3.011739
C	-0.735955	1.707855	4.969799
H	-0.063268	0.043203	3.781903
C	-2.637281	2.919640	4.104826
H	-3.462221	2.169837	2.260857
C	-1.658364	2.748621	5.081177

H	0.022527	1.569080	5.734235
H	-3.366871	3.718500	4.197480
H	-1.619824	3.419852	5.934026
I	-3.792291	-1.673395	2.484298

S-TS-C4

C	2.038538	-2.747526	0.046106
C	3.380997	-2.832437	0.538333
C	1.352070	-3.919655	-0.142232
C	4.187513	-1.714885	0.845662
C	3.921202	-4.135332	0.736551
C	1.982858	-5.164172	0.109184
H	0.316613	-3.929391	-0.479288
C	5.475992	-1.866019	1.308252
H	3.800503	-0.710396	0.763574
C	5.251791	-4.260234	1.201735
H	1.420152	-6.082204	-0.045808
C	6.022924	-3.159964	1.481872
H	5.639249	-5.264351	1.338774
H	7.035514	-3.294522	1.844549
C	-0.117121	0.353522	-2.274897
C	1.281471	-1.006226	-3.831752
C	-0.168862	-0.681825	-3.421126
H	-0.681028	0.060873	-1.385312
H	-0.510950	1.315444	-2.603448
H	-0.646933	-0.193877	-4.279204
C	2.009707	-0.669340	-1.412899
H	3.009478	-0.344359	-1.121497
C	2.065261	-1.594843	-2.658936
H	3.107778	-1.761322	-2.947027
H	1.658419	-2.574167	-2.402096
H	1.273411	-1.716562	-4.662455
C	1.960152	0.298043	-4.244185
H	2.959250	0.101659	-4.644174
H	1.385498	0.798923	-5.029559
C	2.065933	1.202394	-3.007016
H	3.097845	1.327860	-2.674090
H	1.644592	2.190975	-3.186065
N	3.221025	-5.285726	0.514788
N	1.305575	0.630591	-1.831733
O	6.149552	-0.715988	1.582658
C	7.472035	-0.808239	2.064092
H	8.132205	-1.306102	1.342605
H	7.810753	0.218913	2.206660

H	7.518024	-1.338692	3.023636
O	1.245445	-0.686557	0.955560
H	0.288414	-0.414149	1.047136
C	-1.010512	-1.876401	-3.065211
H	-0.715684	-2.483287	-2.209743
C	-2.119357	-2.216266	-3.714265
H	-2.482088	-1.641419	-4.563733
H	-2.707212	-3.070794	-3.392071
C	1.218673	1.710965	-0.756024
H	0.657740	2.519576	-1.220262
H	0.605981	1.307973	0.042327
C	2.528612	2.232158	-0.234751
C	3.135263	3.342573	-0.820999
C	3.134128	1.698344	0.905996
C	4.323885	3.871431	-0.338207
C	4.330481	2.202104	1.402179
H	2.642958	0.865424	1.396948
C	4.921868	3.283307	0.771155
H	4.814093	1.754784	2.262017
F	2.578745	3.946662	-1.884725
F	4.879038	4.925237	-0.931959
F	6.070914	3.790504	1.213706
C	1.336786	-1.422994	-0.232418
H	0.333669	-1.680413	-0.585391
C	-3.709448	4.154962	1.322246
C	-2.759963	3.226420	1.763239
C	-2.264800	3.340592	3.074936
C	-2.715301	4.364547	3.901085
C	-3.657341	5.286880	3.450441
C	-4.154554	5.175938	2.155750
H	-4.109772	4.069265	0.315658
H	-2.320142	4.442304	4.911762
H	-4.002764	6.079392	4.107908
H	-4.896643	5.882005	1.793349
C	-1.224982	2.344172	3.517405
H	-0.239643	2.668233	3.146964
H	-1.161142	2.305886	4.610190
C	-1.536256	0.963202	2.947727
H	-0.732565	0.257485	3.177610
H	-2.448491	0.562414	3.410435
C	-1.709329	1.027609	1.441320
C	-2.277512	2.136462	0.886842
C	-2.392966	2.328985	-0.582270
C	-3.215772	1.507650	-1.407665

C	-1.696220	3.371742	-1.180092
C	-4.015636	0.470115	-0.857498
C	-3.267874	1.718694	-2.816194
C	-1.773610	3.612286	-2.572782
C	-4.766519	-0.349459	-1.657239
H	-4.017626	0.354923	0.220275
C	-4.063001	0.857965	-3.621976
C	-2.535570	2.793586	-3.370916
H	-1.225973	4.436900	-3.016460
C	-4.783630	-0.161592	-3.061212
H	-5.351234	-1.152329	-1.217849
H	-4.089116	1.027306	-4.696057
H	-2.588587	2.974737	-4.441587
H	-5.379038	-0.821430	-3.684387
O	-0.885771	4.102560	-0.363863
C	-0.441760	5.367948	-0.800165
H	0.322070	5.284432	-1.584064
H	-1.274627	5.982748	-1.161685
H	0.001782	5.843912	0.075269
O	-1.239441	0.008324	0.728463
C	-2.087834	-1.823039	0.718049
H	-2.662602	-1.518843	-0.139839
H	-1.098527	-2.211950	0.561159
C	-2.667815	-1.946429	2.044863
C	-1.857172	-2.355671	3.111245
C	-4.000366	-1.597814	2.289321
C	-2.364625	-2.395035	4.401508
H	-0.824033	-2.630498	2.915312
C	-4.507005	-1.633755	3.582027
H	-4.643553	-1.322393	1.459509
C	-3.688422	-2.026078	4.639917
H	-1.730637	-2.712197	5.223686
H	-5.542279	-1.363961	3.765137
H	-4.086707	-2.055802	5.649759
I	-2.716815	-4.402973	-0.382507

S-TS-C5

C	-2.206864	2.412381	-0.519586
C	-3.511139	2.648188	0.022345
C	-1.511652	3.487533	-1.010493
C	-4.312856	1.654690	0.626439
C	-4.015138	3.977927	-0.052788
C	-2.098635	4.778359	-1.002765
H	-0.506984	3.376361	-1.410812

C	-5.567944	1.945544	1.112948
H	-3.944807	0.648857	0.766106
C	-5.313052	4.244644	0.443523
H	-1.525801	5.621759	-1.381822
C	-6.083265	3.260274	1.010585
H	-5.675499	5.264428	0.366727
H	-7.070506	3.502999	1.386686
C	-0.230838	-1.059629	-2.331524
C	-1.888440	-0.131030	-3.938824
C	-0.385459	-0.230388	-3.621358
H	0.422484	-0.617007	-1.577101
H	0.151985	-2.054391	-2.555503
H	0.076477	-0.814953	-4.429325
C	-2.311401	0.036942	-1.436587
H	-3.239172	-0.261078	-0.947155
C	-2.601197	0.647428	-2.832560
H	-3.680651	0.663811	-3.012215
H	-2.266193	1.686114	-2.844347
H	-2.030250	0.376107	-4.897816
C	-2.463385	-1.544690	-3.995421
H	-3.496314	-1.528899	-4.354874
H	-1.882892	-2.165267	-4.685487
C	-2.418619	-2.139018	-2.581666
H	-3.408296	-2.193137	-2.124785
H	-1.982000	-3.137490	-2.568971
N	-3.307216	5.026088	-0.566569
N	-1.570285	-1.291207	-1.661382
O	-6.240890	0.910399	1.685148
C	-7.514745	1.162512	2.235685
H	-8.228020	1.497047	1.471620
H	-7.856875	0.213065	2.649748
H	-7.467775	1.909019	3.038511
O	-1.421748	0.590085	0.800562
H	-0.455740	0.365293	0.925923
C	0.296754	1.117875	-3.616013
H	-0.070245	1.811517	-4.373563
C	1.316254	1.486969	-2.846111
H	1.739361	0.834006	-2.086716
H	1.771128	2.469181	-2.931510
C	-1.287328	-2.097787	-0.395896
H	-0.664757	-2.926654	-0.735302
H	-0.679812	-1.464229	0.241269
C	-2.507943	-2.607681	0.317383
C	-2.985397	-3.892077	0.059649

C	-3.175480	-1.853171	1.286907
C	-4.110125	-4.398118	0.695635
C	-4.312109	-2.332389	1.927153
H	-2.776480	-0.873504	1.527360
C	-4.774600	-3.602589	1.623288
H	-4.845958	-1.727135	2.650314
F	-2.365455	-4.684436	-0.828482
F	-4.544407	-5.623955	0.416106
F	-5.861509	-4.094415	2.213903
C	-1.550834	1.038995	-0.523318
H	-0.563062	1.174435	-0.973454
C	5.012755	-2.719136	1.404336
C	3.690426	-2.378472	1.708081
C	3.114255	-2.884025	2.889804
C	3.866887	-3.692016	3.734750
C	5.186989	-4.017639	3.428278
C	5.755763	-3.530010	2.256011
H	5.464290	-2.335085	0.494350
H	3.410934	-4.077450	4.644321
H	5.763748	-4.647889	4.098784
H	6.783995	-3.775039	2.005112
C	1.662457	-2.570099	3.157426
H	1.037709	-3.281088	2.592267
H	1.424392	-2.715694	4.216545
C	1.310815	-1.151827	2.713581
H	0.227883	-0.989775	2.766427
H	1.768027	-0.414779	3.386884
C	1.776164	-0.892212	1.294754
C	2.893656	-1.508798	0.825257
C	3.269275	-1.373895	-0.609627
C	2.745242	-2.311496	-1.549067
C	4.102422	-0.366864	-1.073232
C	1.966819	-3.430885	-1.133563
C	2.981737	-2.144859	-2.943925
C	4.367239	-0.217861	-2.458876
C	1.427372	-4.301417	-2.046799
H	1.812703	-3.586766	-0.071047
C	2.392604	-3.050436	-3.868031
C	3.801938	-1.073060	-3.367198
H	4.995991	0.591332	-2.810223
C	1.625045	-4.102119	-3.436702
H	0.846073	-5.152980	-1.703102
H	2.573877	-2.899295	-4.929670
H	3.987001	-0.932651	-4.428647

H	1.191862	-4.796027	-4.151137
O	4.629061	0.466192	-0.140887
C	5.426059	1.562317	-0.562834
H	6.337854	1.217216	-1.065259
H	4.860811	2.243951	-1.208172
H	5.692891	2.098388	0.347859
O	1.064068	-0.042408	0.565858
C	1.780204	1.865634	0.572669
H	0.872967	2.148910	0.070274
H	2.617983	1.526264	-0.009456
C	1.923153	2.079721	2.000506
C	0.826782	2.504649	2.761385
C	3.131332	1.766296	2.634766
C	0.942411	2.622488	4.138970
H	-0.112012	2.729929	2.262964
C	3.243829	1.889145	4.014135
H	3.961267	1.400690	2.039283
C	2.151223	2.318040	4.766170
H	0.092340	2.954349	4.727215
H	4.181169	1.644882	4.504253
H	2.241578	2.416450	5.844069
I	2.525769	4.408522	-0.492582

S-TS-C6

C	2.316816	-2.521320	-0.082757
C	3.624015	-2.604436	0.496120
C	1.707989	-3.690430	-0.460819
C	4.341654	-1.497635	1.000634
C	4.220600	-3.895112	0.574268
C	2.386923	-4.926228	-0.312564
H	0.705473	-3.696532	-0.882145
C	5.601701	-1.645090	1.536619
H	3.901643	-0.511644	1.022318
C	5.521256	-4.014915	1.118731
H	1.886004	-5.843606	-0.614552
C	6.208000	-2.923288	1.588571
H	5.954326	-5.008768	1.161561
H	7.199047	-3.054460	2.007607
C	0.108317	0.608220	-2.175496
C	1.769133	-0.404665	-3.728150
C	0.277931	-0.380066	-3.350816
H	-0.509180	0.228158	-1.356468
H	-0.336981	1.543882	-2.510960
H	-0.270001	0.061222	-4.195031



C	2.270354	-0.247186	-1.240219
H	3.171955	0.151991	-0.775216
C	2.613131	-0.957257	-2.574734
H	3.676678	-0.828421	-2.799771
H	2.441881	-2.027217	-2.459859
H	1.923648	-1.006280	-4.627291
C	2.208420	1.037645	-3.979613
H	3.213747	1.067686	-4.409506
H	1.533222	1.527851	-4.688399
C	2.203356	1.781741	-2.637742
H	3.209715	1.930564	-2.241572
H	1.715183	2.753408	-2.711618
N	3.600288	-5.040045	0.164507
N	1.444929	0.999981	-1.587029
O	6.187029	-0.508947	2.004332
C	7.475491	-0.600220	2.570852
H	8.212198	-0.966896	1.844764
H	7.743493	0.414580	2.868228
H	7.484080	-1.248957	3.456013
O	1.359483	-0.636828	1.021966
H	0.380754	-0.462164	1.110634
C	-0.353985	-1.725073	-3.083059
H	-1.265674	-1.704383	-2.484077
C	0.061967	-2.900220	-3.546942
H	0.956960	-3.008688	-4.155683
H	-0.493225	-3.803821	-3.311645
C	1.158009	1.935658	-0.416093
H	0.522194	2.717727	-0.832885
H	0.566749	1.366681	0.293481
C	2.373839	2.537370	0.232570
C	2.859148	3.778082	-0.179808
C	3.021557	1.915387	1.304547
C	3.974716	4.359334	0.407514
C	4.147674	2.471257	1.899450
H	2.618789	0.973250	1.660872
C	4.620204	3.690279	1.441628
H	4.666966	1.962782	2.703118
F	2.259042	4.455451	-1.168602
F	4.417779	5.539397	-0.019140
F	5.698579	4.253473	1.983103
C	1.561647	-1.208737	-0.243513
H	0.600527	-1.471278	-0.697230
C	-4.894836	2.933769	1.058074
C	-3.715537	2.394594	1.584093

C	-3.380431	2.676851	2.922603
C	-4.226238	3.463036	3.696910
C	-5.403126	3.988095	3.165911
C	-5.731548	3.723244	1.840221
H	-5.157155	2.726603	0.024322
H	-3.957895	3.671419	4.730389
H	-6.053898	4.600683	3.782900
H	-6.643892	4.128719	1.411933
C	-2.067008	2.147809	3.442313
H	-1.259750	2.827186	3.124123
H	-2.058004	2.138512	4.537509
C	-1.788633	0.753639	2.888306
H	-0.775015	0.427280	3.144974
H	-2.476809	0.028988	3.340869
C	-1.930090	0.720399	1.378360
C	-2.826491	1.544974	0.767117
C	-2.863243	1.702162	-0.714781
C	-2.278172	2.872713	-1.292479
C	-3.433806	0.764993	-1.565061
C	-1.678594	3.885155	-0.486743
C	-2.236844	3.042176	-2.707195
C	-3.390119	0.929529	-2.973512
C	-1.054432	4.966850	-1.051704
H	-1.713345	3.779888	0.591666
C	-1.579162	4.173352	-3.264102
C	-2.807151	2.039810	-3.526158
H	-3.823585	0.178461	-3.623149
C	-0.991196	5.112800	-2.459107
H	-0.598163	5.718566	-0.414690
H	-1.551523	4.278301	-4.346304
H	-2.779948	2.156811	-4.606656
H	-0.489493	5.972718	-2.892027
O	-4.030903	-0.309861	-0.991674
C	-4.658154	-1.282703	-1.812359
H	-5.486461	-0.843214	-2.381108
H	-3.943641	-1.764806	-2.489189
H	-5.036774	-2.043995	-1.130291
O	-1.152513	-0.127463	0.721899
C	-1.898309	-2.020882	0.515653
H	-0.884553	-2.367693	0.406527
H	-2.420004	-1.622617	-0.333241
C	-2.587815	-2.229333	1.773928
C	-1.920945	-2.834657	2.847012
C	-3.891037	-1.745833	1.950866

C	-2.548352	-2.958283	4.077739
H	-0.913102	-3.213503	2.700915
C	-4.513892	-1.865840	3.186865
H	-4.386990	-1.244464	1.127220
C	-3.844993	-2.471240	4.249200
H	-2.031566	-3.433364	4.905859
H	-5.518457	-1.478341	3.324903
H	-4.334521	-2.566185	5.214062
I	-2.406675	-4.486866	-0.861997

S-TS-C7

C	-3.610728	0.338355	0.083280
C	-4.798847	-0.036570	0.783063
C	-3.647059	1.466021	-0.696785
C	-4.869285	-1.125457	1.680366
C	-5.966758	0.740400	0.539847
C	-4.857237	2.190760	-0.833143
H	-2.748187	1.805049	-1.205359
C	-6.061688	-1.465592	2.283304
H	-3.973954	-1.666068	1.962792
C	-7.176049	0.363226	1.170179
H	-4.878001	3.086707	-1.451720
C	-7.234792	-0.716152	2.014860
H	-8.056732	0.963101	0.965652
H	-8.177088	-0.974764	2.484050
C	-0.812035	-1.944178	-2.279698
C	-2.993733	-3.084904	-2.560623
C	-1.755022	-2.571449	-3.324443
H	-0.935976	-0.861058	-2.237177
H	0.234063	-2.159063	-2.495904
H	-1.260591	-3.430161	-3.795900
C	-2.454705	-1.882973	-0.415468
H	-2.740550	-2.542123	0.407691
C	-3.455999	-2.006222	-1.578100
H	-4.436657	-2.245571	-1.157792
H	-3.563369	-1.041867	-2.083660
H	-3.792475	-3.338750	-3.261924
C	-2.565730	-4.315194	-1.753571
H	-3.363880	-4.608849	-1.064396
H	-2.370262	-5.167920	-2.410324
C	-1.284705	-3.966879	-0.978429
H	-1.293173	-4.344920	0.043742
H	-0.388741	-4.348951	-1.471153
N	-5.984871	1.841043	-0.267520

N	-1.112914	-2.471317	-0.900273
O	-6.025282	-2.527122	3.127112
C	-7.196316	-2.867855	3.836011
H	-8.003393	-3.178552	3.160084
H	-6.923544	-3.707853	4.475853
H	-7.545772	-2.037560	4.462440
O	-1.855158	-0.536656	1.489444
H	-1.065624	0.060222	1.517251
C	-2.074712	-1.569281	-4.398278
H	-2.596183	-0.668839	-4.076399
C	-1.753987	-1.715425	-5.681105
H	-1.223739	-2.594005	-6.042092
H	-2.015138	-0.964156	-6.420225
C	0.019782	-2.113769	0.051634
H	0.084259	-1.024805	0.046401
H	-0.310171	-2.435336	1.040034
C	1.373616	-2.652948	-0.302995
C	1.820793	-3.890694	0.151231
C	2.294467	-1.829270	-0.958355
C	3.117254	-4.325503	-0.077911
C	3.597921	-2.238697	-1.194326
H	1.988327	-0.828094	-1.245299
C	3.999121	-3.488305	-0.753178
H	4.319476	-1.576001	-1.656466
F	0.992527	-4.700915	0.829317
F	3.508785	-5.520867	0.352887
F	5.239443	-3.917175	-0.959853
C	-2.317576	-0.455104	0.166439
H	-1.597573	0.097283	-0.449429
C	0.306152	4.656344	-2.259456
C	0.104916	4.104608	-0.986722
C	-0.426310	4.932014	0.024621
C	-0.786048	6.241853	-0.271958
C	-0.612230	6.769018	-1.550384
C	-0.050590	5.971794	-2.541408
H	0.763195	4.050719	-3.037047
H	-1.199475	6.865539	0.517755
H	-0.896738	7.795425	-1.761871
H	0.116798	6.372979	-3.537165
C	-0.502081	4.389134	1.429307
H	0.478028	4.532009	1.908696
H	-1.228176	4.952798	2.024843
C	-0.825649	2.900408	1.454019
H	-0.680941	2.496327	2.459532

H	-1.881572	2.729983	1.192124
C	0.029523	2.121171	0.477639
C	0.444353	2.703077	-0.680573
C	1.163682	1.902768	-1.709494
C	2.593741	1.818131	-1.719303
C	0.471578	1.244428	-2.703066
C	3.376549	2.462178	-0.724509
C	3.261867	1.059609	-2.721921
C	1.127577	0.502018	-3.715408
C	4.737354	2.303395	-0.684256
H	2.864709	3.065938	0.017815
C	4.676262	0.937214	-2.671284
C	2.493093	0.413466	-3.724408
H	0.527333	-0.014066	-4.460382
C	5.396382	1.527213	-1.665403
H	5.314585	2.766313	0.109222
H	5.177532	0.352708	-3.439527
H	3.001836	-0.168658	-4.488397
H	6.473038	1.401199	-1.615553
O	-0.911576	1.240365	-2.685700
C	-1.534305	1.953090	-3.743338
H	-1.300310	3.020658	-3.678775
H	-1.231464	1.563252	-4.723452
H	-2.610807	1.811488	-3.617631
O	0.260881	0.849490	0.768813
C	1.921715	0.400153	1.728059
H	1.622189	-0.633204	1.684102
H	2.523184	0.788251	0.923104
C	1.696699	1.173216	2.945599
C	2.249260	2.449314	3.089645
C	0.824200	0.689608	3.926782
C	1.923403	3.234362	4.189340
H	2.955091	2.808638	2.347086
C	0.495572	1.475419	5.022832
H	0.392329	-0.301160	3.814362
C	1.040169	2.752946	5.153317
H	2.362324	4.221724	4.297098
H	-0.187577	1.095163	5.776199
H	0.782806	3.368189	6.010406
I	4.399369	-0.817002	2.372835
S-TS-C8			
C	-2.963037	1.526225	-2.271930
C	-4.083913	0.853080	-1.696444

C	-3.122479	2.121183	-3.498693
C	-4.044573	0.143668	-0.471140
C	-5.298047	0.869357	-2.446917
C	-4.380096	2.095450	-4.140336
H	-2.277926	2.590247	-3.994500
C	-5.153185	-0.543846	-0.022632
H	-3.139950	0.064987	0.124642
C	-6.422738	0.172462	-1.942963
H	-4.502879	2.583882	-5.105467
C	-6.360758	-0.525441	-0.766169
H	-7.332602	0.199699	-2.533384
H	-7.234173	-1.061837	-0.413709
C	-0.478923	2.901606	1.141564
C	-1.944518	4.779125	0.467646
C	-1.343401	4.053357	1.688688
H	-1.028605	1.959008	1.133955
H	0.420795	2.758906	1.738873
H	-0.704719	4.761227	2.232127
C	-1.267037	3.023800	-1.210283
H	-0.965883	3.545105	-2.124301
C	-2.454435	3.738838	-0.533137
H	-3.063309	4.207441	-1.309952
H	-3.098374	3.004866	-0.036250
H	-2.751685	5.446562	0.779453
C	-0.814027	5.564287	-0.203684
H	-1.145690	5.950779	-1.172906
H	-0.515134	6.423233	0.404408
C	0.388182	4.622840	-0.376095
H	0.883596	4.741320	-1.339154
H	1.132997	4.767551	0.408295
N	-5.438487	1.503299	-3.643943
N	-0.049882	3.182399	-0.276869
O	-5.013709	-1.204886	1.149007
C	-6.027663	-2.098585	1.555941
H	-6.208626	-2.865315	0.793893
H	-5.645968	-2.583593	2.453671
H	-6.963182	-1.572494	1.787345
O	-0.636661	1.101110	-2.533209
H	-0.215096	0.313723	-2.101487
C	-2.372663	3.527879	2.647924
H	-3.123584	2.859023	2.230835
C	-2.408060	3.827131	3.943585
H	-1.671460	4.485877	4.398725
H	-3.178399	3.429444	4.597370

C	1.094587	2.255303	-0.665734
H	0.719251	1.236756	-0.560850
H	1.299555	2.436344	-1.720754
C	2.325985	2.372450	0.183410
C	3.343644	3.278931	-0.095619
C	2.554830	1.428880	1.188820
C	4.525351	3.294548	0.630631
C	3.730233	1.420043	1.927474
H	1.809067	0.658597	1.360263
C	4.707382	2.359568	1.644005
H	3.908098	0.669616	2.689032
F	3.217211	4.160709	-1.097569
F	5.478635	4.177190	0.340259
F	5.852260	2.381237	2.323888
C	-1.587757	1.568989	-1.617970
H	-1.589359	0.946726	-0.715349
C	-2.340860	-3.248625	2.381879
C	-1.951349	-2.968153	1.066035
C	-2.543080	-3.707385	0.021779
C	-3.533259	-4.640753	0.309360
C	-3.931399	-4.891860	1.621254
C	-3.317134	-4.200378	2.660064
H	-1.850531	-2.734436	3.203354
H	-3.980356	-5.201458	-0.508679
H	-4.695751	-5.635441	1.827979
H	-3.587442	-4.406221	3.692409
C	-1.993032	-3.552160	-1.374536
H	-1.134984	-4.233727	-1.477731
H	-2.733374	-3.862516	-2.119329
C	-1.519807	-2.130321	-1.650031
H	-0.956738	-2.088832	-2.588103
H	-2.382752	-1.461059	-1.778454
C	-0.663938	-1.590114	-0.523036
C	-0.909738	-1.970291	0.759062
C	-0.174232	-1.328939	1.884091
C	1.087599	-1.829317	2.342932
C	-0.716817	-0.241012	2.534201
C	1.696476	-2.967913	1.750871
C	1.765209	-1.180527	3.415554
C	-0.052940	0.405535	3.605419
C	2.938265	-3.395335	2.148216
H	1.168815	-3.499521	0.964986
C	3.038628	-1.660089	3.822908
C	1.161520	-0.055161	4.035054

H	-0.514060	1.278350	4.059743
C	3.621317	-2.730236	3.193008
H	3.396060	-4.241709	1.646351
H	3.545031	-1.160561	4.646399
H	1.681896	0.443445	4.849041
H	4.601875	-3.079490	3.501877
O	-1.918340	0.279039	2.097628
C	-2.985946	0.187527	3.031355
H	-3.202382	-0.859079	3.260930
H	-2.759575	0.741243	3.950652
H	-3.860123	0.620615	2.544294
O	0.283315	-0.718582	-0.857177
C	1.843080	-1.773820	-1.488748
H	1.215664	-2.282508	-2.201414
H	1.945925	-2.182077	-0.500474
C	2.731749	-0.693272	-1.923478
C	2.431390	0.050789	-3.068275
C	3.876953	-0.376306	-1.183144
C	3.252820	1.104152	-3.458347
H	1.548357	-0.193963	-3.651730
C	4.713057	0.653211	-1.591080
H	4.124483	-0.975924	-0.312194
C	4.397792	1.404527	-2.723501
H	3.009751	1.675573	-4.349438
H	5.616304	0.869610	-1.028533
H	5.050348	2.213866	-3.037875
I	3.477629	-4.046356	-1.963307

S-TS-C9

C	-3.376496	-0.880917	2.255882
C	-4.560741	-0.478500	1.564497
C	-3.462339	-1.084264	3.609559
C	-4.613319	-0.217237	0.174748
C	-5.756968	-0.366048	2.328778
C	-4.701360	-0.924618	4.271996
H	-2.572335	-1.342606	4.172475
C	-5.805441	0.089380	-0.443638
H	-3.717122	-0.258319	-0.434868
C	-6.959849	-0.017251	1.667596
H	-4.760073	-1.090353	5.346262
C	-6.997803	0.197817	0.314434
H	-7.856812	0.062016	2.272746
H	-7.938417	0.448200	-0.162157
C	-1.137403	-2.529223	-1.189858



C	-2.816071	-4.235244	-0.517868
C	-2.204937	-3.500559	-1.730850
H	-1.504458	-1.501225	-1.152277
H	-0.236447	-2.536036	-1.803906
H	-1.720226	-4.249842	-2.369255
C	-1.890090	-2.594944	1.176250
H	-1.609181	-3.115374	2.097650
C	-3.167435	-3.219091	0.567677
H	-3.739155	-3.690657	1.371779
H	-3.811005	-2.448427	0.145581
H	-3.709538	-4.784311	-0.825966
C	-1.760332	-5.184131	0.048040
H	-2.113172	-5.615954	0.990060
H	-1.563629	-6.013152	-0.638195
C	-0.466861	-4.387682	0.269026
H	-0.001728	-4.589929	1.233023
H	0.271113	-4.587779	-0.509190
N	-5.816525	-0.589187	3.671322
N	-0.729285	-2.901473	0.211287
O	-5.756166	0.262845	-1.791427
C	-6.930517	0.657591	-2.469329
H	-7.316039	1.610016	-2.085698
H	-6.644348	0.781648	-3.514131
H	-7.712125	-0.108764	-2.398313
O	-1.001434	-0.758036	2.460538
H	-0.538719	0.027960	2.064003
C	-3.205708	-2.752728	-2.570049
H	-3.751463	-1.943159	-2.085977
C	-3.437816	-3.012467	-3.853944
H	-2.908247	-3.801131	-4.384596
H	-4.168305	-2.444572	-4.421713
C	0.535361	-2.140692	0.590851
H	0.309736	-1.088063	0.412931
H	0.662773	-2.293178	1.662107
C	1.771029	-2.508755	-0.176234
C	2.632152	-3.512801	0.260657
C	2.181381	-1.729328	-1.260058
C	3.825608	-3.783739	-0.388817
C	3.376049	-1.973842	-1.921541
H	1.564823	-0.890369	-1.562530
C	4.188618	-3.004104	-1.481410
H	3.707701	-1.341290	-2.736100
F	2.317945	-4.253547	1.334116
F	4.614771	-4.763102	0.039671

F	5.340237	-3.269439	-2.090469
C	-2.027133	-1.096275	1.571101
H	-1.967665	-0.468580	0.670959
C	-0.553730	4.382982	-2.440110
C	-0.440996	3.971392	-1.104656
C	-0.705601	4.913180	-0.089880
C	-1.098904	6.203583	-0.429391
C	-1.224161	6.595550	-1.760558
C	-0.940695	5.678583	-2.766571
H	-0.331193	3.678118	-3.236220
H	-1.302892	6.917831	0.365528
H	-1.530551	7.608261	-2.005445
H	-1.020731	5.967539	-3.810807
C	-0.471974	4.516457	1.346069
H	0.583424	4.700366	1.588704
H	-1.064400	5.144396	2.020419
C	-0.765596	3.040533	1.595613
H	-0.392167	2.739449	2.577549
H	-1.853170	2.860994	1.595172
C	-0.152952	2.150511	0.535915
C	-0.054613	2.591204	-0.747147
C	0.318923	1.654517	-1.842377
C	1.614923	1.708211	-2.450129
C	-0.600095	0.755843	-2.351744
C	2.618262	2.585727	-1.958731
C	1.931694	0.866776	-3.553892
C	-0.289348	-0.084490	-3.449701
C	3.872007	2.605209	-2.512037
H	2.369115	3.236500	-1.126916
C	3.232262	0.926751	-4.121663
C	0.944246	-0.028789	-4.039886
H	-1.062846	-0.758861	-3.807034
C	4.185024	1.767925	-3.607952
H	4.632170	3.266160	-2.108125
H	3.462121	0.283803	-4.968440
H	1.180705	-0.670760	-4.884583
H	5.180587	1.795132	-4.039568
O	-1.866765	0.602817	-1.835426
C	-2.735752	1.734508	-1.920084
H	-2.738685	2.292076	-0.979663
H	-2.418891	2.403256	-2.724510
H	-3.735486	1.350879	-2.129843
O	0.213849	0.934611	0.908691
C	2.125117	0.745787	1.361226

H	2.410823	0.909417	0.333647
H	1.911133	-0.258910	1.679627
C	2.277460	1.794016	2.364918
C	2.813717	3.038094	2.021545
C	1.819922	1.580243	3.670495
C	2.892933	4.052501	2.968570
H	3.205310	3.187725	1.020252
C	1.889110	2.597012	4.612495
H	1.403116	0.612470	3.936035
C	2.423780	3.837162	4.262345
H	3.324848	5.011281	2.698058
H	1.531397	2.424245	5.622997
H	2.484400	4.630001	5.001858
I	4.770281	-0.327068	1.505630

S-TS-C10

C	3.442430	0.606898	-0.401461
C	4.624438	0.180702	-1.083080
C	3.412656	1.881359	0.105248
C	4.754608	-1.072061	-1.723525
C	5.725497	1.083285	-1.097540
C	4.554588	2.713034	-0.006309
H	2.514840	2.257196	0.588300
C	5.944209	-1.443311	-2.313632
H	3.903018	-1.734414	-1.823261
C	6.933111	0.672473	-1.709863
H	4.518602	3.724461	0.395024
C	7.053982	-0.561343	-2.297176
H	7.760545	1.374316	-1.703935
H	7.993334	-0.842096	-2.759341
C	1.016609	-1.364881	2.578107
C	3.292566	-2.293510	2.878012
C	2.067583	-1.745411	3.639421
H	1.071891	-0.303446	2.332463
H	0.004932	-1.584543	2.916693
H	1.669123	-2.543271	4.278801
C	2.510753	-1.550477	0.605079
H	2.795679	-2.336852	-0.097026
C	3.588577	-1.375225	1.689029
H	4.559453	-1.604638	1.241683
H	3.632431	-0.328384	2.005579
H	4.156723	-2.358186	3.543928
C	2.917577	-3.674761	2.332641
H	3.683599	-4.024705	1.633258

H	2.849091	-4.411770	3.138104
C	1.555512	-3.562887	1.629879
H	1.516445	-4.122050	0.695400
H	0.736710	-3.906164	2.264445
N	5.680956	2.335960	-0.556828
N	1.254207	-2.122851	1.295986
O	5.966547	-2.668055	-2.897553
C	7.137580	-3.072823	-3.571796
H	7.991557	-3.153245	-2.886752
H	6.919207	-4.057383	-3.986854
H	7.391617	-2.386691	-4.389375
O	1.704998	-0.668185	-1.478590
H	0.824435	-0.229845	-1.554517
C	2.380379	-0.562359	4.511008
H	2.872212	0.277465	4.022799
C	2.091486	-0.486381	5.807390
H	1.594250	-1.299917	6.331252
H	2.346203	0.390801	6.394743
C	0.032541	-2.037455	0.393205
H	-0.106099	-0.986314	0.139907
H	0.279979	-2.576829	-0.523161
C	-1.256828	-2.512419	0.997520
C	-1.669933	-3.838748	0.929583
C	-2.178998	-1.568404	1.460542
C	-2.939031	-4.229095	1.331207
C	-3.455785	-1.931836	1.868042
H	-1.901021	-0.519089	1.448953
C	-3.826177	-3.265754	1.801236
H	-4.172175	-1.188168	2.198651
F	-0.856990	-4.781417	0.431732
F	-3.304339	-5.505739	1.244904
F	-5.040068	-3.657647	2.177481
C	2.220388	-0.281072	-0.231906
H	1.490014	0.329426	0.312545
C	-0.054996	4.939446	1.335190
C	-0.025471	4.151489	0.177017
C	0.450531	4.737208	-1.014135
C	0.951408	6.034205	-0.996539
C	0.964300	6.789168	0.174722
C	0.437745	6.241122	1.338707
H	-0.487362	4.532929	2.244572
H	1.325944	6.466365	-1.921815
H	1.361733	7.799686	0.169403
H	0.403553	6.825593	2.254051

C	0.302809	3.968986	-2.303241
H	-0.714992	4.140652	-2.684901
H	0.992314	4.350678	-3.063621
C	0.499831	2.471437	-2.104594
H	0.172320	1.923925	-2.994992
H	1.565781	2.233730	-1.974596
C	-0.245882	1.942480	-0.897737
C	-0.482274	2.747561	0.172578
C	-1.114080	2.194187	1.402481
C	-2.537746	2.068386	1.519138
C	-0.340032	1.814812	2.478895
C	-3.405187	2.408890	0.447474
C	-3.113481	1.566270	2.722319
C	-0.903717	1.308353	3.675159
C	-4.760821	2.224109	0.546467
H	-2.976109	2.799351	-0.469215
C	-4.523011	1.413594	2.807559
C	-2.261732	1.194114	3.794342
H	-0.243739	0.989627	4.477436
C	-5.327861	1.722381	1.740646
H	-5.393821	2.444257	-0.306677
H	-4.951647	1.035650	3.733241
H	-2.701656	0.798001	4.705962
H	-6.402411	1.583396	1.808120
O	1.037413	1.839843	2.357103
C	1.739010	2.682013	3.257775
H	1.494089	3.732832	3.076517
H	1.529080	2.426215	4.303478
H	2.801516	2.524444	3.055256
O	-0.560725	0.653508	-0.924670
C	-2.192681	0.302391	-1.974226
H	-2.788976	0.410962	-1.083682
I	-4.749934	0.559997	-3.149805
C	-1.828541	-1.031791	-2.468297
C	-0.814246	-1.172075	-3.420284
C	-2.428126	-2.181106	-1.942922
C	-0.383659	-2.432456	-3.816389
H	-0.348335	-0.284636	-3.839092
C	-2.008808	-3.441990	-2.348671
H	-3.247930	-2.075137	-1.238631
C	-0.977031	-3.571960	-3.277687
H	0.413356	-2.523982	-4.547637
H	-2.490530	-4.327259	-1.943837
H	-0.648861	-4.558396	-3.592362

H	-2.012302	1.177590	-2.576686
S-TS-C11			
C	-3.447310	-0.957423	2.124748
C	-4.612395	-0.523592	1.419455
C	-3.564128	-1.198519	3.469744
C	-4.630698	-0.214436	0.039603
C	-5.821902	-0.411812	2.163475
C	-4.815810	-1.046008	4.110037
H	-2.688871	-1.479755	4.044764
C	-5.798586	0.159126	-0.588222
H	-3.728094	-0.271911	-0.556583
C	-7.001883	-0.010489	1.491972
H	-4.899568	-1.243473	5.177299
C	-7.003741	0.265429	0.149111
H	-7.909874	0.066543	2.080739
H	-7.926866	0.564045	-0.333830
C	-1.191693	-2.628204	-1.317396
C	-2.826655	-4.355771	-0.589525
C	-2.205706	-3.666763	-1.827872
H	-1.592039	-1.613029	-1.288551
H	-0.286746	-2.609976	-1.925929
H	-1.659921	-4.436786	-2.391543
C	-1.947290	-2.654949	1.050252
H	-1.680178	-3.185765	1.969948
C	-3.212078	-3.272286	0.416260
H	-3.838021	-3.675660	1.216558
H	-3.803746	-2.511068	-0.095696
H	-3.708155	-4.933549	-0.881044
C	-1.769333	-5.257219	0.043758
H	-2.117116	-5.623286	1.015206
H	-1.566323	-6.132260	-0.580858
C	-0.483721	-4.436674	0.199880
H	0.006859	-4.595873	1.158831
H	0.238551	-4.654942	-0.588322
N	-5.913274	-0.676974	3.496876
N	-0.774137	-2.957368	0.095765
O	-5.712988	0.407880	-1.922398
C	-6.866844	0.845179	-2.607924
H	-7.250227	1.786186	-2.194818
H	-6.556248	1.008076	-3.640502
H	-7.659076	0.086786	-2.585724
O	-1.075546	-0.851337	2.382975
H	-0.591564	-0.065178	2.011633

C	-3.268966	-3.123289	-2.747993
H	-3.893274	-3.905711	-3.180529
C	-3.536733	-1.856189	-3.054504
H	-2.970059	-1.007577	-2.681223
H	-4.362979	-1.619997	-3.717519
C	0.475632	-2.168948	0.467719
H	0.238627	-1.119735	0.280431
H	0.596621	-2.307277	1.541544
C	1.723732	-2.528786	-0.284050
C	2.593585	-3.520718	0.164424
C	2.138801	-1.746572	-1.363908
C	3.793595	-3.783529	-0.476339
C	3.341204	-1.980530	-2.015097
H	1.517462	-0.914327	-1.672747
C	4.158817	-3.003723	-1.567884
H	3.674594	-1.344933	-2.826530
F	2.285080	-4.257149	1.242294
F	4.588936	-4.752644	-0.037173
F	5.317520	-3.259762	-2.166911
C	-2.084570	-1.164068	1.464765
H	-2.002139	-0.519818	0.578144
C	-0.431683	4.524152	-2.234233
C	-0.368615	4.028411	-0.924513
C	-0.675713	4.902612	0.138160
C	-1.055852	6.212699	-0.133074
C	-1.127475	6.690171	-1.440073
C	-0.805531	5.839133	-2.491436
H	-0.180276	3.869737	-3.064324
H	-1.294221	6.873843	0.697458
H	-1.423418	7.717348	-1.631420
H	-0.845058	6.195889	-3.516903
C	-0.509024	4.410644	1.554514
H	0.534077	4.571847	1.858273
H	-1.131203	4.996282	2.240042
C	-0.818938	2.923517	1.689282
H	-0.498821	2.554234	2.666656
H	-1.905407	2.750635	1.618802
C	-0.153135	2.105463	0.604802
C	0.005046	2.628236	-0.640927
C	0.411735	1.753511	-1.774873
C	1.717974	1.841630	-2.354787
C	-0.490851	0.871747	-2.340275
C	2.705127	2.705530	-1.809439
C	2.061008	1.050011	-3.487355

C	-0.157054	0.086375	-3.471102
C	3.969007	2.755061	-2.336991
H	2.435170	3.321750	-0.958193
C	3.372626	1.139095	-4.025192
C	1.087063	0.176407	-4.035053
H	-0.914724	-0.575581	-3.880364
C	4.309508	1.963223	-3.458425
H	4.716479	3.404318	-1.892481
H	3.622849	0.533994	-4.893851
H	1.341736	-0.423571	-4.904959
H	5.313504	2.012929	-3.867916
O	-1.765204	0.691994	-1.848930
C	-2.639985	1.823113	-1.895418
H	-2.664930	2.330626	-0.927949
H	-2.309405	2.532533	-2.658455
H	-3.633776	1.446207	-2.144808
O	0.198504	0.868520	0.914569
C	2.104464	0.650475	1.372364
H	2.397160	0.853351	0.353942
H	1.884083	-0.365232	1.648796
C	2.252843	1.660039	2.416271
C	2.813524	2.907177	2.127427
C	1.766338	1.408624	3.704396
C	2.889729	3.886851	3.110309
H	3.228411	3.083778	1.140381
C	1.831125	2.391690	4.682162
H	1.327800	0.439712	3.927463
C	2.391366	3.634542	4.386457
H	3.341302	4.847461	2.881769
H	1.449152	2.190433	5.678424
H	2.448294	4.400915	5.153612
I	4.746600	-0.429236	1.476149

S-TS-C12

C	-1.506439	3.146740	-0.593991
C	-2.900112	3.125822	-0.286293
C	-1.047223	4.118045	-1.448661
C	-3.500414	2.197569	0.593773
C	-3.723800	4.098325	-0.927340
C	-1.948771	5.054868	-2.001534
H	0.000571	4.159088	-1.733477
C	-4.856460	2.216716	0.833422
H	-2.926982	1.437607	1.106992
C	-5.121112	4.071969	-0.687983



H	-1.577418	5.825101	-2.675621
C	-5.682492	3.155844	0.161829
H	-5.728947	4.809186	-1.202129
H	-6.753883	3.157160	0.329757
C	0.967821	0.631053	2.154569
C	0.175787	2.645704	3.388893
C	0.018024	1.119170	3.268794
H	0.490879	-0.018935	1.415245
H	1.820101	0.096760	2.572053
H	0.385657	0.685117	4.208812
C	0.476139	2.733869	0.869304
H	1.027500	3.504075	0.324302
C	-0.262556	3.333678	2.093839
H	-0.073571	4.409563	2.157489
H	-1.340296	3.213174	1.959854
H	-0.428487	3.012927	4.223538
C	1.652399	2.957646	3.624456
H	1.793322	4.019418	3.846103
H	2.032203	2.388601	4.478746
C	2.431982	2.588917	2.354314
H	2.771299	3.469620	1.805733
H	3.299624	1.965690	2.571926
N	-3.238883	5.052306	-1.768718
N	1.569188	1.798263	1.397071
O	-5.318336	1.339393	1.745384
C	-6.655637	0.883579	1.622088
H	-6.874346	0.596925	0.588730
H	-6.724563	-0.005124	2.248600
H	-7.369329	1.641180	1.971816
O	0.052058	1.478759	-1.213849
H	-0.037463	0.489859	-1.091332
C	-1.422782	0.684570	3.112486
H	-2.161535	1.359292	3.546637
C	-1.840012	-0.451558	2.558412
H	-1.153785	-1.174235	2.123355
H	-2.896857	-0.700434	2.498533
C	2.476345	1.203788	0.325610
H	3.141153	0.536698	0.873218
H	1.842857	0.602279	-0.314428
C	3.268528	2.193461	-0.482789
C	4.575081	2.512327	-0.114584
C	2.777592	2.744578	-1.672076
C	5.361294	3.374534	-0.866690
C	3.547720	3.609437	-2.440535

H	1.775940	2.467534	-1.985307
C	4.834332	3.922533	-2.030748
H	3.169615	4.036710	-3.362123
F	5.119886	1.983755	0.990772
F	6.600094	3.662523	-0.479111
F	5.596055	4.748066	-2.743361
C	-0.541156	2.077168	-0.094954
H	-1.091704	1.325602	0.477625
C	3.246800	-4.584008	-0.590363
C	2.696418	-3.411616	-1.122408
C	3.218949	-2.909610	-2.331198
C	4.243778	-3.591511	-2.977822
C	4.774214	-4.765322	-2.445849
C	4.273777	-5.256730	-1.244678
H	2.866669	-4.968209	0.352366
H	4.637249	-3.193835	-3.910822
H	5.574044	-5.286301	-2.963638
H	4.681965	-6.166009	-0.812908
C	2.672112	-1.603564	-2.852024
H	3.195523	-0.771707	-2.351286
H	2.871603	-1.499307	-3.923757
C	1.178181	-1.487680	-2.568427
H	0.798899	-0.501771	-2.853283
H	0.620681	-2.214324	-3.174929
C	0.887544	-1.743193	-1.100659
C	1.614004	-2.683146	-0.432519
C	1.335810	-2.948166	1.005216
C	2.231062	-2.432408	2.002237
C	0.186591	-3.585831	1.435713
C	3.467306	-1.823033	1.650560
C	1.874737	-2.466547	3.380273
C	-0.156873	-3.641371	2.812820
C	4.274619	-1.243197	2.599540
H	3.769451	-1.818692	0.608505
C	2.724994	-1.855479	4.338725
C	0.650892	-3.080039	3.757857
H	-1.093295	-4.123259	3.073132
C	3.894726	-1.243136	3.962113
H	5.211901	-0.782435	2.300357
H	2.430923	-1.883887	5.385344
H	0.370642	-3.105845	4.807414
H	4.539180	-0.783327	4.705529
O	-0.745708	-4.151364	0.620831
C	-0.328811	-4.984058	-0.450294

H	-0.016355	-4.405286	-1.323469
H	0.498370	-5.631783	-0.140114
H	-1.199227	-5.593242	-0.701320
O	-0.058503	-1.009193	-0.523293
C	-1.951406	-1.489294	-0.691688
H	-2.176635	-0.630100	-0.080706
H	-1.790310	-2.435397	-0.197813
C	-2.146234	-1.417616	-2.136903
C	-2.317043	-0.178610	-2.763770
C	-2.086377	-2.578425	-2.915828
C	-2.401111	-0.100339	-4.147563
H	-2.379037	0.723684	-2.162911
C	-2.176821	-2.500123	-4.299415
H	-1.993559	-3.541836	-2.423590
C	-2.326285	-1.259657	-4.917984
H	-2.533056	0.865460	-4.625683
H	-2.139100	-3.406418	-4.896371
H	-2.398895	-1.197488	-5.999891
I	-4.660557	-2.117789	0.082713

S-TS-C13

C	-3.042568	-1.250409	0.309227
C	-4.074491	-1.592074	-0.625734
C	-3.365252	-0.382946	1.319386
C	-3.867547	-2.436298	-1.738232
C	-5.370092	-1.045951	-0.403350
C	-4.692710	0.097132	1.450337
H	-2.630331	-0.050600	2.043363
C	-4.904589	-2.740131	-2.595004
H	-2.882562	-2.820480	-1.973284
C	-6.413382	-1.374955	-1.299870
H	-4.936024	0.769517	2.271836
C	-6.196850	-2.202317	-2.371944
H	-7.390919	-0.943894	-1.111360
H	-7.016290	-2.431484	-3.043319
C	0.557842	-3.799112	0.933762
C	-0.671202	-3.642221	3.096588
C	-0.314972	-4.587469	1.933333
H	0.205870	-3.858441	-0.094868
H	1.589298	-4.150591	0.950338
H	0.308894	-5.387663	2.355063
C	-0.808032	-1.753766	1.401991
H	-0.628074	-0.696577	1.615473
C	-1.509504	-2.472211	2.584079

H	-1.682671	-1.760660	3.396759
H	-2.487677	-2.832614	2.256480
H	-1.230725	-4.194045	3.858084
C	0.622256	-3.085367	3.682586
H	0.420496	-2.505671	4.586675
H	1.304061	-3.898256	3.954312
C	1.265184	-2.167329	2.636725
H	1.162110	-1.111640	2.890042
H	2.323391	-2.384122	2.503899
N	-5.668265	-0.217490	0.639429
N	0.611255	-2.335713	1.282773
O	-4.602355	-3.559872	-3.631864
C	-5.597810	-3.826667	-4.595308
H	-5.953653	-2.905768	-5.073867
H	-5.124274	-4.460044	-5.346198
H	-6.450761	-4.362838	-4.159668
O	-1.060940	-1.412263	-1.054032
H	-0.823914	-0.452027	-0.916862
C	-1.537339	-5.264541	1.355583
H	-2.242454	-5.605892	2.114063
C	-1.812818	-5.522406	0.080167
H	-1.163370	-5.236093	-0.743556
H	-2.723386	-6.043902	-0.195974
C	1.432363	-1.570521	0.241503
H	0.957988	-1.769400	-0.715528
H	1.280351	-0.508141	0.451325
C	2.892231	-1.913398	0.206386
C	3.364653	-2.932584	-0.614514
C	3.838720	-1.127136	0.868815
C	4.720877	-3.192229	-0.753939
C	5.200652	-1.367711	0.748830
H	3.494605	-0.295085	1.475241
C	5.633137	-2.402090	-0.066947
H	5.934111	-0.754097	1.258853
F	2.514461	-3.693045	-1.313968
F	5.136293	-4.164673	-1.561200
F	6.931594	-2.655522	-0.214809
C	-1.663741	-1.879067	0.117334
H	-1.841030	-2.947546	-0.039337
C	-0.969994	4.467615	2.840874
C	-1.412212	3.646653	1.793812
C	-2.662426	3.923790	1.206426
C	-3.418297	4.997095	1.665592
C	-2.968396	5.806950	2.705771

C	-1.738517	5.535048	3.294284
H	-0.003782	4.275367	3.298738
H	-4.378846	5.200875	1.197688
H	-3.571731	6.642430	3.047975
H	-1.368345	6.157769	4.103766
C	-3.189614	3.005927	0.132777
H	-3.768143	2.208785	0.614328
H	-3.890494	3.541565	-0.515716
C	-2.082553	2.373099	-0.705446
H	-2.477535	1.519576	-1.268262
H	-1.712397	3.097947	-1.446376
C	-0.897418	1.909961	0.113480
C	-0.584593	2.534782	1.281910
C	0.669974	2.181287	1.999096
C	0.623714	1.479068	3.246975
C	1.912762	2.530072	1.497753
C	-0.615753	1.083931	3.825115
C	1.822984	1.143913	3.940273
C	3.105492	2.204423	2.191024
C	-0.660756	0.384941	5.005278
H	-1.532541	1.376656	3.323724
C	1.745091	0.420492	5.160959
C	3.067962	1.527651	3.380133
H	4.045343	2.511403	1.742354
C	0.534181	0.045208	5.684202
H	-1.620003	0.110463	5.435206
H	2.668912	0.176055	5.679792
H	3.986874	1.286049	3.908633
H	0.487276	-0.495597	6.624951
O	2.078052	3.154194	0.297122
C	1.713775	4.531969	0.215588
H	0.669804	4.687335	0.500306
H	2.366356	5.135473	0.858606
H	1.852880	4.811574	-0.830540
O	-0.141692	0.956273	-0.409990
C	0.629039	1.712747	-2.069361
H	-0.320836	1.656598	-2.574092
H	0.882496	2.590823	-1.505608
C	1.669252	0.736198	-2.390182
C	2.991967	0.952843	-1.983808
C	1.356511	-0.410917	-3.128430
C	3.991414	0.065998	-2.361258
H	3.223388	1.844763	-1.410147
C	2.355527	-1.309155	-3.485449

H	0.329187	-0.585398	-3.434847
C	3.677673	-1.060853	-3.120451
H	5.020678	0.256285	-2.072025
H	2.107493	-2.192475	-4.065852
H	4.461011	-1.750083	-3.424055
I	1.106273	3.641452	-4.125366

S-TS-C14

C	-3.278999	-0.353012	0.102933
C	-4.362571	-0.448923	-0.830858
C	-3.365264	0.605705	1.078121
C	-4.376101	-1.345564	-1.921521
C	-5.478170	0.412902	-0.631399
C	-4.525219	1.413445	1.182461
H	-2.567073	0.763210	1.795141
C	-5.458478	-1.402469	-2.774531
H	-3.518167	-1.967611	-2.146532
C	-6.574891	0.328223	-1.520224
H	-4.586310	2.154284	1.978391
C	-6.576718	-0.556284	-2.568019
H	-7.412869	0.994945	-1.345974
H	-7.430502	-0.592227	-3.234799
C	-0.559133	-3.768220	0.800326
C	-1.820934	-3.304479	2.899971
C	-1.714022	-4.267463	1.705215
H	-0.834319	-3.720487	-0.253626
H	0.318186	-4.409777	0.887258
H	-1.401050	-5.243520	2.100738
C	-1.300264	-1.427487	1.270897
H	-0.833982	-0.461828	1.483323
C	-2.206495	-1.898652	2.435912
H	-2.118271	-1.201741	3.274623
H	-3.245396	-1.876843	2.108283
H	-2.554184	-3.677909	3.619897
C	-0.439934	-3.211805	3.548476
H	-0.489675	-2.663861	4.492786
H	-0.044884	-4.210519	3.763651
C	0.488251	-2.456653	2.589843
H	0.650862	-1.422861	2.896090
H	1.457945	-2.942309	2.497221
N	-5.553314	1.325552	0.380218
N	-0.104692	-2.391767	1.198958
O	-5.371394	-2.295433	-3.791013
C	-6.405722	-2.331967	-4.749824

H	-6.529690	-1.361954	-5.247189
H	-6.102102	-3.075741	-5.487113
H	-7.361069	-2.637256	-4.303834
O	-1.358002	-1.038151	-1.185619
H	-0.878809	-0.178006	-1.026232
C	-2.984759	-4.513435	0.923787
H	-2.833426	-4.958165	-0.060654
C	-4.231170	-4.292801	1.332685
H	-4.465278	-3.863771	2.303176
H	-5.076251	-4.539357	0.698150
C	0.957377	-1.876389	0.225181
H	0.494086	-1.900831	-0.757893
H	1.117064	-0.823432	0.471902
C	2.248875	-2.639824	0.235294
C	2.435614	-3.735036	-0.602546
C	3.354358	-2.187184	0.960662
C	3.658982	-4.382996	-0.700747
C	4.588221	-2.818876	0.882325
H	3.245781	-1.303257	1.581204
C	4.732103	-3.915791	0.046638
H	5.446682	-2.462673	1.439773
F	1.432700	-4.192948	-1.360219
F	3.804028	-5.416728	-1.525448
F	5.902553	-4.540282	-0.062180
C	-2.111130	-1.326167	-0.043481
H	-2.564098	-2.308339	-0.216690
C	0.215144	4.456998	2.956007
C	-0.386210	3.846814	1.845625
C	-1.475334	4.497379	1.232944
C	-1.924782	5.714346	1.735080
C	-1.322086	6.308618	2.841213
C	-0.247350	5.671776	3.451355
H	1.065397	3.978782	3.433757
H	-2.764869	6.204988	1.248344
H	-1.687566	7.259234	3.217970
H	0.239853	6.121200	4.311964
C	-2.180686	3.827870	0.080705
H	-3.000198	3.220115	0.481699
H	-2.648496	4.577682	-0.565712
C	-1.260780	2.932589	-0.744429
H	-1.854428	2.261303	-1.375104
H	-0.649974	3.547300	-1.423071
C	-0.311141	2.104429	0.093452
C	0.116004	2.567229	1.302027

C	1.200138	1.857304	2.033617
C	0.932767	1.168207	3.261082
C	2.505873	1.873103	1.572601
C	-0.380336	1.115947	3.808326
C	1.979379	0.507872	3.968664
C	3.548433	1.223591	2.279285
C	-0.640930	0.436391	4.971971
H	-1.172326	1.654908	3.298174
C	1.678252	-0.192231	5.167909
C	3.296920	0.554609	3.446438
H	4.548298	1.278847	1.859685
C	0.399245	-0.232056	5.661118
H	-1.648169	0.426802	5.379113
H	2.487967	-0.690668	5.695463
H	4.101782	0.062755	3.987215
H	0.184948	-0.758172	6.586781
O	2.863835	2.468288	0.399511
C	2.922108	3.894601	0.384234
H	1.968243	4.334472	0.688434
H	3.720545	4.247717	1.048564
H	3.141719	4.169431	-0.649314
O	0.153009	0.989597	-0.449200
C	1.195458	1.533106	-2.041008
H	0.300248	1.768482	-2.592466
H	1.660239	2.285210	-1.431884
C	1.927419	0.305354	-2.351029
C	3.228276	0.117233	-1.866405
C	1.343072	-0.683755	-3.149992
C	3.949343	-1.013710	-2.224767
H	3.671425	0.889780	-1.246054
C	2.059586	-1.825989	-3.489203
H	0.331703	-0.543572	-3.520562
C	3.370783	-1.983200	-3.043586
H	4.967903	-1.140332	-1.869728
H	1.603789	-2.583800	-4.118865
H	3.938138	-2.864391	-3.331035
I	2.340931	3.296286	-3.983063

S-TS-C15

C	2.259955	-1.035399	1.553260
C	3.322746	-1.993900	1.554248
C	2.094037	-0.253503	2.666824
C	3.521903	-2.954556	0.534630
C	4.211059	-1.974582	2.667967



C	3.020269	-0.345728	3.732417
H	1.265614	0.444503	2.719629
C	4.588138	-3.828348	0.586768
H	2.802513	-3.097520	-0.266466
C	5.301601	-2.876408	2.685270
H	2.892782	0.291666	4.606237
C	5.499913	-3.778103	1.671394
H	5.970064	-2.836886	3.539077
H	6.341347	-4.460017	1.717908
C	1.160450	1.604292	-1.907028
C	1.791883	-0.243983	-3.426670
C	1.033070	1.097544	-3.356526
H	0.291041	1.357209	-1.299725
H	1.301793	2.683984	-1.878256
H	1.521233	1.806547	-4.038196
C	2.107776	-0.516488	-0.955258
H	3.115705	-0.929706	-0.875479
C	1.410872	-1.078537	-2.200595
H	1.687970	-2.131438	-2.309077
H	0.328914	-1.049554	-2.051083
H	1.549859	-0.770637	-4.352607
C	3.290542	0.072529	-3.352755
H	3.865113	-0.848727	-3.215107
H	3.639763	0.541885	-4.277123
C	3.526325	1.038504	-2.177888
H	4.425160	0.797103	-1.610088
H	3.598117	2.076943	-2.509219
N	4.059954	-1.142276	3.737831
N	2.358836	0.980734	-1.221191
O	4.694912	-4.702585	-0.440952
C	5.632638	-5.751609	-0.343409
H	5.479766	-6.343070	0.567520
H	5.461737	-6.384437	-1.214764
H	6.664768	-5.377462	-0.367144
O	0.333860	0.031541	0.671691
H	-0.481487	-0.053102	0.108318
C	-0.418364	0.999929	-3.736361
H	-1.035086	0.370736	-3.095495
C	-0.962454	1.647773	-4.762944
H	-0.378560	2.303753	-5.405877
H	-2.016549	1.539984	-5.001682
C	2.671631	1.711595	0.069024
H	1.751836	1.655252	0.650338
H	3.442452	1.123933	0.569381

C	3.107546	3.141651	-0.090225
C	4.457975	3.466618	-0.199708
C	2.186368	4.193498	-0.034083
C	4.889859	4.783058	-0.288860
C	2.596390	5.518939	-0.121469
H	1.131592	3.958409	0.090366
C	3.946625	5.804164	-0.251399
H	1.885736	6.336082	-0.078276
F	5.386667	2.502373	-0.220195
F	6.184915	5.058765	-0.401438
F	4.372300	7.061616	-0.337517
C	1.338639	-0.881716	0.353673
H	0.930756	-1.883364	0.137385
C	-4.977302	3.118288	0.577492
C	-4.633441	1.999077	-0.193536
C	-5.563046	1.530942	-1.144692
C	-6.777065	2.187758	-1.310693
C	-7.102980	3.304865	-0.544043
C	-6.196973	3.765220	0.405240
H	-4.280295	3.479428	1.328865
H	-7.482467	1.814488	-2.050095
H	-8.056337	3.805284	-0.685521
H	-6.437476	4.630265	1.016984
C	-5.212877	0.290348	-1.924668
H	-5.457926	-0.596471	-1.322237
H	-5.807000	0.228113	-2.842971
C	-3.722991	0.262992	-2.238108
H	-3.440207	-0.679137	-2.715241
H	-3.471852	1.070527	-2.945167
C	-2.890868	0.454657	-0.985511
C	-3.341030	1.305652	-0.018446
C	-2.530701	1.599709	1.195934
C	-2.959181	1.076089	2.467129
C	-1.380209	2.363475	1.174431
C	-4.168814	0.341536	2.593352
C	-2.178595	1.277802	3.637725
C	-0.606988	2.575711	2.345586
C	-4.565052	-0.170499	3.803624
H	-4.780495	0.185031	1.712458
C	-2.607518	0.729741	4.873223
C	-0.983499	2.037518	3.540219
H	0.290880	3.181352	2.261292
C	-3.775897	0.017824	4.959736
H	-5.499644	-0.720045	3.875642

H	-1.991311	0.887812	5.754915
H	-0.385439	2.203165	4.432774
H	-4.097349	-0.397935	5.909779
O	-0.827320	2.948681	0.062421
C	-1.642496	3.524231	-0.948072
H	-1.861056	2.805316	-1.742198
H	-2.581406	3.904710	-0.536628
H	-1.063047	4.355831	-1.362029
O	-1.733534	-0.172511	-0.962046
C	-1.751280	-2.221401	-0.823452
H	-1.340827	-2.259648	-1.815860
H	-1.107081	-2.039051	0.015673
C	-3.127914	-2.602243	-0.582592
C	-3.700885	-2.362538	0.671341
C	-3.911426	-3.157944	-1.604122
C	-5.035805	-2.672780	0.901289
H	-3.098594	-1.922143	1.460035
C	-5.241107	-3.474150	-1.370468
H	-3.457144	-3.362982	-2.569329
C	-5.805371	-3.230881	-0.116359
H	-5.471339	-2.480854	1.876900
H	-5.840439	-3.915386	-2.160643
H	-6.847341	-3.477342	0.064771
I	-0.173869	-4.637109	-0.806167

S-TS-C16

C	-3.376496	-0.880917	2.255882
C	-4.560741	-0.478500	1.564497
C	-3.462339	-1.084264	3.609559
C	-4.613319	-0.217237	0.174748
C	-5.756968	-0.366048	2.328778
C	-4.701360	-0.924618	4.271996
H	-2.572335	-1.342606	4.172475
C	-5.805441	0.089380	-0.443638
H	-3.717122	-0.258319	-0.434868
C	-6.959849	-0.017251	1.667596
H	-4.760073	-1.090353	5.346262
C	-6.997803	0.197817	0.314434
H	-7.856812	0.062016	2.272746
H	-7.938417	0.448200	-0.162157
C	-1.137403	-2.529223	-1.189858
C	-2.816071	-4.235244	-0.517868
C	-2.204937	-3.500559	-1.730850
H	-1.504458	-1.501225	-1.152277

H	-0.236447	-2.536036	-1.803906
H	-1.720226	-4.249842	-2.369255
C	-1.890090	-2.594944	1.176250
H	-1.609181	-3.115374	2.097650
C	-3.167435	-3.219091	0.567677
H	-3.739155	-3.690657	1.371779
H	-3.811005	-2.448427	0.145581
H	-3.709538	-4.784311	-0.825966
C	-1.760332	-5.184131	0.048040
H	-2.113172	-5.615954	0.990060
H	-1.563629	-6.013152	-0.638195
C	-0.466861	-4.387682	0.269026
H	-0.001728	-4.589929	1.233023
H	0.271113	-4.587779	-0.509190
N	-5.816525	-0.589187	3.671322
N	-0.729285	-2.901473	0.211287
O	-5.756166	0.262845	-1.791427
C	-6.930517	0.657591	-2.469329
H	-7.316039	1.610016	-2.085698
H	-6.644348	0.781648	-3.514131
H	-7.712125	-0.108764	-2.398313
O	-1.001434	-0.758036	2.460538
H	-0.538719	0.027960	2.064003
C	-3.205708	-2.752728	-2.570049
H	-3.751463	-1.943159	-2.085977
C	-3.437816	-3.012467	-3.853944
H	-2.908247	-3.801131	-4.384596
H	-4.168305	-2.444572	-4.421713
C	0.535361	-2.140692	0.590851
H	0.309736	-1.088063	0.412931
H	0.662773	-2.293178	1.662107
C	1.771029	-2.508755	-0.176234
C	2.632152	-3.512801	0.260657
C	2.181381	-1.729328	-1.260058
C	3.825608	-3.783739	-0.388817
C	3.376049	-1.973842	-1.921541
H	1.564823	-0.890369	-1.562530
C	4.188618	-3.004104	-1.481410
H	3.707701	-1.341290	-2.736100
F	2.317945	-4.253547	1.334116
F	4.614771	-4.763102	0.039671
F	5.340237	-3.269439	-2.090469
C	-2.027133	-1.096275	1.571101
H	-1.967665	-0.468580	0.670959

C	-0.553730	4.382982	-2.440110
C	-0.440996	3.971392	-1.104656
C	-0.705601	4.913180	-0.089880
C	-1.098904	6.203583	-0.429391
C	-1.224161	6.595550	-1.760558
C	-0.940695	5.678583	-2.766571
H	-0.331193	3.678118	-3.236220
H	-1.302892	6.917831	0.365528
H	-1.530551	7.608261	-2.005445
H	-1.020731	5.967539	-3.810807
C	-0.471974	4.516457	1.346069
H	0.583424	4.700366	1.588704
H	-1.064400	5.144396	2.020419
C	-0.765596	3.040533	1.595613
H	-0.392167	2.739449	2.577549
H	-1.853170	2.860994	1.595172
C	-0.152952	2.150511	0.535915
C	-0.054613	2.591204	-0.747147
C	0.318923	1.654517	-1.842377
C	1.614923	1.708211	-2.450129
C	-0.600095	0.755843	-2.351744
C	2.618262	2.585727	-1.958731
C	1.931694	0.866776	-3.553892
C	-0.289348	-0.084490	-3.449701
C	3.872007	2.605209	-2.512037
H	2.369115	3.236500	-1.126916
C	3.232262	0.926751	-4.121663
C	0.944246	-0.028789	-4.039886
H	-1.062846	-0.758861	-3.807034
C	4.185024	1.767925	-3.607952
H	4.632170	3.266160	-2.108125
H	3.462121	0.283803	-4.968440
H	1.180705	-0.670760	-4.884583
H	5.180587	1.795132	-4.039568
O	-1.866765	0.602817	-1.835426
C	-2.735752	1.734508	-1.920084
H	-2.738685	2.292076	-0.979663
H	-2.418891	2.403256	-2.724510
H	-3.735486	1.350879	-2.129843
O	0.213849	0.934611	0.908691
C	2.125117	0.745787	1.361226
H	2.410823	0.909417	0.333647
H	1.911133	-0.258910	1.679627
C	2.277460	1.794016	2.364918

C	2.813717	3.038094	2.021545
C	1.819922	1.580243	3.670495
C	2.892933	4.052501	2.968570
H	3.205310	3.187725	1.020252
C	1.889110	2.597012	4.612495
H	1.403116	0.612470	3.936035
C	2.423780	3.837162	4.262345
H	3.324848	5.011281	2.698058
H	1.531397	2.424245	5.622997
H	2.484400	4.630001	5.001858
I	4.770281	-0.327068	1.505630

S-TS-C17

C	1.428981	3.133973	0.692482
C	2.841721	3.163707	0.487976
C	0.867643	4.134867	1.447432
C	3.552308	2.211308	-0.277003
C	3.568100	4.224828	1.108631
C	1.680603	5.147756	2.001316
H	-0.199802	4.151686	1.646299
C	4.915717	2.309990	-0.448086
H	3.063908	1.372962	-0.756560
C	4.976329	4.274633	0.950449
H	1.224575	5.937589	2.596103
C	5.641909	3.345744	0.195843
H	5.503596	5.085082	1.442898
H	6.718124	3.410353	0.076444
C	-1.006365	0.439118	-1.983346
C	-0.005173	2.251293	-3.365158
C	0.026931	0.737990	-3.091852
H	-0.604742	-0.179445	-1.173553
H	-1.880939	-0.063772	-2.390857
H	-0.348822	0.238952	-3.996288
C	-0.421658	2.621005	-0.884239
H	-0.944279	3.468577	-0.435444
C	0.396890	3.060562	-2.126069
H	0.243017	4.126957	-2.318075
H	1.460571	2.928730	-1.919579
H	0.655166	2.499404	-4.200077
C	-1.450538	2.620321	-3.707770
H	-1.513920	3.653933	-4.060162
H	-1.831237	1.975300	-4.505847
C	-2.307655	2.455324	-2.443409
H	-2.594651	3.414738	-2.008650

H	-3.213494	1.880850	-2.636730
N	2.981486	5.202296	1.852052
N	-1.549068	1.708850	-1.368323
O	5.485252	1.410036	-1.271481
C	6.823546	1.016573	-1.027429
H	6.989923	0.837631	0.040207
H	6.956926	0.076712	-1.562838
H	7.535808	1.765309	-1.398408
O	-0.111366	1.428033	1.272120
H	-0.039346	0.435506	1.166253
C	1.370355	0.115284	-2.796940
H	1.318942	-0.888477	-2.372992
C	2.568547	0.628732	-3.064795
H	2.700802	1.616999	-3.500865
H	3.472405	0.072881	-2.827968
C	-2.537356	1.281886	-0.289135
H	-3.248302	0.637362	-0.806716
H	-1.975885	0.678966	0.415038
C	-3.248129	2.399334	0.421707
C	-4.482824	2.858139	-0.034475
C	-2.753489	2.943356	1.612213
C	-5.185733	3.855202	0.628701
C	-3.441050	3.940715	2.293411
H	-1.815052	2.555300	1.996163
C	-4.651363	4.395338	1.792887
H	-3.058918	4.364306	3.215088
F	-5.038377	2.337606	-1.137592
F	-6.355739	4.276547	0.158188
F	-5.333494	5.350401	2.419009
C	0.533943	2.010360	0.173748
H	1.141760	1.260116	-0.340977
C	-3.236568	-4.746059	0.772642
C	-2.657416	-3.598632	1.329143
C	-3.064285	-3.196536	2.617405
C	-3.994753	-3.956064	3.317980
C	-4.548158	-5.108112	2.762173
C	-4.170660	-5.495452	1.480818
H	-2.953321	-5.049023	-0.231873
H	-4.295100	-3.637289	4.313830
H	-5.270589	-5.692358	3.324209
H	-4.601368	-6.384190	1.028617
C	-2.514551	-1.903123	3.166287
H	-3.122532	-1.069800	2.777623
H	-2.606072	-1.875482	4.257337

C	-1.065851	-1.692578	2.739661
H	-0.711432	-0.698130	3.028051
H	-0.409121	-2.410370	3.250959
C	-0.908185	-1.867547	1.241816
C	-1.660144	-2.800733	0.590300
C	-1.478408	-2.999394	-0.874350
C	-2.445728	-2.461660	-1.788297
C	-0.345675	-3.589072	-1.406819
C	-3.655036	-1.872366	-1.326873
C	-2.183043	-2.436353	-3.187873
C	-0.076592	-3.552822	-2.800994
C	-4.530564	-1.266573	-2.195811
H	-3.874968	-1.897675	-0.264650
C	-3.105739	-1.805199	-4.062440
C	-0.962506	-2.981740	-3.667467
H	0.858179	-3.986795	-3.140031
C	-4.250884	-1.219637	-3.581659
H	-5.444841	-0.819093	-1.815882
H	-2.884739	-1.789328	-5.127231
H	-0.747395	-2.948046	-4.732292
H	-4.950120	-0.740364	-4.260476
O	0.636106	-4.193489	-0.684988
C	0.296569	-5.051125	0.393503
H	0.145325	-4.497511	1.323914
H	-0.613094	-5.618175	0.170836
H	1.141134	-5.734481	0.501341
O	-0.030186	-1.081726	0.629804
C	1.876456	-1.562093	0.534284
H	2.003940	-0.692132	-0.087829
H	1.652332	-2.501261	0.053437
C	2.247292	-1.511596	1.945474
C	2.456726	-0.281777	2.578375
C	2.311784	-2.689279	2.698371
C	2.700111	-0.229341	3.944424
H	2.422879	0.635538	1.998961
C	2.560384	-2.637021	4.063797
H	2.190548	-3.644913	2.197231
C	2.746586	-1.405751	4.690712
H	2.857524	0.730450	4.426884
H	2.615461	-3.556351	4.638985
H	2.938617	-1.363520	5.758867
I	4.421993	-2.162156	-0.643942

S-TS-C18



C	3.500360	1.068026	-0.215745
C	4.725424	0.829054	-0.912111
C	3.319824	2.293612	0.370578
C	5.003001	-0.354950	-1.631438
C	5.711111	1.855063	-0.857784
C	4.354176	3.260307	0.325929
H	2.380036	2.520441	0.864287
C	6.228994	-0.542223	-2.234163
H	4.234710	-1.104459	-1.779221
C	6.959898	1.631694	-1.484182
H	4.201937	4.231296	0.794572
C	7.226018	0.462024	-2.149621
H	7.699877	2.422838	-1.424441
H	8.192715	0.324387	-2.620155
C	1.358313	-1.373271	2.652022
C	3.728963	-2.091734	2.833530
C	2.459195	-1.762211	3.655822
H	1.288018	-0.297201	2.483094
H	0.378075	-1.725335	2.973717
H	2.148001	-2.684200	4.165790
C	2.829492	-1.237681	0.654378
H	3.196975	-1.938473	-0.098404
C	3.887151	-1.022674	1.749977
H	4.873678	-1.070719	1.281488
H	3.790633	-0.024079	2.189395
H	4.608428	-2.118081	3.482257
C	3.504428	-3.445849	2.158102
H	4.281263	-3.634758	1.410305
H	3.545071	-4.261055	2.886542
C	2.115157	-3.420002	1.506106
H	2.099660	-3.898800	0.528099
H	1.360944	-3.901546	2.130530
N	5.517704	3.055814	-0.237562
N	1.651703	-1.996441	1.305105
O	6.398360	-1.714722	-2.895574
C	7.600140	-1.922966	-3.604508
H	8.468490	-1.945068	-2.933344
H	7.496782	-2.895737	-4.086549
H	7.754126	-1.154925	-4.372900
O	1.929743	-0.337350	-1.377365
H	1.008485	0.016762	-1.441625
C	2.744061	-0.747713	4.731816
H	3.300117	-1.159223	5.573891
C	2.444296	0.548037	4.732503

H	1.894949	1.021166	3.925351
H	2.743172	1.181994	5.562027
C	0.415734	-1.980459	0.418084
H	0.146611	-0.936455	0.255325
H	0.719056	-2.399160	-0.543766
C	-0.799048	-2.669421	0.971482
C	-1.033818	-4.030305	0.798863
C	-1.845218	-1.893817	1.480333
C	-2.243828	-4.613215	1.143588
C	-3.067627	-2.451551	1.831874
H	-1.708584	-0.819872	1.551198
C	-3.257296	-3.813296	1.661974
H	-3.882231	-1.835513	2.195565
F	-0.104025	-4.821597	0.245491
F	-2.435120	-5.916024	0.950640
F	-4.413690	-4.387243	1.981209
C	2.391757	0.035855	-0.107131
H	1.590070	0.525242	0.462083
C	-1.561487	4.879097	1.296747
C	-1.154837	4.128066	0.185233
C	-0.852176	4.811951	-1.009941
C	-0.912282	6.200655	-1.046383
C	-1.288160	6.937866	0.074730
C	-1.624940	6.268272	1.245519
H	-1.839749	4.367367	2.213929
H	-0.673764	6.713412	-1.975543
H	-1.332216	8.021753	0.025808
H	-1.943042	6.823964	2.123123
C	-0.563262	4.006895	-2.253261
H	-1.523611	3.771886	-2.737317
H	0.013429	4.599880	-2.970963
C	0.154730	2.699555	-1.936310
H	0.175358	2.050972	-2.818597
H	1.204661	2.887271	-1.664661
C	-0.507415	1.959657	-0.792707
C	-1.074786	2.654628	0.226311
C	-1.582762	1.944418	1.431671
C	-2.961695	1.571749	1.556577
C	-0.740494	1.671741	2.488140
C	-3.882246	1.772004	0.494154
C	-3.430923	0.961770	2.756455
C	-1.196996	1.057915	3.679902
C	-5.186814	1.362675	0.602881
H	-3.534308	2.229312	-0.426467

C	-4.795418	0.580437	2.853067
C	-2.515382	0.717915	3.813130
H	-0.481646	0.862871	4.474226
C	-5.651826	0.767013	1.797747
H	-5.854069	1.479770	-0.244470
H	-5.146644	0.126423	3.777092
H	-2.873446	0.246631	4.724767
H	-6.689155	0.455834	1.874713
O	0.610157	1.970786	2.412033
C	0.965971	3.220660	2.995615
H	0.615495	4.050875	2.375574
H	0.544812	3.313030	4.004806
H	2.057111	3.239627	3.057801
O	-0.475620	0.633872	-0.844029
C	-2.018221	0.041348	-1.929616
H	-2.646930	0.061303	-1.054462
I	-4.573958	0.010415	-3.171921
C	-1.479250	-1.228151	-2.431283
C	-0.412013	-1.224900	-3.334219
C	-1.974461	-2.452571	-1.970017
C	0.169660	-2.417719	-3.747020
H	-0.024452	-0.278667	-3.701057
C	-1.406871	-3.646162	-2.396686
H	-2.830860	-2.458360	-1.302111
C	-0.324814	-3.632073	-3.276388
H	1.005638	-2.398280	-4.439215
H	-1.809621	-4.591209	-2.044052
H	0.120046	-4.566248	-3.606571
H	-1.944698	0.936356	-2.524974

S-TS-C19

C	-3.134472	0.544359	-1.095615
C	-4.495906	0.443230	-1.519402
C	-2.651034	1.787652	-0.784735
C	-5.124112	-0.763801	-1.904850
C	-5.263461	1.645059	-1.531603
C	-3.494269	2.919562	-0.858055
H	-1.624042	1.915634	-0.462929
C	-6.457940	-0.796802	-2.251256
H	-4.575237	-1.695617	-1.976191
C	-6.628602	1.580824	-1.900999
H	-3.094090	3.901052	-0.607210
C	-7.224358	0.395185	-2.246533
H	-7.188283	2.510314	-1.899595

H	-8.273185	0.383112	-2.519529
C	-1.841180	-3.297291	0.680618
C	-3.100305	-1.968422	2.380182
C	-3.119274	-3.271901	1.556719
H	-2.069452	-3.365774	-0.384842
H	-1.201559	-4.143417	0.934946
H	-3.064001	-4.109906	2.261423
C	-1.808216	-0.796425	0.530733
H	-1.111855	0.013871	0.764379
C	-3.050918	-0.752927	1.456020
H	-3.023280	0.167100	2.045564
H	-3.963093	-0.710234	0.856720
H	-3.997321	-1.922756	3.003668
C	-1.845168	-1.967114	3.247645
H	-1.832885	-1.076618	3.879620
H	-1.829370	-2.844259	3.902856
C	-0.612210	-1.963479	2.334311
H	-0.019297	-1.052326	2.428321
H	0.038075	-2.815187	2.531189
N	-4.757309	2.866737	-1.200844
N	-1.005859	-2.064303	0.876671
O	-6.956706	-2.013341	-2.584382
C	-8.296194	-2.099027	-3.020494
H	-8.466641	-1.496667	-3.921392
H	-8.465948	-3.150272	-3.255567
H	-8.999016	-1.789216	-2.236757
O	-1.144788	-0.587157	-1.864127
H	-0.518434	0.124940	-1.567730
C	-4.366334	-3.444866	0.733810
H	-4.583449	-2.671894	-0.001551
C	-5.208928	-4.465993	0.857088
H	-5.042214	-5.264145	1.577665
H	-6.099712	-4.537290	0.240603
C	0.267233	-2.139116	0.039166
H	-0.053075	-2.224831	-0.996986
H	0.729268	-1.158629	0.160044
C	1.207112	-3.249540	0.403150
C	2.290076	-2.998889	1.240691
C	1.129474	-4.508826	-0.196136
C	3.243252	-3.965729	1.517190
C	2.069692	-5.495734	0.064443
H	0.340504	-4.705799	-0.915199
C	3.122063	-5.214450	0.920786
H	2.024380	-6.466591	-0.413806

F	2.436709	-1.791462	1.797883
F	4.258003	-3.695483	2.330075
F	4.040913	-6.137366	1.190725
C	-2.210568	-0.666126	-0.965989
H	-2.768617	-1.564080	-1.243828
C	0.916573	5.056154	1.856144
C	1.001751	4.369664	0.636459
C	1.182666	5.122809	-0.543043
C	1.241382	6.510973	-0.475636
C	1.137459	7.181328	0.740891
C	0.981396	6.444609	1.909680
H	0.798565	4.497739	2.779513
H	1.378662	7.075000	-1.395661
H	1.185424	8.265791	0.773882
H	0.906596	6.947863	2.869467
C	1.377877	4.388843	-1.845886
H	2.440607	4.132121	-1.954466
H	1.118725	5.032731	-2.693302
C	0.564360	3.102735	-1.879800
H	0.807004	2.512002	-2.763909
H	-0.509929	3.338459	-1.942167
C	0.791130	2.266625	-0.635915
C	0.945922	2.893800	0.564865
C	0.949105	2.106944	1.831113
C	-0.243293	2.033968	2.630431
C	2.076565	1.459039	2.293293
C	-1.436811	2.707599	2.249343
C	-0.248654	1.310801	3.857371
C	2.062029	0.705987	3.494960
C	-2.567134	2.657847	3.025563
H	-1.430397	3.292983	1.337479
C	-1.428778	1.288137	4.648561
C	0.931281	0.631881	4.259864
H	2.978378	0.201957	3.782786
C	-2.566200	1.939439	4.243925
H	-3.462898	3.182622	2.707083
H	-1.409351	0.750082	5.594016
H	0.929931	0.069723	5.190536
H	-3.459640	1.917925	4.860917
O	3.277444	1.505370	1.639132
C	3.922526	2.773898	1.664796
H	3.850112	3.224093	2.661877
H	3.492933	3.458943	0.927352
H	4.972792	2.589277	1.428065

O	0.709362	0.953033	-0.762746
C	2.281385	-0.019761	-1.533728
H	1.580702	-0.649819	-2.054438
H	2.577680	-0.273854	-0.528892
C	3.056436	0.969876	-2.265422
C	2.821517	1.212803	-3.624694
C	4.038207	1.705975	-1.595592
C	3.549480	2.184297	-4.296095
H	2.076310	0.622096	-4.150106
C	4.774291	2.672298	-2.270689
H	4.223234	1.487509	-0.550819
C	4.528060	2.915355	-3.619938
H	3.367886	2.364710	-5.351045
H	5.542750	3.232487	-1.746359
H	5.103295	3.668729	-4.150100
I	3.888596	-2.368929	-2.167618

S-TS-C20

C	3.134328	0.176645	1.098352
C	4.505717	-0.091647	1.405268
C	2.755527	1.486863	0.964546
C	5.040093	-1.387585	1.584008
C	5.383240	1.027212	1.511925
C	3.711014	2.520722	1.098065
H	1.727924	1.751256	0.736605
C	6.379718	-1.579505	1.840379
H	4.417392	-2.269958	1.525233
C	6.753009	0.798837	1.784952
H	3.399525	3.556785	0.969735
C	7.252798	-0.468563	1.943012
H	7.397267	1.668524	1.860645
H	8.308560	-0.606370	2.145811
C	1.316812	-3.356022	-0.927624
C	2.791726	-2.111634	-2.513367
C	2.637437	-3.426476	-1.728296
H	1.455018	-3.557377	0.134100
H	0.578369	-4.062524	-1.304382
H	2.534426	-4.232902	-2.467016
C	1.668219	-0.887701	-0.599391
H	1.095789	0.029058	-0.761400
C	2.897035	-0.939883	-1.540414
H	2.975126	0.004604	-2.086238
H	3.811692	-1.042429	-0.951937
H	3.693247	-2.159674	-3.131846

C	1.558326	-1.916872	-3.389802
H	1.679814	-1.031643	-4.018182
H	1.415450	-2.779512	-4.048942
C	0.338199	-1.730033	-2.479072
H	-0.055560	-0.714897	-2.507162
H	-0.473342	-2.411216	-2.733431
N	4.979460	2.319117	1.351906
N	0.688058	-1.996251	-1.035265
O	6.781205	-2.870910	1.976836
C	8.125818	-3.124343	2.322051
H	8.391534	-2.652804	3.276268
H	8.211201	-4.206893	2.422665
H	8.817285	-2.780961	1.542025
O	1.046591	-0.818975	1.815694
H	0.459725	-0.055449	1.584951
C	3.855818	-3.744994	-0.889437
H	4.790692	-3.321742	-1.256817
C	3.894347	-4.510649	0.198340
H	3.011278	-4.986011	0.620143
H	4.831882	-4.684395	0.717443
C	-0.588631	-1.908185	-0.205201
H	-0.299855	-2.173842	0.809431
H	-0.836153	-0.843847	-0.206558
C	-1.762063	-2.712236	-0.682058
C	-1.921968	-4.048095	-0.316485
C	-2.819924	-2.094775	-1.358322
C	-3.052787	-4.771108	-0.660810
C	-3.969367	-2.795238	-1.700314
H	-2.772443	-1.028694	-1.564407
C	-4.073951	-4.131921	-1.357500
H	-4.808865	-2.300715	-2.172837
F	-0.969264	-4.674913	0.393820
F	-3.162841	-6.051161	-0.313747
F	-5.156924	-4.836308	-1.672303
C	2.092991	-0.927435	0.894584
H	2.560401	-1.896215	1.086233
C	-0.724096	5.039990	-1.745592
C	-0.445752	4.340112	-0.564259
C	-0.086021	5.075900	0.582092
C	-0.014399	6.463311	0.521997
C	-0.290990	7.147981	-0.659457
C	-0.647199	6.428232	-1.794627
H	-1.007199	4.490246	-2.638800
H	0.263765	7.016180	1.416659

H	-0.229738	8.231736	-0.690064
H	-0.869578	6.945339	-2.723646
C	0.245075	4.312071	1.838644
H	1.298440	3.995479	1.803920
H	0.145130	4.954588	2.719718
C	-0.638173	3.076708	1.975714
H	-0.308477	2.446565	2.806775
H	-1.668486	3.382121	2.203809
C	-0.643720	2.241538	0.709686
C	-0.529119	2.863111	-0.498852
C	-0.519671	2.126406	-1.791501
C	0.658869	2.138971	-2.615916
C	-1.642472	1.492192	-2.287704
C	1.876859	2.712150	-2.158482
C	0.637807	1.561719	-3.917632
C	-1.674047	0.941658	-3.594358
C	3.012283	2.683131	-2.927738
H	1.894865	3.181340	-1.182293
C	1.824896	1.559415	-4.698757
C	-0.567174	0.984030	-4.397449
H	-2.599893	0.484059	-3.930546
C	2.989858	2.097387	-4.215029
H	3.931501	3.116633	-2.545601
H	1.791019	1.120395	-5.693361
H	-0.593081	0.560872	-5.398399
H	3.891446	2.086504	-4.820186
O	-2.766276	1.334955	-1.526487
C	-3.715927	2.392926	-1.605212
H	-3.277182	3.330443	-1.243232
H	-4.064488	2.526462	-2.637541
H	-4.551307	2.090503	-0.970003
O	-0.769395	0.935484	0.855075
C	-2.629990	0.435240	1.440067
H	-3.020682	1.224299	0.822047
H	-2.461893	-0.518484	0.973544
C	-2.546302	0.564556	2.892505
C	-1.739364	-0.309999	3.626689
C	-3.212639	1.601398	3.555913
C	-1.581435	-0.135877	4.996413
H	-1.209160	-1.109060	3.116778
C	-3.062830	1.769017	4.924599
H	-3.871383	2.252900	2.989207
C	-2.241054	0.904201	5.647237
H	-0.942616	-0.811579	5.556693



H	-3.590107	2.571256	5.431695
H	-2.119556	1.038515	6.718010
I	-5.349766	-0.410899	1.087189

S-TS-C21

C	2.483543	2.610582	-1.991470
C	3.524152	1.628293	-1.973403
C	2.764347	3.821225	-2.571829
C	3.364569	0.317092	-1.477109
C	4.795120	2.017145	-2.489709
C	4.057765	4.094417	-3.079642
H	1.995950	4.585981	-2.651980
C	4.420775	-0.571721	-1.475497
H	2.406495	-0.039372	-1.120489
C	5.862671	1.089541	-2.453852
H	4.263506	5.062856	-3.532244
C	5.692592	-0.176128	-1.955145
H	6.820079	1.415613	-2.846368
H	6.524968	-0.870409	-1.948095
C	-0.546297	3.951781	0.729297
C	1.603544	3.762519	1.979174
C	0.607002	4.765213	1.367355
H	-0.731092	4.227719	-0.308459
H	-1.480897	4.097637	1.271723
H	0.186458	5.356238	2.189093
C	1.080568	2.123828	0.110366
H	1.160890	1.046615	0.276532
C	2.193892	2.860679	0.894798
H	2.853066	2.115937	1.350608
H	2.809900	3.450268	0.214635
H	2.406526	4.309517	2.480329
C	0.843513	2.892333	2.977216
H	1.536614	2.237588	3.508076
H	0.338091	3.516869	3.721319
C	-0.178959	2.040471	2.213253
H	0.082993	0.982604	2.189485
H	-1.180705	2.130059	2.631889
N	5.049648	3.244299	-3.029553
N	-0.271766	2.473996	0.768403
O	4.152415	-1.811975	-1.002871
C	5.204345	-2.742937	-0.837818
H	5.973439	-2.353421	-0.159277
H	4.746568	-3.629850	-0.400194
H	5.659804	-3.002845	-1.800807

O	0.402100	1.413984	-2.171098
H	0.332894	0.541454	-1.714421
C	1.233745	5.721514	0.390404
H	1.684334	5.287331	-0.500927
C	1.272711	7.039419	0.561994
H	0.834376	7.514633	1.437039
H	1.744369	7.693979	-0.164397
C	-1.386628	1.689290	0.093811
H	-1.439905	2.032578	-0.939160
H	-1.032078	0.656210	0.079073
C	-2.731615	1.750814	0.756445
C	-3.658695	2.725703	0.400955
C	-3.171255	0.703479	1.573172
C	-4.968582	2.691285	0.856223
C	-4.477670	0.645024	2.040734
H	-2.494468	-0.114630	1.800021
C	-5.368869	1.643602	1.678950
H	-4.825092	-0.183629	2.646122
F	-3.311663	3.717480	-0.429911
F	-5.830579	3.635925	0.490366
F	-6.628519	1.620347	2.102814
C	1.083122	2.379144	-1.427332
H	0.557379	3.328600	-1.600841
C	2.684038	-3.971638	1.736816
C	1.959841	-3.600650	0.594746
C	1.997632	-4.467293	-0.519179
C	2.767172	-5.625229	-0.478567
C	3.503829	-5.965457	0.654385
C	3.450289	-5.133591	1.766680
H	2.654493	-3.348938	2.623635
H	2.780635	-6.277352	-1.349028
H	4.098077	-6.874299	0.669317
H	4.001768	-5.385816	2.668011
C	1.147373	-4.139511	-1.718694
H	0.129978	-4.524692	-1.548383
H	1.530871	-4.642478	-2.612507
C	1.082888	-2.634418	-1.931609
H	0.387238	-2.384510	-2.736638
H	2.069405	-2.256168	-2.231411
C	0.665729	-1.923178	-0.660108
C	1.129288	-2.371010	0.538472
C	0.843348	-1.660503	1.819106
C	1.885494	-0.942184	2.498818
C	-0.392681	-1.733835	2.434883

C	3.156617	-0.743100	1.892697
C	1.672894	-0.415532	3.804975
C	-0.613998	-1.184938	3.723416
C	4.152325	-0.058039	2.541659
H	3.332789	-1.163917	0.909490
C	2.733823	0.264595	4.463177
C	0.394990	-0.558037	4.403154
H	-1.603775	-1.296356	4.156185
C	3.944631	0.448687	3.846596
H	5.111076	0.087201	2.052019
H	2.562457	0.646382	5.467079
H	0.225748	-0.157356	5.399340
H	4.745932	0.973625	4.358125
O	-1.474453	-2.296845	1.820260
C	-1.533770	-3.724839	1.850641
H	-1.652986	-4.074645	2.883814
H	-0.627114	-4.159207	1.417700
H	-2.401850	-4.001183	1.249606
O	-0.123435	-0.865712	-0.807593
C	-1.920820	-1.580449	-1.266545
H	-1.478686	-2.471746	-1.679939
H	-2.168408	-1.601058	-0.217419
C	-2.451135	-0.549605	-2.169297
C	-1.801479	-0.274748	-3.375608
C	-3.587540	0.195735	-1.828873
C	-2.250401	0.744230	-4.207110
H	-0.914790	-0.838245	-3.647576
C	-4.038536	1.212234	-2.659689
H	-4.141783	-0.069304	-0.934667
C	-3.365290	1.495279	-3.848028
H	-1.724123	0.954186	-5.132821
H	-4.928544	1.773591	-2.389788
H	-3.719958	2.289182	-4.498867
I	-4.189812	-3.403019	-1.172152

S-TS-C22

C	3.311088	-1.981742	-1.745871
C	4.275457	-1.000431	-1.358937
C	3.677046	-2.892139	-2.705876
C	4.014010	0.046005	-0.445865
C	5.558086	-1.065196	-1.980765
C	4.985138	-2.879374	-3.239834
H	2.968301	-3.625741	-3.079920
C	4.964695	1.010307	-0.185327

H	3.049554	0.161402	0.036895
C	6.524906	-0.081051	-1.661226
H	5.268370	-3.620989	-3.984809
C	6.242973	0.941796	-0.793642
H	7.492445	-0.157247	-2.146028
H	6.995111	1.693367	-0.582060
C	0.427428	-3.179664	1.447201
C	1.742563	-5.194894	0.847108
C	1.093493	-4.438848	2.029722
H	1.062912	-2.293062	1.488475
H	-0.505184	-2.943803	1.959881
H	0.307667	-5.085652	2.444012
C	1.401935	-3.360320	-0.839249
H	1.128821	-3.864917	-1.770959
C	2.446678	-4.177096	-0.052587
H	3.106331	-4.677533	-0.764050
H	3.078612	-3.510452	0.546422
H	2.452308	-5.942024	1.211826
C	0.620090	-5.850428	0.042303
H	1.002731	-6.230046	-0.910799
H	0.188968	-6.699299	0.581193
C	-0.467821	-4.793043	-0.186387
H	-0.898822	-4.839859	-1.184999
H	-1.278751	-4.882881	0.537711
N	5.904960	-2.012977	-2.895635
N	0.098139	-3.402114	-0.014089
O	4.591140	1.992183	0.666194
C	5.402683	3.139875	0.803526
H	5.578359	3.619960	-0.166648
H	4.838263	3.820222	1.441079
H	6.364322	2.900159	1.275705
O	1.063863	-1.417865	-2.238686
H	0.670985	-0.574248	-1.888072
C	2.084354	-4.200885	3.138118
H	2.358957	-5.112917	3.668231
C	2.661077	-3.055231	3.488723
H	2.431021	-2.113922	3.002014
H	3.390201	-3.029022	4.292861
C	-0.917066	-2.372245	-0.495598
H	-0.470217	-1.387358	-0.350736
H	-1.031224	-2.532865	-1.567389
C	-2.237149	-2.386895	0.220658
C	-3.283217	-3.232501	-0.137984
C	-2.505486	-1.398696	1.172191

C	-4.528764	-3.149667	0.465860
C	-3.747086	-1.287001	1.783686
H	-1.731798	-0.673592	1.400701
C	-4.750715	-2.171997	1.428642
H	-3.950689	-0.500565	2.501330
F	-3.129561	-4.147158	-1.106205
F	-5.506654	-3.973303	0.094578
F	-5.958300	-2.096075	1.984535
C	1.877385	-1.943363	-1.225482
H	1.836411	-1.316937	-0.325653
C	1.819263	3.732532	2.351320
C	1.549537	3.329863	1.037727
C	1.950434	4.171924	-0.020403
C	2.615196	5.360679	0.258183
C	2.888106	5.746777	1.570423
C	2.483585	4.926832	2.618421
H	1.489177	3.109864	3.178392
H	2.909676	6.005625	-0.566772
H	3.399248	6.684426	1.768106
H	2.673435	5.217253	3.647912
C	1.564991	3.791122	-1.428997
H	0.549122	4.167001	-1.627432
H	2.228932	4.274752	-2.153350
C	1.581435	2.276355	-1.613875
H	1.182427	1.997914	-2.594345
H	2.613493	1.902480	-1.577787
C	0.771602	1.594900	-0.528177
C	0.808410	2.089640	0.736663
C	0.072600	1.412036	1.837786
C	-1.203948	1.894152	2.280085
C	0.615260	0.325755	2.489588
C	-1.851746	2.979827	1.631594
C	-1.865248	1.265062	3.374418
C	-0.029490	-0.295802	3.586645
C	-3.105261	3.385325	2.013543
H	-1.354544	3.483666	0.808416
C	-3.147967	1.729861	3.769798
C	-1.240976	0.167272	4.022677
H	0.454572	-1.143004	4.065166
C	-3.761181	2.756032	3.096919
H	-3.592062	4.188328	1.469450
H	-3.639396	1.249931	4.613504
H	-1.743503	-0.308781	4.860807
H	-4.749323	3.092273	3.396321

O	1.822896	-0.210622	2.082620
C	2.947386	0.333717	2.772195
H	3.084333	1.386128	2.515636
H	2.822936	0.216416	3.856841
H	3.820202	-0.229324	2.435667
O	0.004843	0.569062	-0.882544
C	-1.599253	1.514091	-1.631699
H	-0.950062	2.009618	-2.332178
H	-1.752685	1.951437	-0.661412
C	-2.457923	0.418055	-2.083212
C	-2.049235	-0.411869	-3.131704
C	-3.697895	0.192650	-1.472785
C	-2.861551	-1.460453	-3.553595
H	-1.088390	-0.241876	-3.608388
C	-4.522437	-0.829511	-1.919843
H	-4.026046	0.864019	-0.685372
C	-4.102228	-1.666071	-2.954433
H	-2.534590	-2.102973	-4.365905
H	-5.497857	-0.974053	-1.465349
H	-4.745836	-2.470876	-3.297158
I	-3.170976	3.826901	-2.231886

S-TS-C23

C	-3.222857	0.048432	-0.601200
C	-4.553527	-0.164767	-1.082760
C	-2.929028	1.275693	-0.068368
C	-4.999819	-1.364483	-1.680501
C	-5.484578	0.904108	-0.923598
C	-3.923870	2.277503	0.015188
H	-1.935616	1.498220	0.301316
C	-6.312014	-1.524459	-2.067131
H	-4.327169	-2.193407	-1.857067
C	-6.822607	0.714568	-1.343622
H	-3.667641	3.248303	0.437630
C	-7.240859	-0.469285	-1.895808
H	-7.509924	1.543037	-1.208167
H	-8.275556	-0.583045	-2.197881
C	-1.067439	-3.668136	0.421770
C	-2.581340	-3.010304	2.302071
C	-2.367890	-4.043315	1.180345
H	-1.222126	-3.579801	-0.655775
H	-0.275656	-4.401014	0.582503
H	-2.183281	-5.012743	1.663087
C	-1.588925	-1.248338	0.769039

H	-1.058793	-0.347349	1.088508
C	-2.749369	-1.600739	1.731713
H	-2.779016	-0.870837	2.544838
H	-3.697275	-1.521878	1.198027
H	-3.458257	-3.281972	2.896185
C	-1.333541	-3.007932	3.184008
H	-1.483321	-2.353168	4.046474
H	-1.121219	-4.014447	3.559313
C	-0.154982	-2.479528	2.356044
H	0.168655	-1.487395	2.672783
H	0.703304	-3.147817	2.398589
N	-5.161445	2.111546	-0.378412
N	-0.523483	-2.353551	0.895782
O	-6.633234	-2.735121	-2.596282
C	-7.937668	-2.924387	-3.100489
H	-8.174269	-2.198779	-3.888486
H	-7.952171	-3.929322	-3.523885
H	-8.693334	-2.858088	-2.307309
O	-1.192665	-0.741549	-1.655136
H	-0.697811	0.085258	-1.396756
C	-3.524227	-4.248291	0.228948
H	-3.264804	-4.761294	-0.698478
C	-4.795516	-3.911409	0.427310
H	-5.136366	-3.403088	1.325184
H	-5.550155	-4.118186	-0.325160
C	0.725188	-1.969528	0.108606
H	0.365380	-1.806717	-0.904866
H	1.038700	-1.004164	0.513772
C	1.836132	-2.977756	0.111804
C	2.870252	-2.908760	1.040861
C	1.957111	-3.915663	-0.918288
C	3.967421	-3.753877	0.983305
C	3.042575	-4.775706	-0.997120
H	1.198092	-3.946952	-1.693773
C	4.044837	-4.684250	-0.044405
H	3.147352	-5.489599	-1.805084
F	2.824452	-2.013837	2.033195
F	4.928330	-3.666565	1.895917
F	5.100282	-5.490991	-0.092402
C	-2.141927	-1.031668	-0.670246
H	-2.614470	-1.968758	-0.973126
C	0.054264	4.957888	2.299015
C	0.086143	4.407290	1.010178
C	-0.190329	5.250722	-0.086008

C	-0.521241	6.583619	0.132674
C	-0.570233	7.114026	1.420055
C	-0.271165	6.295019	2.503472
H	0.287654	4.330290	3.154029
H	-0.735038	7.219968	-0.723439
H	-0.828517	8.157746	1.572261
H	-0.292205	6.694446	3.513554
C	-0.030701	4.692117	-1.476799
H	1.027746	4.770729	-1.766529
H	-0.597371	5.287580	-2.200714
C	-0.438069	3.225796	-1.552140
H	-0.151495	2.797164	-2.514525
H	-1.532237	3.130527	-1.479645
C	0.183288	2.408096	-0.437638
C	0.416033	2.988143	0.776189
C	0.943185	2.146525	1.887986
C	0.058049	1.604759	2.878766
C	2.282491	1.813421	1.967277
C	-1.324250	1.941010	2.907435
C	0.546963	0.711260	3.875179
C	2.765022	0.901062	2.939047
C	-2.171322	1.413091	3.849349
H	-1.697661	2.656357	2.183547
C	-0.352417	0.179650	4.838246
C	1.921882	0.360194	3.866978
H	3.819760	0.650103	2.911188
C	-1.682893	0.515654	4.827801
H	-3.220034	1.695797	3.849718
H	0.039032	-0.495772	5.596087
H	2.297368	-0.338954	4.609566
H	-2.357490	0.111605	5.577334
O	3.234496	2.278763	1.108361
C	3.348116	3.686072	0.941969
H	3.130171	4.206997	1.880716
H	2.670119	4.056727	0.168949
H	4.384043	3.870368	0.649355
O	0.387213	1.121348	-0.665513
C	2.124906	0.609887	-1.503267
H	1.716962	-0.378071	-1.605414
H	2.647730	0.881938	-0.600045
C	2.166536	1.474899	-2.673849
C	1.446617	1.135282	-3.825653
C	2.851201	2.692510	-2.624334
C	1.400499	2.008399	-4.903571



H	0.913181	0.189420	-3.859681
C	2.807472	3.564556	-3.705422
H	3.434186	2.932462	-1.741246
C	2.076243	3.227669	-4.842511
H	0.838940	1.741783	-5.793831
H	3.344957	4.507142	-3.662834
H	2.040339	3.911013	-5.685853
I	4.513209	-0.915309	-1.925580

S-TS-C24

C	2.249391	-0.896561	1.667158
C	3.281514	-1.883494	1.753733
C	2.107598	-0.015570	2.707033
C	3.457929	-2.922879	0.810433
C	4.158863	-1.809015	2.873656
C	3.025014	-0.050412	3.784282
H	1.302634	0.710842	2.696555
C	4.488825	-3.830053	0.944968
H	2.751792	-3.094401	0.003302
C	5.211893	-2.748801	2.977226
H	2.918256	0.665581	4.597999
C	5.386533	-3.732829	2.038042
H	5.871703	-2.668722	3.834912
H	6.199515	-4.441154	2.149833
C	1.066503	1.402445	-2.033844
C	1.878026	-0.528712	-3.360896
C	1.007935	0.734236	-3.428730
H	0.194348	1.160497	-1.427717
H	1.142106	2.486768	-2.113430
H	1.449363	1.424850	-4.162822
C	2.126988	-0.543115	-0.865988
H	3.156832	-0.876031	-0.712898
C	1.517660	-1.269331	-2.071346
H	1.866024	-2.305621	-2.072860
H	0.431659	-1.302570	-1.966631
H	1.723233	-1.163324	-4.235413
C	3.344102	-0.092196	-3.286591
H	3.980508	-0.951920	-3.054677
H	3.683102	0.318402	-4.242375
C	3.475176	0.986842	-2.201332
H	4.371185	0.864012	-1.592957
H	3.482975	1.993049	-2.625714
N	4.030193	-0.885810	3.869455
N	2.287123	0.934194	-1.268636

O	4.575314	-4.782128	-0.012161
C	5.477677	-5.850152	0.172810
H	5.300704	-6.365549	1.124785
H	5.291276	-6.542456	-0.648670
H	6.521607	-5.512276	0.129625
O	0.320184	0.092912	0.711190
H	-0.496925	-0.027205	0.153596
C	-0.432073	0.518606	-3.828234
H	-1.092624	1.360291	-3.620217
C	-0.946048	-0.565440	-4.400689
H	-0.363180	-1.455006	-4.622876
H	-2.000032	-0.605108	-4.656809
C	2.531715	1.805188	-0.049431
H	1.588701	1.800745	0.496321
H	3.279488	1.278201	0.544584
C	2.983450	3.209276	-0.343373
C	4.341829	3.519700	-0.386570
C	2.072217	4.260814	-0.488085
C	4.792624	4.814481	-0.603427
C	2.501067	5.565626	-0.705045
H	1.009860	4.044857	-0.406079
C	3.859432	5.832992	-0.764786
H	1.796944	6.382378	-0.814077
F	5.261445	2.560830	-0.217764
F	6.095089	5.073622	-0.648568
F	4.302636	7.070312	-0.970641
C	1.333324	-0.827451	0.455885
H	0.934967	-1.843476	0.300951
C	-4.979336	3.150971	0.564671
C	-4.635920	2.005836	-0.168072
C	-5.587071	1.476738	-1.064793
C	-6.816801	2.105259	-1.223604
C	-7.140219	3.251440	-0.499635
C	-6.215883	3.767744	0.401928
H	-4.268057	3.557679	1.278572
H	-7.536706	1.686485	-1.923763
H	-8.105350	3.730179	-0.636209
H	-6.454133	4.654943	0.982123
C	-5.241577	0.201949	-1.789705
H	-5.451119	-0.653378	-1.130516
H	-5.866555	0.079827	-2.681157
C	-3.763113	0.175102	-2.153662
H	-3.483348	-0.785694	-2.590987
H	-3.548531	0.944155	-2.914361

C	-2.891515	0.448544	-0.943341
C	-3.324145	1.349220	-0.011451
C	-2.453025	1.750263	1.126761
C	-2.762308	1.299946	2.456805
C	-1.344547	2.557586	0.966704
C	-3.913799	0.510133	2.718739
C	-1.915182	1.628468	3.550669
C	-0.511795	2.906687	2.059947
C	-4.191803	0.063075	3.986118
H	-4.572939	0.259124	1.895247
C	-2.223394	1.146344	4.848299
C	-0.779017	2.444939	3.315623
H	0.338170	3.556256	1.871071
C	-3.336664	0.377206	5.066343
H	-5.083197	-0.532309	4.163823
H	-1.558027	1.400975	5.669623
H	-0.136519	2.715131	4.150108
H	-3.564588	0.011312	6.062855
O	-0.897706	3.056606	-0.234509
C	-1.810053	3.604156	-1.172918
H	-2.152007	2.849536	-1.886161
H	-2.682498	4.038609	-0.676910
H	-1.263453	4.390597	-1.703827
O	-1.728811	-0.159220	-0.915643
C	-1.726581	-2.213238	-0.879801
H	-1.461657	-2.211800	-1.923171
H	-0.971630	-2.044224	-0.138731
C	-3.062990	-2.585531	-0.451321
C	-3.472687	-2.294701	0.854300
C	-3.966320	-3.181935	-1.341208
C	-4.764564	-2.601341	1.264707
H	-2.780724	-1.812031	1.538204
C	-5.252773	-3.494491	-0.927235
H	-3.637246	-3.424795	-2.347638
C	-5.653616	-3.203188	0.377997
H	-5.072730	-2.370468	2.279723
H	-5.944156	-3.968480	-1.616857
H	-6.661286	-3.446561	0.701654
I	-0.246380	-4.654640	-1.006440

S-TS-C25

C	-1.689132	1.803716	1.392238
C	-2.252026	3.115670	1.305766
C	-1.778054	1.140825	2.587064

C	-2.131156	3.950590	0.170697
C	-2.934483	3.609823	2.452580
C	-2.477595	1.733092	3.666307
H	-1.309679	0.170111	2.702791
C	-2.667551	5.220449	0.161665
H	-1.564982	3.645130	-0.702154
C	-3.498834	4.906726	2.402317
H	-2.558821	1.193822	4.608686
C	-3.376178	5.701039	1.290418
H	-4.019646	5.258955	3.286528
H	-3.811484	6.693559	1.292678
C	-1.622398	-1.396694	-1.775894
C	-1.749053	0.405144	-3.474068
C	-1.391967	-1.081364	-3.267996
H	-0.702622	-1.350012	-1.196170
H	-2.068354	-2.381184	-1.641362
H	-2.072042	-1.689310	-3.878971
C	-1.888647	0.983111	-1.036311
H	-2.731714	1.675705	-0.962655
C	-1.118272	1.219897	-2.343826
H	-1.134533	2.290809	-2.566727
H	-0.067547	0.947658	-2.207930
H	-1.392294	0.748379	-4.448115
C	-3.272564	0.534851	-3.368398
H	-3.561195	1.590140	-3.328716
H	-3.767584	0.091872	-4.237602
C	-3.734000	-0.200339	-2.098296
H	-4.506785	0.343825	-1.554504
H	-4.111300	-1.200609	-2.319895
N	-3.055330	2.907437	3.615300
N	-2.569270	-0.390535	-1.153773
O	-2.464003	5.945284	-0.967799
C	-2.881595	7.294044	-0.987448
H	-2.406382	7.873082	-0.186081
H	-2.564752	7.690967	-1.952424
H	-3.972070	7.382582	-0.903154
O	-0.320733	0.022884	0.593321
H	0.508230	-0.123214	0.057706
C	0.021137	-1.412472	-3.660042
H	0.801688	-0.885810	-3.111826
C	0.340257	-2.294089	-4.603881
H	-0.416497	-2.848696	-5.155609
H	1.376300	-2.492587	-4.862163
C	-3.045783	-0.874769	0.205242

H	-2.138615	-1.134478	0.752626
H	-3.504820	-0.009005	0.684430
C	-4.010622	-2.027281	0.166815
C	-5.383872	-1.788814	0.187519
C	-3.581720	-3.358620	0.193923
C	-6.310062	-2.822014	0.202619
C	-4.492093	-4.409619	0.208570
H	-2.515354	-3.570399	0.219035
C	-5.850360	-4.134748	0.211220
H	-4.163347	-5.442164	0.232859
F	-5.851906	-0.533016	0.189022
F	-7.612189	-2.557469	0.213429
F	-6.745136	-5.118713	0.226109
C	-0.966729	1.190014	0.207658
H	-0.238530	1.935147	-0.137953
C	3.314166	-4.580444	0.886433
C	3.428182	-3.504612	-0.004402
C	4.526579	-3.482442	-0.887047
C	5.442557	-4.529030	-0.882205
C	5.305981	-5.602469	-0.005170
C	4.239600	-5.618953	0.886890
H	2.493958	-4.596916	1.598206
H	6.283202	-4.496374	-1.571776
H	6.032495	-6.409395	-0.013245
H	4.126972	-6.437856	1.591639
C	4.713464	-2.274951	-1.770896
H	5.267177	-1.506635	-1.209294
H	5.322006	-2.525956	-2.646353
C	3.366514	-1.703011	-2.196574
H	3.496268	-0.767779	-2.748903
H	2.861927	-2.406572	-2.877351
C	2.463345	-1.470353	-0.999940
C	2.454693	-2.389396	-0.000209
C	1.515411	-2.278163	1.153240
C	1.918076	-1.485226	2.286279
C	0.278221	-2.892798	1.200403
C	3.150875	-0.780310	2.294824
C	1.065177	-1.343268	3.414530
C	-0.546932	-2.794155	2.354263
C	3.490908	0.048505	3.335710
H	3.827209	-0.880670	1.452720
C	1.448447	-0.499752	4.486741
C	-0.167329	-2.044650	3.427541
H	-1.484615	-3.341724	2.357016

C	2.630935	0.193431	4.446564
H	4.420544	0.606772	3.285990
H	0.777311	-0.401575	5.337089
H	-0.807998	-1.977752	4.304022
H	2.909229	0.854547	5.261464
O	-0.351383	-3.606823	0.209688
C	0.313279	-4.187284	-0.900040
H	0.595519	-3.440231	-1.646912
H	1.199266	-4.747445	-0.593766
H	-0.416201	-4.875559	-1.336262
O	1.712937	-0.368164	-1.030737
C	2.907858	1.134803	-0.605746
H	2.686282	1.041343	0.446069
H	3.751474	0.589900	-0.992238
C	2.289895	2.198374	-1.410228
C	2.330047	2.134527	-2.806710
C	1.609516	3.259621	-0.800853
C	1.693297	3.099766	-3.578784
H	2.858568	1.317373	-3.287833
C	0.977134	4.229336	-1.571404
H	1.625705	3.345812	0.282376
C	1.011809	4.148158	-2.963191
H	1.737445	3.038266	-4.662258
H	0.463627	5.054988	-1.088070
H	0.521386	4.908828	-3.563601
I	5.096917	2.603940	0.479161

S-TS-C26

C	3.228377	0.268576	1.065081
C	4.609804	0.044686	1.358308
C	2.805530	1.563579	0.925129
C	5.184521	-1.229560	1.572968
C	5.455295	1.191032	1.419266
C	3.726755	2.630051	1.037223
H	1.766965	1.786845	0.707738
C	6.536128	-1.377039	1.799244
H	4.580990	-2.128994	1.606037
C	6.838671	1.008492	1.657611
H	3.374308	3.654135	0.921074
C	7.379434	-0.238803	1.836171
H	7.458456	1.898351	1.693643
H	8.443797	-0.341143	2.012697
C	1.495435	-3.336637	-0.874908
C	2.838617	-2.055230	-2.551697

C	2.727911	-3.405380	-1.813520
H	1.764234	-3.478169	0.173973
H	0.753767	-4.095550	-1.129721
H	2.536448	-4.178961	-2.566483
C	1.751067	-0.861182	-0.590134
H	1.144812	0.033442	-0.755579
C	2.961433	-0.901907	-1.555875
H	3.022893	0.049992	-2.090333
H	3.890975	-1.000873	-0.990862
H	3.714705	-2.072741	-3.205569
C	1.566614	-1.851041	-3.369560
H	1.633369	-0.917058	-3.931531
H	1.434302	-2.666403	-4.087996
C	0.370599	-1.786566	-2.410629
H	-0.132698	-0.819558	-2.429551
H	-0.367465	-2.558312	-2.629355
N	5.007448	2.468106	1.257089
N	0.799665	-2.011964	-0.978438
O	6.975357	-2.648105	1.978545
C	8.335993	-2.852961	2.292828
H	8.616930	-2.338922	3.220394
H	8.452414	-3.928370	2.431156
H	8.994476	-2.522435	1.479561
O	1.207802	-0.792612	1.857186
H	0.573035	-0.061426	1.640560
C	3.977442	-3.789496	-1.069314
H	4.346255	-3.083783	-0.326832
C	4.649895	-4.918250	-1.273327
H	4.326262	-5.654030	-2.006568
H	5.552583	-5.145064	-0.714441
C	-0.434409	-1.971342	-0.093307
H	-0.067487	-2.106132	0.921432
H	-0.781362	-0.940154	-0.170094
C	-1.522283	-2.959794	-0.392330
C	-2.593445	-2.613316	-1.215176
C	-1.589831	-4.186545	0.276997
C	-3.680208	-3.456050	-1.402242
C	-2.664769	-5.048108	0.106613
H	-0.792962	-4.458706	0.963223
C	-3.703838	-4.673410	-0.732585
H	-2.726909	-5.995538	0.628553
F	-2.589299	-1.442491	-1.851244
F	-4.667941	-3.107462	-2.210080
F	-4.745112	-5.478541	-0.915354

C	2.218063	-0.865851	0.895535
H	2.727305	-1.815656	1.079034
C	-0.398112	5.174785	-1.442195
C	-0.600746	4.402881	-0.288881
C	-0.834710	5.078195	0.928557
C	-0.814804	6.468191	0.969043
C	-0.583730	7.220564	-0.179825
C	-0.385981	6.564844	-1.389449
H	-0.248851	4.684114	-2.398115
H	-0.992283	6.968930	1.918238
H	-0.569103	8.305252	-0.129325
H	-0.220116	7.132190	-2.300821
C	-1.172888	4.263744	2.151890
H	-2.253074	4.047137	2.141130
H	-0.973559	4.834084	3.065420
C	-0.408433	2.948387	2.155393
H	-0.725668	2.302233	2.975799
H	0.665376	3.141936	2.304698
C	-0.592481	2.214145	0.842000
C	-0.621444	2.921614	-0.322352
C	-0.642026	2.231853	-1.644221
C	0.530053	2.200060	-2.473764
C	-1.790074	1.632153	-2.122749
C	1.765205	2.758669	-2.043085
C	0.480526	1.608789	-3.769034
C	-1.843913	1.050839	-3.415130
C	2.887906	2.709158	-2.829701
H	1.800425	3.249026	-1.077850
C	1.654597	1.587234	-4.569931
C	-0.740108	1.044110	-4.223261
H	-2.780840	0.600764	-3.726691
C	2.835326	2.113829	-4.112057
H	3.817710	3.137358	-2.467320
H	1.596750	1.143883	-5.561733
H	-0.783348	0.598893	-5.214248
H	3.724676	2.089445	-4.734797
O	-2.905768	1.534825	-1.350269
C	-3.810943	2.626164	-1.420581
H	-4.171402	2.769719	-2.447709
H	-3.337122	3.551598	-1.069395
H	-4.647729	2.355100	-0.774178
O	-0.665977	0.892332	0.901255
C	-2.511335	0.331856	1.373066
H	-2.444777	-0.438156	0.629452



H	-2.922393	1.270684	1.037153
C	-2.380260	0.027886	2.794045
C	-1.868306	-1.202223	3.218605
C	-2.728541	0.985298	3.754054
C	-1.678827	-1.459200	4.569374
H	-1.644652	-1.968083	2.482435
C	-2.543354	0.728617	5.105572
H	-3.166828	1.925063	3.429446
C	-2.010002	-0.492111	5.516148
H	-1.277630	-2.416689	4.887350
H	-2.823318	1.476190	5.841295
H	-1.863514	-0.693038	6.573187
I	-5.235612	-0.573966	1.013940

S-TS-C27

C	-1.806366	3.255686	0.969186
C	-3.144568	3.156362	1.470471
C	-1.133000	4.430566	1.186045
C	-3.940356	1.993975	1.386094
C	-3.694074	4.312258	2.098301
C	-1.770574	5.511795	1.841771
H	-0.113078	4.551139	0.834310
C	-5.228764	1.969149	1.873751
H	-3.546680	1.078694	0.972390
C	-5.023628	4.261718	2.581083
H	-1.225298	6.441000	1.998422
C	-5.784456	3.125318	2.474098
H	-5.418290	5.157548	3.048794
H	-6.796733	3.120305	2.861881
C	0.337142	1.279601	-2.292848
C	-1.078351	3.115045	-3.207718
C	0.362519	2.729633	-2.829698
H	0.899602	1.136377	-1.367172
H	0.744918	0.578218	-3.021814
H	0.952552	2.697455	-3.755709
C	-1.800439	1.835686	-1.133337
H	-2.766813	1.369546	-0.940134
C	-1.974650	3.133222	-1.965311
H	-3.021367	3.246364	-2.265210
H	-1.733932	3.993099	-1.341103
H	-1.094684	4.091932	-3.697770
C	-1.613354	2.042654	-4.156312
H	-2.566814	2.352096	-4.593647
H	-0.913257	1.873235	-4.980897

C	-1.815054	0.756099	-3.347555
H	-2.863046	0.580128	-3.098145
H	-1.444046	-0.125141	-3.869117
N	-3.005763	5.477200	2.271381
N	-1.073438	0.822311	-2.030659
O	-5.889899	0.791630	1.744554
C	-7.210705	0.696276	2.232501
H	-7.882617	1.394204	1.717196
H	-7.530596	-0.325646	2.026321
H	-7.256837	0.876480	3.313754
O	-1.041995	0.991476	1.060370
H	-0.084397	0.730103	1.152155
C	1.080713	3.690677	-1.910196
H	1.915111	3.263506	-1.354192
C	0.831505	4.993046	-1.789349
H	0.023188	5.494322	-2.316523
H	1.442986	5.616661	-1.143779
C	-0.980860	-0.595562	-1.469626
H	-0.371770	-1.151842	-2.186096
H	-0.411501	-0.503645	-0.555433
C	-2.298808	-1.277428	-1.251622
C	-2.824447	-2.123337	-2.224924
C	-2.980605	-1.189828	-0.036605
C	-4.004782	-2.822412	-2.024655
C	-4.172896	-1.864337	0.182856
H	-2.540760	-0.594007	0.753989
C	-4.676117	-2.679503	-0.815705
H	-4.702397	-1.777501	1.123377
F	-2.193517	-2.285070	-3.398158
F	-4.486951	-3.611458	-2.981043
F	-5.818241	-3.342637	-0.645020
C	-1.100925	2.118738	0.233268
H	-0.086992	2.477959	0.020649
C	6.123217	0.784723	0.074534
C	5.009716	0.627953	0.912461
C	5.210696	0.739814	2.302839
C	6.472666	1.047927	2.802916
C	7.561725	1.230188	1.955967
C	7.380992	1.083300	0.584677
H	6.007474	0.656389	-0.997024
H	6.603325	1.137668	3.879278
H	8.539367	1.469207	2.364090
H	8.221047	1.198290	-0.094945
C	4.064807	0.433245	3.232061

H	4.057307	-0.647052	3.431612
H	4.206357	0.929963	4.198267
C	2.723386	0.817714	2.624863
H	1.903040	0.434041	3.233861
H	2.620206	1.914193	2.600132
C	2.574998	0.326399	1.200675
C	3.664882	0.311948	0.377216
C	3.495607	0.175435	-1.098562
C	3.130115	-1.046281	-1.734214
C	3.680032	1.296874	-1.896904
C	3.014368	-2.258441	-1.002729
C	2.877927	-1.085319	-3.137039
C	3.518519	1.245426	-3.301654
C	2.552086	-3.405720	-1.591058
H	3.300967	-2.242206	0.042869
C	2.398885	-2.289664	-3.724529
C	3.110105	0.080857	-3.903228
H	3.693549	2.131819	-3.902226
C	2.210878	-3.414467	-2.966493
H	2.423239	-4.308062	-1.002526
H	2.184977	-2.300070	-4.791016
H	2.961459	0.046473	-4.979975
H	1.819593	-4.322222	-3.414078
O	3.981665	2.460927	-1.250212
C	4.651020	3.473661	-1.967453
H	5.502389	3.068572	-2.527640
H	3.974862	4.001328	-2.654298
H	5.016315	4.178291	-1.219104
O	1.341436	0.042591	0.795186
C	0.641500	-1.777068	1.258541
H	1.150037	-2.149851	0.389820
H	-0.365618	-1.411104	1.147948
C	1.107539	-2.066732	2.603436
C	2.304033	-2.758824	2.820406
C	0.366305	-1.616255	3.704412
C	2.755887	-2.989201	4.113945
H	2.858637	-3.146962	1.972410
C	0.822874	-1.838032	4.995462
H	-0.567145	-1.086370	3.534080
C	2.021391	-2.521879	5.201630
H	3.681629	-3.533029	4.273998
H	0.244690	-1.484897	5.843707
H	2.377198	-2.699523	6.212095
I	-0.719052	-4.292276	0.580360

## S-TS-C28

C	-3.597020	0.288616	0.090938
C	-4.779589	-0.133006	0.773328
C	-3.644453	1.457424	-0.625366
C	-4.838707	-1.270352	1.609234
C	-5.953896	0.647793	0.577863
C	-4.860220	2.179857	-0.716871
H	-2.750081	1.830541	-1.117748
C	-6.026203	-1.651911	2.196871
H	-3.938461	-1.819294	1.857953
C	-7.157908	0.227615	1.190864
H	-4.889800	3.108484	-1.284820
C	-7.205616	-0.897240	1.974712
H	-8.043599	0.831525	1.023151
H	-8.144135	-1.188201	2.432385
C	-0.792226	-1.839448	-2.405215
C	-2.967039	-2.978578	-2.740701
C	-1.735113	-2.414733	-3.479550
H	-0.923557	-0.761262	-2.302338
H	0.254447	-2.034497	-2.636893
H	-1.236644	-3.242459	-3.999665
C	-2.427569	-1.893324	-0.534329
H	-2.705398	-2.599052	0.252141
C	-3.432771	-1.959270	-1.698251
H	-4.409988	-2.228569	-1.288175
H	-3.548966	-0.969219	-2.149247
H	-3.766878	-3.198982	-3.451989
C	-2.527118	-4.248520	-2.004597
H	-3.320343	-4.585602	-1.329757
H	-2.328409	-5.062171	-2.708274
C	-1.245368	-3.934403	-1.216155
H	-1.246972	-4.368472	-0.216454
H	-0.348798	-4.282161	-1.732619
N	-5.983036	1.791262	-0.167264
N	-1.083713	-2.444257	-1.055971
O	-5.978894	-2.758212	2.980480
C	-7.144580	-3.146077	3.673801
H	-7.952250	-3.424708	2.984733
H	-6.863303	-4.018202	4.265138
H	-7.497240	-2.354254	4.346534
O	-1.829584	-0.650181	1.439936
H	-1.044133	-0.050081	1.497791
C	-2.066232	-1.357016	-4.495059

H	-1.724091	-1.542600	-5.512326
C	-2.744447	-0.244477	-4.226454
H	-2.899533	0.099129	-3.206032
H	-3.165299	0.368312	-5.017830
C	0.050379	-2.131771	-0.089971
H	0.107221	-1.043749	-0.035155
H	-0.273233	-2.509903	0.880339
C	1.406472	-2.640731	-0.478961
C	1.864161	-3.898458	-0.095624
C	2.318829	-1.775439	-1.091156
C	3.162672	-4.310568	-0.353328
C	3.624126	-2.161778	-1.354300
H	2.004516	-0.762153	-1.321092
C	4.035869	-3.430956	-0.984506
H	4.339117	-1.469344	-1.781740
F	1.044386	-4.750905	0.539661
F	3.564324	-5.525084	0.009171
F	5.278294	-3.838784	-1.219239
C	-2.298021	-0.498888	0.125212
H	-1.584446	0.091903	-0.461820
C	0.279875	4.757730	-2.023796
C	0.087759	4.134984	-0.782813
C	-0.445055	4.901315	0.274760
C	-0.815161	6.222930	0.052492
C	-0.650314	6.821261	-1.195432
C	-0.087214	6.084160	-2.231161
H	0.737924	4.199366	-2.835423
H	-1.229672	6.798971	0.877059
H	-0.942860	7.855720	-1.348711
H	0.073252	6.541021	-3.203801
C	-0.511227	4.281015	1.647513
H	0.469831	4.404206	2.130410
H	-1.238778	4.805617	2.276048
C	-0.824277	2.790908	1.590985
H	-0.672597	2.332865	2.572039
H	-1.880056	2.627629	1.324005
C	0.032280	2.073071	0.569776
C	0.438245	2.721143	-0.555989
C	1.158894	1.984195	-1.630317
C	2.589457	1.910539	-1.650141
C	0.467310	1.376866	-2.656216
C	3.371847	2.504184	-0.624152
C	3.258721	1.213488	-2.695701
C	1.124295	0.696353	-3.710548

C	4.733883	2.353228	-0.597836
H	2.858870	3.062242	0.152364
C	4.674134	1.098676	-2.657203
C	2.490348	0.618278	-3.729539
H	0.524601	0.217966	-4.480700
C	5.394261	1.637291	-1.622902
H	5.311137	2.775683	0.217888
H	5.176300	0.561200	-3.458493
H	2.999987	0.082999	-4.526477
H	6.471969	1.516475	-1.584129
O	-0.915698	1.361880	-2.633932
C	-1.547757	2.127525	-3.648159
H	-1.320964	3.191544	-3.525472
H	-1.246249	1.794706	-4.649475
H	-2.622714	1.971430	-3.526461
O	0.273721	0.788928	0.789240
C	1.941603	0.299187	1.715927
H	1.649128	-0.732287	1.615954
H	2.537015	0.735553	0.931449
C	1.716220	1.002058	2.975228
C	2.260439	2.272180	3.187628
C	0.851183	0.458627	3.931389
C	1.933648	2.992812	4.330305
H	2.960668	2.677117	2.463466
C	0.521601	1.180202	5.070479
H	0.425786	-0.527490	3.765910
C	1.057790	2.452444	5.269448
H	2.366099	3.975837	4.490914
H	-0.155757	0.753931	5.804189
H	0.799675	3.017451	6.160237
I	4.430346	-0.933890	2.283072

S-TS-C29

C	2.288158	-2.580934	-0.166809
C	3.598278	-2.701309	0.398764
C	1.652329	-3.730219	-0.560870
C	4.342697	-1.618868	0.917135
C	4.168972	-4.005060	0.447834
C	2.307074	-4.982086	-0.441433
H	0.646337	-3.708140	-0.973283
C	5.603994	-1.801803	1.439062
H	3.923156	-0.624720	0.960875
C	5.471505	-4.161336	0.978384
H	1.784927	-5.883338	-0.755767

C	6.184431	-3.092791	1.462084
H	5.884498	-5.164400	0.999061
H	7.176128	-3.251817	1.869784
C	0.126375	0.631128	-2.181851
C	1.752798	-0.386253	-3.767620
C	0.265688	-0.338398	-3.376618
H	-0.491754	0.248534	-1.364480
H	-0.302531	1.581707	-2.496063
H	-0.280287	0.129528	-4.207654
C	2.278362	-0.285220	-1.281780
H	3.191880	0.086865	-0.817570
C	2.595129	-0.977194	-2.632135
H	3.659129	-0.865820	-2.864237
H	2.403007	-2.045406	-2.535440
H	1.887287	-0.974077	-4.679018
C	2.219345	1.051263	-3.996415
H	3.221369	1.068866	-4.434628
H	1.548292	1.568156	-4.690015
C	2.240966	1.770256	-2.641091
H	3.253506	1.891233	-2.251238
H	1.772166	2.752838	-2.692725
N	3.521885	-5.129355	0.022627
N	1.475700	0.984674	-1.598217
O	6.216421	-0.686661	1.922359
C	7.507535	-0.814580	2.475594
H	8.230358	-1.182588	1.736345
H	7.798777	0.188872	2.789187
H	7.510405	-1.479686	3.348560
O	1.379057	-0.698238	0.980885
H	0.404900	-0.505417	1.081473
C	-0.391310	-1.675039	-3.128025
H	0.187947	-2.547082	-3.435250
C	-1.562523	-1.881501	-2.532369
H	-2.199682	-1.068811	-2.190452
H	-1.922833	-2.894997	-2.380381
C	1.217996	1.904074	-0.407755
H	0.594782	2.706496	-0.804405
H	0.621296	1.334137	0.296475
C	2.451378	2.468826	0.241002
C	2.958436	3.706875	-0.152793
C	3.095362	1.814018	1.295538
C	4.090639	4.254349	0.435153
C	4.237657	2.335765	1.890503
H	2.676456	0.873797	1.638049

C	4.731107	3.553237	1.450989
H	4.753278	1.802014	2.680020
F	2.363895	4.414536	-1.123569
F	4.554098	5.432895	0.026346
F	5.825365	4.084267	1.993097
C	1.558662	-1.250531	-0.296653
H	0.588532	-1.485032	-0.746536
C	-4.800349	2.997311	1.138428
C	-3.627882	2.424629	1.643905
C	-3.275654	2.675115	2.984340
C	-4.098553	3.463791	3.780488
C	-5.268941	4.022407	3.269751
C	-5.614022	3.788947	1.942394
H	-5.075670	2.814750	0.103420
H	-3.817188	3.647453	4.815192
H	-5.901750	4.636516	3.903682
H	-6.521501	4.220746	1.529789
C	-1.968942	2.109955	3.482500
H	-1.150697	2.778596	3.169677
H	-1.950779	2.080137	4.577215
C	-1.723896	0.720951	2.900480
H	-0.715014	0.369370	3.142054
H	-2.422867	0.002140	3.345753
C	-1.878891	0.718641	1.391499
C	-2.763417	1.572455	0.803544
C	-2.809596	1.757854	-0.674825
C	-2.205648	2.926814	-1.236085
C	-3.406457	0.848416	-1.537080
C	-1.578620	3.911734	-0.417239
C	-2.172942	3.121650	-2.647757
C	-3.371440	1.038163	-2.942600
C	-0.937301	4.990841	-0.967748
H	-1.606308	3.787183	0.659318
C	-1.497029	4.249389	-3.189602
C	-2.770614	2.146453	-3.479903
H	-3.825716	0.308246	-3.602053
C	-0.883111	5.161592	-2.372735
H	-0.460322	5.721177	-0.321106
H	-1.476490	4.373837	-4.269894
H	-2.750249	2.282926	-4.558266
H	-0.367631	6.019040	-2.794219
O	-4.020507	-0.224559	-0.978262
C	-4.674519	-1.169055	-1.811080
H	-5.498485	-0.702352	-2.364241



H	-3.975826	-1.652911	-2.503007
H	-5.062800	-1.935041	-1.139783
O	-1.124460	-0.132494	0.712646
C	-1.910580	-2.006224	0.478261
H	-0.905102	-2.371458	0.353740
H	-2.431245	-1.581751	-0.358478
C	-2.593438	-2.223968	1.738586
C	-1.929957	-2.862533	2.794365
C	-3.884935	-1.717479	1.936000
C	-2.549231	-2.996233	4.028154
H	-0.931362	-3.258983	2.632344
C	-4.499539	-1.847754	3.175086
H	-4.377539	-1.190934	1.126171
C	-3.834122	-2.486235	4.220099
H	-2.035223	-3.497008	4.842754
H	-5.494749	-1.442570	3.329180
H	-4.317235	-2.589127	5.187377
I	-2.481046	-4.435365	-0.939932

S-TS-C30

C	1.660408	3.230171	-1.886072
C	2.948964	2.741088	-1.497375
C	1.622528	4.290611	-2.755436
C	3.151877	1.634581	-0.646299
C	4.089547	3.436583	-1.994561
C	2.821259	4.888920	-3.215057
H	0.671072	4.683990	-3.104583
C	4.421456	1.247565	-0.269219
H	2.326956	1.020598	-0.309319
C	5.379493	3.011736	-1.596258
H	2.771694	5.727877	-3.906947
C	5.554549	1.947552	-0.748833
H	6.228219	3.560739	-1.990296
H	6.555066	1.643253	-0.463639
C	-2.031803	3.681257	0.309913
C	-0.145065	4.539493	1.695737
C	-1.329896	4.969330	0.808955
H	-2.204935	3.685166	-0.765502
H	-3.000879	3.543668	0.791388
H	-2.040821	5.509252	1.444786
C	0.219402	2.565083	0.138655
H	0.654929	1.622707	0.474515
C	0.882410	3.754192	0.877198
H	1.664577	3.366921	1.537269

H	1.374770	4.414124	0.161983
H	0.325614	5.427182	2.126630
C	-0.688848	3.627892	2.793635
H	0.084858	3.402486	3.530556
H	-1.516125	4.115325	3.320167
C	-1.156892	2.317459	2.148926
H	-0.471826	1.491337	2.344274
H	-2.149979	2.022590	2.485077
N	4.013931	4.500568	-2.845377
N	-1.229404	2.454199	0.643652
O	4.489593	0.178543	0.556137
C	5.748955	-0.374445	0.885800
H	6.367649	0.345634	1.436092
H	5.535412	-1.235846	1.518246
H	6.279315	-0.709506	-0.013087
O	0.059169	1.429007	-2.071922
H	0.456292	0.643300	-1.610561
C	-0.937802	5.890328	-0.314637
H	-1.466752	6.839451	-0.387857
C	-0.001405	5.603065	-1.213972
H	0.552956	4.667388	-1.183122
H	0.246263	6.291458	-2.016067
C	-1.874531	1.201415	0.062855
H	-1.907401	1.354430	-1.014486
H	-1.159648	0.399284	0.265488
C	-3.224857	0.850147	0.606318
C	-4.383747	1.330074	0.004194
C	-3.361397	-0.101614	1.618646
C	-5.641974	0.914870	0.411405
C	-4.608675	-0.533320	2.044277
H	-2.469376	-0.534113	2.059723
C	-5.742070	-0.021855	1.433159
H	-4.716197	-1.288493	2.813467
F	-4.304413	2.215820	-0.997488
F	-6.731641	1.401144	-0.172703
F	-6.954474	-0.413465	1.815061
C	0.333172	2.631421	-1.417105
H	-0.429913	3.334161	-1.772772
C	3.475046	-3.020975	2.393708
C	3.040323	-2.779501	1.083150
C	3.847406	-3.225316	0.014742
C	5.051070	-3.868925	0.277703
C	5.479858	-4.093878	1.585832
C	4.681620	-3.670707	2.643630

H	2.863343	-2.692917	3.229027
H	5.660772	-4.207895	-0.557205
H	6.421082	-4.602281	1.772781
H	4.994699	-3.844373	3.669439
C	3.327620	-3.037542	-1.386161
H	2.623935	-3.851449	-1.610121
H	4.140562	-3.111660	-2.116533
C	2.587888	-1.712836	-1.538010
H	2.070803	-1.672803	-2.499619
H	3.299112	-0.876463	-1.520923
C	1.577708	-1.508576	-0.430475
C	1.785897	-2.063428	0.793756
C	0.793667	-1.862500	1.885257
C	0.923438	-0.781276	2.814986
C	-0.256201	-2.742340	2.055075
C	1.977611	0.167250	2.695717
C	0.006707	-0.647619	3.897792
C	-1.178324	-2.606456	3.122258
C	2.114920	1.185918	3.606646
H	2.697243	0.050756	1.891095
C	0.175886	0.418417	4.822227
C	-1.049371	-1.587142	4.026844
H	-1.987753	-3.326969	3.188476
C	1.209600	1.310615	4.688009
H	2.939613	1.886842	3.509073
H	-0.523804	0.505427	5.649965
H	-1.753958	-1.485880	4.848415
H	1.339643	2.107545	5.415055
O	-0.472582	-3.765588	1.171602
C	0.247316	-4.956085	1.454069
H	-0.001200	-5.334603	2.454383
H	1.328649	-4.793565	1.385720
H	-0.063680	-5.687225	0.705862
O	0.534537	-0.733229	-0.684449
C	-1.066213	-1.640684	-1.425728
H	-1.271287	-2.098459	-0.471621
H	-1.459034	-0.665581	-1.644082
C	-0.511535	-2.428081	-2.515154
C	-0.121049	-3.753224	-2.300926
C	-0.289496	-1.831884	-3.762921
C	0.484511	-4.473751	-3.324136
H	-0.307548	-4.202242	-1.331049
C	0.321211	-2.551320	-4.779839
H	-0.592397	-0.800284	-3.918522

C	0.711767	-3.873267	-4.560581
H	0.781522	-5.505192	-3.158262
H	0.492154	-2.086221	-5.745879
H	1.186275	-4.437094	-5.358545
I	-3.891073	-2.166555	-1.782169

S-TS-C31

C	3.498579	0.769162	0.252575
C	4.884015	0.850339	0.596020
C	2.904126	1.881586	-0.288880
C	5.631421	-0.214308	1.151854
C	5.545748	2.087509	0.338442
C	3.655635	3.062168	-0.489008
H	1.857796	1.872854	-0.579370
C	6.972868	-0.072206	1.435615
H	5.174222	-1.166161	1.396280
C	6.922863	2.203784	0.645233
H	3.168715	3.938359	-0.914835
C	7.629654	1.157064	1.177862
H	7.399986	3.156614	0.441686
H	8.683497	1.281788	1.398133
C	2.048031	-3.380403	-0.690769
C	3.136827	-2.376490	-2.717207
C	3.081900	-3.631246	-1.815641
H	2.523874	-3.224304	0.279793
H	1.352823	-4.211300	-0.579277
H	2.733791	-4.469260	-2.431730
C	2.132436	-0.903042	-0.928018
H	1.484686	-0.116116	-1.319625
C	3.343170	-1.128182	-1.865700
H	3.459855	-0.248364	-2.503746
H	4.266224	-1.212695	-1.282975
H	3.950645	-2.484148	-3.439103
C	1.794490	-2.216522	-3.429772
H	1.766191	-1.254786	-3.951625
H	1.639590	-3.006541	-4.170895
C	0.680784	-2.270134	-2.379684
H	-0.045455	-1.467252	-2.500380
H	0.138794	-3.216146	-2.403105
N	4.927626	3.176992	-0.198255
N	1.238933	-2.151665	-0.981150
O	7.589675	-1.159543	1.960725
C	8.947269	-1.054677	2.331466
H	9.099121	-0.277581	3.091043

H	9.216106	-2.023644	2.753254
H	9.589289	-0.848326	1.465652
O	1.734103	-0.324211	1.496074
H	1.056664	0.353956	1.236166
C	4.418581	-4.003883	-1.234330
H	4.874916	-3.277183	-0.560695
C	5.055119	-5.143002	-1.488603
H	4.633534	-5.899515	-2.146926
H	6.022219	-5.361696	-1.046876
C	0.072893	-1.988459	-0.009757
H	0.478497	-2.169468	0.983862
H	-0.189440	-0.931265	-0.083657
C	-1.150998	-2.806723	-0.291897
C	-1.315861	-4.093577	0.208661
C	-2.236991	-2.219725	-0.945822
C	-2.498157	-4.796410	0.034168
C	-3.429888	-2.899483	-1.134307
H	-2.152030	-1.191781	-1.281755
C	-3.551536	-4.186506	-0.638296
H	-4.280553	-2.422634	-1.606464
F	-0.314955	-4.692869	0.873748
F	-2.620132	-6.032239	0.509419
F	-4.679981	-4.872818	-0.795401
C	2.663925	-0.495108	0.473546
H	3.322333	-1.299023	0.813483
C	-1.653685	4.519888	-2.513772
C	-1.281508	4.107604	-1.226585
C	-1.061225	5.093525	-0.243202
C	-1.186867	6.438643	-0.573217
C	-1.542203	6.836737	-1.860440
C	-1.782430	5.868728	-2.829157
H	-1.845847	3.772964	-3.279099
H	-1.011917	7.188001	0.195691
H	-1.638280	7.891887	-2.098399
H	-2.070802	6.159630	-3.835375
C	-0.770277	4.646835	1.166603
H	-1.724904	4.452308	1.675492
H	-0.270745	5.442408	1.729849
C	0.059122	3.367770	1.198261
H	0.111767	2.967697	2.212898
H	1.093417	3.583378	0.891200
C	-0.508253	2.308082	0.274461
C	-1.121401	2.680058	-0.881433
C	-1.631108	1.667437	-1.847155

C	-3.026652	1.336806	-1.873992
C	-0.809218	1.067599	-2.779789
C	-3.924458	1.858755	-0.904153
C	-3.538078	0.438059	-2.853452
C	-1.321224	0.210767	-3.784921
C	-5.240127	1.474852	-0.881129
H	-3.539872	2.555712	-0.166818
C	-4.911398	0.077657	-2.818649
C	-2.653648	-0.098049	-3.823711
H	-0.626065	-0.193818	-4.515916
C	-5.742046	0.572471	-1.847365
H	-5.903554	1.859527	-0.113315
H	-5.289075	-0.609894	-3.571906
H	-3.043425	-0.767136	-4.586189
H	-6.785467	0.275402	-1.814745
O	0.563163	1.218115	-2.753161
C	1.072083	2.406854	-3.343095
H	0.737185	3.295757	-2.800454
H	0.760885	2.482957	-4.392824
H	2.160536	2.332412	-3.288270
O	-0.335735	1.039882	0.613023
C	-1.759583	0.247281	1.723797
H	-2.478113	0.353281	0.926321
H	-1.173458	-0.653111	1.772115
C	-1.767795	1.146366	2.871506
C	-0.771230	1.031591	3.847912
C	-2.708094	2.176293	2.965350
C	-0.709118	1.943307	4.892612
H	-0.035782	0.236059	3.767399
C	-2.648603	3.084478	4.015607
H	-3.501358	2.237523	2.226222
C	-1.645369	2.974211	4.976095
H	0.068014	1.852092	5.645287
H	-3.387848	3.876563	4.087367
H	-1.598209	3.686309	5.794627
I	-3.750717	-1.618660	2.619750

S-TS-C32

C	-2.044212	2.948947	-0.565152
C	-3.400732	2.952284	-0.117517
C	-1.678890	3.884955	-1.498137
C	-3.922328	2.036963	0.823437
C	-4.278892	3.914658	-0.692791
C	-2.628171	4.812439	-1.985343

H	-0.668460	3.904895	-1.893299
C	-5.252898	2.052932	1.176676
H	-3.301340	1.270048	1.266863
C	-5.643599	3.907087	-0.312119
H	-2.323877	5.553192	-2.722706
C	-6.131846	3.001931	0.595376
H	-6.293433	4.644458	-0.771641
H	-7.183493	3.020290	0.857457
C	0.639956	0.575484	2.092088
C	-0.385547	2.414134	3.422361
C	-0.373019	0.889902	3.210398
H	0.256554	-0.076763	1.303520
H	1.532315	0.104510	2.498908
H	0.028594	0.446201	4.132328
C	-0.067452	2.659571	0.911010
H	0.391853	3.503635	0.389988
C	-0.857299	3.137658	2.158017
H	-0.739772	4.218482	2.284989
H	-1.922247	2.958304	2.009545
H	-1.042859	2.667716	4.259395
C	1.047025	2.857314	3.713458
H	1.074015	3.906602	4.021338
H	1.475699	2.264128	4.527318
C	1.867953	2.677550	2.429896
H	2.081712	3.630447	1.941659
H	2.815043	2.170633	2.611653
N	-3.883245	4.839505	-1.611340
N	1.123754	1.839669	1.415214
O	-5.636165	1.124805	2.087138
C	-7.013797	0.974416	2.360871
H	-7.579616	0.744432	1.449943
H	-7.089778	0.134513	3.051844
H	-7.432434	1.870180	2.836763
O	-0.324669	1.455100	-1.225719
H	-0.247700	0.467920	-1.144938
C	-1.746472	0.289013	3.017061
H	-2.555443	0.805143	3.535852
C	-2.020591	-0.831829	2.352696
H	-1.259101	-1.411449	1.836348
H	-3.033507	-1.221746	2.311685
C	2.119217	1.417194	0.338512
H	2.864511	0.806041	0.848417
H	1.574290	0.781710	-0.345339
C	2.791884	2.538425	-0.403079

C	4.033449	3.013145	0.017952
C	2.269147	3.059612	-1.592116
C	4.717641	3.999557	-0.679153
C	2.937791	4.046601	-2.307075
H	1.326952	2.656387	-1.949785
C	4.156928	4.514746	-1.842103
H	2.535064	4.450898	-3.228643
F	4.614770	2.522707	1.120952
F	5.895424	4.435648	-0.241214
F	4.821800	5.460180	-2.501716
C	-1.002958	1.933048	-0.098691
H	-1.499007	1.104453	0.415536
C	4.206583	-3.735219	-0.453821
C	3.452697	-2.707240	-1.030674
C	3.844780	-2.205841	-2.284289
C	4.977289	-2.713099	-2.912352
C	5.731195	-3.725023	-2.321455
C	5.336305	-4.239818	-1.090556
H	3.896555	-4.150779	0.501164
H	5.270777	-2.312184	-3.880040
H	6.610206	-4.116173	-2.824969
H	5.900059	-5.045062	-0.627875
C	2.997847	-1.114459	-2.884925
H	3.272205	-0.149026	-2.430363
H	3.177707	-1.026017	-3.961495
C	1.521808	-1.384320	-2.600602
H	0.901476	-0.554137	-2.952154
H	1.196348	-2.283035	-3.145976
C	1.282440	-1.565122	-1.111004
C	2.249573	-2.166269	-0.360163
C	2.198470	-2.242186	1.123306
C	1.158521	-2.918269	1.839470
C	3.188254	-1.609446	1.856847
C	0.179898	-3.702874	1.174700
C	1.095310	-2.829424	3.260831
C	3.166197	-1.574964	3.271987
C	-0.842157	-4.304206	1.864279
H	0.260679	-3.838094	0.102646
C	0.015482	-3.444298	3.949272
C	2.127498	-2.149636	3.956154
H	3.954624	-1.050023	3.803552
C	-0.938958	-4.153185	3.267854
H	-1.582813	-4.882488	1.319020
H	-0.033721	-3.348420	5.031350



H	2.090211	-2.100055	5.041651
H	-1.762312	-4.617977	3.801453
O	4.129146	-0.868311	1.181685
C	5.489871	-1.164449	1.441904
H	5.766677	-0.947779	2.481564
H	5.705176	-2.213112	1.212532
H	6.071206	-0.522826	0.778401
O	0.136263	-1.086839	-0.630545
C	-1.415888	-2.159249	-1.215586
H	-1.647706	-2.332760	-0.180276
H	-0.783050	-2.875976	-1.715000
C	-2.186972	-1.195408	-1.996446
C	-3.212353	-0.459454	-1.393560
C	-1.899865	-0.980593	-3.349460
C	-3.936436	0.469465	-2.129085
H	-3.466037	-0.651475	-0.354422
C	-2.606531	-0.032818	-4.076986
H	-1.129918	-1.575000	-3.832004
C	-3.626685	0.694965	-3.467645
H	-4.747457	1.016002	-1.658978
H	-2.375791	0.126354	-5.125983
H	-4.189725	1.427699	-4.037932
I	-3.233335	-4.397430	-1.361091

S-TS-C33

C	4.039003	-0.014344	-1.804697
C	4.176153	-1.358938	-1.331051
C	5.025200	0.476485	-2.621523
C	3.236883	-2.013776	-0.503211
C	5.346398	-2.070289	-1.731747
C	6.143391	-0.321072	-2.962368
H	4.955581	1.484333	-3.023191
C	3.438058	-3.317951	-0.094991
H	2.311830	-1.542327	-0.194041
C	5.527735	-3.401326	-1.287227
H	6.916882	0.084840	-3.612121
C	4.601721	-4.021786	-0.490060
H	6.426404	-3.915819	-1.610658
H	4.760951	-5.046690	-0.175601
C	2.604069	3.626593	0.154439
C	4.025238	2.384003	1.788283
C	3.771348	3.772099	1.157643
H	2.957093	3.586995	-0.877982
H	1.900970	4.454487	0.224741

H	3.465523	4.456935	1.958077
C	2.701687	1.135138	0.035039
H	2.168452	0.307382	0.508510
C	4.088295	1.329384	0.686612
H	4.414733	0.365400	1.086740
H	4.825493	1.614938	-0.068972
H	4.960153	2.401494	2.354153
C	2.839432	2.041744	2.688842
H	2.888185	0.994261	2.999832
H	2.829712	2.664488	3.588768
C	1.555053	2.279875	1.891614
H	0.828153	1.484524	2.033050
H	1.077633	3.225156	2.152425
N	6.315703	-1.544842	-2.535081
N	1.840376	2.357747	0.409121
O	2.465295	-3.856194	0.672670
C	2.519762	-5.229260	1.003888
H	3.400053	-5.458593	1.618353
H	1.612134	-5.432146	1.572288
H	2.526421	-5.854544	0.103070
O	1.706661	0.463181	-2.171947
H	1.080060	-0.082405	-1.628115
C	4.978899	4.359984	0.481800
H	5.397892	3.787888	-0.346792
C	5.545494	5.510906	0.830993
H	5.153990	6.116027	1.645809
H	6.422667	5.891896	0.317515
C	0.516863	2.325825	-0.347656
H	0.723407	2.630219	-1.372794
H	0.208502	1.278899	-0.355034
C	-0.590631	3.126456	0.272314
C	-0.800578	4.467775	-0.021799
C	-1.538563	2.481364	1.072587
C	-1.886663	5.165527	0.487800
C	-2.632281	3.154629	1.597061
H	-1.432384	1.415942	1.253891
C	-2.797176	4.498094	1.299424
H	-3.370719	2.639127	2.201126
F	0.046469	5.129760	-0.825215
F	-2.057903	6.451003	0.187400
F	-3.837448	5.180156	1.775052
C	2.843109	0.890784	-1.493449
H	3.110127	1.861070	-1.938403
C	-0.816028	-4.225793	2.442296

C	-0.757812	-3.749745	1.126956
C	-0.851015	-4.678239	0.068829
C	-0.964537	-6.034812	0.350043
C	-1.000812	-6.500254	1.664616
C	-0.932948	-5.587514	2.711593
H	-0.781472	-3.519073	3.266957
H	-1.039124	-6.740054	-0.474575
H	-1.096878	-7.563340	1.864264
H	-0.978901	-5.930548	3.741443
C	-0.886241	-4.148946	-1.343770
H	-1.918532	-3.852051	-1.586255
H	-0.604828	-4.931248	-2.056403
C	0.029840	-2.937299	-1.485244
H	-0.065169	-2.484165	-2.476556
H	1.076164	-3.248317	-1.382234
C	-0.286473	-1.901964	-0.423879
C	-0.642821	-2.311585	0.819198
C	-0.958798	-1.332551	1.892164
C	-2.322270	-1.001332	2.195016
C	0.033902	-0.749837	2.649268
C	-3.398262	-1.512961	1.421131
C	-2.621075	-0.105966	3.262436
C	-0.261102	0.101112	3.744108
C	-4.690062	-1.115463	1.655366
H	-3.193012	-2.212542	0.617062
C	-3.971571	0.262046	3.503055
C	-1.557716	0.418691	4.042371
H	0.564492	0.505476	4.324510
C	-4.981962	-0.218904	2.709074
H	-5.482347	-1.486718	1.013302
H	-4.189378	0.940787	4.324846
H	-1.786648	1.086303	4.868978
H	-6.009494	0.081502	2.890433
O	1.364199	-0.931018	2.326612
C	2.021019	-1.947419	3.070952
H	1.550925	-2.918589	2.896590
H	2.011093	-1.712423	4.144170
H	3.049699	-1.979877	2.707107
O	-0.256576	-0.621512	-0.784552
C	-2.027199	-0.443645	-1.720345
H	-1.719150	-1.214371	-2.404694
H	-2.504174	-0.725370	-0.798544
I	-4.591356	-1.500598	-2.541757
C	-2.081324	0.946028	-2.173719

C	-3.035276	1.827695	-1.649106
C	-1.177968	1.407628	-3.136380
C	-3.090129	3.143078	-2.087001
H	-3.760014	1.453582	-0.932529
C	-1.212236	2.736374	-3.548192
H	-0.428532	0.732395	-3.535793
C	-2.170559	3.604578	-3.029159
H	-3.850901	3.811659	-1.695634
H	-0.500884	3.088414	-4.289458
H	-2.209022	4.636706	-3.365591

S-TS-C34

C	2.173952	-2.845829	-0.806895
C	3.507988	-2.870503	-0.294934
C	1.886809	-3.654244	-1.876825
C	3.954989	-2.072152	0.780192
C	4.439018	-3.739205	-0.934306
C	2.887754	-4.484833	-2.431282
H	0.897517	-3.647877	-2.321933
C	5.260572	-2.124309	1.212675
H	3.302867	-1.351902	1.256692
C	5.774509	-3.774582	-0.464899
H	2.645095	-5.124066	-3.278610
C	6.186774	-2.992818	0.584616
H	6.462743	-4.444321	-0.969705
H	7.217573	-3.043443	0.916326
C	-0.735405	-0.994156	2.047462
C	0.407567	-2.888625	3.182057
C	0.277719	-1.353783	3.147761
H	-0.393277	-0.222253	1.353561
H	-1.678510	-0.663108	2.472283
H	-0.174234	-1.056591	4.104713
C	0.165491	-2.863011	0.649710
H	-0.214902	-3.671577	0.019659
C	0.960380	-3.424276	1.858153
H	0.920170	-4.518231	1.857615
H	2.011736	-3.154246	1.764231
H	1.065298	-3.187636	4.003582
C	-0.990566	-3.473597	3.375084
H	-0.936752	-4.551198	3.554549
H	-1.483200	-3.020126	4.240977
C	-1.797334	-3.204333	2.097469
H	-1.930977	-4.105060	1.495166
H	-2.781409	-2.788043	2.310417

N	4.119052	-4.540747	-1.988814
N	-1.096717	-2.200000	1.210995
O	5.579590	-1.290453	2.236196
C	6.925254	-1.222117	2.655748
H	7.588346	-0.916716	1.836622
H	6.955070	-0.465248	3.440147
H	7.272019	-2.178853	3.066774
O	0.357729	-1.393663	-1.314449
H	0.242177	-0.421588	-1.116914
C	1.598210	-0.625257	3.069811
H	2.406740	-1.090064	3.635788
C	1.833336	0.534552	2.458885
H	1.092040	1.073915	1.872415
H	2.817738	0.988057	2.519250
C	-2.096463	-1.709116	0.168887
H	-2.845515	-1.150206	0.732714
H	-1.555014	-1.011530	-0.452946
C	-2.722582	-2.775243	-0.682034
C	-3.957901	-3.321470	-0.338888
C	-2.150973	-3.171722	-1.895871
C	-4.591747	-4.261676	-1.139452
C	-2.767694	-4.110459	-2.714234
H	-1.216678	-2.704080	-2.190291
C	-3.983268	-4.653105	-2.326887
H	-2.329722	-4.418488	-3.656557
F	-4.578804	-2.946032	0.788419
F	-5.765017	-4.771033	-0.777282
F	-4.600174	-5.554539	-3.086364
C	1.063931	-1.957864	-0.244894
H	1.497955	-1.165063	0.371427
C	-4.339218	3.432312	0.230443
C	-3.598219	2.451443	-0.440181
C	-4.138737	1.878001	-1.606063
C	-5.394306	2.272550	-2.055366
C	-6.130120	3.238490	-1.371847
C	-5.594018	3.821768	-0.228175
H	-3.920256	3.902136	1.116038
H	-5.800968	1.820156	-2.957174
H	-7.106471	3.540705	-1.738724
H	-6.146329	4.591113	0.303985
C	-3.320702	0.828886	-2.315791
H	-3.484217	-0.147925	-1.833004
H	-3.644843	0.722659	-3.356344
C	-1.835256	1.178286	-2.248345

H	-1.228162	0.370269	-2.671569
H	-1.643714	2.074426	-2.856831
C	-1.394630	1.433419	-0.815435
C	-2.266219	2.033005	0.040514
C	-1.923202	2.281216	1.466300
C	-0.960533	3.268083	1.857682
C	-2.538026	1.547190	2.458444
C	-0.394403	4.171215	0.920001
C	-0.564355	3.374134	3.221749
C	-2.177518	1.674578	3.821021
C	0.570221	5.072434	1.295271
H	-0.741060	4.150037	-0.108543
C	0.441584	4.308944	3.581327
C	-1.192699	2.549717	4.190322
H	-2.669979	1.042303	4.555246
C	1.007266	5.128820	2.639202
H	1.002226	5.730624	0.547507
H	0.749325	4.368103	4.622578
H	-0.890788	2.632271	5.231146
H	1.778121	5.838597	2.923401
O	-3.433089	0.549619	2.114482
C	-4.785444	0.779608	2.481286
H	-4.890755	0.913587	3.565509
H	-5.182846	1.657447	1.962369
H	-5.339109	-0.108955	2.171223
O	-0.160603	1.047867	-0.486049
C	1.138385	2.271621	-1.343571
H	0.995373	2.962000	-0.532957
H	0.518627	2.367041	-2.219418
C	2.351891	1.463209	-1.396123
C	3.335348	1.615944	-0.410422
C	2.557852	0.545482	-2.430958
C	4.512898	0.886528	-0.477006
H	3.185914	2.355462	0.371136
C	3.733499	-0.193057	-2.491464
H	1.795431	0.421643	-3.194160
C	4.715608	-0.015768	-1.521219
H	5.273035	1.012384	0.288064
H	3.884245	-0.908463	-3.294048
H	5.632423	-0.596760	-1.566552
I	2.144281	4.736518	-2.463749
S-TS-C35			
C	-0.707973	-2.815019	0.525169

C	-1.998998	-3.373573	0.277091
C	-0.007515	-3.278927	1.608065
C	-2.858155	-2.950780	-0.761569
C	-2.455473	-4.384085	1.173311
C	-0.554045	-4.290273	2.429593
H	0.958672	-2.855908	1.859843
C	-4.113955	-3.494952	-0.912375
H	-2.583529	-2.151114	-1.437103
C	-3.746961	-4.931266	0.986952
H	0.013960	-4.651204	3.285438
C	-4.567917	-4.503010	-0.026217
H	-4.069929	-5.696606	1.684857
H	-5.553961	-4.939722	-0.136555
C	1.104394	-0.492805	-2.808774
C	0.600656	-2.790461	-3.669306
C	0.209410	-1.301847	-3.779882
H	0.542081	0.156811	-2.131585
H	1.819651	0.131175	-3.350456
H	0.472864	-0.992257	-4.800977
C	1.007008	-2.381897	-1.199454
H	1.681371	-2.930900	-0.538483
C	0.360551	-3.318765	-2.251179
H	0.770157	-4.329750	-2.160736
H	-0.710903	-3.398881	-2.060770
H	0.016185	-3.374358	-4.386291
C	2.091004	-2.909162	-3.970713
H	2.389416	-3.958626	-4.046255
H	2.331557	-2.430879	-4.925508
C	2.853715	-2.236987	-2.824372
H	3.326473	-2.963522	-2.162003
H	3.627033	-1.558069	-3.180914
N	-1.727751	-4.837535	2.232256
N	1.933015	-1.417412	-1.947308
O	-4.858598	-2.997593	-1.933920
C	-6.196438	-3.422943	-2.060199
H	-6.777926	-3.195975	-1.156968
H	-6.610327	-2.864816	-2.900799
H	-6.265501	-4.497088	-2.274781
O	0.431585	-0.708640	0.502249
H	0.001715	0.158230	0.262298
C	-1.282761	-1.096557	-3.651531
H	-1.866651	-1.817852	-4.224921
C	-1.928466	-0.149008	-2.976616
H	-1.425846	0.601324	-2.372868

H	-3.013799	-0.115487	-2.973919
C	2.809059	-0.554825	-1.035110
H	3.400102	0.080771	-1.697195
H	2.121464	0.053719	-0.467099
C	3.697932	-1.296906	-0.078026
C	4.993026	-1.665558	-0.433191
C	3.311770	-1.486909	1.253469
C	5.860582	-2.260091	0.472095
C	4.163884	-2.077546	2.177052
H	2.333267	-1.131607	1.559627
C	5.433106	-2.465980	1.777856
H	3.869884	-2.216538	3.210885
F	5.448726	-1.450502	-1.674491
F	7.084447	-2.617255	0.092239
F	6.273020	-3.038759	2.637596
C	-0.087011	-1.706823	-0.323510
H	-0.847986	-1.282212	-0.981052
C	-4.637492	2.718204	1.459935
C	-3.768805	2.690330	0.361857
C	-4.118519	3.425865	-0.785244
C	-5.305877	4.149465	-0.816130
C	-6.166980	4.161963	0.278983
C	-5.824481	3.442824	1.419949
H	-4.375516	2.166707	2.358570
H	-5.560717	4.709580	-1.713578
H	-7.091138	4.731528	0.242297
H	-6.478669	3.451060	2.287744
C	-3.179649	3.366172	-1.961749
H	-3.378467	2.446196	-2.532632
H	-3.351561	4.208874	-2.640438
C	-1.733026	3.352711	-1.477166
H	-1.040864	3.213824	-2.312845
H	-1.494147	4.321305	-1.018950
C	-1.506936	2.231405	-0.477407
C	-2.509523	1.912400	0.389063
C	-2.441564	0.766155	1.332303
C	-1.492384	0.680874	2.395987
C	-3.374711	-0.250388	1.204947
C	-0.505944	1.682051	2.592318
C	-1.498812	-0.437308	3.274803
C	-3.442450	-1.314921	2.133382
C	0.473684	1.540637	3.540345
H	-0.553119	2.561199	1.961519
C	-0.477599	-0.556890	4.253903



C	-2.518267	-1.409336	3.138936
H	-4.190913	-2.091270	2.012949
C	0.501118	0.395138	4.373013
H	1.234150	2.308257	3.657663
H	-0.484709	-1.426654	4.907183
H	-2.540728	-2.256600	3.819225
H	1.284427	0.289216	5.117811
O	-4.198805	-0.205263	0.116583
C	-5.547574	-0.566393	0.306887
H	-5.669526	-1.645601	0.472129
H	-5.985827	-0.016476	1.148451
H	-6.065744	-0.290635	-0.613144
O	-0.350825	1.583810	-0.556126
C	1.435514	2.538448	-0.242189
H	1.458548	2.034897	0.710461
H	1.764072	2.017645	-1.122195
C	1.172079	3.963963	-0.334405
C	1.297407	4.616188	-1.568242
C	0.746079	4.692419	0.781957
C	0.974202	5.958012	-1.690858
H	1.657713	4.058842	-2.428259
C	0.411324	6.035018	0.657537
H	0.691064	4.208202	1.751176
C	0.517924	6.667260	-0.579147
H	1.076963	6.455688	-2.650052
H	0.073858	6.589995	1.527028
H	0.259678	7.717541	-0.675641
I	4.285231	2.563791	0.158898

S-TS-C36

C	-1.589968	-2.490931	1.189413
C	-3.003801	-2.671949	1.299324
C	-0.802577	-2.975831	2.202163
C	-3.940401	-2.204713	0.348887
C	-3.487036	-3.336576	2.464509
C	-1.388604	-3.636059	3.305917
H	0.271702	-2.825508	2.182253
C	-5.292785	-2.378956	0.537478
H	-3.626834	-1.653904	-0.527660
C	-4.883878	-3.497635	2.630345
H	-0.750718	-4.017434	4.101248
C	-5.775791	-3.032084	1.698106
H	-5.223976	-4.001435	3.528956
H	-6.838753	-3.170302	1.859063

C	-0.216909	-1.417910	-2.945607
C	-1.424221	-3.605589	-3.033671
C	-1.474787	-2.129658	-3.482653
H	-0.420488	-0.521059	-2.357577
H	0.454058	-1.125167	-3.756541
H	-1.400931	-2.143179	-4.579215
C	-0.291552	-2.832374	-0.891020
H	0.400459	-3.426857	-0.288925
C	-1.408671	-3.714260	-1.508290
H	-1.268205	-4.758619	-1.213156
H	-2.376955	-3.408353	-1.112815
H	-2.292609	-4.136455	-3.434466
C	-0.131688	-4.217819	-3.563618
H	-0.109061	-5.294786	-3.374951
H	-0.047109	-4.072972	-4.645297
C	1.039072	-3.541297	-2.840172
H	1.521701	-4.203381	-2.119498
H	1.803400	-3.191493	-3.532638
N	-2.677712	-3.817889	3.449421
N	0.584756	-2.331352	-2.052732
O	-6.099382	-1.888789	-0.442580
C	-7.492950	-1.885211	-0.225129
H	-7.757442	-1.326253	0.681682
H	-7.930546	-1.389564	-1.092563
H	-7.897734	-2.902809	-0.154177
O	0.068424	-0.912007	0.601650
H	0.030848	-0.008873	0.181801
C	-2.789995	-1.462310	-3.162824
H	-3.657910	-2.060693	-3.442326
C	-2.995826	-0.252760	-2.649682
H	-2.211779	0.423605	-2.320478
H	-4.006097	0.114865	-2.506382
C	1.829675	-1.550687	-1.640080
H	2.298711	-1.278280	-2.588276
H	1.460489	-0.642631	-1.180124
C	2.825773	-2.266923	-0.772461
C	3.895455	-2.946555	-1.358620
C	2.827126	-2.143455	0.621455
C	4.900137	-3.528355	-0.602849
C	3.833133	-2.704350	1.397976
H	2.035832	-1.571302	1.091987
C	4.859048	-3.399611	0.782201
H	3.856769	-2.559439	2.471174
F	3.988082	-3.046524	-2.696790

F	5.894637	-4.182196	-1.198293
F	5.835314	-3.954181	1.493654
C	-0.899953	-1.743025	0.044763
H	-1.639669	-1.157475	-0.511469
C	-3.074419	4.449206	0.075325
C	-2.267856	3.742002	-0.825052
C	-2.297375	4.104850	-2.186013
C	-3.119559	5.144302	-2.606293
C	-3.921775	5.839081	-1.702878
C	-3.895354	5.486202	-0.357655
H	-3.047037	4.187919	1.129569
H	-3.134398	5.412846	-3.660677
H	-4.556956	6.649661	-2.047863
H	-4.507340	6.024206	0.360918
C	-1.467662	3.303328	-3.159276
H	-2.051908	2.425891	-3.477559
H	-1.267102	3.887318	-4.064361
C	-0.159437	2.830631	-2.529021
H	0.344710	2.102489	-3.173146
H	0.535850	3.673663	-2.416207
C	-0.390661	2.194078	-1.173129
C	-1.393991	2.644627	-0.373144
C	-1.607038	2.051138	0.976185
C	-0.785739	2.414653	2.089690
C	-2.607134	1.126211	1.179465
C	0.168331	3.462719	1.999125
C	-0.926562	1.735057	3.330980
C	-2.787402	0.480820	2.426453
C	0.997782	3.756761	3.050871
H	0.230294	4.019695	1.069520
C	-0.050549	2.057761	4.400483
C	-1.945726	0.758529	3.467472
H	-3.571306	-0.262855	2.527729
C	0.903169	3.031183	4.260601
H	1.742994	4.540373	2.955425
H	-0.146119	1.510601	5.334959
H	-2.055246	0.235840	4.413985
H	1.587748	3.251833	5.072809
O	-3.408954	0.774488	0.118712
C	-4.773010	1.120227	0.267937
H	-5.206482	0.677989	1.174216
H	-4.892623	2.210113	0.296356
H	-5.295266	0.708912	-0.597734
O	0.425617	1.195989	-0.840466

C	2.137904	1.591496	0.054995
H	1.647143	1.946966	0.945493
H	2.374427	0.544677	-0.000669
C	2.737894	2.520729	-0.898136
C	3.305189	2.040986	-2.083441
C	2.676463	3.900987	-0.683677
C	3.779055	2.921385	-3.045919
H	3.379389	0.968124	-2.239337
C	3.151361	4.784090	-1.645670
H	2.276257	4.273537	0.252916
C	3.694710	4.296875	-2.832724
H	4.220861	2.538666	-3.961242
H	3.101195	5.853918	-1.467914
H	4.064872	4.987550	-3.584563
I	4.303016	1.338395	1.928204

S-TS-C37

C	1.385677	3.308664	0.993937
C	2.799736	3.430210	0.862948
C	0.723742	4.235650	1.762512
C	3.616800	2.521328	0.139530
C	3.419541	4.544049	1.504726
C	1.440176	5.289583	2.366705
H	-0.345658	4.152641	1.925740
C	4.966127	2.738208	0.016475
H	3.209963	1.639535	-0.341125
C	4.821875	4.727617	1.372363
H	0.908639	6.022184	2.971740
C	5.579050	3.853806	0.642209
H	5.259052	5.591043	1.862745
H	6.647207	4.002344	0.517237
C	-0.737956	0.709500	-2.018169
C	0.320194	2.639295	-3.196095
C	0.367542	1.111947	-3.024295
H	-0.396361	0.055651	-1.210134
H	-1.557114	0.191005	-2.517532
H	0.074567	0.672538	-3.988311
C	-0.314779	2.833929	-0.744674
H	-0.902313	3.632485	-0.289308
C	0.597256	3.368993	-1.876597
H	0.438183	4.443509	-2.010384
H	1.641947	3.240347	-1.589898
H	1.041972	2.954649	-3.953702
C	-1.097013	3.004562	-3.635595

H	-1.159464	4.065889	-3.893213
H	-1.383315	2.434122	-4.524809
C	-2.059824	2.705446	-2.475766
H	-2.447051	3.617044	-2.018467
H	-2.912457	2.104689	-2.794810
N	2.734855	5.460217	2.242233
N	-1.374844	1.924965	-1.378931
O	5.713334	1.897120	-0.751492
C	6.524443	0.989016	-0.012651
H	5.903422	0.337770	0.611141
H	7.046057	0.375565	-0.747085
H	7.252510	1.527963	0.609085
O	-0.127245	1.551222	1.398879
H	-0.154363	0.570355	1.198306
C	1.706300	0.504983	-2.682825
H	1.673651	-0.545219	-2.388297
C	2.897937	1.089054	-2.783104
H	3.026327	2.125205	-3.088557
H	3.801262	0.538532	-2.535447
C	-2.409252	1.438844	-0.346573
H	-2.626153	0.400730	-0.600887
H	-1.897243	1.468915	0.611630
C	-3.699789	2.206217	-0.296144
C	-3.825732	3.371033	0.455680
C	-4.842396	1.727155	-0.944313
C	-5.030786	4.053641	0.554852
C	-6.061210	2.389489	-0.857997
H	-4.759994	0.808789	-1.517997
C	-6.146151	3.551246	-0.106381
H	-6.949169	2.017179	-1.355534
F	-2.768494	3.880636	1.100577
F	-5.113751	5.167553	1.274416
F	-7.295970	4.212481	-0.002053
C	0.570168	2.183591	0.364627
H	1.235793	1.475014	-0.139670
C	-3.110490	-4.827019	0.766630
C	-2.697818	-3.604750	1.311090
C	-3.085912	-3.284626	2.626928
C	-3.854465	-4.181913	3.359388
C	-4.256979	-5.398221	2.810223
C	-3.883588	-5.715566	1.508372
H	-2.815404	-5.084179	-0.247175
H	-4.145368	-3.923613	4.375332
H	-4.856550	-6.088728	3.395792

H	-4.187556	-6.660490	1.067036
C	-2.686241	-1.934351	3.165989
H	-3.398191	-1.178851	2.794890
H	-2.752095	-1.917175	4.258994
C	-1.284261	-1.553034	2.701658
H	-1.051645	-0.519621	2.978014
H	-0.532871	-2.182062	3.197565
C	-1.142712	-1.706174	1.200355
C	-1.871353	-2.653577	0.544065
C	-1.742210	-2.791055	-0.936072
C	-0.661012	-3.554716	-1.490495
C	-2.587800	-2.143750	-1.815436
C	0.188899	-4.336771	-0.661727
C	-0.392925	-3.523180	-2.886772
C	-2.360578	-2.160277	-3.214211
C	1.279264	-4.986427	-1.180971
H	-0.034971	-4.396571	0.398728
C	0.744865	-4.203573	-3.394885
C	-1.272295	-2.803328	-3.735318
H	-3.064068	-1.628619	-3.848365
C	1.573651	-4.905549	-2.561213
H	1.933663	-5.556157	-0.529105
H	0.953588	-4.144976	-4.460016
H	-1.084477	-2.790507	-4.805862
H	2.459664	-5.394847	-2.951038
O	-3.644916	-1.343611	-1.434400
C	-4.616233	-1.872508	-0.539289
H	-4.716356	-2.953924	-0.664888
H	-4.358746	-1.657976	0.500852
H	-5.564077	-1.386563	-0.787709
O	-0.281334	-0.901830	0.591536
C	1.622281	-1.469442	0.447189
H	1.806759	-0.526073	-0.039298
H	1.339979	-2.307632	-0.166723
C	1.957151	-1.644794	1.855183
C	1.945287	-2.921179	2.428750
C	2.209526	-0.529895	2.662110
C	2.166358	-3.078930	3.790501
H	1.782552	-3.785430	1.792556
C	2.425444	-0.688493	4.024402
H	2.218165	0.462961	2.222176
C	2.399829	-1.961553	4.591606
H	2.159874	-4.071969	4.229135
H	2.615158	0.182024	4.644749

H	2.570114	-2.084878	5.657042
I	4.146301	-2.104614	-0.719462