

Supporting Information

**Mechanisms and Origins of Stereoselectivity in NHC-Catalyzed Oxidative
Reaction of Enals and Pyrroles: A Density Functional Theory Study**

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1. Computational Details

1.1 Global reactivity indexes (GRI) analysis

To disclose the role of the NHC, we performed the global reactivity index (GRI) analyses. The molecular global electrophilicity character is described with the electrophilicity index ω , which can be calculated from the expression $\omega = (\mu^2/2\eta)$ (eV), in which μ and η are the electronic chemical potential and the chemical hardness, respectively. The values of μ and η can be calculated from the following expressions $\mu \approx (E_H + E_L)/2$ and $\eta \approx (E_H - E_L)$, in which E_H is and E_L are the one-electron energies of the frontier molecular orbital HOMO and LUMO, respectively. Within the Kohn–Sham scheme, Domingo and coworkers introduce relative nucleophilicity index N , defined as $N = E_H(\text{Nu}) - E_H(\text{TCE})$. This nucleophilicity scale takes tetracyanoethylene (TCE) as a reference.

1.2 Distortion-interaction analysis

In distortion-interaction analysis, the transition state was divided into two fragments, followed by single point energy calculations on each fragment. The activation energy ΔE^\ddagger was divided into $\Delta E_{\text{dist}}^\ddagger$ and $\Delta E_{\text{int}}^\ddagger$, where $\Delta E_{\text{dist}}^\ddagger$ and $\Delta E_{\text{int}}^\ddagger$ are distortion energy and interaction energy, respectively. The distortion energy $\Delta E_{\text{dist}}^\ddagger$ of each fragment is the energy difference between the distorted fragment and the corresponding optimized structure without the other fragment. The interaction energy $\Delta E_{\text{int}}^\ddagger$ can be calculated using $\Delta E_{\text{int}}^\ddagger = \Delta E^\ddagger - \Delta E_{\text{dist}}^\ddagger$.

1.3 Calculation of enantiomeric excess (ee)

The extent of enantioselectivity, in terms of enantiomeric excess (ee %), was calculated by using the Boltzmann distribution of diastereomeric transition states with the following equations:

$$\frac{[R]}{[S]} = \frac{\exp(-G_{[R]}^\ddagger)}{\exp(-G_{[S]}^\ddagger)} = \exp(\Delta G^\ddagger / RT) \quad (1)$$

$$ee = \frac{[R]-[S]}{[R]+[S]} \times 100\% = \frac{\frac{[R]}{[S]} - 1}{\frac{[R]}{[S]} + 1} \times 100\% \quad (2)$$

Where G^\ddagger is the Gibbs free energy barrier of the competing diastereomeric transition state and ΔG^\ddagger is the Gibbs free energy difference between the two diastereomeric transition states.

2. Test results of computational methods

Table S1 Different computational levels for single-point energies.

Level	Functional	Basis set	Solvent model
L1	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
L2	M06-2X-D3	6-311++G(2df,2pd)	SMD
L3	ω B97X-D	6-311++G(2df,2pd)	IEFPCM
L4	M06-2X-D3	6-311++G(d,p)	IEFPCM
L5	M06-2X	6-31G(d,p)	IEFPCM
L6	M06-2X-D3	def2-TZVP	IEFPCM

It should be noted that the single-point energies of L1~L5 were based on the geometries optimized at IEF-PCM(toluene)M06-2X/6-31G(d,p) level, and the single-point energy of L6 was based on the geometries optimized at IEF-PCM(toluene)M06-2X/def2-SVP level.

Table S2 Relative energies (kcal/mol) at different computational levels.

	L1	L2	L3	L4	L5	L6
TS4RR	3.7	3.9	2.8	3.9	3.4	7.1
TS4RS	0.0	0.0	0.0	0.0	0.0	0.0
TS4SR	3.6	2.7	2.0	3.7	4.1	4.1
TS4SS	6.6	5.3	3.7	7.0	7.5	8.1

3. Additionally computational results

Fig. S1 The deprotonation of **Pre-NHC** to generate **NHC**. Energies and distances are given in kcal/mol and Å, respectively.

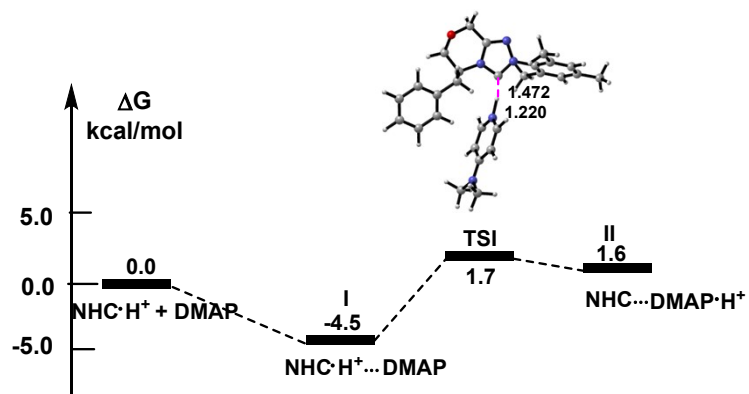


Fig. S2 The deprotonation of **Pre-R2** to generate **R2**. Energies and distances are given in kcal/mol and Å, respectively.

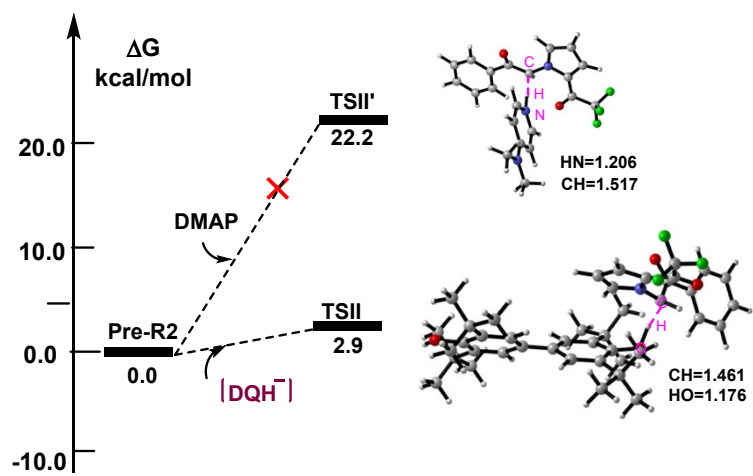
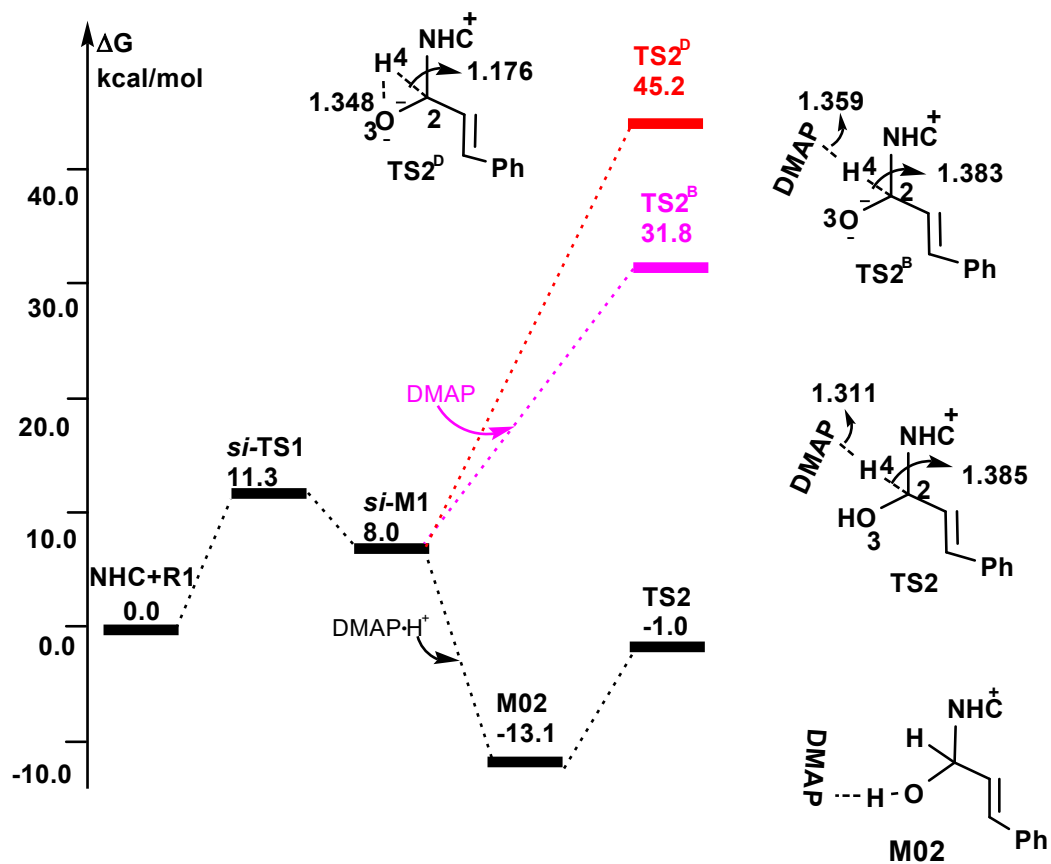


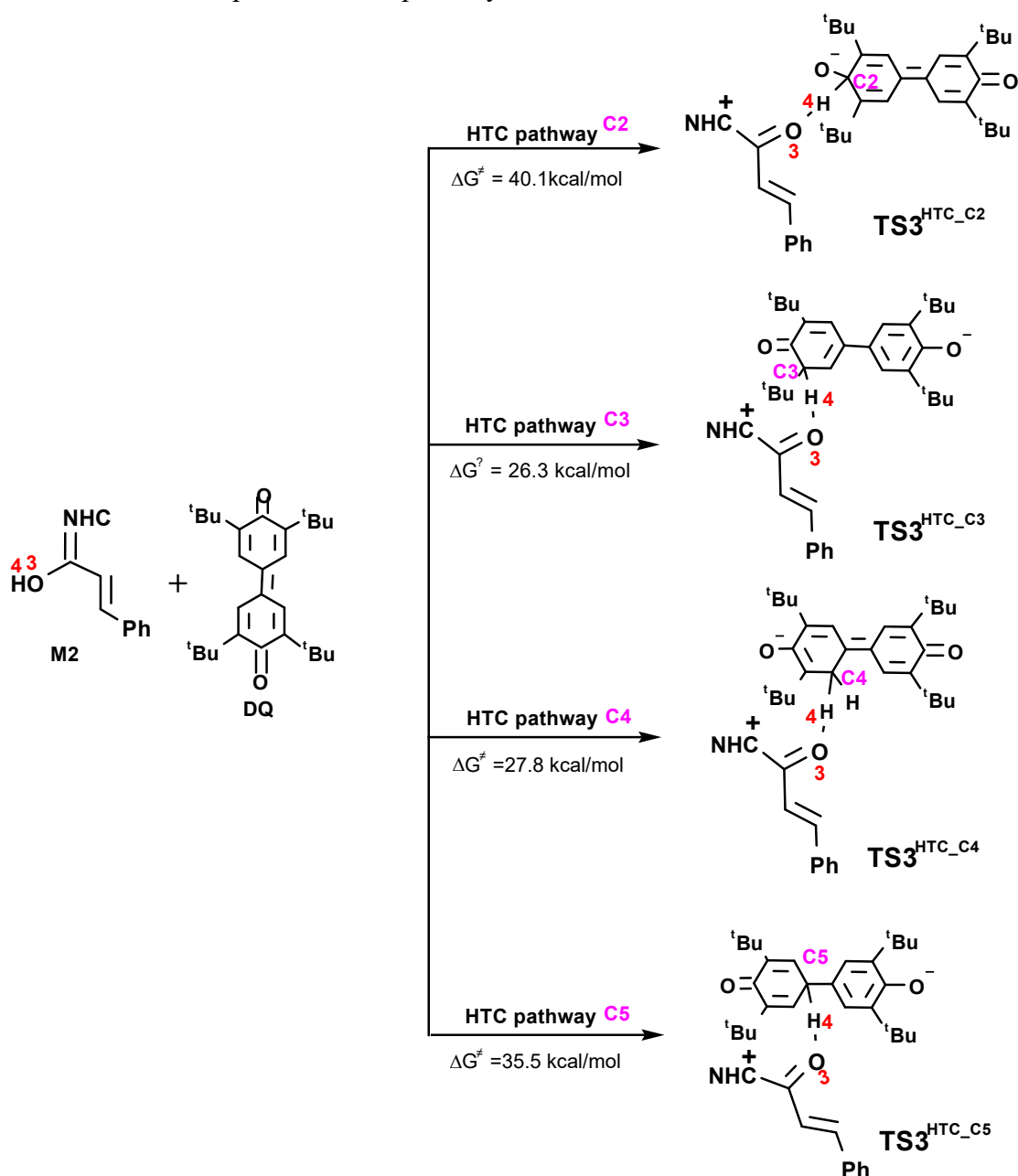
Fig. S3 Possible pathways for [1,2]-proton transfer. Energies and distances are given in kcal/mol and Å, respectively.



4. Possible pathways for the oxidation process (M2 → M3).

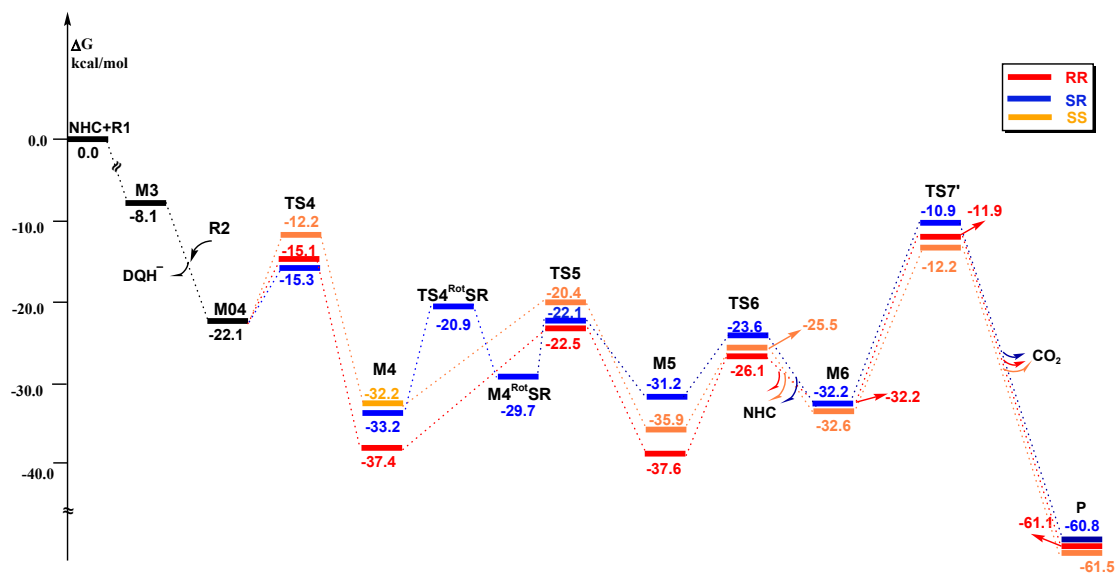
As presented in Scheme S1, four possible HTC pathways corresponding to the hydride H4 transfers from the O3 atom to four different types of carbon atoms (C2, C3, C4 and C5) of DQ have been investigated. The energy barriers are calculated to be 40.1 (TS3^{HTC_C2}), 26.3 (TS3^{HTC_C3}), 27.8 (TS3^{HTC_C4}) and 35.5 (TS3^{HTC_C5}), which are much higher than the HTO pathway (TS3, 12.3 kcal/mol). Therefore, the HTC pathways can be ruled out.

Scheme S1. Other possible HTC pathways.



5. Unfavorable pathways for the reaction of M3 and R2.

Fig. S4 Unfavorable pathways for the reaction of M3 and R2. Energies are given in kcal/mol.



It should be noted that TS7' (*i.e.* TS7RR', TS7SR' and TS7SS') corresponds to the transition state for direct decarboxylation of M6.

6. Conformational search of TS4.

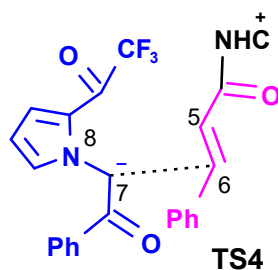
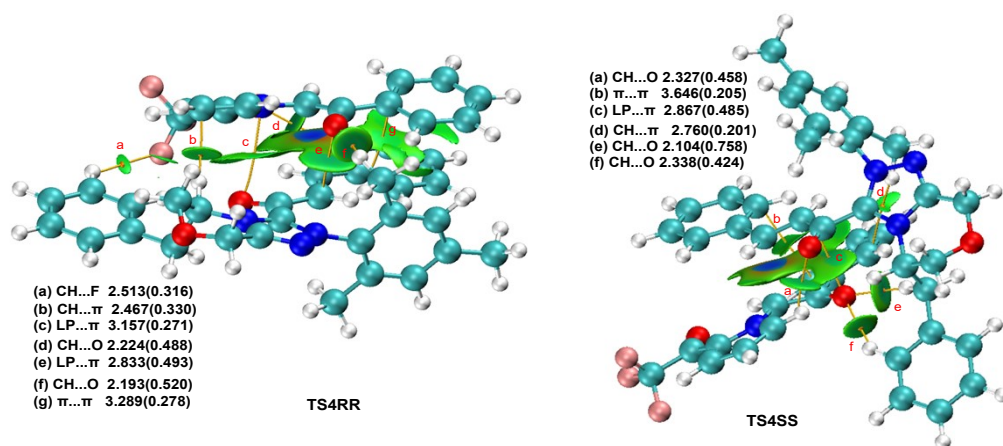


Table S3. Energies of different conformations of the stereoselective transition states.

species	Dihedral angle C5-C6-C7-N8	Free energies (a.u.)	relative energies (kcal/mol)
TS4RR	-71.75	-2518.7413179	0.0
TS4RR'	-144.61	-2518.7400772	0.8
TS4RR''	70.25	-2518.7413504	0.0
TS4RR'''	131.03	-2518.7365735	3.0
TS4RS	78.63	-2518.7472606	0.0
TS4RS'	-47.74	-2518.7424075	3.0
TS4RS''	-98.36	-2518.7320108	9.6
TS4RS'''	171.53	-2518.7397611	4.7
TS4SR	54.56	-2518.7415346	0.0
TS4SR'	38.43	-2518.7321354	5.9
TS4SR''	146.22	-2518.7271208	9.0
TS4SR'''	-145.41	-2518.7353066	3.9
TS4SS	74.23	-2518.7384829	0.0
TS4SS'	110.06	-2518.7366673	1.1
TS4SS''	147.24	-2518.7235251	9.4
TS4SS'''	-9.15	-2518.7217146	10.5

7. NCI and AIM analyses for TS4RR and TS4SS.

Fig. S5 NCI and AIM analyses for **TS4RR** and **TS4SS** (isosurface = 0.008). Distances are given in Å. The Laplacian of electron density ($\nabla^2\rho$, 10^{-1} a.u.) are given in parentheses. The blue, green, and red regions represent strong, weak, and repulsive interactions, respectively.



8. Coordinates

DMAP

C	-1.94847700	1.12920100	0.00155900
C	-0.56426000	1.19695200	0.00115300
C	0.18374300	0.00025300	0.00016500
C	-0.56360700	-1.19681600	-0.00018000
C	-1.94785600	-1.12980000	0.00034200
H	-2.52001600	2.05558200	0.00229500
H	-0.08253100	2.16624300	0.00192200
H	-0.08130600	-2.16584300	-0.00104900
H	-2.51888600	-2.05649400	0.00000800
C	2.26934200	-1.25736600	0.00014800
C	2.26936000	1.25821900	-0.00242700
H	2.03473300	-1.85553200	-0.88866900
H	3.33963100	-1.05569200	0.00171300
H	2.03237000	-1.85583800	0.88808300
H	2.03058300	1.85658000	-0.88993900
H	2.03668900	1.85653500	0.88680800
H	3.33963200	1.05649000	-0.00621000
N	1.54947100	0.00042500	-0.00031100
N	-2.66387600	-0.00049300	0.00115000

DMAP·H⁺

C	1.87814500	1.17875300	-0.00170300
C	0.51514300	1.21653700	-0.00116000
C	-0.23553100	0.00017900	0.00008300
C	0.51480300	-1.21639100	0.00082900
C	1.87781900	-1.17900200	0.00024300
H	2.48603700	2.07424100	-0.00264100
H	0.02870700	2.18125000	-0.00171200
H	0.02807400	-2.18095600	0.00197700
H	2.48546400	-2.07465800	0.00077900
C	-2.30504500	-1.26291500	0.00188200
C	-2.30465400	1.26388700	0.00041800
H	-2.06899000	-1.84821100	0.89511900
H	-3.37081200	-1.04914200	0.00123800
H	-2.06842700	-1.85025600	-0.88984400
H	-2.06769500	1.85046800	0.89256300
H	-2.06857300	1.84979500	-0.89240000
H	-3.37048500	1.05044400	0.00099000
N	-1.56888200	0.00037200	0.00055100
N	2.54208500	-0.00021500	-0.00104400
H	3.55404000	-0.00034600	-0.00139100

NHC·H⁺

C	8. 17762700	-0. 11167400	-2. 94086300
C	9. 56065000	0. 39821200	-2. 53008500
H	7. 75930100	-0. 75164800	-2. 15867900
H	9. 53506200	0. 80639100	-1. 51036600
N	7. 32643400	1. 10014400	-3. 03452300
O	9. 98808400	1. 38164400	-3. 45563600
C	7. 82428600	2. 36055100	-3. 24854600
C	9. 30729000	2. 60233400	-3. 28463200
H	9. 55589200	3. 25091500	-4. 12570400
H	9. 60793600	3. 10041700	-2. 35250200
N	6. 85825500	3. 23150100	-3. 35684300
C	5. 99495000	1. 21856600	-3. 03222600
N	5. 72352400	2. 49937500	-3. 21732000
C	4. 41983400	3. 11306300	-3. 27814600
C	3. 94234400	3. 50219600	-4. 53147500
C	3. 71950100	3. 29719900	-2. 08442500
C	2. 68205100	4. 09312900	-4. 56672000
C	2. 46271700	3. 89034800	-2. 17977000
C	1. 93114300	4. 29353000	-3. 40637400
H	2. 27750800	4. 40543500	-5. 52553500
H	1. 88857500	4. 04858700	-1. 27075300
H	10. 27808800	-0. 42190000	-2. 56878900
C	8. 17374200	-0. 82492400	-4. 30286000
H	7. 14129100	-1. 09333100	-4. 55336200
H	8. 52556200	-0. 11281800	-5. 05575200
C	9. 05216100	-2. 05191400	-4. 29137100
C	8. 58350700	-3. 25857200	-3. 76704100
C	10. 36125300	-1. 98225500	-4. 77401900
C	9. 40814500	-4. 37940300	-3. 73017500
H	7. 56321600	-3. 32617000	-3. 39688000
C	11. 18737800	-3. 10240600	-4. 73802800
H	10. 73219700	-1. 04364000	-5. 17910000
C	10. 71124400	-4. 30280400	-4. 21639500
H	9. 03123800	-5. 31412000	-3. 32832700
H	12. 20024400	-3. 03783300	-5. 12139300
H	11. 35214200	-5. 17773300	-4. 19280100
C	0. 58464800	4. 96312900	-3. 47119200
H	0. 68980900	6. 04115900	-3. 31347700
H	0. 11456800	4. 81412500	-4. 44516900
H	-0. 08497800	4. 57959100	-2. 69869300
C	4. 75847600	3. 29668600	-5. 77917600
H	5. 63463500	3. 95154200	-5. 78363900
H	5. 11753000	2. 26539200	-5. 85791200

H	4. 16242200	3. 51693700	-6. 66512600
C	4. 29336300	2. 88134000	-0. 75483800
H	4. 26088300	1. 79488700	-0. 62200900
H	5. 33406500	3. 20234900	-0. 65270400
H	3. 72106300	3. 32777200	0. 05890200
H	5. 26783000	0. 42979000	-2. 90150800
I			
C	2. 00305500	-0. 16790600	0. 18322900
C	3. 43684000	0. 04132700	0. 67834000
H	1. 43236700	-0. 75453000	0. 90944600
H	3. 44471700	0. 29325100	1. 74765100
N	1. 39268800	1. 17807500	0. 13190100
O	4. 06304100	1. 06386300	-0. 07650700
C	2. 08877300	2. 35824300	0. 15632000
C	3. 58572700	2. 34219100	0. 27465800
H	4. 02203200	3. 06869800	-0. 41157700
H	3. 87293700	2. 60671100	1. 30193100
N	1. 27830900	3. 37710100	0. 08480900
C	0. 09858600	1. 49499500	0. 01095600
N	0. 03956600	2. 81752400	-0. 00696700
C	-1. 14889000	3. 62541100	-0. 07850900
C	-1. 24355300	4. 57332700	-1. 10504300
C	-2. 15268200	3. 41812500	0. 87286100
C	-2. 40215000	5. 34255700	-1. 14895800
C	-3. 29114900	4. 21841800	0. 77605100
C	-3. 43179700	5. 18501600	-0. 21790900
H	-2. 50595500	6. 08256800	-1. 93818400
H	-4. 08544600	4. 08240000	1. 50473900
H	4. 00762100	-0. 87579400	0. 52496800
C	1. 92793100	-0. 82808400	-1. 19951100
H	0. 89278600	-0. 76321300	-1. 55504100
H	2. 56318100	-0. 26374300	-1. 88957500
C	2. 35359400	-2. 27468500	-1. 12596200
C	1. 51196300	-3. 20795800	-0. 51400400
C	3. 58372000	-2. 69772700	-1. 63100500
C	1. 88890200	-4. 54259700	-0. 41462900
H	0. 55148200	-2. 88548100	-0. 12096800
C	3. 96332400	-4. 03536500	-1. 53279600
H	4. 24402800	-1. 97824200	-2. 10857100
C	3. 11727800	-4. 95945700	-0. 92553300
H	1. 22053600	-5. 25640000	0. 05814400
H	4. 91950000	-4. 35474600	-1. 93381100
H	3. 41307600	-6. 00070700	-0. 85254200
C	-4. 65678400	6. 05769000	-0. 28319500

H	-4.43224100	7.05982300	0.09462500
H	-5.00637000	6.16613000	-1.31263100
H	-5.46990600	5.64658000	0.31749500
C	-0.15762100	4.75630900	-2.13267100
H	0.69354300	5.29820700	-1.71334900
H	0.21566800	3.79510100	-2.49775200
H	-0.54103000	5.32036700	-2.98370400
C	-2.04680000	2.38058000	1.96294100
H	-2.28347000	1.37801600	1.58803200
H	-1.04486700	2.35128700	2.40106500
H	-2.75539000	2.60783600	2.76024600
H	-0.71689300	0.76023700	-0.03538000
C	-1.89077500	-1.88438000	-0.71388300
C	-2.16629000	-3.22439300	-0.52334800
C	-1.95864500	-3.80403900	0.75212800
C	-1.48601200	-2.93023600	1.76203200
C	-1.24921700	-1.60495200	1.45104400
H	-2.04414600	-1.44371300	-1.69605100
H	-2.53211300	-3.80930300	-1.35657300
H	-1.30658800	-3.27653500	2.77106400
H	-0.88642100	-0.93267000	2.22835500
C	-1.96925600	-5.66306800	2.31929700
C	-2.66362600	-5.97615600	-0.08330400
H	-2.59846900	-5.16491000	3.06495300
H	-2.22025700	-6.72193400	2.31448800
H	-0.92102100	-5.55933600	2.62220000
H	-3.63422800	-5.64074500	-0.46470000
H	-1.95003000	-5.99917700	-0.91452000
H	-2.77772500	-6.98929300	0.29728500
N	-2.19187000	-5.11738800	0.99082000
N	-1.42778400	-1.05886300	0.23832700

TSI

C	7.87892800	0.04444900	-3.04604300
C	9.33189600	0.41900400	-2.74582500
H	7.45913300	-0.52907500	-2.21270300
H	9.42750500	0.80374400	-1.72074200
N	7.13554400	1.30766700	-3.13536000
O	9.77679400	1.38547600	-3.68130800
C	7.71508700	2.52988200	-3.35516700
C	9.20907500	2.65516200	-3.43611000
H	9.48981600	3.31282700	-4.25956600
H	9.59251800	3.08041600	-2.49812100
N	6.80706000	3.45752800	-3.43525200

C	5. 79071900	1. 45583400	-3. 08964300
N	5. 63286800	2. 76959000	-3. 26751200
C	4. 37978400	3. 46988500	-3. 30875000
C	3. 94405600	3. 97632100	-4. 53610600
C	3. 65143000	3. 61029900	-2. 12552500
C	2. 72006600	4. 64152800	-4. 55641600
C	2. 43207800	4. 28176100	-2. 19968800
C	1. 95320900	4. 80448100	-3. 40161500
H	2. 35551800	5. 04017200	-5. 49975600
H	1. 84566000	4. 40551700	-1. 29262600
H	9. 96934900	-0. 46036500	-2. 85479500
C	7. 73076500	-0. 74850000	-4. 35458600
H	6. 67841800	-0. 71666700	-4. 65929600
H	8. 31694700	-0. 24323800	-5. 12933300
C	8. 16366500	-2. 18238200	-4. 17964600
C	7. 27828400	-3. 10414300	-3. 61296600
C	9. 44536800	-2. 60680400	-4. 53417400
C	7. 66474100	-4. 42314600	-3. 40308600
H	6. 27380500	-2. 78273600	-3. 34329300
C	9. 83615100	-3. 92771600	-4. 32356400
H	10. 13792700	-1. 89983500	-4. 98489500
C	8. 94773800	-4. 83751300	-3. 75704300
H	6. 96396600	-5. 12925300	-2. 96788100
H	10. 83391000	-4. 24612200	-4. 60696800
H	9. 25172400	-5. 86652600	-3. 59617600
C	0. 64845700	5. 55576100	-3. 44634200
H	0. 81321200	6. 62088900	-3. 25545300
H	0. 17343900	5. 46484300	-4. 42560300
H	-0. 04637500	5. 18734900	-2. 68850600
C	4. 76669200	3. 80488200	-5. 78511900
H	5. 66974900	4. 42019300	-5. 74452400
H	5. 08910600	2. 76569400	-5. 90761400
H	4. 19085600	4. 09303800	-6. 66561600
C	4. 15864700	3. 05840400	-0. 81855600
H	4. 07284000	1. 96706800	-0. 78729800
H	5. 21176700	3. 31027800	-0. 66469400
H	3. 58281600	3. 46492200	0. 01414500
H	4. 91162700	0. 28464500	-2. 93783400
C	3. 86690600	-1. 35837400	-3. 99424100
C	3. 35638500	-2. 63176000	-4. 02676800
C	3. 34191400	-3. 41344100	-2. 83743300
C	3. 87154500	-2. 79989500	-1. 66751800
C	4. 35969300	-1. 51807900	-1. 73605300
H	3. 89669600	-0. 73767300	-4. 88522400

H	2.97491400	-3.01774700	-4.96170000
H	3.89901100	-3.32106700	-0.72067000
H	4.77654500	-1.02454600	-0.86249800
C	2.86956000	-5.43739700	-1.58355400
C	2.33222000	-5.26424500	-4.04231400
H	2.28365400	-4.93859400	-0.80530300
H	2.42909500	-6.41412100	-1.77076900
H	3.89205000	-5.58313400	-1.21936200
H	1.48870000	-4.68520800	-4.43098400
H	3.10636500	-5.32875600	-4.81382300
H	1.98336400	-6.27037700	-3.82077900
N	2.85741500	-4.66702900	-2.82055400
N	4.36313800	-0.80375900	-2.87454100

I

C	2.29113400	-0.05694900	0.29417300
C	3.74291000	0.29030700	0.63010100
H	1.85163900	-0.64434200	1.10739200
H	3.82120900	0.65512500	1.66410300
N	1.56296500	1.21351500	0.21707900
O	4.22307000	1.26624700	-0.27731200
C	2.16569100	2.42977800	0.02472100
C	3.66204400	2.53835300	-0.02620700
H	3.96678400	3.20439900	-0.83419800
H	4.03269300	2.94623100	0.92466800
N	1.27431800	3.37157100	-0.05806800
C	0.21368900	1.37122100	0.24123500
N	0.08739100	2.69417700	0.08011100
C	-1.14998300	3.41866300	0.02169800
C	-1.54658700	3.95533700	-1.20653400
C	-1.90422000	3.55906100	1.18884100
C	-2.75256300	4.65169600	-1.24502400
C	-3.10555500	4.26132200	1.09750800
C	-3.54227400	4.81651700	-0.10558200
H	-3.08415200	5.07473900	-2.18994000
H	-3.71028600	4.38456400	1.99242800
H	4.37062200	-0.59574300	0.51896400
C	2.15916500	-0.82017200	-1.03318800
H	1.10978300	-0.78123500	-1.34642100
H	2.74946800	-0.29330400	-1.78993200
C	2.59939800	-2.25586100	-0.89505500
C	1.74054300	-3.18941400	-0.30667200
C	3.86514600	-2.67263900	-1.31058900
C	2.13637800	-4.51143800	-0.13634100

H	0.74825300	-2.87548200	0.01250200
C	4.26534100	-3.99686500	-1.14124600
H	4.53790400	-1.95616700	-1.77569500
C	3.40279600	-4.91814100	-0.55360000
H	1.45615600	-5.22565400	0.31786900
H	5.25045200	-4.30858500	-1.47219300
H	3.71410700	-5.94929900	-0.42443300
C	-4.82440200	5.60483400	-0.16953200
H	-4.62717500	6.67035400	-0.01501700
H	-5.30645900	5.49711200	-1.14372800
H	-5.52663600	5.28294100	0.60225500
C	-0.70027800	3.78129400	-2.43942600
H	0.21379400	4.37741100	-2.37154700
H	-0.39615900	2.73715900	-2.56487700
H	-1.25072000	4.09077100	-3.32898200
C	-1.44007700	2.97720100	2.49865900
H	-1.52646200	1.88571100	2.50143300
H	-0.39141700	3.22280000	2.68894800
H	-2.04047600	3.36692600	3.32196600
H	-0.76862300	0.05167400	0.37337800
C	-1.71435900	-1.53665800	-0.69509300
C	-2.18671900	-2.82234200	-0.70674700
C	-2.18546200	-3.58618000	0.49635200
C	-1.68669800	-2.93872200	1.66411100
C	-1.23323800	-1.64815600	1.58280300
H	-1.69144900	-0.92287900	-1.58943000
H	-2.55011200	-3.23533100	-1.63689600
H	-1.65566200	-3.44330400	2.61939700
H	-0.83734600	-1.12220100	2.44554100
C	-2.59652100	-5.60894900	1.77363600
C	-3.12495800	-5.48313700	-0.69104000
H	-3.21342700	-5.12811900	2.53868500
H	-2.99145500	-6.60542400	1.59060000
H	-1.57272100	-5.70596400	2.14889200
H	-3.98358600	-4.93561600	-1.09108700
H	-2.34318000	-5.53209200	-1.45545800
H	-3.44276400	-6.49656600	-0.45778700
N	-2.62657900	-4.85245300	0.52672600
N	-1.24338700	-0.95991500	0.42648600

NHC

C	1.89510100	0.45302400	0.54455900
C	2.53562300	1.83388800	0.41760800
H	1.98531800	0.09402600	1.57452400

H	2.17461800	2.49537000	1.21890800
N	0.47356500	0.61679400	0.24914300
O	2.23566700	2.39290700	-0.85152600
C	-0.01579000	1.66643500	-0.48778300
C	0.87996300	2.78494100	-0.93587900
H	0.67314300	3.04668500	-1.97478500
H	0.69764800	3.67075400	-0.30951500
N	-1.29455800	1.54462000	-0.66338500
C	-0.52559800	-0.26658800	0.56846500
N	-1.57408800	0.35943300	-0.00770100
C	-2.92987300	-0.09732400	0.02278800
C	-3.28311200	-1.22637100	-0.71985200
C	-3.85595900	0.60845000	0.79605400
C	-4.61213600	-1.64667700	-0.67036800
C	-5.17328400	0.15521200	0.81078400
C	-5.56963600	-0.96718300	0.08217200
H	-4.90577500	-2.52570700	-1.23942800
H	-5.90617400	0.68748400	1.41304000
H	3.62191300	1.75436900	0.48660100
C	2.50219800	-0.57601600	-0.42239400
H	1.89546500	-1.48458200	-0.35245500
H	2.40083000	-0.18251100	-1.43934900
C	3.94689500	-0.87338300	-0.11136500
C	4.28192600	-1.77674400	0.90109500
C	4.97533900	-0.22374500	-0.79895400
C	5.61380700	-2.02830300	1.21738300
H	3.48911700	-2.29166800	1.43895600
C	6.30916600	-0.47272700	-0.48533500
H	4.72312800	0.48237300	-1.58691500
C	6.63131200	-1.37634000	0.52403000
H	5.85797600	-2.73630700	2.00306600
H	7.09659300	0.03675500	-1.03190300
H	7.67027300	-1.57355800	0.76793400
C	-7.00781900	-1.41817900	0.08979800
H	-7.46969100	-1.25123500	1.06604800
H	-7.59240100	-0.86146600	-0.65013100
H	-7.09112100	-2.47996500	-0.15293400
C	-2.25766200	-1.96145000	-1.54102000
H	-1.75894300	-1.28051700	-2.23793800
H	-1.48207300	-2.38789200	-0.89929000
H	-2.72636100	-2.76371100	-2.11381500
C	-3.42951800	1.81033600	1.59595200
H	-2.54296000	1.57984900	2.19510800
H	-3.16641000	2.64343000	0.93812600

H	-4.22956100	2.13131100	2.26552200
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R1

C	-0.07762600	1.30779700	-0.00004100
C	1.12770800	0.71705600	-0.00026600
H	-0.10017400	2.39904400	0.00016500
C	-1.39223700	0.65992400	-0.00004100
C	-2.53942200	1.46362000	0.00022300
C	-1.54565300	-0.73415400	-0.00030500
C	-3.80812600	0.89418800	0.00022400
H	-2.42935200	2.54474700	0.00043100
C	-2.81157600	-1.30264300	-0.00030400
H	-0.67090700	-1.37643900	-0.00050900
C	-3.94667700	-0.49068000	-0.00004000
H	-4.68686000	1.53049900	0.00042400
H	-2.91710000	-2.38251600	-0.00051200
H	-4.93505200	-0.93876600	-0.00004200
C	2.33965200	1.54450800	-0.00023200
O	3.46865400	1.10256800	-0.00042600
H	2.15561700	2.64007600	-0.00001000
H	1.27020500	-0.35962100	-0.00048000

Pre-R2

C	-4.15915800	-0.50439200	0.16847300
C	-4.18874000	-1.62538800	1.00039500
H	-4.55591700	-2.60118000	0.71915300
C	-3.65580400	-1.25111100	2.23938800
H	-3.52756400	-1.87405500	3.11111900
C	-3.31727000	0.08891200	2.14171400
H	-2.88918100	0.76236000	2.87215200
N	-3.61556100	0.53972900	0.90003300
C	-4.60006400	-0.39805300	-1.20123100
O	-4.50097500	0.57001300	-1.93485000
C	-5.25131200	-1.67635300	-1.78262600
F	-5.65834800	-1.46932400	-3.02701800
F	-6.30580700	-2.05720900	-1.04998900
F	-4.37536100	-2.69152300	-1.78964000
C	-3.40823300	1.93204900	0.50319600
H	-3.68972800	2.04348500	-0.54243200
H	-4.02903100	2.58313000	1.12133500
C	-1.94775100	2.31846300	0.75503800
O	-1.69188100	3.11484600	1.63531400
C	-0.88014000	1.66361900	-0.05261200
C	0.44624400	1.82453700	0.36181400

C	-1.16655800	0.91955300	-1.20108100
C	1.47697600	1.23938200	-0.36020100
H	0.64506000	2.41135200	1.25251500
C	-0.12974400	0.34058900	-1.92648900
H	-2.18901100	0.80582100	-1.54871100
C	1.18839000	0.49610200	-1.50526600
H	2.50486700	1.36065100	-0.03489200
H	-0.35271200	-0.23089900	-2.82112000
H	1.99408300	0.03832900	-2.07045200

TSII

C	2.97558200	2.61611800	-0.11723800
C	1.82219000	3.33425200	-0.46921600
H	1.69329700	4.40158200	-0.36420600
C	0.89322400	2.41578000	-0.95809800
H	-0.10595000	2.61509300	-1.31591700
C	1.49501000	1.16007600	-0.88697100
H	1.10585100	0.18326500	-1.14043900
N	2.73553600	1.27751800	-0.38102500
C	4.18911100	3.12416100	0.46091900
O	5.18707600	2.51175900	0.79957000
C	4.20395700	4.65918000	0.68144400
F	5.35634600	5.04804500	1.22042900
F	3.21684900	5.04867600	1.50596100
F	4.04312500	5.32982000	-0.47086300
C	3.61299200	0.14717900	-0.14808600
H	4.32064100	0.37294200	0.64608800
H	2.79717600	-0.88263700	0.49030200
C	4.26130900	-0.35165500	-1.35106500
O	3.96099700	-0.04227000	-2.50312000
C	5.33990100	-1.38613200	-1.12439800
C	6.27642300	-1.59368800	-2.13889800
C	5.41372900	-2.15134600	0.04424900
C	7.28950200	-2.53351500	-1.98248500
H	6.18633000	-1.00320300	-3.04515500
C	6.42100500	-3.10090800	0.19485100
H	4.66274800	-2.03035800	0.82032600
C	7.36384400	-3.28922900	-0.81331100
H	8.02036100	-2.68157300	-2.77196800
H	6.46396900	-3.70031700	1.09906200
H	8.14958600	-4.02885900	-0.69141700
H	-7.70372100	-0.20040200	-1.05416500
C	-5.50337600	-1.19968200	-0.63502700
C	-4.17507100	-1.51489900	-0.34017500

C	-3.25816900	-0.56089300	0.09947200
C	-3.70354100	0.75543500	0.24244700
C	-5.01572800	1.14117000	-0.02614500
C	-5.90527600	0.14082600	-0.46673200
H	-3.83385800	-2.53961000	-0.42588400
H	-2.97952300	1.49824700	0.55657500
C	-1.85583600	-0.92185800	0.41531200
C	-1.20110000	-0.34271900	1.50479300
C	-1.16041500	-1.87091500	-0.33392400
C	0.12637300	-0.62412300	1.81689800
H	-1.77293800	0.32859400	2.13623400
C	0.17226100	-2.19611600	-0.07726600
H	-1.67912100	-2.34530700	-1.16024400
C	0.85559500	-1.49430800	0.95647400
O	-7.19508100	0.54244200	-0.72059900
O	2.17702000	-1.65529900	1.12313700
C	-5.46810200	2.60025400	0.14274800
C	-5.96087700	3.17043900	-1.20034300
C	-6.58424800	2.69247000	1.19986900
C	-4.31604600	3.49485600	0.62055900
H	-5.16106500	3.12632100	-1.94664400
H	-6.82223500	2.62086800	-1.58003000
H	-6.24634900	4.22062800	-1.07131700
H	-6.22409200	2.31783900	2.16349200
H	-6.88091400	3.73922300	1.33223600
H	-7.46320500	2.11694200	0.90971000
H	-4.68510400	4.51878500	0.73361200
H	-3.92404100	3.17075100	1.58962800
H	-3.48979700	3.51394000	-0.09698500
C	-6.48554800	-2.28623600	-1.11034700
C	-7.64866800	-2.45025600	-0.10703000
C	-6.99863200	-1.97270400	-2.53333400
C	-5.81121200	-3.66269600	-1.20251500
H	-7.25508900	-2.79427300	0.85367600
H	-8.20954100	-1.53438300	0.09650500
H	-8.35657200	-3.20012900	-0.47528100
H	-6.15771100	-1.97287800	-3.23254600
H	-7.70993800	-2.74179600	-2.85172600
H	-7.49157300	-1.00270700	-2.64397000
H	-6.54535200	-4.39741900	-1.54733200
H	-4.98004000	-3.65889700	-1.91350200
H	-5.43557000	-3.99379900	-0.23043800
C	0.87245200	-3.30777000	-0.87606800
C	1.39150100	-4.37681300	0.10253200

C	-0.08725500	-3.99949000	-1.85358500
C	2.05165500	-2.76145300	-1.69384200
H	2.08309900	-3.93067500	0.81869000
H	0.55875500	-4.83266200	0.64928800
H	1.91242400	-5.16804000	-0.44949900
H	-0.44340600	-3.31342900	-2.62935300
H	0.44137600	-4.81779800	-2.35291000
H	-0.95729700	-4.42361500	-1.34106200
H	2.46112500	-3.54989500	-2.33691600
H	1.74712800	-1.92729900	-2.33530200
H	2.84383100	-2.41703600	-1.03333200
C	0.77175900	-0.03459000	3.08069400
C	1.33551000	-1.17275900	3.94978700
C	1.89422800	0.95107300	2.72065500
C	-0.24633600	0.73168400	3.93719500
H	0.52794700	-1.83435600	4.28222500
H	2.06305900	-1.75955100	3.38885700
H	1.82188000	-0.75560500	4.83970700
H	1.52271700	1.72072300	2.03473500
H	2.26224200	1.44501200	3.62844100
H	2.72884900	0.43543400	2.24696000
H	0.24553400	1.07123700	4.85440100
H	-0.63009300	1.61765500	3.42052500
H	-1.09514300	0.10215400	4.22367200

II

C	1.44992000	2.24580800	0.03176100
C	0.13039400	2.59334700	-0.33246400
H	-0.40015400	3.46990900	0.00980400
C	-0.32678400	1.61904700	-1.20736000
H	-1.29702000	1.55996900	-1.68005500
C	0.70030700	0.68211800	-1.36170300
H	0.75664400	-0.21745100	-1.95114100
N	1.76846900	1.05415600	-0.62649600
C	2.35786600	3.00212200	0.83238700
O	3.51663100	2.74743800	1.13650500
C	1.77623100	4.32596300	1.39278600
F	2.67522200	4.95791900	2.14379700
F	0.69080200	4.10921500	2.15975100
F	1.40188200	5.16752700	0.41478300
C	2.99026200	0.33526300	-0.53527900
H	3.66474400	0.71075600	0.21351400
H	2.69158100	-1.62819800	0.76214400
C	3.40191400	-0.49568800	-1.57444600

O	2.76742700	-0.73592900	-2.63943300
C	4.73602900	-1.19782000	-1.38836100
C	5.25201800	-1.87758300	-2.49502200
C	5.46060500	-1.23505200	-0.18991700
C	6.46273100	-2.55837200	-2.42008500
H	4.66474900	-1.85605800	-3.40634900
C	6.67142600	-1.91683900	-0.11131700
H	5.07626400	-0.74157900	0.69846300
C	7.18059700	-2.57975400	-1.22648900
H	6.84649600	-3.07764400	-3.29399400
H	7.21625300	-1.93629000	0.82807400
H	8.12405400	-3.11370900	-1.16167500
H	-7.49068500	0.11862700	-1.12517600
C	-5.38477500	-1.06439200	-0.68480100
C	-4.09489100	-1.49042800	-0.36081800
C	-3.09088200	-0.60634300	0.02874200
C	-3.40048800	0.75429100	0.08870000
C	-4.66392900	1.25093700	-0.22399800
C	-5.65070400	0.31756700	-0.60083500
H	-3.85867600	-2.54744500	-0.38304900
H	-2.60352400	1.43601700	0.36076900
C	-1.73301100	-1.08765100	0.38458200
C	-1.02695500	-0.48583200	1.42779400
C	-1.14977800	-2.16343500	-0.28396400
C	0.25747400	-0.89325100	1.78551500
H	-1.51671200	0.30664200	1.98116800
C	0.13870700	-2.61249400	0.01727400
H	-1.71122400	-2.63581200	-1.08194400
C	0.84638000	-1.91361500	1.01301000
O	-6.89361800	0.82958200	-0.88044500
O	2.15621800	-2.27245400	1.27025600
C	-4.95850300	2.75837800	-0.16775100
C	-5.39615300	3.27190500	-1.55200000
C	-6.04989600	3.05008100	0.87821600
C	-3.71112900	3.55834400	0.23471800
H	-4.61009900	3.08342800	-2.29036300
H	-6.31444800	2.79238500	-1.89052100
H	-5.56448700	4.35370400	-1.50610200
H	-5.72695300	2.70905700	1.86713100
H	-6.22893600	4.12971100	0.93363200
H	-6.98862100	2.55525100	0.62879000
H	-3.96450400	4.62255500	0.26215100
H	-3.34337400	3.27540600	1.22610500
H	-2.89718500	3.42665700	-0.48603000

C	-6.46825900	-2.07637600	-1.10025100
C	-7.63269100	-2.07988600	-0.08549400
C	-6.96522900	-1.78902100	-2.53444000
C	-5.92470700	-3.51258000	-1.12470600
H	-7.26313000	-2.39603600	0.89408100
H	-8.11446800	-1.10938200	0.06262800
H	-8.40477200	-2.78708200	-0.40597700
H	-6.13482400	-1.89498300	-3.23803800
H	-7.74250700	-2.50943200	-2.80979700
H	-7.37607000	-0.78744800	-2.68767300
H	-6.72515400	-4.19230800	-1.43251700
H	-5.10057600	-3.61994900	-1.83578300
H	-5.57619000	-3.83003400	-0.13799100
C	0.72212300	-3.87374600	-0.64428800
C	0.95069600	-4.93027200	0.45311800
C	-0.25574300	-4.46955700	-1.66665500
C	2.04578800	-3.60673600	-1.38097500
H	1.66661200	-4.56853400	1.19332200
H	0.00985400	-5.17199800	0.95968500
H	1.34600900	-5.85017100	0.00671700
H	-0.44367300	-3.77780900	-2.49415100
H	0.18024400	-5.38131500	-2.08650800
H	-1.21487000	-4.73771000	-1.21081800
H	2.34262300	-4.51365900	-1.92201900
H	1.95854900	-2.78631800	-2.09890500
H	2.84972000	-3.35726900	-0.68762000
C	0.91923600	-0.37566000	3.07698500
C	0.90343600	-1.53570900	4.08968100
C	2.37042800	0.10200000	2.90228700
C	0.13375200	0.80175900	3.67349700
H	-0.12179800	-1.86530900	4.28831600
H	1.47574500	-2.38406800	3.70425100
H	1.35270100	-1.21458800	5.03702900
H	2.45967300	0.80954800	2.07930700
H	2.69103900	0.61242300	3.81773600
H	3.05386900	-0.72795300	2.72568000
H	0.63241100	1.13516000	4.58880500
H	0.09874900	1.64926000	2.97981500
H	-0.89008400	0.52385000	3.94098600

TSII'

C	-4.59364800	0.49649100	-0.27765100
C	-4.90392600	-0.79491900	0.17597500
H	-5.78268800	-1.35867700	-0.09961900

C	-3.87596800	-1.19295900	1.02517100
H	-3.78922300	-2.13067900	1.55316300
C	-2.95131900	-0.14800200	1.07512100
H	-2.03135800	-0.04488300	1.62650800
N	-3.37603300	0.86410700	0.28956100
C	-5.35191700	1.33589400	-1.15592700
O	-5.07524900	2.45786400	-1.55876700
C	-6.69906000	0.73369200	-1.62788600
F	-7.34011500	1.58505400	-2.42214500
F	-7.50167000	0.45777600	-0.58750700
F	-6.51637600	-0.40928600	-2.30494300
C	-2.75016800	2.14474800	0.07873600
H	-2.67553500	2.39799600	-0.97171200
H	-3.85698400	3.04364400	0.59760300
C	-1.69727600	2.56394200	0.94895300
O	-1.40223100	2.03777300	2.03595200
C	-0.98088000	3.83411200	0.54926900
C	0.21760900	4.12690100	1.20338900
C	-1.46742400	4.72633200	-0.41235400
C	0.93285400	5.27746300	0.88930900
H	0.56839700	3.43186300	1.95880900
C	-0.75537600	5.88139600	-0.72210200
H	-2.41301800	4.53357500	-0.91101800
C	0.44818000	6.15704700	-0.07655200
H	1.86812100	5.48998300	1.39782400
H	-1.14358700	6.57031700	-1.46568400
H	1.00325900	7.05686800	-0.32261800
C	-4.58129800	3.35502000	2.58702300
C	-5.48078000	3.84993200	3.50037400
C	-6.61570800	4.56994000	3.04446000
C	-6.74966400	4.73141200	1.64017800
C	-5.80108600	4.19929100	0.79908000
H	-3.69564400	2.79767300	2.88098400
H	-5.30585400	3.67536100	4.55265900
H	-7.58770600	5.26168500	1.20958600
H	-5.87370000	4.28061700	-0.28026300
C	-8.68938800	5.78754000	3.40119200
C	-7.35501500	4.88399400	5.33795900
H	-9.29928000	5.14543400	2.75669300
H	-9.30058800	6.10634100	4.24319900
H	-8.39439200	6.67663700	2.83386600
H	-7.36496000	3.82071300	5.60115600
H	-6.41341800	5.32257200	5.68490500
H	-8.17349900	5.37522300	5.86052800

N	-7.52609300	5.07490200	3.90587800
N	-4.73829100	3.52721300	1.26418300

H'

C	-0.22119200	-1.96389600	-0.82468800
C	-0.77043600	-3.05147500	-0.11703200
H	-1.72036800	-3.51853900	-0.32970100
C	0.12763200	-3.38703500	0.88681200
H	0.02560800	-4.17492200	1.61804800
C	1.21791900	-2.51518800	0.78211800
H	2.11617900	-2.42153000	1.37082900
N	1.01728900	-1.66761500	-0.24800300
C	-0.83944600	-1.14109200	-1.80999100
O	-0.39993200	-0.11820300	-2.33109900
C	-2.29760400	-1.51842500	-2.16098900
F	-2.75568200	-0.75827000	-3.15127600
F	-3.09456800	-1.32117200	-1.09487800
F	-2.42806700	-2.79987500	-2.52748100
C	1.88686200	-0.61919000	-0.65653000
H	1.91302000	-0.44304600	-1.71813600
H	0.34222200	0.72683100	-0.27804600
C	2.75566300	-0.01592600	0.24596300
O	2.84453100	-0.28092400	1.48230100
C	3.63891700	1.08138600	-0.30229800
C	4.78045600	1.41759000	0.42932100
C	3.35696400	1.79199400	-1.47443300
C	5.63735100	2.42145100	-0.01096200
H	4.97077400	0.87384300	1.34855100
C	4.21073800	2.79886700	-1.91419800
H	2.45343500	1.57518100	-2.03776500
C	5.35680200	3.11436300	-1.18657200
H	6.52518300	2.66647500	0.56436400
H	3.97622400	3.34509200	-2.82279500
H	6.02203000	3.90032400	-1.53057500
C	-0.12988200	0.74255100	1.70735800
C	-1.07152700	1.01256600	2.66518600
C	-2.33991500	1.53781100	2.29360400
C	-2.56895200	1.75416500	0.90482000
C	-1.58562200	1.46126400	-0.00001300
H	0.85751000	0.33011700	1.91916700
H	-0.82633800	0.80753400	3.69737400
H	-3.51054400	2.13738700	0.53847400
H	-1.70885000	1.57990600	-1.07023400
C	-4.58065100	2.33009800	2.79396600

C	-3.01867900	1.57430300	4.62382100
H	-5.08660700	1.62941600	2.12208000
H	-5.20348600	2.47133000	3.67467100
H	-4.47472200	3.29496200	2.28773200
H	-2.82531300	0.51398600	4.81553200
H	-2.15821500	2.15911700	4.96346700
H	-3.88920400	1.87591600	5.20219800
N	-3.28416400	1.81198100	3.21072000
N	-0.39562500	0.97958600	0.40521900

R2

C	-5.41731700	-4.24176800	-1.19634600
C	-5.91300700	-5.55363100	-1.36708600
H	-6.95594300	-5.81803200	-1.45640800
C	-4.82160500	-6.40608200	-1.39435500
H	-4.83431100	-7.48001900	-1.51227300
C	-3.66784900	-5.62365800	-1.24031700
H	-2.61963100	-5.87340600	-1.20575400
N	-4.02222100	-4.32371500	-1.11922800
C	-6.16372200	-3.02850700	-1.12561000
O	-5.77006300	-1.87793900	-0.97316500
C	-7.69809200	-3.21092000	-1.26348400
F	-8.32199800	-2.03519500	-1.21000000
F	-8.20002100	-3.98013000	-0.28132000
F	-8.03646300	-3.79155900	-2.42799100
C	-3.15095300	-3.22813100	-0.94843000
H	-3.65310500	-2.29137300	-0.80076200
C	-1.77461200	-3.37417600	-0.91085900
O	-1.11033000	-4.45120700	-0.98660800
C	-0.99053600	-2.09041500	-0.72434900
C	-1.48785700	-0.81231200	-1.00659400
C	0.32309000	-2.20255500	-0.25954700
C	-0.70323700	0.31847000	-0.80122000
H	-2.48888100	-0.70137500	-1.41195800
C	1.10944500	-1.07403500	-0.05071400
H	0.69977500	-3.20319100	-0.07506000
C	0.59830200	0.19453900	-0.31729200
H	-1.10691600	1.30125800	-1.02851600
H	2.12531600	-1.18252300	0.31978000
H	1.20963600	1.07809300	-0.15789500

DQ

C	2.80643900	1.28430300	-0.00086700
C	1.45915900	1.23616200	-0.07539300

C	0.69362900	0.00068100	-0.09206100
C	1.46162500	-1.23336300	-0.09415000
C	2.80900800	-1.28001100	-0.02084800
C	3.56820700	0.00216300	0.08365800
H	0.91797800	2.16918300	-0.11896900
H	0.92287200	-2.16640900	-0.16121800
C	-0.69358700	-0.00055400	-0.09196500
C	-1.45911600	-1.23603200	-0.07495500
C	-1.46157800	1.23349100	-0.09416600
C	-2.80638900	-1.28415500	-0.00030400
H	-0.91793600	-2.16906100	-0.11835700
C	-2.80895600	1.28015700	-0.02076100
H	-0.92282900	2.16652600	-0.16140300
C	-3.56815500	-0.00199700	0.08398300
O	4.78571000	0.00229500	0.23129100
O	-4.78565600	-0.00210000	0.23162700
C	3.58788600	-2.59500100	-0.02768200
C	4.58207900	-2.60867200	-1.20471200
C	4.34695700	-2.76184900	1.30262500
C	2.65492400	-3.80074100	-0.19002200
H	4.05346200	-2.49246100	-2.15645700
H	5.32037300	-1.81280100	-1.11116400
H	5.10627100	-3.56982400	-1.22447200
H	3.64834400	-2.76075700	2.14553000
H	4.87343800	-3.72212900	1.30056100
H	5.07600000	-1.96527400	1.44688800
H	3.25443500	-4.71503800	-0.20518400
H	1.94614600	-3.88403700	0.64068500
H	2.09153700	-3.75580600	-1.12802100
C	3.58273700	2.60076600	0.01530900
C	4.33998000	2.74730200	1.34898700
C	4.57834600	2.63538200	-1.16019300
C	2.64750500	3.80718400	-0.12843900
H	3.64062000	2.72934000	2.19108300
H	5.07158300	1.95082700	1.48027200
H	4.86324900	3.70922200	1.36414100
H	4.05091800	2.53438200	-2.11433700
H	5.10139400	3.59734900	-1.16316400
H	5.31729400	1.83872400	-1.07878600
H	3.24544500	4.72261900	-0.13077500
H	2.08310000	3.77499100	-1.06635100
H	1.93965100	3.87695900	0.70426600
C	-3.58782200	2.59515400	-0.02772300
C	-4.34683800	2.76217000	1.30259200

C	-2.65485500	3.80086700	-0.19024300
C	-4.58205700	2.60869600	-1.20471900
H	-5.07587000	1.96560900	1.44699800
H	-3.64819200	2.76121800	2.14546200
H	-4.87333500	3.72244300	1.30041700
H	-2.09150300	3.75580900	-1.12825800
H	-3.25436100	4.71515800	-0.20552000
H	-1.94604500	3.88426300	0.64042600
H	-5.10622500	3.56985800	-1.22458900
H	-4.05347900	2.49232600	-2.15646700
H	-5.32036500	1.81284900	-1.11103200
C	-3.58268800	-2.60061400	0.01624200
C	-4.33985800	-2.74681300	1.34999800
C	-4.57836100	-2.63552500	-1.15919800
C	-2.64746300	-3.80706900	-0.12725400
H	-3.64045400	-2.72860900	2.19205200
H	-5.07147200	-1.95031900	1.48111000
H	-4.86310400	-3.70874100	1.36543900
H	-4.05098500	-2.53477000	-2.11339600
H	-5.10141500	-3.59749100	-1.16189100
H	-5.31730300	-1.83884500	-1.07793900
H	-3.24540300	-4.72250500	-0.12931300
H	-2.08311100	-3.77511800	-1.06520500
H	-1.93956000	-3.87662500	0.70542500

DQH⁻

H	-5.27768000	0.77015100	-0.13187900
C	-2.86065600	1.16271100	-0.33469400
C	-1.46509900	1.13017600	-0.37431400
C	-0.71898900	-0.01250000	-0.06819300
C	-1.43938600	-1.16722800	0.26415900
C	-2.83203600	-1.21443200	0.30085000
C	-3.53182100	-0.02773100	0.00709000
H	-0.92030800	2.01842300	-0.66819300
H	-0.87263900	-2.05035300	0.53176100
C	0.75661400	0.00241200	-0.07308200
C	1.50545000	-1.14648700	-0.36918300
C	1.47591100	1.16270300	0.25048600
C	2.89115800	-1.17694200	-0.34311400
H	0.96042900	-2.04194800	-0.65583200
C	2.86032200	1.21030700	0.29508500
H	0.90738600	2.05033600	0.51512600
C	3.63931900	0.01822400	0.00696800
O	-4.90880800	-0.09119200	0.07557500

O	4.91365100	0.02084300	0.06203400
C	-3.57253800	-2.50923800	0.67381800
C	-4.39425700	-2.30503200	1.95970500
C	-4.49296000	-2.94996400	-0.47981300
C	-2.59757600	-3.66468000	0.93894000
H	-3.73599600	-2.01935400	2.78665900
H	-5.15080700	-1.53074700	1.83451700
H	-4.89496100	-3.24146500	2.23242500
H	-3.90430300	-3.12562100	-1.38620500
H	-4.99560000	-3.88752800	-0.21487400
H	-5.25192200	-2.19901800	-0.69859800
H	-3.17078200	-4.56418500	1.18512400
H	-1.98217300	-3.88808200	0.06179500
H	-1.93257800	-3.45090100	1.78118400
C	-3.62543500	2.45958900	-0.65971000
C	-4.53263100	2.27182700	-1.89486000
C	-4.42973300	2.93757000	0.56957600
C	-2.67256200	3.61217200	-1.01089600
H	-3.91676900	2.02964600	-2.76554600
H	-5.27134000	1.47066900	-1.80473100
H	-5.07533100	3.19958900	-2.10527500
H	-3.74127000	3.16770500	1.38775500
H	-4.98695600	3.84766800	0.32300300
H	-5.14380800	2.20801200	0.96170500
H	-3.26057000	4.51058700	-1.22378200
H	-1.99449100	3.84107000	-0.18394800
H	-2.07319600	3.38399400	-1.89653500
C	3.59991100	2.49700300	0.67964200
C	4.54981200	2.91549200	-0.45745600
C	2.64642400	3.66975600	0.93789800
C	4.41173300	2.26499800	1.96664900
H	5.24723600	2.10546900	-0.67128000
H	3.97641200	3.14106900	-1.36378900
H	5.10905200	3.81732400	-0.17545600
H	1.96691200	3.46553100	1.77252400
H	3.22903100	4.56256500	1.19198000
H	2.04170800	3.90382400	0.05449000
H	4.98102600	3.16608400	2.23003000
H	3.73842800	2.03248500	2.79963200
H	5.09807100	1.43023400	1.82268500
C	3.66644900	-2.45889800	-0.66912100
C	4.60844600	-2.21760200	-1.86230700
C	4.49641400	-2.88531400	0.55590600
C	2.74366400	-3.62843000	-1.03349700

H	4.02900300	-1.95459400	-2.75460400
H	5.29230300	-1.40056200	-1.63051700
H	5.18367300	-3.12583400	-2.08504100
H	3.83447600	-3.11795800	1.39790600
H	5.08379500	-3.78388800	0.32528400
H	5.16685100	-2.07511700	0.84422100
H	3.34986700	-4.51457300	-1.25356100
H	2.06579800	-3.88252800	-0.21098900
H	2.13758500	-3.40815100	-1.91921700

CO₂

C	0.00548500	0.00000000	0.00004700
O	-0.00204100	0.00000000	1.21926100
O	0.01924500	0.00000000	-1.21911000

re-TS1

C	-3.04701300	-0.90569500	0.11969200
C	-3.92654600	-2.15417700	0.14929500
H	-2.95711000	-0.46613200	1.11769500
H	-3.70557800	-2.76299700	1.03741800
N	-1.69717600	-1.35151300	-0.24062800
O	-3.73202700	-2.92238400	-1.02962100
C	-1.38950300	-2.58910900	-0.73819000
C	-2.48232300	-3.57900600	-1.02125700
H	-2.33824400	-4.03494900	-2.00203900
H	-2.46246300	-4.37189200	-0.25943400
N	-0.10306100	-2.72987900	-0.86546700
C	-0.55643100	-0.64778700	-0.05689300
N	0.38765700	-1.51406100	-0.43589500
C	1.80539900	-1.35301500	-0.26502700
C	2.57304900	-0.84787700	-1.31089400
C	2.34398300	-1.69394500	0.97872800
C	3.94596400	-0.71805800	-1.09967600
C	3.71762600	-1.53932700	1.14666100
C	4.53319400	-1.06549300	0.11521500
H	4.56504600	-0.31060800	-1.89515100
H	4.16300900	-1.79145800	2.10649500
H	-4.97804100	-1.85945700	0.17409800
C	-3.55745500	0.14645700	-0.87255300
H	-2.72146300	0.80141400	-1.14166300
H	-3.88660600	-0.35688100	-1.78848800
C	-4.67107300	0.96594400	-0.26582900
C	-4.42152600	1.71100800	0.89391600
C	-5.94677800	0.99220800	-0.82852500

C	-5.43306800	2.47351900	1.46778300
H	-3.43397900	1.67469400	1.35662700
C	-6.95996200	1.75775900	-0.25313600
H	-6.14745200	0.41258700	-1.72609900
C	-6.70428300	2.50062000	0.89511200
H	-5.22879800	3.04724100	2.36629400
H	-7.94812000	1.77090600	-0.70238700
H	-7.49206400	3.09627300	1.34532500
C	6.02108000	-0.94224500	0.31591500
H	6.25244300	-0.59367000	1.32603100
H	6.51205300	-1.91161600	0.17965400
H	6.45448900	-0.23641600	-0.39588000
C	1.92057000	-0.40737400	-2.59169000
H	1.30192900	-1.20260600	-3.01778600
H	1.26615100	0.45224700	-2.40327900
H	2.67038900	-0.11201600	-3.32787600
C	1.44786700	-2.17069400	2.09213900
H	0.70333800	-1.40858600	2.35578000
H	0.89908700	-3.06966800	1.79343200
H	2.03169600	-2.40465700	2.98390300
C	1.41226800	2.05915700	0.11502300
C	0.83127200	1.32602600	1.06727200
H	0.78177000	2.44432600	-0.68976400
C	2.85295100	2.31570400	-0.02526500
C	3.35670300	2.69439500	-1.27530100
C	3.75431400	2.13784800	1.03289200
C	4.72404500	2.85642400	-1.47718200
H	2.66435000	2.84482200	-2.10027800
C	5.11837000	2.30781500	0.83523900
H	3.38214100	1.86878500	2.01679000
C	5.61084800	2.65758500	-0.42244300
H	5.09599000	3.14174400	-2.45638500
H	5.80453500	2.16846200	1.66527400
H	6.67806400	2.78743200	-0.57338000
C	-0.63462200	1.00373500	1.03852400
O	-1.25282900	0.70073900	2.08745300
H	-1.15000600	1.58458100	0.24010400
H	1.39695900	0.88124700	1.88441900

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C	-2.85123500	-1.24091200	0.27087500
C	-3.71856100	-2.45071100	-0.06549200
H	-2.89922500	-0.99375000	1.33294000
H	-3.55349200	-3.25970500	0.66089200

N	-1.46088400	-1.62718300	-0.02556500
O	-3.44043400	-2.91141300	-1.38059700
C	-1.12379700	-2.65400700	-0.87099400
C	-2.18307800	-3.54600600	-1.44998200
H	-1.96730100	-3.75536700	-2.49875900
H	-2.19638900	-4.49757300	-0.89800400
N	0.16527300	-2.72881800	-1.02408900
C	-0.33073200	-0.99780600	0.37215000
N	0.62885400	-1.69724900	-0.24040300
C	2.03151200	-1.40154800	-0.18262300
C	2.56159000	-0.54593600	-1.14869500
C	2.78873900	-1.92713900	0.86534700
C	3.90813400	-0.20488600	-1.03913200
C	4.12879500	-1.55185900	0.93921100
C	4.70009600	-0.68660800	0.00186900
H	4.33346800	0.49315400	-1.75656300
H	4.73970900	-1.93734800	1.75253600
H	-4.77136600	-2.16313800	-0.04191900
C	-3.21755700	0.00185500	-0.55227600
H	-2.42780100	0.74002200	-0.38441500
H	-3.23356000	-0.27166500	-1.61316100
C	-4.54373100	0.57259700	-0.11616200
C	-4.61424400	1.29857900	1.07832000
C	-5.70863500	0.36148800	-0.85563700
C	-5.83343700	1.80438000	1.51828200
H	-3.69748300	1.45618100	1.64332100
C	-6.92940900	0.86954600	-0.41422400
H	-5.65707700	-0.20255100	-1.78440900
C	-6.99332100	1.59142700	0.77436300
H	-5.87901700	2.37035900	2.44367100
H	-7.82839200	0.70141100	-0.99920000
H	-7.94280600	1.98840400	1.11968100
C	6.13869800	-0.25977500	0.13712000
H	6.30200400	0.24873200	1.09278000
H	6.81148200	-1.12192700	0.10554800
H	6.42173300	0.42828300	-0.66213600
C	1.68019000	0.03893500	-2.21643000
H	1.20734500	-0.74495200	-2.81562600
H	0.87941400	0.62982000	-1.75500200
H	2.25343300	0.69318900	-2.87523900
C	2.15967700	-2.84266200	1.88164300
H	1.39425500	-2.31675800	2.46228800
H	1.67079200	-3.69054300	1.39284800
H	2.91038200	-3.22647600	2.57414600

C	1. 76986500	1. 60960600	1. 09703700
C	0. 45083100	1. 48705600	0. 92331600
H	2. 24543400	0. 94833300	1. 82558000
C	2. 69499000	2. 50325200	0. 38358300
C	4. 02104800	2. 59258900	0. 82647800
C	2. 32710300	3. 22164100	-0. 76174600
C	4. 95350500	3. 37220200	0. 15160500
H	4. 31960000	2. 02517200	1. 70477100
C	3. 25756100	4. 00237200	-1. 43856900
H	1. 30964100	3. 15579300	-1. 13613100
C	4. 57465500	4. 07969700	-0. 98734500
H	5. 97665700	3. 42370400	0. 51142900
H	2. 95620100	4. 54933100	-2. 32655000
H	5. 29950200	4. 68578200	-1. 52118600
C	-0. 35593400	0. 47425200	1. 69036700
O	-1. 54897200	0. 71299600	1. 99318600
H	0. 29697900	-0. 09155000	2. 39440500
H	-0. 11689600	2. 12156400	0. 24352600

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C	-3. 07829800	-0. 87065800	0. 08822000
C	-3. 95124900	-2. 12188200	0. 11959500
H	-2. 94778200	-0. 43340000	1. 08385300
H	-3. 72227100	-2. 73711400	1. 00079200
N	-1. 72881100	-1. 32470700	-0. 27866400
O	-3. 76189800	-2. 87891700	-1. 06905200
C	-1. 41813000	-2. 56646900	-0. 75295100
C	-2. 51666400	-3. 54010900	-1. 07382600
H	-2. 36796300	-3. 96700800	-2. 06704900
H	-2. 49883300	-4. 35459700	-0. 33554400
N	-0. 12922300	-2. 73878700	-0. 80795800
C	-0. 57594500	-0. 67279500	-0. 03103100
N	0. 38005300	-1. 54639900	-0. 35444800
C	1. 79007700	-1. 43589700	-0. 08426300
C	2. 65612600	-1. 06991100	-1. 11167900
C	2. 20220600	-1. 65728300	1. 23190300
C	4. 00373600	-0. 92037000	-0. 78792000
C	3. 55834500	-1. 49311900	1. 50536100
C	4. 46789300	-1. 12311900	0. 51108100
H	4. 69808200	-0. 59902100	-1. 56053600
H	3. 91081600	-1. 64191000	2. 52326300
H	-5. 00272900	-1. 82880700	0. 15338800
C	-3. 60497500	0. 18184800	-0. 89578800
H	-2. 76584900	0. 78476100	-1. 25826400

H	-4.04005100	-0.32348600	-1.76518800
C	-4.61319600	1.08041800	-0.21941000
C	-4.23058700	1.80821900	0.91577300
C	-5.91641000	1.19922800	-0.70066200
C	-5.14574000	2.64612300	1.54436700
H	-3.22062800	1.69369300	1.31796400
C	-6.83116600	2.03995700	-0.06856000
H	-6.21564100	0.63212700	-1.57863900
C	-6.44611700	2.76625500	1.05378400
H	-4.84419000	3.20722400	2.42333300
H	-7.84252700	2.12502000	-0.45357400
H	-7.15633100	3.42166700	1.54800900
C	5.92690800	-0.94505400	0.84081000
H	6.05166900	-0.47531500	1.82006700
H	6.44061100	-1.91174200	0.86929100
H	6.42124200	-0.31751600	0.09605900
C	2.12808700	-0.77630600	-2.48755600
H	1.57837900	-1.63051800	-2.89383800
H	1.43671300	0.07405900	-2.45032300
H	2.94224000	-0.52423400	-3.16892500
C	1.19911100	-1.99692300	2.30337500
H	0.46321900	-1.18981200	2.43528200
H	0.64520800	-2.90454300	2.03962400
H	1.70218700	-2.16948300	3.25625200
C	1.41483900	1.94354800	-0.27155500
C	0.86201600	1.23654000	0.71665400
H	0.79772200	2.21855600	-1.12965100
C	2.84855400	2.26393800	-0.38084200
C	3.39962100	2.49313800	-1.64718300
C	3.70648300	2.25718000	0.72762200
C	4.77096000	2.66927100	-1.81094200
H	2.74406900	2.51157200	-2.51459100
C	5.07357200	2.44097900	0.56715900
H	3.29604600	2.10759200	1.72171000
C	5.61498300	2.63614600	-0.70431000
H	5.17991400	2.83430500	-2.80310600
H	5.72290200	2.43211200	1.43748400
H	6.68442300	2.77602100	-0.82732800
C	-0.56584100	0.71462300	0.69453600
O	-1.15843100	0.54532700	1.87313000
H	-1.11138800	1.36725700	-0.04061400
H	1.44735700	0.92554000	1.58045000

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C	-2.50043700	-1.89437300	0.06290700
C	-3.07765000	-3.19426200	-0.48590100
H	-2.56907100	-1.81913700	1.14800400
H	-2.74339800	-4.05683700	0.10839700
N	-1.05382700	-1.91447800	-0.25255500
O	-2.70904400	-3.36871500	-1.84833700
C	-0.50295200	-2.70566000	-1.22640700
C	-1.34632700	-3.69880200	-1.97331100
H	-1.08763000	-3.68485500	-3.03313500
H	-1.14853800	-4.70551000	-1.57644600
N	0.77670900	-2.49647800	-1.33964500
C	-0.06727900	-1.15661400	0.26307600
N	1.02873300	-1.53306300	-0.40188900
C	2.34641200	-0.98515500	-0.23839200
C	2.73969700	0.04191200	-1.10149500
C	3.14032300	-1.45332400	0.80699000
C	3.97202600	0.63900400	-0.86168800
C	4.36720500	-0.81768500	1.00992700
C	4.78956100	0.23338600	0.19667200
H	4.28669200	1.46640800	-1.49311700
H	5.00197300	-1.15155700	1.82680100
H	-4.16782900	-3.14292100	-0.45149000
C	-3.14333500	-0.65200800	-0.56624600
H	-2.49170900	0.19527600	-0.33840700
H	-3.20242000	-0.78711300	-1.65208800
C	-4.50368100	-0.39838900	0.03398000
C	-4.57663900	0.10452000	1.33867600
C	-5.68023300	-0.67663400	-0.66199100
C	-5.81630700	0.32953300	1.92809600
H	-3.64185800	0.30879400	1.86093500
C	-6.92161800	-0.45075700	-0.06814100
H	-5.62345600	-1.06564900	-1.67630900
C	-6.99072300	0.05345600	1.22708100
H	-5.86935500	0.72450700	2.93808400
H	-7.83194900	-0.66704000	-0.61870100
H	-7.95646400	0.23135000	1.68998900
C	6.10538700	0.92631700	0.43611500
H	6.49057900	0.71723800	1.43623100
H	6.85580600	0.59765600	-0.28985600
H	5.99393800	2.00916800	0.32538800
C	1.82818400	0.52151800	-2.19612600
H	1.56142900	-0.29243200	-2.87640900
H	0.90065300	0.91674000	-1.76520400
H	2.30322600	1.31927600	-2.76904700

C	2. 68262800	-2. 58792800	1. 68483100
H	1. 85381300	-2. 28193900	2. 33213800
H	2. 33713600	-3. 43288500	1. 08225300
H	3. 49882400	-2. 93034400	2. 32272500
C	1. 37210200	1. 78611500	1. 04962500
C	0. 17168500	1. 23436400	0. 85330100
H	2. 08614000	1. 23948400	1. 67028700
C	1. 89337500	3. 03873200	0. 47881600
C	3. 17344700	3. 46880200	0. 85346200
C	1. 18593000	3. 80378000	-0. 45828500
C	3. 72891600	4. 62667700	0. 31905200
H	3. 73630200	2. 87632000	1. 57147000
C	1. 73836500	4. 96166300	-0. 99332900
H	0. 19593200	3. 48853500	-0. 77442900
C	3. 01185400	5. 37903900	-0. 60814800
H	4. 72091800	4. 94238400	0. 62770900
H	1. 17360100	5. 54115600	-1. 71702000
H	3. 44060300	6. 28286900	-1. 02873000
C	-0. 24055900	-0. 11655600	1. 44279200
O	-1. 45090800	-0. 17355000	1. 95370700
H	0. 61187800	-0. 41606100	2. 11466400
H	-0. 60526100	1. 73012700	0. 26991400

M02

C	-2. 36788900	-1. 78688500	1. 27177100
C	-3. 18879900	-3. 00195500	1. 70446200
H	-2. 09595900	-1. 18674800	2. 14017700
H	-2. 75199700	-3. 47009700	2. 59878300
N	-1. 10481800	-2. 31108600	0. 68440600
O	-3. 28204000	-3. 94695400	0. 65463900
C	-0. 96383900	-3. 60763600	0. 26228300
C	-2. 05961300	-4. 61356100	0. 46302300
H	-2. 14376700	-5. 24677200	-0. 42099200
H	-1. 81143200	-5. 24513300	1. 32870900
N	0. 20319000	-3. 80224100	-0. 27641300
C	0. 04523300	-1. 67101000	0. 37940200
N	0. 82070000	-2. 59005200	-0. 19610000
C	2. 12691400	-2. 45722700	-0. 79900700
C	2. 18022000	-2. 08045000	-2. 14285400
C	3. 25376100	-2. 73932200	-0. 02665600
C	3. 44439500	-1. 95717600	-2. 71567700
C	4. 49267000	-2. 61199400	-0. 65249100
C	4. 60787000	-2. 22019500	-1. 98776400
H	3. 52150600	-1. 65427600	-3. 75649500

H	5.39134500	-2.81231000	-0.07469200
H	-4.20175900	-2.67415800	1.94386100
C	-3.09269700	-0.90776800	0.24351800
H	-2.39053600	-0.16049600	-0.14002600
H	-3.41482800	-1.53000500	-0.59771600
C	-4.27418800	-0.21367200	0.87536600
C	-4.06262200	0.84869700	1.75888200
C	-5.57795600	-0.63883100	0.61653000
C	-5.14180600	1.47876000	2.37030700
H	-3.04573200	1.18115200	1.95936900
C	-6.65915100	-0.00709400	1.22776900
H	-5.74613500	-1.46484600	-0.07140600
C	-6.44200900	1.05189600	2.10475100
H	-4.96930300	2.30574300	3.05144600
H	-7.66962600	-0.34109100	1.01618000
H	-7.28309400	1.54606400	2.57963700
C	5.96213700	-2.10424800	-2.63548600
H	5.94800200	-1.38493700	-3.45667800
H	6.71850500	-1.79215500	-1.91157100
H	6.27417600	-3.07047400	-3.04423500
C	0.92319600	-1.79941900	-2.92361300
H	0.23210200	-2.64633200	-2.87696600
H	0.39708400	-0.91899200	-2.53666600
H	1.15837200	-1.60772600	-3.97083700
C	3.13939800	-3.10218000	1.42652700
H	2.89286600	-2.21132000	2.01440400
H	2.35577300	-3.84526100	1.60071600
H	4.08432500	-3.50189300	1.79726500
C	2.40422000	0.76733400	1.57105400
C	1.76005600	0.18529500	0.55828100
H	1.83592800	1.00997100	2.46674300
C	3.82912600	1.13160500	1.59535200
C	4.31597800	1.88502400	2.66944100
C	4.72562500	0.72667100	0.59648500
C	5.66029600	2.23705300	2.74298300
H	3.62850900	2.20403100	3.44918800
C	6.06724800	1.07691400	0.67008600
H	4.37787500	0.12237500	-0.23622900
C	6.53975800	1.83421400	1.74222000
H	6.01894900	2.82648600	3.58041400
H	6.74981200	0.75547200	-0.11055500
H	7.58888900	2.10559300	1.79640600
C	0.29811600	-0.18312900	0.64468000
O	-0.31580800	0.16712400	1.84261000

H	0.11652900	-0.37311800	2.57650000
H	2.25128200	0.00483600	-0.39231700
C	0.36011100	-2.76500900	3.68213000
C	0.95156300	-3.79816100	4.37952400
C	2.16111700	-3.55933000	5.07708900
C	2.66430700	-2.23708400	5.00746000
C	1.98429900	-1.28645800	4.27474300
H	-0.57365300	-2.95181300	3.15537400
H	0.47761600	-4.77075600	4.38274500
H	3.57402700	-1.95071600	5.51793300
H	2.38368800	-0.27748700	4.21731800
C	4.04145700	-4.23998200	6.45858300
C	2.22397500	-5.86904900	5.83098000
H	3.89769200	-3.48607100	7.24017900
H	4.41209000	-5.15105600	6.92427500
H	4.80222500	-3.87847700	5.75845300
H	1.22591900	-5.85287100	6.28258200
H	2.15110800	-6.31725200	4.83365600
H	2.86361600	-6.50129300	6.44355900
N	2.79505800	-4.53373800	5.76939500
N	0.84626300	-1.51831000	3.59900900
H	-0.23491500	0.34329200	-0.16242700

TS2

C	-3.08545900	-0.94722500	1.33776700
C	-4.02243900	-2.14478400	1.48711100
H	-2.87709000	-0.51702800	2.31491500
H	-3.67597300	-2.80905300	2.29142800
N	-1.81502700	-1.45446400	0.77076600
O	-4.11908700	-2.85796900	0.26801600
C	-1.76191800	-2.61563500	0.03203700
C	-2.92737200	-3.56085000	0.00352600
H	-3.00626900	-4.01566100	-0.98427900
H	-2.76822500	-4.35378300	0.74836100
N	-0.62021400	-2.75444200	-0.56061900
C	-0.62189800	-0.81863900	0.60538600
N	0.08978500	-1.64046700	-0.18951000
C	1.35904600	-1.38543300	-0.80849500
C	1.35490800	-0.72126900	-2.03708000
C	2.52633500	-1.78908300	-0.15685000
C	2.59320200	-0.41587600	-2.60095200
C	3.73816600	-1.46960300	-0.76607400
C	3.78989800	-0.77145500	-1.97605100
H	2.62286400	0.10307600	-3.55563200

H	4.66495300	-1.76793300	-0.28203900
H	-5.02220400	-1.78141400	1.73384000
C	-3.65244800	0.12078200	0.39134500
H	-2.83403100	0.78689800	0.09712200
H	-4.01164300	-0.38159500	-0.51311800
C	-4.75594000	0.91547600	1.04371000
C	-4.44404000	1.84266200	2.04455400
C	-6.09189800	0.72383600	0.68800200
C	-5.45180200	2.57004200	2.67049100
H	-3.40226100	1.98356500	2.32744100
C	-7.10164100	1.45045800	1.31603600
H	-6.34030300	0.00391400	-0.08806200
C	-6.78320500	2.37465600	2.30698300
H	-5.19981700	3.28894500	3.44369600
H	-8.13662200	1.29373400	1.02993900
H	-7.56951300	2.94021500	2.79604600
C	5.11545500	-0.39337600	-2.58179500
H	5.48496100	0.53769600	-2.13954900
H	5.86656900	-1.16527600	-2.40091100
H	5.02868200	-0.23984800	-3.65927400
C	0.06138400	-0.37844000	-2.72902900
H	-0.44278500	-1.28960000	-3.06584900
H	-0.63241200	0.15045700	-2.06566600
H	0.24547200	0.25547800	-3.59839400
C	2.46286000	-2.48161200	1.17699500
H	2.11757900	-1.78857300	1.95414400
H	1.76892100	-3.32602000	1.15173200
H	3.44770200	-2.84867000	1.46816600
C	1.50733600	1.84038700	2.15408000
C	1.12140900	0.89770000	1.28020100
H	0.75601700	2.35598000	2.74908700
C	2.89502500	2.28508200	2.35849600
C	3.13142600	3.43327600	3.12447800
C	3.99950800	1.60739800	1.81997400
C	4.42406900	3.90334400	3.33379800
H	2.28670100	3.96414700	3.55605500
C	5.28988100	2.07718500	2.02698800
H	3.85357400	0.69637300	1.24441500
C	5.50940200	3.22874600	2.78282800
H	4.58320200	4.79720200	3.92850200
H	6.13152400	1.53817000	1.60303900
H	6.51896700	3.59137300	2.94543700
C	-0.29290000	0.53055600	1.05388000
O	-1.16239300	0.98375300	2.07089800

H	-0.76531900	0.76213700	2.92796700
H	1.86204200	0.44638000	0.63029800
C	-1.85224800	3.36869500	-0.48107100
C	-1.95439800	4.55952700	-1.16109200
C	-0.92646000	4.94354900	-2.06263600
C	0.16648800	4.04640000	-2.19829800
C	0.17456200	2.87815800	-1.47532900
H	-2.62113400	3.05986000	0.22306900
H	-2.81738500	5.18745900	-0.98729200
H	0.99886100	4.26552500	-2.85271400
H	1.00271900	2.17521300	-1.55195200
C	0.10695900	6.46965200	-3.64411200
C	-2.12024700	6.99386000	-2.58471600
H	0.22548300	5.73342300	-4.44589800
H	-0.11509300	7.43458900	-4.09505000
H	1.05353200	6.55365400	-3.09983000
H	-3.05448900	6.49456500	-2.86222100
H	-2.20062500	7.34583600	-1.55083200
H	-1.98892800	7.85812400	-3.23241000
N	-0.98157700	6.10181900	-2.75035600
N	-0.81523200	2.53073600	-0.63827100
H	-0.62660700	1.44072800	0.06468400

M2

C	-3.02621000	-0.63892100	0.51016000
C	-4.15830600	-1.64974800	0.68065300
H	-3.06974500	0.08939500	1.32090800
H	-4.17881600	-2.02364500	1.71479300
N	-1.76392800	-1.37821000	0.61811800
O	-4.01754400	-2.73213600	-0.22403100
C	-1.67478900	-2.70069800	0.23126400
C	-2.91436200	-3.53712500	0.13531900
H	-2.78334700	-4.30427500	-0.62839800
H	-3.10141700	-4.02727000	1.10284300
N	-0.46436600	-3.08941200	0.03454700
C	-0.46997200	-0.85996000	0.59257500
N	0.30863400	-1.97260300	0.31197000
C	1.69424600	-1.98202200	-0.01691100
C	2.06826200	-1.82329200	-1.35425800
C	2.63018500	-2.06395800	1.01818300
C	3.42927500	-1.74096500	-1.64578100
C	3.97939900	-1.96854200	0.68438000
C	4.39519100	-1.80564500	-0.63936000
H	3.74151600	-1.60337000	-2.67833300

H	4.72353600	-2.00905600	1.47639600
H	-5.11157500	-1.16556800	0.45836400
C	-3.09503100	0.08405900	-0.84475200
H	-2.16059900	0.64105900	-0.97593500
H	-3.14712200	-0.67345600	-1.63460700
C	-4.27776200	1.01535500	-0.92117400
C	-4.29373200	2.18798700	-0.15900100
C	-5.38840200	0.71341900	-1.71172300
C	-5.38938600	3.04404500	-0.19411200
H	-3.43615800	2.42398200	0.46685600
C	-6.48709900	1.56954800	-1.75101100
H	-5.38900400	-0.20034900	-2.30070600
C	-6.48938700	2.73745500	-0.99363000
H	-5.38524300	3.95190700	0.40077100
H	-7.34120900	1.32239900	-2.37353900
H	-7.34409300	3.40536900	-1.02396900
C	5.86200700	-1.70835100	-0.97106800
H	6.40702900	-1.17945800	-0.18521300
H	6.30534900	-2.70483200	-1.06715100
H	6.01987300	-1.18280800	-1.91559700
C	1.01332100	-1.68842200	-2.41940700
H	0.38091700	-2.57990900	-2.45702800
H	0.35892100	-0.83585000	-2.20256900
H	1.46646300	-1.53487200	-3.40016500
C	2.16553600	-2.17690100	2.44381900
H	1.61955000	-1.27260900	2.73598600
H	1.48387100	-3.02318000	2.56562400
H	3.01176700	-2.30305200	3.12117100
C	1.60924000	2.20150700	1.14676300
C	1.23754100	0.96648400	0.73452900
H	0.89126900	2.82530400	1.67567100
C	2.94680000	2.77300800	0.98650500
C	3.21785100	4.03849400	1.53094100
C	3.99548200	2.11519000	0.31696700
C	4.47467800	4.62301200	1.42090400
H	2.42271000	4.56507000	2.05281600
C	5.25090600	2.69877000	0.20940800
H	3.83224300	1.13628300	-0.12656400
C	5.50236100	3.95611200	0.75912500
H	4.65076700	5.60279300	1.85478800
H	6.04215000	2.16795900	-0.31238500
H	6.48466800	4.40833100	0.66932100
C	-0.08776500	0.43587500	0.85352400
O	-1.08586500	1.29893100	1.31224400

H	-0.99629900	2.11712100	0.80241400
H	1.97550000	0.33893500	0.24987300

TS2^D

C	-2.89710200	-0.43128900	0.48509700
C	-3.85509300	-1.26542900	1.32910500
H	-2.69742000	0.53500700	0.94346800
H	-3.53519400	-1.28446700	2.38084600
N	-1.61975100	-1.17378500	0.44863700
O	-3.94002000	-2.58728500	0.81649100
C	-1.55010900	-2.53132800	0.63913200
C	-2.76001800	-3.31302900	1.06858000
H	-2.81269100	-4.25183400	0.51510700
H	-2.66629000	-3.54311100	2.14037100
N	-0.34589300	-2.98262900	0.48967200
C	-0.35999300	-0.73789500	0.14704900
N	0.39392200	-1.86423200	0.18334400
C	1.78155400	-2.00178800	-0.13797100
C	2.15739100	-1.97975200	-1.48191700
C	2.70185700	-2.10404600	0.90897200
C	3.52059000	-2.04558600	-1.76884900
C	4.05146500	-2.17261700	0.57341100
C	4.47724800	-2.14005300	-0.75767300
H	3.84131500	-2.01820400	-2.80719800
H	4.78975800	-2.23936100	1.36892300
H	-4.85581900	-0.83301100	1.26845900
C	-3.42490500	-0.22955600	-0.94285800
H	-2.59602700	0.12803000	-1.55872700
H	-3.76249700	-1.19540200	-1.33349600
C	-4.54074100	0.78536100	-0.96285200
C	-4.23258500	2.14123200	-0.80583500
C	-5.87504500	0.40051700	-1.09952400
C	-5.24708500	3.09266100	-0.79425400
H	-3.18817300	2.42718400	-0.69470100
C	-6.89143900	1.35439700	-1.08683400
H	-6.11689200	-0.65298000	-1.22132400
C	-6.57844100	2.70193600	-0.93526900
H	-5.00014700	4.14330900	-0.67678900
H	-7.92564700	1.04373600	-1.19785000
H	-7.36849600	3.44636600	-0.92758400
C	5.94418300	-2.22835600	-1.08976500
H	6.54630900	-1.68602900	-0.35659200
H	6.27843400	-3.27082800	-1.08480000
H	6.15092200	-1.81618900	-2.07957700

C	1. 12206300	-1. 85416000	-2. 56639100
H	0. 33803100	-2. 60816800	-2. 44729200
H	0. 64365400	-0. 86932400	-2. 52314200
H	1. 57578700	-1. 97570600	-3. 55097900
C	2. 23242800	-2. 07142600	2. 33754600
H	1. 74328100	-1. 11497500	2. 55426600
H	1. 50414100	-2. 86410600	2. 52999700
H	3. 07154300	-2. 18990800	3. 02438800
C	1. 63495400	2. 37592500	0. 30369100
C	1. 37677400	1. 07690000	0. 08610500
H	0. 79413400	3. 06450800	0. 28230100
C	2. 96169900	2. 93430700	0. 59395100
C	3. 05918500	4. 24292100	1. 08808200
C	4. 15375600	2. 21680300	0. 39896600
C	4. 29171800	4. 80958900	1. 39535700
H	2. 14728300	4. 81514000	1. 23757700
C	5. 38488200	2. 78142300	0. 70692400
H	4. 11825400	1. 21115000	-0. 01218800
C	5. 46291100	4. 08024200	1. 20925500
H	4. 33750600	5. 82402300	1. 77978200
H	6. 29297600	2. 20807600	0. 54459300
H	6. 42694200	4. 51993900	1. 44414000
C	0. 01688700	0. 60433700	-0. 21288700
O	-1. 03416800	1. 58813700	-0. 17201400
H	-0. 48786500	0. 94098400	-1. 22117200
H	2. 18071500	0. 34911600	0. 12764800

TS2^B

C	-3. 05543000	-0. 85715700	1. 22411500
C	-4. 03208200	-2. 02093500	1. 35773900
H	-2. 83721200	-0. 39930100	2. 18658900
H	-3. 72874200	-2. 69377400	2. 17318200
N	-1. 79194400	-1. 41251900	0. 71247800
O	-4. 12366900	-2. 74661900	0. 13905000
C	-1. 74623200	-2. 55972900	-0. 03893500
C	-2. 93869400	-3. 46835000	-0. 10824500
H	-3. 00989000	-3. 91480800	-1. 10112500
H	-2. 81752500	-4. 27404000	0. 63167400
N	-0. 58367900	-2. 75896500	-0. 56484100
C	-0. 55967200	-0. 80449100	0. 63174300
N	0. 17385800	-1. 68826600	-0. 12071200
C	1. 41693300	-1. 43148300	-0. 77318900
C	1. 37981200	-0. 85692800	-2. 04680300
C	2. 61470300	-1. 75396900	-0. 12861800

C	2. 59674700	-0. 56568500	-2. 66475800
C	3. 80553100	-1. 44614600	-0. 78392900
C	3. 81505800	-0. 84226300	-2. 04398200
H	2. 59100600	-0. 11870600	-3. 65651200
H	4. 74963100	-1. 68101800	-0. 29737100
H	-5. 02946000	-1. 62944100	1. 57124100
C	-3. 57331700	0. 21274200	0. 25126400
H	-2. 71489000	0. 82822500	-0. 03215600
H	-3. 96692700	-0. 28218600	-0. 64406500
C	-4. 62649200	1. 07986800	0. 89477200
C	-4. 27020100	1. 90393900	1. 97098900
C	-5. 95147400	1. 06903300	0. 45690600
C	-5. 22746200	2. 70637400	2. 58375900
H	-3. 23311500	1. 89108900	2. 30603600
C	-6. 90933600	1. 87407400	1. 07215300
H	-6. 23344500	0. 42750500	-0. 37461200
C	-6. 54845100	2. 69595600	2. 13557800
H	-4. 94356400	3. 34196900	3. 41720900
H	-7. 93628800	1. 85740300	0. 72010700
H	-7. 29299900	3. 32332000	2. 61589700
C	5. 11966100	-0. 48358600	-2. 70696700
H	5. 52033800	0. 44610700	-2. 28992900
H	5. 86923500	-1. 26318600	-2. 55031500
H	4. 99187400	-0. 33941500	-3. 78197500
C	0. 06201300	-0. 59789900	-2. 73031300
H	-0. 41934500	-1. 54342500	-2. 99793100
H	-0. 63125800	-0. 05736300	-2. 07539200
H	0. 20485600	-0. 01079000	-3. 64017600
C	2. 59915300	-2. 36337200	1. 24600000
H	2. 21991100	-1. 64126700	1. 97865300
H	1. 94349300	-3. 23763800	1. 27789300
H	3. 60405600	-2. 66349800	1. 54780600
C	1. 49520200	1. 79017700	2. 28295200
C	1. 14726300	0. 84261400	1. 39470000
H	0. 68849200	2. 24427800	2. 85350500
C	2. 85978600	2. 25662800	2. 54351700
C	3. 06601300	3. 29246000	3. 46832300
C	3. 99593900	1. 71385100	1. 91588800
C	4. 34061100	3. 77088000	3. 75284200
H	2. 20259100	3. 72415700	3. 96796500
C	5. 26886900	2. 19171500	2. 19821500
H	3. 88167400	0. 90346800	1. 19964800
C	5. 45282900	3. 22498900	3. 11773000
H	4. 46537100	4. 57268100	4. 47471800

H	6.12802500	1.75229700	1.69912300
H	6.44943100	3.59464100	3.33700600
C	-0.27690100	0.51463500	1.14782600
O	-1.20456100	1.09393900	1.90996800
H	1.90213000	0.38485200	0.76300400
C	-1.48401800	3.25894900	-0.24634900
C	-1.76174900	4.45855400	-0.86709900
C	-1.05916900	4.81984700	-2.04195900
C	-0.07675400	3.90770600	-2.50183200
C	0.12583300	2.73129200	-1.81384500
H	-1.96876700	2.93703000	0.67075500
H	-2.51315200	5.10550000	-0.43520000
H	0.52461900	4.11628100	-3.37631900
H	0.88309100	2.01768000	-2.13390500
C	-0.55414000	6.32401000	-3.88595800
C	-2.30135400	6.90718500	-2.17030300
H	-0.68269600	5.56463300	-4.66506500
H	-0.91578200	7.27405600	-4.27521900
H	0.51590100	6.42426300	-3.67008100
H	-3.29206500	6.44162100	-2.12629000
H	-2.03469400	7.25357600	-1.16541100
H	-2.35958200	7.77356000	-2.82693400
N	-1.30897500	5.98347300	-2.69291800
N	-0.56949800	2.39870600	-0.72091400
H	-0.34071200	1.25966800	-0.01561300

TS3

C	-3.50538400	-2.40941800	-1.41500000
C	-4.53681000	-3.49899200	-1.44010900
C	-5.95841800	-2.12408200	-0.24007600
C	-4.96369800	-0.97412400	0.02304000
C	-2.49944700	-0.62677200	-0.60510300
H	-4.03679300	-4.46892200	-1.42159400
H	-4.82642800	-0.82028000	1.09283300
N	-2.38572700	-2.34991800	-2.06872500
N	-1.77172500	-1.21750500	-1.59940400
N	-3.65939500	-1.36032500	-0.54961600
C	-0.64433700	-0.66996600	-2.29725400
C	-0.80181000	0.56080000	-2.95187600
C	0.57238300	-1.35737700	-2.27542100
C	0.34581800	1.17010200	-3.45367300
C	1.69224900	-0.70156300	-2.78684400
C	1.60537100	0.57462800	-3.34189900
H	0.25478400	2.14333600	-3.93057900

H	2.65865200	-1.19811400	-2.72839500
O	-5.32802100	-3.38716000	-0.28074000
H	-5.15177800	-3.43237900	-2.34897500
H	-6.69723200	-2.14940500	0.56154700
C	-2.15120000	1.21419300	-3.10626700
H	-2.93925500	0.46831600	-3.25007000
H	-2.40868100	1.81660600	-2.22893700
H	-2.14548800	1.87427300	-3.97557700
C	2.84185700	1.28342500	-3.82783700
H	2.93054400	1.21858500	-4.91722500
H	2.80913600	2.34367800	-3.56034400
H	3.74138900	0.84258300	-3.38927800
C	0.66588500	-2.76550500	-1.76553400
H	0.19751700	-2.86465800	-0.78481000
H	0.14454500	-3.44878800	-2.44258200
H	1.71096500	-3.06687000	-1.69677800
C	-2.16548900	0.48582300	0.23281000
O	-3.05371700	0.87890100	1.11357500
C	-0.95117300	1.22908900	-0.03106800
C	-0.87472400	2.56748500	0.08195400
H	-0.07886500	0.65076100	-0.32838800
C	0.32527000	3.36291100	-0.16573400
C	1.53323400	2.79077400	-0.60170200
C	0.27482800	4.75402900	0.01109500
C	2.63410100	3.59213100	-0.86847900
H	1.61647300	1.71627600	-0.74441100
C	1.38689000	5.55216700	-0.23792900
H	-0.65404000	5.20793500	0.34826700
C	2.57229500	4.97472400	-0.68484000
H	3.54824800	3.12750500	-1.22337500
H	1.32467600	6.62546600	-0.08918300
H	3.44082900	5.59145800	-0.89223000
H	-2.62644700	0.57523800	2.21355400
C	0.24284700	0.88520900	2.83870300
C	1.41639500	0.65940500	2.17592000
C	1.69369400	-0.55343700	1.45741100
C	0.71697600	-1.58319500	1.57482900
C	-0.50616800	-1.40979800	2.18485300
C	-0.81404500	-0.10243400	2.72073800
H	2.19419700	1.40777000	2.23142400
H	0.95064700	-2.55838000	1.17424500
C	2.90895200	-0.73326200	0.73628400
C	3.28460500	-2.01645700	0.21496400
C	3.85522600	0.33087000	0.54328000

C	4. 38669200	-2. 22694100	-0. 55754200
H	2. 67358300	-2. 87104300	0. 47521200
C	4. 99793800	0. 19556700	-0. 19019200
H	3. 65806700	1. 28780300	1. 01168400
C	5. 22841300	-1. 06746400	-0. 92336200
O	-2. 01086100	0. 19653600	3. 14357800
O	6. 11359500	-1. 15967300	-1. 78793900
C	-1. 39433400	-2. 64150100	2. 45330400
C	-2. 88353800	-2. 33555100	2. 68020400
C	-1. 31932700	-3. 65621500	1. 30085700
C	-0. 84358100	-3. 30564900	3. 73027900
H	-3. 06089200	-1. 84369400	3. 63526300
H	-3. 26740400	-1. 68330800	1. 89707100
H	-3. 44617900	-3. 27470300	2. 65306100
H	-0. 31677700	-4. 06607100	1. 15145000
H	-1. 97808700	-4. 50138300	1. 52233400
H	-1. 65153400	-3. 20975500	0. 35707800
H	-1. 44667100	-4. 18334200	3. 98819000
H	0. 19389900	-3. 62421500	3. 59115700
H	-0. 87821400	-2. 60606300	4. 57118100
C	0. 05172000	2. 10344900	3. 75489600
C	-1. 06389400	3. 05382300	3. 28348000
C	-0. 27847100	1. 58343800	5. 16822500
C	1. 33547800	2. 93837200	3. 84944100
H	-0. 73243000	3. 62567900	2. 41365800
H	-1. 98311400	2. 52710100	3. 03079700
H	-1. 27936900	3. 76810600	4. 08606400
H	0. 50139500	0. 89909400	5. 51834700
H	-0. 33008700	2. 42645300	5. 86553600
H	-1. 23622400	1. 06120400	5. 18217900
H	1. 16135400	3. 77925800	4. 52763200
H	2. 17510400	2. 35696000	4. 24414000
H	1. 62019500	3. 35224900	2. 87498800
C	6. 07916500	1. 27789100	-0. 25208300
C	6. 22254300	1. 84373000	-1. 67657600
C	5. 78899000	2. 43179000	0. 71615300
C	7. 42599100	0. 66148700	0. 17913800
H	6. 48512500	1. 05100700	-2. 37777800
H	5. 29078700	2. 31003000	-2. 01382200
H	7. 00616100	2. 60976000	-1. 69349700
H	5. 71103600	2. 07308000	1. 74796400
H	6. 61344700	3. 15001900	0. 67154000
H	4. 86944200	2. 97178500	0. 47359400
H	8. 19801600	1. 43872900	0. 18636000

H	7.35044400	0.24853600	1.19051100
H	7.73468800	-0.13050200	-0.50295800
C	4.79205600	-3.61460300	-1.05867800
C	4.66597000	-3.68131100	-2.59245700
C	6.24851200	-3.90890900	-0.65046500
C	3.91828900	-4.72122000	-0.45447000
H	3.62633700	-3.52899000	-2.90530600
H	5.29132400	-2.92178900	-3.06257000
H	4.97847000	-4.66980800	-2.94782000
H	6.35464200	-3.87171900	0.43891100
H	6.52804200	-4.91402600	-0.98433800
H	6.93421600	-3.18864200	-1.09587400
H	4.27598000	-5.69209600	-0.81019800
H	3.97117700	-4.72313500	0.63930600
H	2.86686600	-4.63431100	-0.74863800
H	-1.77499000	3.11062200	0.36513300
H	-6.48540600	-1.94546300	-1.19074900
C	-5.46381000	0.32970300	-0.61840500
H	-5.66100000	0.14734700	-1.68167400
H	-4.67849600	1.08461000	-0.53666200
C	-6.70920300	0.81128500	0.08572400
C	-7.97771300	0.64905700	-0.47309400
C	-6.59264100	1.40028400	1.34919600
C	-9.11338900	1.06769200	0.21741700
H	-8.07734100	0.20146300	-1.45904200
C	-7.72532000	1.81745600	2.03988100
H	-5.60138600	1.53565200	1.77650900
C	-8.98936000	1.65048700	1.47536100
H	-10.09418900	0.94033000	-0.22962100
H	-7.62217700	2.27687700	3.01777000
H	-9.87339300	1.97689800	2.01353200

M3

C	-3.55241500	-2.31597300	-1.79196500
C	-4.55340200	-3.43318700	-1.78864400
C	-5.98775700	-2.10672600	-0.55511800
C	-5.02721600	-0.92721700	-0.31369600
C	-2.60305500	-0.45368000	-1.02636200
H	-4.03256000	-4.39183000	-1.79312300
H	-4.83675200	-0.80886900	0.75527700
N	-2.43933400	-2.25971900	-2.43866400
N	-1.86987600	-1.05887100	-2.03771600
N	-3.75610000	-1.23184100	-0.97069300
C	-0.65308600	-0.59891400	-2.60854500

C	-0.65807900	0.60173900	-3.33575300
C	0.53129000	-1.28983100	-2.33375300
C	0.56891500	1.14648400	-3.70728800
C	1.73639700	-0.71534400	-2.74019200
C	1.77631800	0.51280400	-3.40016300
H	0.58423100	2.09621100	-4.23732400
H	2.66800300	-1.22669700	-2.50840000
O	-5.32037700	-3.35070400	-0.60730100
H	-5.20256600	-3.37853200	-2.67511300
H	-6.71339900	-2.15397200	0.25813400
C	-1.95006600	1.31463000	-3.62668400
H	-2.72682100	0.60632600	-3.92918400
H	-2.31144500	1.83697200	-2.73288600
H	-1.81294000	2.05031900	-4.42117200
C	3.09191200	1.15272600	-3.75960500
H	3.19349200	1.26895800	-4.84316000
H	3.16264800	2.15172600	-3.31614100
H	3.93626200	0.55633200	-3.40187900
C	0.49647900	-2.58962800	-1.57966900
H	-0.10252400	-2.48415100	-0.66849000
H	0.03420600	-3.38090400	-2.17626600
H	1.50886100	-2.89797000	-1.30698500
C	-2.26043300	0.59804300	-0.20780600
O	-3.20014900	1.02573800	0.72951300
C	-1.03427700	1.33184100	-0.31632000
C	-0.81750200	2.56443700	0.19587100
H	-0.22366800	0.84860700	-0.84788500
C	0.44540200	3.28411100	0.05708900
C	1.61407200	2.67322600	-0.43426700
C	0.51965700	4.64814900	0.38961500
C	2.78225400	3.40342000	-0.60349200
H	1.61891100	1.61572200	-0.68661700
C	1.69854000	5.37208200	0.24022800
H	-0.37315500	5.14605200	0.76088800
C	2.84166300	4.75535900	-0.26283800
H	3.65777100	2.89920500	-1.00049000
H	1.71964300	6.42405700	0.50849900
H	3.76303900	5.31459100	-0.39207800
H	-2.78361100	0.91811000	1.60356700
C	0.62356600	1.02992500	2.87376000
C	1.77519000	0.80488600	2.20251200
C	2.05965900	-0.43882100	1.50175800
C	1.09774000	-1.51532000	1.68668400
C	-0.09581800	-1.35225000	2.29477000

C	-0.46474500	0.01881300	2.74541900
H	2.54786200	1.56024200	2.22988500
H	1.34926400	-2.49613200	1.31126100
C	3.21479500	-0.62755900	0.75969800
C	3.56000000	-1.93027300	0.20661000
C	4.17739300	0.44201800	0.52811300
C	4.57079200	-2.12548100	-0.66562400
H	2.99156700	-2.78936100	0.53326400
C	5.23213600	0.31709000	-0.30851500
H	4.04291000	1.37421800	1.06089800
C	5.33851500	-0.93047600	-1.12254800
O	-1.63161300	0.29443400	3.03059000
O	6.04285600	-0.97433200	-2.12600400
C	-1.06784700	-2.50725700	2.53979300
C	-2.29774100	-2.37535200	1.62549000
C	-0.40681100	-3.86133800	2.25087500
C	-1.50450500	-2.50873800	4.01784400
H	-2.77733000	-1.40137000	1.73995900
H	-2.00387700	-2.49432400	0.57682800
H	-3.02659100	-3.15911900	1.86131200
H	0.49190700	-4.00971700	2.85875200
H	-1.11376600	-4.66056100	2.49086600
H	-0.13727900	-3.97400200	1.19512800
H	-2.12986900	-3.38656000	4.20868300
H	-0.63247300	-2.56470500	4.67832100
H	-2.07727500	-1.61591500	4.26817700
C	0.43655300	2.20307300	3.83874800
C	-0.75223700	3.11782200	3.49612400
C	0.21288300	1.59372400	5.23847100
C	1.69037400	3.08448900	3.88291200
H	-0.54429000	3.68370400	2.58731800
H	-1.67707200	2.55794900	3.36829200
H	-0.88558200	3.83464800	4.31403400
H	1.04661700	0.94133200	5.51767400
H	0.14195300	2.39552500	5.98042500
H	-0.71323700	1.01433400	5.27194300
H	1.52739500	3.89910900	4.59459100
H	2.57337800	2.52630000	4.21102700
H	1.89466400	3.53228400	2.90298100
C	6.33429600	1.36835300	-0.44617800
C	6.33727200	2.01044500	-1.84599900
C	6.18480100	2.47565400	0.60489300
C	7.69483700	0.68192400	-0.20610400
H	6.50269600	1.26257200	-2.62093100

H	5.39269200	2.52249900	-2.05271800
H	7.13864400	2.75531200	-1.89745300
H	6.20032200	2.06599300	1.62031300
H	7.02361600	3.17134400	0.51019400
H	5.26366300	3.05273600	0.48032400
H	8.48999600	1.43341800	-0.24216600
H	7.72117200	0.20726700	0.78041700
H	7.90001500	-0.07267000	-0.96667900
C	4.94135500	-3.49787900	-1.22389500
C	4.57808000	-3.57226800	-2.71892700
C	6.45169400	-3.73986700	-1.03920900
C	4.19454000	-4.62006100	-0.49263800
H	3.49674100	-3.46441000	-2.85944000
H	5.08798600	-2.79483300	-3.28831200
H	4.87258800	-4.54980600	-3.11559100
H	6.72614500	-3.67468400	0.01895800
H	6.70439700	-4.74441000	-1.39284700
H	7.04345200	-3.01710700	-1.60165300
H	4.52859100	-5.58458100	-0.88515600
H	4.39622400	-4.60515600	0.58352600
H	3.11133600	-4.56538600	-0.64591400
H	-1.63624600	3.08383200	0.68791700
H	-6.53590000	-1.94787000	-1.49820400
C	-5.63288100	0.37219200	-0.87016600
H	-5.90610600	0.20643000	-1.91918700
H	-4.86931600	1.15250900	-0.83688000
C	-6.83487700	0.79499300	-0.06143500
C	-8.13791100	0.54383500	-0.49508500
C	-6.64243000	1.41727400	1.17648800
C	-9.22989700	0.90578900	0.29158800
H	-8.29879100	0.06970300	-1.46048100
C	-7.73095400	1.77931100	1.96350700
H	-5.62608600	1.62133600	1.50498700
C	-9.02843000	1.52310500	1.52286700
H	-10.23770000	0.70890900	-0.06053800
H	-7.56806300	2.26573600	2.92018800
H	-9.87849300	1.80749400	2.13470800

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C	-3.39934800	-0.47714200	-3.46332500
C	-4.49133300	-1.34031500	-4.02070000
C	-5.80156800	-0.82481200	-2.17975500
C	-4.75857200	-0.01692900	-1.38993600
C	-2.35221000	0.67734900	-1.93937600

H	-4.04579500	-2.16774000	-4.57415800
H	-4.45466400	-0.55528200	-0.49390500
N	-2.22189000	-0.23940100	-3.97194100
N	-1.58323100	0.48667500	-3.01877500
N	-3.53415600	0.08594200	-2.22419100
C	-0.18464800	0.80799700	-3.15030900
C	0.18722700	1.88357700	-3.96199000
C	0.72027000	0.04929400	-2.40848000
C	1.54061800	2.21064800	-3.99185300
C	2.05880700	0.43696600	-2.44951900
C	2.48706200	1.50485300	-3.23732700
H	1.86489100	3.04157600	-4.61375300
H	2.78052200	-0.11629000	-1.85427700
O	-5.22494400	-1.86585200	-2.94175400
H	-5.13472700	-0.76040200	-4.69751200
H	-6.49390100	-1.27857100	-1.46981000
C	-0.84290300	2.65970100	-4.73884700
H	-1.37001000	2.01344400	-5.44655300
H	-1.59487900	3.09833500	-4.07286900
H	-0.37141900	3.47050100	-5.29546600
C	3.94901000	1.85850000	-3.30156800
H	4.38091300	1.50138200	-4.24246300
H	4.09612700	2.94160500	-3.26158900
H	4.50124500	1.40095200	-2.47569800
C	0.26856900	-1.13645100	-1.60344500
H	-0.22820300	-0.83212500	-0.67552300
H	-0.42889700	-1.75999100	-2.17320700
H	1.13023800	-1.74500900	-1.32061200
C	-2.00868400	1.34778900	-0.65635200
O	-2.67112900	1.00304600	0.34452700
C	-1.00727900	2.39074700	-0.67447300
C	-0.60349100	2.99801500	0.46220600
H	-0.62310400	2.71403500	-1.63519500
C	0.33187600	4.11566900	0.51247900
C	1.23879200	4.37666500	-0.52769500
C	0.30602200	4.97516600	1.62157800
C	2.07144500	5.48609400	-0.46860300
H	1.31560600	3.68506600	-1.36397000
C	1.14017900	6.08606300	1.67606500
H	-0.39476900	4.77908000	2.42862000
C	2.02100400	6.34649000	0.62858300
H	2.77971900	5.67005500	-1.27019000
H	1.10496800	6.74619600	2.53621400
H	2.67859800	7.20846600	0.67228000

H	-2.15993100	-0.00314800	1.44197000
C	-1.28414700	0.41471400	3.16575300
C	0.04177100	0.46607200	2.84597700
C	0.68256900	-0.49752300	1.99939300
C	-0.08583100	-1.65826200	1.66592100
C	-1.42419700	-1.76567500	1.91358300
C	-2.18124500	-0.61303800	2.51562600
H	0.65884300	1.24768900	3.27039200
H	0.40568200	-2.45901700	1.13149900
C	1.99192300	-0.29966500	1.48386600
C	2.71996600	-1.35398100	0.84756100
C	2.65063200	0.96701400	1.56689400
C	3.93930100	-1.18416500	0.25701900
H	2.29326600	-2.34923800	0.86669500
C	3.88018200	1.21568100	1.02455200
H	2.12958300	1.77794100	2.06291300
C	4.54443400	0.16161300	0.24031300
O	-3.42062800	-0.75036400	2.89577100
O	5.58122400	0.39587700	-0.41472900
C	-2.21065800	-2.99824400	1.48287100
C	-3.32918000	-2.56603800	0.52132900
C	-1.34141400	-4.03867100	0.76772000
C	-2.81949400	-3.65282800	2.73714300
H	-3.98875200	-1.85966500	1.03077300
H	-2.89430200	-2.09738700	-0.37316500
H	-3.90698300	-3.43800700	0.19598600
H	-0.52778500	-4.39824200	1.40562500
H	-1.96214200	-4.90037100	0.50404900
H	-0.90722500	-3.64456100	-0.15862500
H	-3.43275800	-4.51186500	2.44305700
H	-2.02493900	-4.01304600	3.39881200
H	-3.43354600	-2.92818400	3.27204200
C	-1.91167900	1.40464800	4.14244300
C	-3.08374400	2.15628700	3.48496800
C	-2.43250000	0.60397000	5.35236600
C	-0.90092400	2.43687500	4.65474100
H	-2.74858700	2.75200600	2.62868600
H	-3.84102700	1.45091100	3.14518500
H	-3.52524300	2.84082700	4.21781100
H	-1.60424800	0.09980900	5.86125000
H	-2.90581700	1.28726800	6.06645500
H	-3.15820400	-0.13872300	5.02034100
H	-1.40759700	3.12476500	5.33835500
H	-0.07968000	1.96473500	5.20307000

H	-0.46822000	3.03045100	3.84140300
C	4.59577600	2.55689700	1.20470100
C	4.81495000	3.24839200	-0.15252000
C	3.79445500	3.50731700	2.10076600
C	5.96042600	2.31688300	1.87768400
H	5.51248300	2.67834200	-0.76562000
H	3.86389600	3.33751200	-0.68779900
H	5.21366000	4.25848700	0.00275200
H	3.63125200	3.07938400	3.09609000
H	4.34899300	4.44341000	2.22355100
H	2.82207300	3.75588700	1.66491400
H	6.48065200	3.27263600	2.00944900
H	5.82554300	1.86456300	2.86575200
H	6.58191400	1.65933800	1.26877300
C	4.69747700	-2.34433200	-0.39539300
C	4.83686700	-2.10308000	-1.91015300
C	6.09530700	-2.47358300	0.23736800
C	3.97440300	-3.68256900	-0.20280700
H	3.85175900	-2.10382600	-2.39225800
H	5.32969200	-1.15001200	-2.10606500
H	5.42807900	-2.90793900	-2.36207200
H	6.00984900	-2.66628700	1.31190500
H	6.63222200	-3.31337000	-0.21778600
H	6.67283800	-1.56157500	0.08732800
H	4.56101800	-4.47902200	-0.67110700
H	3.85544200	-3.93083500	0.85709800
H	2.98353300	-3.68452700	-0.67180200
H	-1.02693500	2.65555000	1.40536200
H	-6.36936900	-0.15111100	-2.84057700
C	-5.33511100	1.34630900	-0.99346300
H	-5.77385600	1.83054100	-1.87302300
H	-4.54290400	1.99175000	-0.61120500
C	-6.37664400	1.13524400	0.08449500
C	-7.72311600	1.42101700	-0.13972100
C	-5.98134400	0.61243800	1.32163800
C	-8.66713300	1.19945100	0.86200300
H	-8.03536600	1.82363000	-1.10044100
C	-6.92583900	0.38849800	2.31802300
H	-4.93687200	0.37068200	1.52453400
C	-8.27013800	0.68319700	2.09227800
H	-9.71193500	1.42940700	0.67809600
H	-6.59840300	-0.01742400	3.27012000
H	-9.00585900	0.51041300	2.87129500

TS3^{HCT3}

C	-5.52808100	0.32362600	0.08983800
C	-6.61621100	1.22541500	0.59345500
C	-5.27792700	3.03945200	0.08287100
C	-3.98939600	2.27493300	-0.26714100
C	-3.48209100	-0.24110200	-0.46090200
H	-7.14509300	0.73014500	1.40869100
H	-3.20912500	2.49093000	0.46142100
N	-5.57542800	-0.96333700	-0.08580000
N	-4.30693200	-1.30532400	-0.44801400
N	-4.28244600	0.82444200	-0.17128900
C	-4.03817600	-2.66576000	-0.82065200
C	-3.90218700	-2.95387700	-2.18237500
C	-3.97118900	-3.63509200	0.18260500
C	-3.62068100	-4.27351800	-2.52983200
C	-3.69893600	-4.94111100	-0.22121800
C	-3.50916100	-5.27564200	-1.56288400
H	-3.49417800	-4.52445400	-3.57979600
H	-3.61893600	-5.71551100	0.53772100
O	-6.02603900	2.40003300	1.09501300
H	-7.33099900	1.45102600	-0.21073700
H	-5.00734300	4.03225600	0.44451900
C	-4.02935100	-1.87500500	-3.22602600
H	-4.93404300	-1.27978500	-3.06782800
H	-3.17234600	-1.19159100	-3.20162800
H	-4.07819600	-2.31402900	-4.22331400
C	-3.21701900	-6.69973500	-1.95646400
H	-2.84479500	-6.76037800	-2.98092400
H	-2.47229600	-7.14305300	-1.29077500
H	-4.12270700	-7.31056800	-1.89049600
C	-4.17074200	-3.27675300	1.62965800
H	-3.53910600	-2.42891400	1.91159400
H	-5.21417200	-3.00517700	1.81720500
H	-3.91308200	-4.12537300	2.26634600
C	-2.03223500	-0.14591300	-0.63005400
O	-1.52141200	0.97367100	-0.25773900
C	-1.22974300	-1.19880500	-1.16970400
C	0.12249000	-1.05351800	-1.21996900
H	-1.70082500	-2.12632300	-1.47007400
C	1.08604000	-2.02858600	-1.70523800
C	0.72009200	-3.24672400	-2.30632600
C	2.45188100	-1.74891600	-1.53467200
C	1.69040500	-4.16218000	-2.68734600
H	-0.32929300	-3.47961100	-2.47068700

C	3.42196900	-2.66771000	-1.91676900
H	2.75083700	-0.80546000	-1.08428100
C	3.04428700	-3.88087600	-2.48805200
H	1.39397000	-5.10078100	-3.14478100
H	4.47058600	-2.42960300	-1.76652800
H	3.79806700	-4.60300800	-2.78493300
H	-0.78414300	0.89599900	0.83068100
C	-0.21295100	0.72766300	1.97710200
C	1.14238500	1.11393600	1.73972900
C	2.15275800	0.21525100	1.42526200
C	1.84274100	-1.18892600	1.59612300
C	0.60321900	-1.68906700	1.84513300
C	-0.52441400	-0.73919700	1.95835100
H	1.38978100	2.16789100	1.79780300
H	2.65660200	-1.89085500	1.46373900
C	3.45340600	0.63760200	0.96319800
C	4.58611300	-0.21779800	0.98654400
C	3.63367400	1.92591200	0.39277300
C	5.82070400	0.15146900	0.51500700
H	4.47694000	-1.20050700	1.43056200
C	4.83001000	2.37346600	-0.10376200
H	2.75924600	2.56190200	0.30560000
C	6.00901000	1.49885800	-0.04262500
O	-1.70700500	-1.10776400	1.93865300
O	7.12629100	1.88134100	-0.45883000
C	0.34738100	-3.18087500	2.07879100
C	-0.25782700	-3.35361300	3.48500400
C	-0.62247400	-3.75842700	1.03515200
C	1.64558500	-3.99251300	2.00633500
H	0.41052700	-2.94058600	4.24776600
H	-1.22577900	-2.85299600	3.55775700
H	-0.40099900	-4.41861000	3.69713900
H	-0.15570300	-3.78327000	0.04626000
H	-0.88406500	-4.78803600	1.30905800
H	-1.53533100	-3.16872900	0.98027500
H	1.41957800	-5.04649400	2.19477900
H	2.10595500	-3.92108500	1.01386100
H	2.37503600	-3.66655200	2.75522700
C	-1.03901800	1.65916800	2.91665600
C	-2.52211500	1.27674100	3.03189100
C	-0.41659800	1.57787000	4.32012000
C	-0.96404200	3.10939100	2.41180300
H	-2.98966900	1.16337200	2.05179800
H	-2.65735100	0.33346400	3.56111800

H	-3.04580900	2.06567700	3.58235000
H	0.62726400	1.90458600	4.30820300
H	-0.97195800	2.21338700	5.01855500
H	-0.44834500	0.54935700	4.69539700
H	-1.59991800	3.74655700	3.03410800
H	0.04689000	3.52171700	2.46055400
H	-1.31051100	3.19130700	1.37517600
C	4.97269500	3.75599300	-0.74512500
C	5.44340600	3.61310500	-2.20436600
C	3.64593100	4.52530100	-0.75870700
C	5.99129600	4.59562900	0.04779900
H	6.40198200	3.09642700	-2.24854300
H	4.70833900	3.04705200	-2.78694100
H	5.54961200	4.60405500	-2.66124600
H	3.26255400	4.69125600	0.25427500
H	3.80297000	5.50485900	-1.22158800
H	2.87797100	4.00051900	-1.33803800
H	6.10737700	5.58099600	-0.41883200
H	5.64220600	4.74474300	1.07534200
H	6.95926000	4.09567200	0.07231200
C	7.02094000	-0.79688600	0.56904200
C	7.56938400	-1.03053400	-0.85121700
C	8.12724300	-0.19382000	1.45423000
C	6.65051900	-2.16490600	1.15404900
H	6.80458500	-1.49331000	-1.48536600
H	7.87593900	-0.08774100	-1.30362600
H	8.43066400	-1.70766100	-0.81220900
H	7.76115700	-0.05535400	2.47721800
H	8.98822500	-0.87174400	1.48952700
H	8.44897600	0.77005400	1.06050800
H	7.53543700	-2.80916600	1.15165900
H	6.30031500	-2.08491200	2.18875000
H	5.87153100	-2.66365900	0.56568000
H	0.54224800	-0.11476100	-0.85931700
H	-5.89980700	3.15433100	-0.81905100
C	-3.50809200	2.65185800	-1.67828600
H	-4.36067400	2.61377200	-2.36644200
H	-2.76877400	1.92523200	-2.01937800
C	-2.88617300	4.02859400	-1.66554700
C	-3.62653800	5.16714500	-1.98769100
C	-1.54876200	4.17205000	-1.28223800
C	-3.04330800	6.43077200	-1.92454200
H	-4.66332100	5.06448100	-2.30032600
C	-0.96555600	5.43366500	-1.21789800

H	-0.97091700	3.28211800	-1.04113900
C	-1.71291300	6.56607900	-1.53745100
H	-3.62751400	7.30825100	-2.18241300
H	0.07468200	5.53254500	-0.92340800
H	-1.25753800	7.54983700	-1.48917200

TS3^{HCT4}

C	-4.22903200	2.24326700	0.58119400
C	-4.81131300	3.50950700	1.13653900
C	-2.94770000	4.65127900	0.37579800
C	-2.14023000	3.42860000	-0.11109400
C	-2.60859200	0.90658100	-0.06105700
H	-5.38800700	3.27756200	2.03327800
H	-1.17717200	3.37112100	0.39100700
N	-4.79917200	1.08550500	0.44751500
N	-3.79764300	0.25948000	0.01054300
N	-2.90614500	2.21042000	0.22855900
C	-4.12494900	-1.04307900	-0.49417300
C	-4.05727400	-1.23561600	-1.88183000
C	-4.49846300	-2.05247900	0.39632300
C	-4.29851000	-2.51833000	-2.36458300
C	-4.73326800	-3.31918400	-0.14282900
C	-4.61228200	-3.57682900	-1.50689800
H	-4.24113200	-2.69571900	-3.43586200
H	-5.00733300	-4.12707700	0.53102400
O	-3.75075200	4.36080100	1.50031300
H	-5.47257000	3.98905700	0.40064700
H	-2.25668100	5.44481200	0.66183900
C	-3.70249600	-0.11212400	-2.82005000
H	-4.17937500	0.82612200	-2.51983000
H	-2.61878500	0.05197800	-2.84241400
H	-4.02485900	-0.35120700	-3.83469500
C	-4.79817100	-4.96912200	-2.05018900
H	-5.27198200	-4.95062000	-3.03454900
H	-3.82777300	-5.46555100	-2.15955700
H	-5.40887500	-5.57910700	-1.38161900
C	-4.61890500	-1.80390900	1.87197700
H	-3.62974100	-1.69599800	2.33222400
H	-5.18612200	-0.89190100	2.07494900
H	-5.12253800	-2.64441600	2.35359300
C	-1.27093500	0.42430200	-0.35852800
O	-0.32062800	1.28250900	-0.29787800
C	-1.03044000	-0.92537600	-0.81983500
C	0.17140500	-1.26549200	-1.33646300

H	-1.81281200	-1.66709900	-0.71052300
C	0.53205900	-2.59123100	-1.83387000
C	-0.42596200	-3.57492400	-2.13081100
C	1.88814000	-2.90137100	-2.02489500
C	-0.03549200	-4.83713500	-2.56017800
H	-1.48498800	-3.34330200	-2.03938000
C	2.27667300	-4.16584200	-2.45624400
H	2.63881400	-2.13955200	-1.82294300
C	1.31675200	-5.14163900	-2.71773200
H	-0.78921000	-5.58662400	-2.78131300
H	3.33068300	-4.38670300	-2.59799200
H	1.61874300	-6.12762300	-3.05520900
H	0.37790200	0.92270600	0.90545700
C	-0.44759800	-0.07541000	2.58004800
C	0.75901500	0.36523500	1.92582400
C	1.72190800	-0.63356700	1.39879200
C	1.30500000	-2.01426500	1.42235600
C	0.15195200	-2.44928600	1.98977700
C	-0.77363900	-1.47970900	2.64922300
H	1.25133400	1.19727300	2.43133900
H	1.93920000	-2.73728600	0.92861300
C	2.92772000	-0.24145800	0.82970600
C	3.90456900	-1.19601400	0.36271300
C	3.24099800	1.15323500	0.62942100
C	5.02443600	-0.85170900	-0.31932000
H	3.73567600	-2.24058500	0.58777200
C	4.33953900	1.58598900	-0.03636300
H	2.53649000	1.88410700	1.00533900
C	5.27219000	0.58243600	-0.61544400
O	-1.75117600	-1.90200500	3.30420200
O	6.22543600	0.93292700	-1.31730400
C	-0.21548500	-3.93429500	2.00368300
C	-1.59593900	-4.13939400	1.35193300
C	0.79963700	-4.78778300	1.23204100
C	-0.24293100	-4.44214000	3.45949200
H	-2.37076500	-3.58829400	1.88546400
H	-1.57858700	-3.81557800	0.30551600
H	-1.84998400	-5.20559200	1.36408600
H	1.79662300	-4.73893900	1.68339800
H	0.47696400	-5.83307900	1.25965400
H	0.87503400	-4.48799100	0.18142400
H	-0.48152100	-5.51152200	3.46452800
H	0.73959500	-4.31346600	3.92579500
H	-0.98763600	-3.90688400	4.04695300

C	-1.18372800	0.89974200	3.50497300
C	-2.71884500	0.76088500	3.45361800
C	-0.72557800	0.60668500	4.94915500
C	-0.83556400	2.35849800	3.17051200
H	-3.08075900	0.71126300	2.42418400
H	-3.05017400	-0.14411100	3.95853700
H	-3.17863600	1.63119100	3.93550900
H	0.35530400	0.74901700	5.05075700
H	-1.22749600	1.28762400	5.64655300
H	-0.97504500	-0.42104400	5.22264000
H	-1.47967500	3.03295900	3.74143100
H	0.19942400	2.61330300	3.41462600
H	-0.99196000	2.55574500	2.10804600
C	4.63613000	3.07143200	-0.24688300
C	4.57944800	3.40803500	-1.74832800
C	3.61721700	3.95909100	0.47721200
C	6.02932600	3.41612600	0.31281200
H	5.32055900	2.83525700	-2.30589600
H	3.58497400	3.18687600	-2.15289100
H	4.77990600	4.47612800	-1.89481500
H	3.61413600	3.77381800	1.55665800
H	3.87936900	5.01009300	0.31896900
H	2.59955100	3.81253900	0.09944800
H	6.21808000	4.48802600	0.18794600
H	6.07949300	3.18609900	1.38225300
H	6.81072900	2.86057000	-0.20432800
C	6.02614000	-1.89325100	-0.82120200
C	6.04676800	-1.88650000	-2.36121800
C	7.43441200	-1.58769400	-0.27902100
C	5.64827100	-3.30674400	-0.36269800
H	5.05759400	-2.14243100	-2.75899100
H	6.33674800	-0.90784300	-2.74400700
H	6.76075100	-2.63392800	-2.72477400
H	7.43322200	-1.59753600	0.81595100
H	8.13427700	-2.35681000	-0.62365700
H	7.78698000	-0.61566900	-0.62222200
H	6.38602000	-4.01740700	-0.74700900
H	5.63906400	-3.39041300	0.72928000
H	4.66511200	-3.61165400	-0.73894500
H	0.94312000	-0.49895100	-1.37729000
H	-3.58270300	5.02508500	-0.44284600
C	-1.90741200	3.49687900	-1.62897000
H	-2.87413300	3.62867200	-2.13010500
H	-1.47387900	2.55027500	-1.95999500

C	-0.96611800	4.62790200	-1.96453100
C	-1.43445000	5.85731500	-2.43035400
C	0.40776100	4.45331800	-1.76629200
C	-0.54699500	6.89948500	-2.69151600
H	-2.49924000	5.99739700	-2.60123600
C	1.29458400	5.49307000	-2.02670300
H	0.76936500	3.48708200	-1.41669500
C	0.81795600	6.71959600	-2.48803300
H	-0.92290900	7.84927800	-3.05825700
H	2.35934900	5.34389100	-1.87463800
H	1.51066000	7.52926300	-2.69340700

TS3^{HCT5}

C	4.25626300	-1.82487400	-0.16126900
C	4.83381400	-3.11217300	0.34698500
C	2.81253400	-4.14180000	-0.07921600
C	2.01930900	-2.88638200	-0.51249200
C	2.66263200	-0.40717900	-0.65673200
H	5.55394700	-2.89269100	1.13623900
H	1.16392000	-2.71027700	0.14347900
N	4.87287200	-0.69785700	-0.35900900
N	3.88514300	0.17885800	-0.69456100
N	2.91344500	-1.71851300	-0.39584900
C	4.23133900	1.47011300	-1.21813500
C	3.83495600	1.77437800	-2.53259300
C	4.93705600	2.37476000	-0.41806800
C	4.06857200	3.06577300	-2.99192800
C	5.14043900	3.65771900	-0.93275300
C	4.69328400	4.03098600	-2.19766000
H	3.75803200	3.32459900	-4.00114900
H	5.66994400	4.38162900	-0.31804100
O	3.79535300	-3.88294100	0.89470000
H	5.34503500	-3.65023700	-0.46471500
H	2.12030000	-4.87362600	0.33914100
C	3.17446900	0.76623500	-3.43842100
H	3.38840000	1.01329100	-4.47958000
H	3.53633500	-0.24891200	-3.25095300
H	2.08637300	0.76676900	-3.31403800
C	4.86835100	5.43824900	-2.70313600
H	5.16156200	5.44525700	-3.75574000
H	3.92621600	5.99067300	-2.62228900
H	5.62460600	5.97620100	-2.12849400
C	5.52335100	2.02431800	0.92406600
H	5.36691000	2.84187400	1.63162500

H	5.10757600	1.11207100	1.34496000
H	6.60239400	1.87485400	0.81715400
C	1.34804300	0.22245800	-0.79840500
O	0.33059600	-0.52883900	-0.96233800
C	1.23614500	1.65487100	-0.72181500
C	0.03319500	2.27557200	-0.77962900
H	2.12628500	2.23466200	-0.51764000
C	-0.15910600	3.70968600	-0.60750200
C	0.90486100	4.62925200	-0.65720400
C	-1.45459600	4.18885100	-0.35915400
C	0.67544100	5.97971900	-0.44101500
H	1.91112000	4.28844500	-0.88906100
C	-1.67820100	5.54349700	-0.13436700
H	-2.28132400	3.48154200	-0.32859700
C	-0.61516800	6.44156800	-0.17268200
H	1.50330400	6.68037600	-0.48629200
H	-2.68471600	5.89541200	0.07164000
H	-0.78923600	7.49882000	-0.00127400
H	-0.63256200	-0.42964300	0.02052600
C	-0.25151400	-2.36573100	2.09063800
C	-1.29377400	-1.85194600	1.40113700
C	-1.39518900	-0.42364500	1.03252200
C	-0.53535600	0.45288500	1.83761000
C	0.57432000	0.00717600	2.46490800
C	0.89105500	-1.44234500	2.35642000
H	-2.12497900	-2.48921400	1.10677900
H	-0.74728300	1.51637400	1.80633400
C	-2.70198300	0.07381100	0.56283900
C	-3.24795700	1.29883100	1.00693800
C	-3.43747200	-0.65446000	-0.40152200
C	-4.44509300	1.80112900	0.54489900
H	-2.72531100	1.84039600	1.78806100
C	-4.62712100	-0.21289600	-0.93358800
H	-3.01895600	-1.59872900	-0.74397600
C	-5.17971300	1.07237900	-0.49309800
O	2.04800400	-1.85477100	2.44596400
O	-6.24750000	1.52383800	-0.97428400
C	1.50794200	0.91231200	3.26471800
C	2.86644200	1.04895300	2.56259000
C	0.91376100	2.31638100	3.42326100
C	1.71478900	0.30492900	4.66352700
H	3.32469400	0.06962700	2.40290900
H	2.74436900	1.54898400	1.59441000
H	3.54026100	1.66210400	3.17201000

H	-0.06824300	2.28510100	3.90683200
H	1.57893600	2.92362600	4.04447200
H	0.80796400	2.82254600	2.45659600
H	2.35664300	0.95843500	5.26330000
H	0.75661200	0.19812300	5.18235300
H	2.18891600	-0.67676200	4.59730100
C	-0.29294600	-3.80353500	2.63846700
C	-0.73764100	-4.80022700	1.55744000
C	1.03685400	-4.29300900	3.23198100
C	-1.33753400	-3.81412400	3.77229600
H	-1.73619900	-4.57823100	1.17159400
H	-0.05504500	-4.80745300	0.70084500
H	-0.76625000	-5.80997700	1.98038700
H	1.36509500	-3.65814100	4.05853800
H	0.88541800	-5.30652800	3.61885700
H	1.84710400	-4.30763200	2.50131900
H	-1.40814800	-4.81489900	4.21203700
H	-1.05793900	-3.11038200	4.56291600
H	-2.32589500	-3.52941100	3.39965400
C	-5.39427100	-1.00918400	-1.99085900
C	-5.46622900	-0.20114700	-3.29911900
C	-4.71885600	-2.34817200	-2.29933200
C	-6.81905700	-1.32007300	-1.49448600
H	-5.95440900	0.75774100	-3.12526900
H	-4.45892200	-0.02287300	-3.69103000
H	-6.03115800	-0.75992400	-4.05452600
H	-4.67467900	-2.97822800	-1.40329800
H	-5.29861600	-2.88446100	-3.05738800
H	-3.70224100	-2.21880000	-2.68819600
H	-7.35595600	-1.90354300	-2.25164300
H	-6.78050600	-1.91275500	-0.57400100
H	-7.36576500	-0.39893100	-1.29773600
C	-5.06104700	3.08054800	1.11808200
C	-5.26296600	4.12804000	0.00588100
C	-6.42611500	2.75280300	1.75269400
C	-4.18316700	3.70856200	2.20825000
H	-4.31096500	4.37591500	-0.47637200
H	-5.94357100	3.74629800	-0.75396000
H	-5.67612900	5.04936700	0.43379200
H	-6.30238700	2.03731600	2.57259600
H	-6.87589700	3.66508100	2.16202000
H	-7.09978800	2.32663500	1.00911200
H	-4.66995200	4.61460400	2.58365500
H	-4.04461800	3.02981200	3.05660000

H	-3.19410000	3.99428000	1.83283800
H	-0.86552100	1.67395500	-0.92087100
H	3.29133900	-4.58793500	-0.96546500
C	1.54369400	-3.05642400	-1.96798900
H	2.39408700	-3.37542000	-2.58251900
H	1.18495200	-2.09914800	-2.34695400
C	0.42822200	-4.07281200	-2.01750800
C	0.68992400	-5.43300300	-2.19690600
C	-0.88961300	-3.65697800	-1.80618200
C	-0.34225200	-6.36680700	-2.14525300
H	1.70807100	-5.76572700	-2.38430200
C	-1.92240800	-4.58838300	-1.76292500
H	-1.09267300	-2.59548200	-1.67428400
C	-1.65018200	-5.94560400	-1.92315700
H	-0.12460600	-7.42086500	-2.28474800
H	-2.94205600	-4.25540100	-1.60110600
H	-2.45689800	-6.67020800	-1.88253900

TS3'

C	0.85126000	-3.39225200	-0.26707300
C	1.23645600	-4.32799700	-1.41016100
H	1.35377900	-2.43015800	-0.38579800
H	1.15590500	-3.81551400	-2.37946800
N	-0.59965900	-3.13791800	-0.42272000
O	0.41053400	-5.48196600	-1.38601400
C	-1.42216600	-3.95711500	-1.15402600
C	-0.89478900	-5.19504700	-1.82443200
H	-1.52769200	-6.05072300	-1.58319600
H	-0.92108600	-5.03557200	-2.91201500
N	-2.62301000	-3.47525700	-1.24624900
C	-1.34440100	-2.06506000	-0.04143500
N	-2.57311000	-2.30528400	-0.54035500
C	-3.73527400	-1.46827400	-0.45854500
C	-4.51229600	-1.50893000	0.69790800
C	-3.98256000	-0.59607000	-1.52383400
C	-5.58304500	-0.61716300	0.77661200
C	-5.05385900	0.28112200	-1.39289500
C	-5.85930100	0.28720200	-0.24910000
H	-6.20314900	-0.61923800	1.66901700
H	-5.25513000	0.98880500	-2.19301300
H	2.26523000	-4.66366500	-1.26677300
C	1.17663900	-4.01477400	1.09644700
H	0.64070600	-3.45960500	1.86932100
H	0.82358400	-5.05100400	1.10538500

C	2. 66627600	-3. 94991100	1. 34387500
C	3. 29033700	-2. 70412100	1. 47756400
C	3. 44784600	-5. 10397000	1. 40452000
C	4. 66392000	-2. 61065000	1. 67386800
H	2. 68638700	-1. 80060500	1. 41849800
C	4. 82535900	-5. 01607000	1. 60370100
H	2. 97482400	-6. 07681500	1. 29493500
C	5. 43428900	-3. 77202600	1. 73795000
H	5. 11976500	-1. 63043800	1. 77473100
H	5. 42108900	-5. 92230800	1. 65000600
H	6. 50667200	-3. 70518300	1. 89099800
C	-6. 98268600	1. 28253100	-0. 12481100
H	-6. 58439600	2. 30106800	-0. 08120900
H	-7. 65060400	1. 23011700	-0. 98888800
H	-7. 57161700	1. 10704200	0. 77740300
C	-4. 16953200	-2. 44267700	1. 82676800
H	-3. 99162500	-3. 45787900	1. 46091600
H	-3. 26007300	-2. 10675300	2. 33761500
H	-4. 97643900	-2. 47372200	2. 56002700
C	-3. 08317800	-0. 59368600	-2. 72868600
H	-2. 03552600	-0. 50579600	-2. 42261000
H	-3. 18883400	-1. 52426800	-3. 29458300
H	-3. 31707000	0. 24695800	-3. 38290100
C	-0. 96844600	1. 48285500	1. 27383500
C	-1. 52862800	0. 27026400	0. 75219600
H	-0. 06613600	1. 34878500	1. 87351700
C	-1. 88371400	2. 48568200	1. 88204300
C	-1. 32809100	3. 53739900	2. 62266300
C	-3. 27558300	2. 45473700	1. 71762600
C	-2. 13356500	4. 53005100	3. 16949700
H	-0. 25005900	3. 57993800	2. 73675700
C	-4. 07972000	3. 44614300	2. 26927500
H	-3. 74963200	1. 64766400	1. 16529400
C	-3. 51496300	4. 49149700	2. 99639400
H	-1. 67850800	5. 33812700	3. 73441500
H	-5. 15679000	3. 39640900	2. 13593500
H	-4. 14516100	5. 26246500	3. 42832300
C	-0. 87898300	-0. 92369100	0. 70114100
O	0. 34419400	-1. 13434300	1. 30864000
H	0. 34287200	-0. 65482600	2. 14836400
H	-2. 49013700	0. 33687100	0. 26416600
C	0. 80330500	1. 29197100	-0. 77576000
C	0. 56024400	0. 56591300	-1. 92780700
H	-0. 26675200	0. 73041300	-2. 60188200

C	1. 62616300	-0. 35540800	-2. 09560200
H	1. 76804900	-1. 04823300	-2. 91318200
C	2. 48658900	-0. 16809300	-1. 03817600
H	3. 41964800	-0. 65322300	-0. 78314800
N	1. 98871600	0. 83459900	-0. 24870000
C	0. 02106700	2. 40350900	-0. 12738900
O	0. 65538100	3. 35271600	0. 43759700
C	-1. 10438400	2. 90166000	-1. 06350500
F	-1. 75688100	3. 93747600	-0. 54428500
F	-2. 02919000	1. 96043800	-1. 37770600
F	-0. 58310900	3. 31327500	-2. 23550200
C	2. 62175100	1. 24100500	0. 99532000
H	2. 14985700	2. 17332500	1. 31700900
H	2. 50036600	0. 46608100	1. 75934300
C	4. 12143200	1. 43228100	0. 78591600
O	4. 90637200	0. 71500400	1. 37958100
C	4. 58358200	2. 48397300	-0. 16355700
C	5. 94238600	2. 51073000	-0. 49731200
C	3. 70694900	3. 43322400	-0. 70189100
C	6. 42648100	3. 47567200	-1. 36913100
H	6. 59940200	1. 76554700	-0. 06078700
C	4. 20266300	4. 40210000	-1. 57097800
H	2. 64970400	3. 43610000	-0. 43798500
C	5. 55384100	4. 42275400	-1. 90702400
H	7. 47950900	3. 49391800	-1. 63089600
H	3. 52676800	5. 14232700	-1. 98603600
H	5. 93074900	5. 17831900	-2. 58956600

M3'

C	0. 64488700	3. 46058000	0. 29678300
C	0. 93960300	4. 47860600	1. 39461300
H	1. 19265900	2. 53424900	0. 48261700
H	0. 82857000	4. 02430400	2. 38954400
N	-0. 79991000	3. 14709600	0. 42824400
O	0. 07663200	5. 59701800	1. 25596900
C	-1. 69264400	3. 99477900	1. 02956100
C	-1. 24427500	5. 29660900	1. 63458400
H	-1. 88705600	6. 11000800	1. 29351700
H	-1. 33480400	5. 21348400	2. 72705800
N	-2. 88381300	3. 47390000	1. 08163000
C	-1. 48439700	2. 02684700	0. 09983200
N	-2. 74504300	2. 25282500	0. 49015300
C	-3. 87985600	1. 37234500	0. 39076000
C	-4. 57059700	1. 30603300	-0. 81731700

C	-4.20501000	0.60386000	1.51367600
C	-5.65026700	0.42266600	-0.88179800
C	-5.28757800	-0.26151600	1.39667900
C	-6.02014500	-0.36343500	0.20883000
H	-6.20628900	0.34325900	-1.81204200
H	-5.55932000	-0.88122500	2.24728400
H	1.96240800	4.84167400	1.28227600
C	0.97160900	4.01316300	-1.10157100
H	0.43123300	3.42317500	-1.84423700
H	0.62450500	5.04997900	-1.15768600
C	2.45828700	3.91725500	-1.35485400
C	3.00711700	2.71005200	-1.79893600
C	3.31460400	4.98981400	-1.09826700
C	4.38093200	2.56418900	-1.96383900
H	2.34107400	1.88180700	-2.02442500
C	4.69123800	4.85319600	-1.27026000
H	2.89982700	5.94018200	-0.76891700
C	5.22669600	3.63997400	-1.69468000
H	4.78437500	1.60867300	-2.28910300
H	5.34469300	5.69634200	-1.07009500
H	6.29907200	3.53285600	-1.82096100
C	-7.17237900	-1.32901800	0.11711300
H	-6.82241900	-2.35616100	0.25682200
H	-7.91241700	-1.12701900	0.89640300
H	-7.66871800	-1.26464400	-0.85292500
C	-4.13750800	2.12063600	-2.00562800
H	-3.98235800	3.16884900	-1.73458800
H	-3.19606200	1.73322900	-2.41118800
H	-4.88728800	2.07535000	-2.79625400
C	-3.36561900	0.67419100	2.76117200
H	-2.35200600	0.30619900	2.56071600
H	-3.28555000	1.70108700	3.12869700
H	-3.79521700	0.05388800	3.54824200
C	-0.83621300	-1.61956900	-0.92393400
C	-1.46146900	-0.38640600	-0.39154600
H	-0.14696400	-1.35218100	-1.73430400
C	-1.84796500	-2.60902400	-1.47273800
C	-1.38584100	-3.70807600	-2.20776500
C	-3.22648300	-2.46260900	-1.29317200
C	-2.27778200	-4.63807900	-2.72902200
H	-0.31561900	-3.83218400	-2.32183700
C	-4.11981300	-3.39162000	-1.82328700
H	-3.63521500	-1.61284200	-0.75470100
C	-3.65061000	-4.48605300	-2.54090000

H	-1.89785400	-5.48696000	-3.28958100
H	-5.18716000	-3.24788200	-1.67867500
H	-4.34581100	-5.20920700	-2.95598900
C	-0.92565900	0.83759800	-0.52780900
O	0.23434600	1.10244300	-1.20545200
H	0.91440500	0.47690900	-0.89763000
H	-2.33840700	-0.48874700	0.23202400
C	1.12293400	-1.19755700	0.67995800
C	1.03583200	-0.41358900	1.81281400
H	0.27689900	-0.51019700	2.57528400
C	2.11885600	0.50738000	1.80474800
H	2.35640900	1.24413200	2.55983000
C	2.83880500	0.27333100	0.65933500
H	3.73878800	0.73057200	0.27198900
N	2.22884300	-0.75318800	-0.03152700
C	0.22929300	-2.32490900	0.13357100
O	0.88904900	-3.30789000	-0.44921800
C	-0.58494400	-2.88155300	1.32476800
F	-1.32495300	-3.93279100	0.97370600
F	-1.44677100	-1.97444600	1.87393800
F	0.21960300	-3.28045700	2.32199700
C	2.81463400	-1.34060900	-1.23918300
H	2.26902500	-2.27580100	-1.41929100
H	2.71572400	-0.65641800	-2.08887000
C	4.30632500	-1.57639200	-1.02602500
O	5.11302600	-0.98403000	-1.72074400
C	4.73155000	-2.50449800	0.06062900
C	6.08368300	-2.51088700	0.42263600
C	3.82372900	-3.35691700	0.70094900
C	6.53166000	-3.35946300	1.42516700
H	6.76421700	-1.84264700	-0.09528000
C	4.28589900	-4.20892500	1.70218500
H	2.76933500	-3.38419200	0.41414100
C	5.62944200	-4.20978200	2.06648700
H	7.57941200	-3.36283700	1.70831800
H	3.58620000	-4.87452300	2.19731500
H	5.97845500	-4.87577500	2.84989000

M3^{SET}

C	-3.03591000	-0.59486200	0.40442400
C	-4.10566200	-1.67648000	0.55718200
H	-2.99722100	0.01140200	1.30933600
H	-4.01173700	-2.17537400	1.53156000
N	-1.73740700	-1.30207900	0.26970200

O	-4.00449900	-2.62055800	-0.49282600
C	-1.65054800	-2.60608500	-0.14329200
C	-2.88106000	-3.44862000	-0.31592300
H	-2.77152900	-4.07724100	-1.20043800
H	-2.99988600	-4.09499000	0.56552700
N	-0.41625500	-2.97113200	-0.33123600
C	-0.46378300	-0.81928000	0.30599200
N	0.31873200	-1.86661200	-0.03480400
C	1.75299300	-1.91421100	-0.11430100
C	2.33446500	-1.87371200	-1.38296200
C	2.48845600	-1.93964700	1.07470100
C	3.72747600	-1.82873700	-1.44109500
C	3.87471200	-1.88698200	0.96000800
C	4.50921400	-1.82182600	-0.28404700
H	4.21048000	-1.79005400	-2.41376900
H	4.47652600	-1.89588200	1.86514700
H	-5.09082500	-1.21287300	0.48863800
C	-3.25264200	0.28716800	-0.83368700
H	-2.38226600	0.94221900	-0.94951200
H	-3.30312200	-0.36552600	-1.71105200
C	-4.51205200	1.10806500	-0.71082700
C	-4.54847700	2.21795700	0.13756000
C	-5.66645600	0.75200900	-1.41069600
C	-5.71460000	2.96309200	0.27852300
H	-3.65288100	2.50125900	0.68633900
C	-6.83493500	1.49708000	-1.27272800
H	-5.64708500	-0.11384500	-2.06785100
C	-6.86062600	2.60396400	-0.42868600
H	-5.72910000	3.82676500	0.93523900
H	-7.72365100	1.21379400	-1.82690800
H	-7.76986000	3.18642600	-0.32319000
C	6.00979100	-1.72928900	-0.36190500
H	6.35758700	-0.79134300	0.08243800
H	6.48020700	-2.54667600	0.19088000
H	6.35784700	-1.76866000	-1.39540000
C	1.48644400	-1.85301400	-2.62662400
H	0.95206600	-2.79928600	-2.74877700
H	0.73546800	-1.05641400	-2.58245800
H	2.10515200	-1.68868200	-3.50931000
C	1.81097200	-1.98026700	2.41769700
H	1.41869100	-0.99342000	2.68919600
H	0.97735500	-2.68778100	2.42341400
H	2.51930600	-2.27959600	3.19110700
C	1.72401000	2.15855900	1.00332500

C	1. 24309300	1. 00888000	0. 43232600
H	1. 10517000	2. 70774800	1. 71199300
C	3. 04929600	2. 70672000	0. 78956900
C	3. 38036300	3. 92058300	1. 41574800
C	4. 02346600	2. 06834800	-0. 00277000
C	4. 63722100	4. 48705800	1. 25192100
H	2. 63735600	4. 41822200	2. 03290800
C	5. 27749500	2. 63699100	-0. 16267300
H	3. 80868900	1. 12002700	-0. 48790300
C	5. 58898400	3. 84721200	0. 46122000
H	4. 87513200	5. 42555200	1. 74074300
H	6. 01986500	2. 13692700	-0. 77604900
H	6. 57228000	4. 28668400	0. 33133400
C	-0. 05090200	0. 50537900	0. 65759000
O	-1. 01830000	1. 22792600	1. 26959900
H	-0. 82743800	2. 17237800	1. 17908600
H	1. 88483400	0. 43933100	-0. 22615600

M3^{HAT}

C	-3. 02815700	-0. 65040900	0. 40671200
C	-4. 06966000	-1. 69145400	0. 80670200
H	-2. 98623800	0. 15854700	1. 13653100
H	-3. 95588000	-1. 96724300	1. 86520400
N	-1. 72588200	-1. 33160200	0. 41938200
O	-3. 95931800	-2. 84546900	-0. 01328300
C	-1. 58981200	-2. 68225200	0. 26192400
C	-2. 79469900	-3. 57800600	0. 29154700
H	-2. 68552700	-4. 36992100	-0. 45062200
H	-2. 87554200	-4. 03794300	1. 28772600
N	-0. 35136700	-3. 04533200	0. 14263700
C	-0. 46194500	-0. 78139600	0. 39128900
N	0. 35847200	-1. 86699300	0. 22003200
C	1. 75844600	-1. 88678000	-0. 06330200
C	2. 20235700	-1. 43031300	-1. 30930100
C	2. 63079400	-2. 32919500	0. 93388200
C	3. 57750200	-1. 39811200	-1. 52985400
C	3. 99797300	-2. 28584100	0. 66402300
C	4. 48767800	-1. 81731100	-0. 55643300
H	3. 94801300	-1. 03240100	-2. 48459400
H	4. 69640900	-2. 61377600	1. 42992600
H	-5. 06908400	-1. 28017100	0. 65151300
C	-3. 29219100	-0. 07083700	-0. 99200200
H	-2. 38813800	0. 45888700	-1. 30380100
H	-3. 47258400	-0. 90192400	-1. 68259200

C	-4.46050600	0.88141000	-0.97216600
C	-4.29753700	2.15456800	-0.41447200
C	-5.71300900	0.50992800	-1.46339400
C	-5.37019800	3.03838200	-0.35716900
H	-3.31734700	2.43399300	-0.03335400
C	-6.78784700	1.39533800	-1.40643800
H	-5.84375100	-0.47875800	-1.89757600
C	-6.61786700	2.66129900	-0.85324200
H	-5.23338800	4.02573300	0.07302400
H	-7.75587100	1.09562700	-1.79574700
H	-7.45320800	3.35300600	-0.80995100
C	5.96886800	-1.77451200	-0.83000500
H	6.54362300	-1.82752300	0.09702900
H	6.27132900	-2.61697800	-1.46018300
H	6.24387800	-0.85622700	-1.35539800
C	1.22743400	-0.94669400	-2.34815000
H	0.36393300	-1.61462600	-2.42037800
H	0.85367200	0.05052500	-2.08918900
H	1.70611800	-0.88763100	-3.32697200
C	2.09613100	-2.78810100	2.26333700
H	1.52856700	-1.98582500	2.74685500
H	1.41754600	-3.63657000	2.13914800
H	2.91040700	-3.08264500	2.92712300
C	1.55065000	2.35113800	0.69400500
C	1.21601600	1.04671700	0.67916300
H	0.74558300	3.07959400	0.61931000
C	2.91449000	2.87284300	0.81110500
C	3.10562300	4.23883100	1.06428500
C	4.05271500	2.06083600	0.66815100
C	4.38257100	4.77497000	1.19146200
H	2.23488100	4.88112400	1.16651900
C	5.32746800	2.59652000	0.79552900
H	3.93899300	1.00481700	0.43533500
C	5.50050800	3.95540200	1.06083000
H	4.50505600	5.83489700	1.39162100
H	6.19363300	1.95158000	0.67967000
H	6.49825100	4.37119100	1.15765200
C	-0.17728400	0.61811700	0.55043900
O	-1.14020100	1.44037300	0.57520800
H	1.98523300	0.29214200	0.79344300

M04

C	3.95671300	0.35074600	0.19940000
C	4.90946600	0.46737600	1.38464200

H	3.31858200	-0.52617600	0.30977200
H	4.37289800	0.32167000	2.33318500
N	3.06458600	1.52963300	0.27310700
O	5.55477800	1.73325200	1.36768200
C	3.38374400	2.65845100	0.97331400
C	4.67416700	2.76607300	1.73546600
H	5.15829000	3.71987800	1.51849400
H	4.44265900	2.72664300	2.80971800
N	2.41655500	3.52894700	0.93582600
C	1.81391600	1.70057600	-0.20123900
N	1.44872100	2.92223600	0.19412400
C	0.18196900	3.57984600	0.02492100
C	-0.17502100	4.04607200	-1.24097700
C	-0.64049200	3.69196300	1.15196500
C	-1.45055600	4.59449200	-1.37995400
C	-1.89909300	4.25536500	0.95688500
C	-2.32904600	4.68765800	-0.30010300
H	-1.76408800	4.95079600	-2.35768600
H	-2.56685900	4.34646500	1.81041900
H	5.68517800	-0.29520600	1.29203400
C	4.70885400	0.31386000	-1.13532300
H	3.98930800	0.47594100	-1.94110500
H	5.44217100	1.12698400	-1.15026700
C	5.38916400	-1.02397100	-1.30895200
C	4.61811500	-2.19029900	-1.36024100
C	6.77898500	-1.12546500	-1.38889000
C	5.23030700	-3.43147900	-1.49947700
H	3.53386900	-2.12241100	-1.28871600
C	7.39206400	-2.36865300	-1.53263000
H	7.38379600	-0.22330800	-1.34095700
C	6.61807600	-3.52439600	-1.58961100
H	4.61878900	-4.32811200	-1.53268100
H	8.47368300	-2.43289200	-1.59796000
H	7.09366800	-4.49364100	-1.70101800
C	-3.72543900	5.22234200	-0.47845700
H	-4.45227500	4.40476300	-0.42462400
H	-3.97722400	5.93717400	0.30908200
H	-3.84377900	5.71543400	-1.44508800
C	0.74874000	3.91228200	-2.42211700
H	1.78392700	4.13501000	-2.15020000
H	0.71658400	2.89497800	-2.82956100
H	0.44729100	4.59534000	-3.21766800
C	-0.19643900	3.21013200	2.50799200
H	0.21582300	2.19654600	2.44719800

H	0.57315800	3.87102300	2.91700300
H	-1.04463100	3.19795800	3.19524100
C	-0.95912100	-0.29948000	-1.81435000
C	-0.33200200	0.77003000	-1.28369700
H	-0.35161100	-1.16524000	-2.06859800
C	-2.39457900	-0.39657800	-2.07189600
C	-2.94755600	-1.65367600	-2.35004400
C	-3.24093800	0.71994600	-2.02258500
C	-4.31360900	-1.79706100	-2.55970800
H	-2.29952400	-2.52573900	-2.36472000
C	-4.60457000	0.57725100	-2.24005300
H	-2.82905100	1.70486000	-1.81771600
C	-5.14446200	-0.67993000	-2.50652000
H	-4.73256200	-2.78062600	-2.74789700
H	-5.25120900	1.44796400	-2.19535300
H	-6.21282200	-0.79171500	-2.66068600
C	1.09176400	0.64804900	-1.01312000
O	1.78787400	-0.27496900	-1.41726300
H	-0.88149100	1.63073600	-0.92919500
C	-3.68008100	-1.06645200	0.96115400
C	-4.50932700	0.04404900	1.16654400
H	-5.58842900	0.02396200	1.14451100
C	-3.68577400	1.14986300	1.36918800
H	-3.98979600	2.17130100	1.54720500
C	-2.36858600	0.70325000	1.29414500
H	-1.42752400	1.21068500	1.41403900
N	-2.35736400	-0.63220400	1.05142900
C	-4.07996900	-2.41886000	0.68647100
C	-1.21580200	-1.45884500	0.96811900
H	-1.44307500	-2.50784600	0.87994800
C	0.07296500	-1.01531400	1.16255600
O	0.45051500	0.20341300	1.33630300
C	1.14628200	-2.06665700	1.18455400
C	1.13090200	-3.21316400	0.38248600
C	2.22188300	-1.87448800	2.05824200
C	2.16431000	-4.14354600	0.46040900
H	0.31411300	-3.36230000	-0.31833800
C	3.25662500	-2.80167600	2.13624800
H	2.22244000	-0.97745100	2.67171800
C	3.23108700	-3.94154700	1.33466500
H	2.14269700	-5.02549000	-0.17322600
H	4.07984200	-2.64064800	2.82694600
H	4.04081900	-4.66275200	1.38449000
C	-5.60625000	-2.67894000	0.79049700

F	-6.06345400	-2.37962600	2.01575000
F	-5.88123600	-3.95710000	0.55092500
F	-6.31028300	-1.94070300	-0.08391000
O	-3.37920100	-3.37771300	0.40654400

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C	3.03385500	2.00421400	0.52493000
C	3.79271600	2.77438900	1.60067800
H	2.87832700	0.96517200	0.81572000
H	3.35264600	2.59856200	2.59304100
N	1.69361300	2.63430100	0.44489700
O	3.79386400	4.16273500	1.29918000
C	1.45916100	3.92199400	0.83548600
C	2.52802200	4.74060400	1.50271300
H	2.54151800	5.74831800	1.08427400
H	2.29219000	4.80842100	2.57487300
N	0.21997200	4.26182500	0.62192500
C	0.52747700	2.14014600	-0.02253300
N	-0.34751300	3.14636600	0.08810800
C	-1.73356900	3.18037700	-0.30116100
C	-2.04230200	3.17788700	-1.66278400
C	-2.69797400	3.18203100	0.71158700
C	-3.39233200	3.11740100	-2.00724600
C	-4.03035100	3.12644600	0.30911600
C	-4.39444200	3.06909000	-1.03793700
H	-3.66319500	3.09722400	-3.05958800
H	-4.80502600	3.11161100	1.07278900
H	4.83353300	2.44554700	1.60873900
C	3.73602600	2.06713800	-0.83861600
H	3.01764500	1.76039200	-1.60184100
H	4.04562300	3.09972500	-1.03126700
C	4.92155400	1.13215500	-0.84819100
C	4.70897200	-0.24823100	-0.94394800
C	6.22546100	1.61358100	-0.72350600
C	5.78821800	-1.12625800	-0.92076600
H	3.69183800	-0.62409700	-1.03326700
C	7.30627300	0.73350600	-0.69914500
H	6.39463400	2.68563900	-0.65025900
C	7.08886500	-0.63750700	-0.79804500
H	5.61024000	-2.19377500	-1.00699400
H	8.31589600	1.12100400	-0.60573900
H	7.92951000	-1.32381300	-0.78264500
C	-5.84245500	2.92326100	-1.42406300
H	-6.00127000	3.15577000	-2.47875800

H	-6.17320100	1.89336800	-1.25097500
H	-6.47946800	3.57733200	-0.82345200
C	-0.97080700	3.18297500	-2.71968100
H	-0.15066800	3.85833200	-2.46027100
H	-0.55541700	2.17751800	-2.85073900
H	-1.38525600	3.50067400	-3.67757100
C	-2.31640200	3.19416200	2.16633400
H	-1.78963900	2.26678300	2.41598300
H	-1.67441300	4.04720400	2.39982200
H	-3.21252100	3.25589100	2.78706300
C	-1.09856300	-1.12645100	-0.98664000
C	-0.92516700	0.21748400	-0.73120200
H	-0.20660500	-1.72075600	-1.17085200
C	-2.37549500	-1.72443300	-1.39942300
C	-2.43659600	-3.10110100	-1.65560400
C	-3.53861800	-0.95653500	-1.56346200
C	-3.62883700	-3.69706000	-2.05173300
H	-1.53911600	-3.69821600	-1.52459000
C	-4.72986400	-1.55611000	-1.95075700
H	-3.51365000	0.11626500	-1.39019100
C	-4.78051500	-2.92765800	-2.19663300
H	-3.65837400	-4.76464800	-2.24602500
H	-5.62491000	-0.95124800	-2.06102700
H	-5.71363500	-3.39223500	-2.50046300
C	0.38460100	0.72353100	-0.55644800
O	1.45542000	0.15337900	-0.80699300
H	-1.77394600	0.83242600	-0.46903300
C	1.58146700	-2.54933200	0.87021800
C	2.80680100	-2.04587300	1.32142900
H	3.78040300	-2.40769500	1.02562600
C	2.52882700	-1.02593100	2.23056800
H	3.24303300	-0.44351100	2.79526300
C	1.14564100	-0.90062200	2.30293500
H	0.52567600	-0.23505800	2.87714600
N	0.56305500	-1.82358000	1.49021600
C	1.37064200	-3.63103800	-0.04297400
O	0.31130000	-4.14244000	-0.37271500
C	2.66034500	-4.21137200	-0.67636100
F	2.36636100	-5.16964000	-1.54580600
F	3.47150500	-4.73187700	0.25763100
F	3.35964100	-3.26439700	-1.32653300
C	-0.82715300	-2.00234900	1.29409200
H	-1.11584500	-3.00237000	1.01440900
C	-1.72876700	-1.01573900	1.73812300

O	-1.36766600	0.14362300	2.06623200
C	-3.19976200	-1.29994100	1.63266600
C	-3.74803500	-2.57567000	1.46126300
C	-4.05954800	-0.19777900	1.66633300
C	-5.11988100	-2.73553000	1.30013700
H	-3.10847400	-3.45222300	1.44874200
C	-5.43184000	-0.35625000	1.50840000
H	-3.61850700	0.78289100	1.80903700
C	-5.96681200	-1.62829800	1.31974100
H	-5.53034100	-3.72996000	1.15402500
H	-6.08390800	0.51287000	1.53035300
H	-7.03704700	-1.76004300	1.19193000

TS4RR'

C	-1.83556200	2.90279200	0.56881800
C	-2.17496500	3.54378900	1.90994300
H	-0.78162200	2.62586800	0.52720500
H	-1.76324000	2.94402600	2.73322900
N	-2.60556300	1.64249800	0.53183500
O	-3.58578800	3.67755700	2.04002400
C	-3.75665300	1.43026200	1.23730500
C	-4.22225200	2.44010200	2.24844900
H	-5.29897900	2.59255300	2.16136700
H	-4.00283700	2.04697000	3.25195700
N	-4.26982700	0.26239300	0.96731900
C	-2.37174300	0.53242600	-0.18398300
N	-3.39252000	-0.28533100	0.07446900
C	-3.71594900	-1.50494000	-0.61926900
C	-4.10880300	-1.40124400	-1.95502400
C	-3.61391900	-2.72128400	0.06266600
C	-4.40948200	-2.58822400	-2.62365900
C	-3.92827100	-3.87422200	-0.65131700
C	-4.32473400	-3.82730600	-1.99115900
H	-4.71799300	-2.53892800	-3.66437900
H	-3.85625100	-4.83585600	-0.14900500
H	-1.75278800	4.54890600	1.95264800
C	-2.24149900	3.77681100	-0.62757800
H	-2.25089500	3.13978700	-1.51524600
H	-3.25186000	4.16162400	-0.45304600
C	-1.25971500	4.90448400	-0.82515300
C	-0.05859400	4.66175000	-1.50074300
C	-1.51154200	6.18300600	-0.32461000
C	0.86743700	5.68536500	-1.67563800
H	0.12955800	3.66567100	-1.89697400

C	-0.58083400	7.20655200	-0.49354700
H	-2.44800800	6.37846500	0.19308300
C	0.61000100	6.95909500	-1.16996200
H	1.78875700	5.49500000	-2.21735400
H	-0.78971300	8.19703900	-0.10209900
H	1.33343900	7.75599200	-1.30818800
C	-4.65935000	-5.09909700	-2.72560600
H	-3.82984000	-5.80933900	-2.67042200
H	-5.53482600	-5.58299300	-2.28265200
H	-4.87381100	-4.90503300	-3.77793200
C	-4.19696000	-0.06726800	-2.65096700
H	-4.73382200	0.66515800	-2.03981500
H	-3.20236600	0.34013400	-2.86398700
H	-4.72474800	-0.16992000	-3.59987000
C	-3.12732000	-2.78130300	1.48429600
H	-2.06026100	-2.53478000	1.54436900
H	-3.65841900	-2.07086700	2.12281100
H	-3.25949300	-3.78431700	1.89327500
C	0.74693500	-1.24745900	-1.15638300
C	-0.58941300	-0.99191900	-0.88219300
H	1.28796500	-0.48551900	-1.71533500
C	1.30661500	-2.61209100	-1.19756500
C	2.67730800	-2.78421600	-1.43813300
C	0.51487200	-3.74871400	-0.98715500
C	3.24873800	-4.04847300	-1.43660800
H	3.29753600	-1.90481100	-1.59602100
C	1.08707200	-5.01805200	-0.98911800
H	-0.55544800	-3.64565600	-0.83198100
C	2.45350400	-5.17232700	-1.20692300
H	4.31477700	-4.15823100	-1.60570300
H	0.46143900	-5.88919800	-0.82231500
H	2.89810100	-6.16222000	-1.20263600
C	-1.12931200	0.30592600	-1.01509500
O	-0.70418000	1.28449700	-1.64982400
H	-1.16674500	-1.72146800	-0.32750100
C	4.14677800	0.62709900	-0.15090900
C	4.47149800	1.83230500	-0.78440800
H	5.46992100	2.14734800	-1.04792800
C	3.27944700	2.51805900	-1.02142300
H	3.16074000	3.47702400	-1.50243400
C	2.24393400	1.72957600	-0.53293800
H	1.17552200	1.87461900	-0.55573600
N	2.75902900	0.59533700	0.00495900
C	5.04696600	-0.41661500	0.26329400

O	4.77873300	-1.50452300	0.74532500
C	6.54747000	-0.10143700	0.03658900
F	7.30663300	-1.09576900	0.48135900
F	6.91722600	1.02006800	0.67117800
F	6.81326100	0.07077600	-1.26834600
C	2.02850900	-0.44364800	0.63281200
H	2.65086000	-1.28821000	0.87644400
C	0.88242400	-0.17029700	1.41488300
O	0.19580300	0.87057900	1.33406800
C	0.37056800	-1.27928200	2.29261600
C	0.79408400	-2.61102900	2.19911600
C	-0.60100800	-0.94418800	3.24326200
C	0.25329100	-3.58051700	3.04063000
H	1.53743800	-2.90721900	1.46600200
C	-1.11888600	-1.90701100	4.10197400
H	-0.92852700	0.08917700	3.29357200
C	-0.69591900	-3.23182300	3.99903400
H	0.58200700	-4.61081000	2.94756800
H	-1.85826400	-1.62907700	4.84695300
H	-1.10437500	-3.98825000	4.66181400

TS4RR''

C	2.82094000	1.52605800	0.07485300
C	3.48093100	2.21106800	1.26603000
H	2.55043600	0.49915400	0.31442900
H	2.86628300	2.06608900	2.16445600
N	1.55434000	2.25979600	-0.13652600
O	3.65213600	3.59524000	0.98032400
C	1.37545000	3.56159700	0.23135900
C	2.43445700	4.29836200	1.00253100
H	2.60427300	5.28489500	0.56799600
H	2.06317600	4.42160100	2.03001400
N	0.16881600	3.97130000	-0.04971300
C	0.38398400	1.82685200	-0.63270600
N	-0.43682600	2.87645500	-0.58568200
C	-1.76802800	2.98867300	-1.12387300
C	-1.90276000	3.10033500	-2.50913400
C	-2.84710800	2.99347000	-0.23814100
C	-3.19626400	3.21919900	-3.01183500
C	-4.11920500	3.11457400	-0.79417300
C	-4.31174600	3.22473800	-2.17251600
H	-3.33527600	3.31212000	-4.08584300
H	-4.98133100	3.12016200	-0.13225000
H	4.47526200	1.79315900	1.42839000

C	3. 67117300	1. 58283200	-1. 20036000
H	3. 04023200	1. 27080500	-2. 03724400
H	3. 99882400	2. 61419600	-1. 36529300
C	4. 85058700	0. 65367000	-1. 06253500
C	4. 64320600	-0. 72739400	-1. 13764200
C	6. 13122800	1. 13617700	-0. 79237500
C	5. 70049000	-1. 60909500	-0. 93771300
H	3. 64166200	-1. 09356000	-1. 36057100
C	7. 19326300	0. 25384100	-0. 60181100
H	6. 29475500	2. 20937300	-0. 72738300
C	6. 97857900	-1. 11945700	-0. 67012400
H	5. 52977600	-2. 68049800	-0. 98358000
H	8. 18634500	0. 64075700	-0. 39618700
H	7. 80228300	-1. 80862900	-0. 51484300
C	-5. 69969100	3. 32124100	-2. 74887000
H	-6. 06669700	2. 32806500	-3. 02677400
H	-6. 40021400	3. 74510200	-2. 02655600
H	-5. 71077000	3. 94089000	-3. 64827100
C	-0. 70099200	3. 07884100	-3. 41621200
H	0. 08904100	3. 74018700	-3. 04759400
H	-0. 28483100	2. 06809400	-3. 49275700
H	-0. 97626200	3. 40144800	-4. 42108100
C	-2. 64357900	2. 80749800	1. 24075700
H	-2. 39366600	1. 76204900	1. 46755900
H	-1. 83159600	3. 43019500	1. 62251000
H	-3. 55576000	3. 04961800	1. 78827700
C	-1. 46054600	-1. 41115100	-1. 11589900
C	-1. 19346000	-0. 08597100	-0. 86369900
H	-0. 69886800	-1. 98345400	-1. 64058500
C	-2. 73667500	-2. 06211900	-0. 86850500
C	-2. 91404600	-3. 39629800	-1. 26479300
C	-3. 79652800	-1. 40828500	-0. 21327300
C	-4. 11940000	-4. 05115400	-1. 03899600
H	-2. 09109000	-3. 91710800	-1. 74559800
C	-4. 99849700	-2. 06334100	0. 00974400
H	-3. 67884900	-0. 38368600	0. 12915900
C	-5. 16487000	-3. 38534200	-0. 40630000
H	-4. 23598100	-5. 08472700	-1. 34721800
H	-5. 80728900	-1. 54790600	0. 51775700
H	-6. 10584700	-3. 89584600	-0. 22694900
C	0. 12215000	0. 40544400	-1. 07929200
O	1. 10136600	-0. 21697000	-1. 49950800
H	-1. 92551600	0. 56404500	-0. 40472800
C	-1. 20263400	-0. 75494400	2. 56129900

C	-2.34031400	-0.69662100	3.40786100
H	-2.59474100	0.12011500	4.06152200
C	-3.04335000	-1.87355100	3.24562300
H	-3.96069200	-2.15996900	3.73794700
C	-2.35602000	-2.65508600	2.30837400
H	-2.56670100	-3.62964100	1.89872900
N	-1.24579100	-1.99885500	1.89766700
C	-0.14444300	0.17760600	2.41820100
O	0.85728300	0.10143800	1.70149500
C	-0.12861000	1.45094400	3.30182300
F	0.34842800	2.47914900	2.56797900
F	0.71176000	1.27642300	4.32478600
F	-1.29877300	1.86446500	3.80106400
C	-0.31610800	-2.46423400	0.95306800
H	0.46238500	-1.76649200	0.70411700
C	-0.37165500	-3.76829400	0.43336600
O	-1.24392200	-4.62620400	0.70735600
C	0.64708400	-4.12832900	-0.62619900
C	1.83595500	-3.42837300	-0.86546100
C	0.35154600	-5.23773300	-1.42538000
C	2.69221900	-3.82651500	-1.88822100
H	2.10620800	-2.57644600	-0.24796700
C	1.20468900	-5.63132600	-2.45116000
H	-0.56417700	-5.78460100	-1.22598000
C	2.37914000	-4.92391200	-2.68851400
H	3.61721000	-3.28663700	-2.06558800
H	0.95250000	-6.49175200	-3.06353300
H	3.05079800	-5.22582100	-3.48606200

TS4RR'''

C	4.08064700	0.67023500	0.25529300
C	5.08142100	1.09686800	1.32206800
H	3.67230400	-0.31537900	0.47200000
H	4.66500400	0.93831900	2.32884800
N	2.95638100	1.63010600	0.35032600
O	5.44092000	2.45974800	1.14557500
C	3.10029400	2.88447200	0.87103800
C	4.39219900	3.32347800	1.50230400
H	4.65149100	4.32866100	1.16438700
H	4.25552900	3.34668500	2.59431200
N	1.98580400	3.55578900	0.80772200
C	1.67161800	1.50871400	-0.05178200
N	1.10822300	2.69014400	0.22969200
C	-0.23640700	3.13305700	-0.03734900

C	-0.51075800	3.67485100	-1.29396700
C	-1.19596900	2.95485300	0.95730000
C	-1.82422800	4.06249900	-1.53811100
C	-2.49932600	3.34764900	0.65861900
C	-2.82839400	3.90301200	-0.57732500
H	-2.07452800	4.49049000	-2.50647400
H	-3.27673900	3.17960400	1.39777800
H	5.99521400	0.50831100	1.21616400
C	4.68530100	0.68884700	-1.15410100
H	3.86367100	0.63329100	-1.87263500
H	5.22755000	1.62966900	-1.30122800
C	5.59855400	-0.50086200	-1.32594200
C	5.03783900	-1.77727400	-1.44736600
C	6.98675100	-0.36337000	-1.31622800
C	5.85955000	-2.89360600	-1.56383400
H	3.95402000	-1.87970700	-1.44713800
C	7.80933800	-1.48258400	-1.43294100
H	7.42535500	0.62777100	-1.21985300
C	7.24644300	-2.74927800	-1.55654800
H	5.41549800	-3.87976100	-1.66496600
H	8.88852900	-1.36281100	-1.42829000
H	7.88575000	-3.62214400	-1.64785500
C	-4.24531700	4.30294300	-0.89773700
H	-4.68031000	3.61702400	-1.63208400
H	-4.87649100	4.27679200	-0.00742000
H	-4.28098600	5.31071600	-1.32245500
C	0.56537300	3.78786900	-2.34076000
H	1.45739700	4.28502700	-1.94578000
H	0.86375800	2.79461900	-2.69735400
H	0.20787200	4.35780700	-3.20065000
C	-0.83757500	2.28641400	2.25515800
H	-0.49989500	1.26088400	2.06042600
H	-0.03511800	2.82325700	2.77228300
H	-1.70937800	2.22380500	2.90726800
C	-0.84201800	-1.08455400	-1.18200700
C	-0.28836400	0.12316300	-0.76689800
H	-0.14683000	-1.89626500	-1.38909300
C	-2.18765800	-1.24190200	-1.71519000
C	-2.63583500	-2.53127100	-2.04495200
C	-3.05975300	-0.15341500	-1.89540500
C	-3.92906000	-2.73137300	-2.50941900
H	-1.96681700	-3.37355000	-1.87861900
C	-4.34798900	-0.35814400	-2.36970300
H	-2.72946400	0.85328800	-1.65134100

C	-4.79048000	-1.64800100	-2.66600700
H	-4.27261800	-3.73733600	-2.72966800
H	-5.01952500	0.48723500	-2.48783200
H	-5.80394800	-1.80496800	-3.02302200
C	1.11145800	0.23240100	-0.65455000
O	1.97053500	-0.60312600	-0.98204200
H	-0.93411900	0.94083200	-0.48197400
C	-3.98048100	-1.78504700	0.85239700
C	-5.10023600	-2.61506100	0.69799200
H	-6.12527700	-2.28447700	0.65713700
C	-4.64471300	-3.93135700	0.63631100
H	-5.24403400	-4.82306300	0.52359100
C	-3.25982100	-3.90085100	0.72762600
H	-2.52430400	-4.68812200	0.68931200
N	-2.84789700	-2.61291300	0.88437900
C	-3.90353300	-0.36040000	0.97723100
O	-2.92595600	0.31784700	1.27271300
C	-5.18997000	0.47442000	0.76040000
F	-5.68211000	0.85501900	1.94672500
F	-6.17439500	-0.13078700	0.08787900
F	-4.88260900	1.58828600	0.07810200
C	-1.52768400	-2.16966700	1.00875200
H	-1.43026200	-1.20556400	1.47235500
C	-0.42548700	-3.04877500	0.84491400
O	-0.47595100	-4.16333300	0.29026100
C	0.91056600	-2.55746200	1.35181000
C	1.06682500	-1.50000500	2.25397900
C	2.04330100	-3.26902100	0.94516900
C	2.32981400	-1.16744800	2.74345300
H	0.19956800	-0.96656000	2.62913100
C	3.30261300	-2.94056900	1.43024300
H	1.89806100	-4.09332700	0.25462500
C	3.44879300	-1.89449000	2.34278700
H	2.43027300	-0.36467900	3.47045000
H	4.17458500	-3.50367100	1.11005100
H	4.43141700	-1.65606300	2.74402600

TS4RS

C	3.87726900	0.40111200	0.34635900
C	4.79093000	0.55903200	1.55697500
H	3.23209700	-0.47155300	0.45816100
H	4.22152800	0.45797400	2.49208400
N	2.99256800	1.58784300	0.34499600
O	5.44906500	1.81750600	1.51109900

C	3. 30415700	2. 74663600	0. 99855900
C	4. 56759200	2. 87366600	1. 80252700
H	5. 07015200	3. 81211000	1. 56270100
H	4. 29801200	2. 88214400	2. 86852900
N	2. 35172400	3. 62677500	0. 88322300
C	1. 76776500	1. 75205000	-0. 19688500
N	1. 40485900	2. 99601100	0. 13389000
C	0. 13756300	3. 63444200	-0. 08599900
C	-0. 20032600	4. 05376700	-1. 37173000
C	-0. 72080300	3. 73922600	1. 01507400
C	-1. 48466500	4. 56897200	-1. 55326000
C	-1. 98856400	4. 26199300	0. 77820500
C	-2. 39196800	4. 66563600	-0. 49838500
H	-1. 78335700	4. 89040800	-2. 54738200
H	-2. 68404300	4. 34834100	1. 60951400
H	5. 56334300	-0. 21163300	1. 52281400
C	4. 66472800	0. 33072700	-0. 96637900
H	3. 95764700	0. 46732900	-1. 78743700
H	5. 39197000	1. 14926700	-0. 98291600
C	5. 35786500	-1. 00291500	-1. 10455200
C	4. 59630200	-2. 16746000	-1. 25089200
C	6. 75042000	-1. 09903600	-1. 07593100
C	5. 22538400	-3. 40087600	-1. 38924800
H	3. 50897100	-2. 09858900	-1. 25833900
C	7. 37924000	-2. 33519500	-1. 21025500
H	7. 34454800	-0. 19676100	-0. 95316400
C	6. 61656500	-3. 48848500	-1. 37221600
H	4. 62346600	-4. 29637400	-1. 50841000
H	8. 46281100	-2. 39546000	-1. 19073200
H	7. 10350200	-4. 45218500	-1. 48261200
C	-3. 79103600	5. 17785500	-0. 71889100
H	-4. 52113500	4. 38727100	-0. 51872300
H	-4. 01518400	6. 00848200	-0. 04410100
H	-3. 93273400	5. 52056200	-1. 74528300
C	0. 74993900	3. 89538700	-2. 52755400
H	1. 77243600	4. 16068500	-2. 24636300
H	0. 75296900	2. 85727300	-2. 87845100
H	0. 44477600	4. 52997600	-3. 36075500
C	-0. 29451200	3. 28754100	2. 38792200
H	0. 17852500	2. 29927200	2. 35505500
H	0. 42674900	3. 98869700	2. 81728800
H	-1. 15947600	3. 22986600	3. 05162900
C	-1. 01092300	-0. 43555600	-1. 45580700
C	-0. 35131600	0. 74246600	-1. 12952700

H	-0.39132400	-1.25259500	-1.81625000
C	-2.43698000	-0.48903700	-1.81928600
C	-2.99208200	-1.70752900	-2.22968600
C	-3.27130300	0.63334600	-1.73337800
C	-4.34503700	-1.81179700	-2.52864200
H	-2.35667800	-2.58844000	-2.27748800
C	-4.62572300	0.52939000	-2.02889900
H	-2.86660800	1.59319900	-1.42543200
C	-5.16770400	-0.69173400	-2.42294300
H	-4.76045500	-2.76930500	-2.82630500
H	-5.26251400	1.40454300	-1.94532100
H	-6.22790900	-0.77356800	-2.63916700
C	1.04956100	0.65752200	-0.95211300
O	1.76169800	-0.30029200	-1.29330600
H	-0.89843100	1.62006800	-0.82045600
C	-3.68212000	-1.10182500	1.07976400
C	-4.47064700	-0.03432000	1.52382500
H	-5.54155800	-0.06623700	1.65574800
C	-3.62260600	1.04785100	1.75903300
H	-3.89830900	2.03056300	2.11229300
C	-2.32937800	0.63128900	1.45781600
H	-1.38433800	1.14079000	1.50787100
N	-2.35602300	-0.66680100	1.06170600
C	-4.11841400	-2.43002200	0.73904100
C	-1.25493300	-1.43016200	0.60953300
H	-1.53899100	-2.44154400	0.36561300
C	0.06271300	-1.17468200	1.07403200
O	0.44577900	-0.06926200	1.52390500
C	1.05982200	-2.29423600	0.95958500
C	0.94261100	-3.35205000	0.05166400
C	2.14291800	-2.28273000	1.84499900
C	1.88537100	-4.37526900	0.03701600
H	0.12059600	-3.37391000	-0.65766200
C	3.08492800	-3.30654200	1.83257200
H	2.21796900	-1.45929800	2.54932500
C	2.95524100	-4.36011500	0.93097600
H	1.78465900	-5.18766100	-0.67616100
H	3.91642200	-3.28738400	2.53058300
H	3.68811000	-5.16061200	0.91890300
C	-5.64559200	-2.66448200	0.87123500
F	-6.04369900	-2.51753300	2.14490400
F	-5.96374900	-3.89346600	0.47982500
F	-6.35860400	-1.80120600	0.13182200
O	-3.44675300	-3.38556300	0.38793000

TS4RS'

C	-3.71327300	0.05316300	-0.19051800
C	-4.85798900	-0.22468800	0.77928200
H	-3.09330600	0.88488000	0.14732600
H	-4.48463500	-0.29283400	1.81114500
N	-2.86483400	-1.15869300	-0.16441700
O	-5.52020200	-1.42734600	0.41188900
C	-3.34236400	-2.39172600	0.17646500
C	-4.74135500	-2.56420700	0.69513700
H	-5.21392500	-3.42726200	0.22363100
H	-4.68200800	-2.74296300	1.77882100
N	-2.41429000	-3.30159700	0.07783500
C	-1.55960100	-1.30375400	-0.45750600
N	-1.31122900	-2.61013900	-0.31991500
C	-0.10134200	-3.31921600	-0.65206300
C	0.22890800	-3.44351800	-2.00441800
C	0.70201700	-3.79286700	0.38570000
C	1.44221100	-4.05473500	-2.30680700
C	1.90363600	-4.40279000	0.02538000
C	2.29676100	-4.52437800	-1.30714100
H	1.73193600	-4.15725000	-3.34933400
H	2.55661500	-4.77369900	0.81163400
H	-5.59253600	0.57968400	0.71162500
C	-4.20877600	0.31324800	-1.61955500
H	-3.34893900	0.23495100	-2.28874800
H	-4.94372200	-0.45373000	-1.88524800
C	-4.80733200	1.69506700	-1.71213700
C	-3.96132100	2.80973500	-1.68964000
C	-6.18745400	1.88754000	-1.77843100
C	-4.49399600	4.09422000	-1.73707600
H	-2.88556900	2.65239000	-1.63244300
C	-6.72089200	3.17455500	-1.82837400
H	-6.84699500	1.02295500	-1.79436400
C	-5.87474700	4.27931100	-1.80734900
H	-3.83075500	4.95378100	-1.72491000
H	-7.79607000	3.31233600	-1.88476400
H	-6.28793700	5.28208500	-1.84799400
C	3.63647900	-5.11156900	-1.66263500
H	3.59606000	-5.64665300	-2.61404100
H	4.37819000	-4.31203900	-1.76297100
H	3.98726500	-5.79962600	-0.89057500
C	-0.66562700	-2.90080500	-3.08732600
H	-1.71591000	-3.14700900	-2.90430700

H	-0.58033100	-1.81000000	-3.15200600
H	-0.38142800	-3.31394400	-4.05614400
C	0.34947300	-3.56440300	1.82966000
H	0.69489900	-2.57423600	2.14913000
H	-0.72624100	-3.62092300	2.00691200
H	0.84264100	-4.30428400	2.46289900
C	1.70563700	0.53652900	-0.99927000
C	0.72803500	-0.37888900	-0.62791000
H	1.38900100	1.40207600	-1.58110300
C	3.11980500	0.14952900	-1.10553100
C	3.96756500	0.87645600	-1.95092700
C	3.65313000	-0.93258300	-0.38882700
C	5.30595200	0.52690400	-2.09121300
H	3.56743400	1.73414100	-2.48623900
C	4.99047200	-1.28171300	-0.53034500
H	3.02566400	-1.49010600	0.30164800
C	5.82140100	-0.55655500	-1.38493800
H	5.94887100	1.11059900	-2.74226100
H	5.39003900	-2.11680800	0.03778700
H	6.86742900	-0.82736100	-1.48814100
C	-0.64383200	-0.15624200	-0.85821400
O	-1.21693800	0.82524100	-1.35483100
H	1.02267000	-1.29917700	-0.14575000
C	-0.37371400	1.39252400	1.86905000
C	-1.66824800	1.93884700	1.86182100
H	-2.51132400	1.55685900	2.41887500
C	-1.64303500	3.06122500	1.03933300
H	-2.47084600	3.71398800	0.80264500
C	-0.34160100	3.20474800	0.56313900
H	0.09818300	3.93433300	-0.09474500
N	0.43309900	2.21520500	1.07331800
C	0.07650500	0.21748000	2.55184600
C	1.80953600	2.01407400	0.86747900
H	2.23365900	1.29456800	1.54384600
C	2.61620400	3.00821600	0.23853400
O	2.16454900	3.92003200	-0.47898600
C	4.11091400	2.88777400	0.39448000
C	4.74989900	1.93253600	1.19260400
C	4.89413000	3.78428000	-0.34028000
C	6.13884200	1.86690800	1.23493800
H	4.17838000	1.21857100	1.77580100
C	6.28128900	3.72493900	-0.29137100
H	4.38133900	4.51805800	-0.95256800
C	6.90911100	2.75934700	0.49321600

H	6.62056300	1.11075600	1.84719600
H	6.87471000	4.42725300	-0.86893500
H	7.99285700	2.70418300	0.52975100
C	-1.03300700	-0.53562100	3.33468600
F	-1.66990300	0.24493200	4.21390600
F	-0.52992500	-1.56974800	3.99738800
F	-1.97194000	-1.01859100	2.48382800
O	1.19315000	-0.28210700	2.57903700

TS4RS''

C	3.24890300	1.19219100	-0.25053400
C	4.30277700	1.77984000	0.68219700
H	2.92883500	0.21291800	0.09262600
H	3.99779700	1.66956700	1.73137600
N	2.06722400	2.08202200	-0.15514300
O	4.51833000	3.14860800	0.36688400
C	2.14106900	3.36151300	0.31874800
C	3.44162300	3.94372100	0.79585700
H	3.57119600	4.94611800	0.38459600
H	3.41090700	4.01380800	1.89274900
N	0.96735600	3.92755900	0.34132100
C	0.76983100	1.83910600	-0.44471000
N	0.12745900	2.97037500	-0.13513600
C	-1.28534900	3.23362200	-0.19385600
C	-1.82838100	3.69274100	-1.39407700
C	-2.04154400	2.94532500	0.94264400
C	-3.20972700	3.86241400	-1.43811400
C	-3.41931800	3.13329100	0.84670900
C	-4.01781400	3.58034600	-0.33310100
H	-3.66730300	4.21158300	-2.36030700
H	-4.04032900	2.91618100	1.71124900
H	5.24737400	1.25491300	0.52788000
C	3.74285600	1.07731400	-1.69698800
H	2.87434000	0.92203700	-2.34174100
H	4.23826800	2.01154400	-1.98169200
C	4.68355200	-0.09957100	-1.81437900
C	4.17887900	-1.39709900	-1.66457300
C	6.05057900	0.07699500	-2.02925500
C	5.03127100	-2.49334500	-1.73461800
H	3.11329600	-1.53953000	-1.49475200
C	6.90419700	-1.02318300	-2.10299500
H	6.44953000	1.08233300	-2.14212400
C	6.39609500	-2.31035100	-1.95564400
H	4.62369300	-3.49340500	-1.61801600

H	7.96535300	-0.87177000	-2.27415800
H	7.05970500	-3.16741800	-2.01117300
C	-5.51378000	3.72395500	-0.43071000
H	-5.78862000	4.64803900	-0.94516900
H	-5.93961100	2.89155700	-1.00046400
H	-5.97780500	3.72571200	0.55738000
C	-0.95455900	3.92600800	-2.59609600
H	-0.08605600	4.54079500	-2.34370300
H	-0.58769400	2.97089600	-2.98872200
H	-1.51394900	4.42390100	-3.38894400
C	-1.38547500	2.40704100	2.18427000
H	-2.13120800	2.20139300	2.95455400
H	-0.84057700	1.47941300	1.96941800
H	-0.66177500	3.12237500	2.58721900
C	-1.56365200	-0.99605200	-1.34109000
C	-1.12523400	0.29959100	-1.06289500
H	-0.81774500	-1.70407000	-1.69644400
C	-2.96056100	-1.31972900	-1.63649700
C	-3.27062400	-2.58500200	-2.15464900
C	-4.00802900	-0.40822800	-1.41468900
C	-4.58378400	-2.92609100	-2.46250400
H	-2.47083000	-3.30333100	-2.30561000
C	-5.31627300	-0.75144400	-1.72068000
H	-3.80419800	0.56689400	-0.98093000
C	-5.60883800	-2.00913000	-2.25032400
H	-4.80438200	-3.90977800	-2.86430300
H	-6.11616400	-0.04132400	-1.53531700
H	-6.63463600	-2.27395400	-2.48742200
C	0.26107700	0.50776600	-0.95160700
O	1.14986100	-0.33091200	-1.18221100
H	-1.83049800	1.08320700	-0.84225400
C	1.43767200	-2.38114900	1.08193600
C	2.39149300	-3.34301700	0.70754200
H	3.43992300	-3.31471200	0.96693300
C	1.74561200	-4.28675100	-0.08462300
H	2.18013700	-5.15953500	-0.54824000
C	0.40395700	-3.90964800	-0.16680000
H	-0.44052300	-4.39462200	-0.62783500
N	0.21478300	-2.76403000	0.52836800
C	1.67871100	-1.16638000	1.78961300
C	-1.01738500	-2.10496300	0.73914300
H	-0.90048600	-1.16149400	1.24009800
C	-2.22910400	-2.84324200	0.80577800
O	-2.36431400	-4.00971000	0.39171500

C	-3.44719000	-2.09803600	1.28845000
C	-3.41387200	-0.83880400	1.89896600
C	-4.68474100	-2.70440000	1.06077700
C	-4.59747400	-0.20165800	2.26041700
H	-2.46848000	-0.34957700	2.11266800
C	-5.86669300	-2.06599500	1.41684600
H	-4.68856400	-3.67848700	0.58429600
C	-5.82759200	-0.80837800	2.01448900
H	-4.55833400	0.76680000	2.75091900
H	-6.82116400	-2.54642400	1.22325200
H	-6.74837600	-0.30706200	2.29704000
C	3.04805400	-1.10937700	2.52060300
F	3.23191000	-2.15523100	3.32872900
F	3.14039500	0.00180500	3.25276100
F	4.07647100	-1.09317000	1.64608000
O	0.97091100	-0.16788000	1.88344400

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C	-1.52644300	3.14587400	0.11552400
C	-2.24151800	4.23428000	0.91066000
H	-0.66062800	2.76206100	0.65320200
H	-2.38830500	3.92375800	1.95449000
N	-2.49049500	2.02317700	0.00288500
O	-3.49368300	4.53926300	0.31302100
C	-3.84343400	2.18661900	0.11067000
C	-4.42726700	3.50800700	0.52131700
H	-5.31553300	3.72450300	-0.07373700
H	-4.71799100	3.44746900	1.58083400
N	-4.47876000	1.07541100	-0.13129700
C	-2.27381000	0.72494700	-0.29516000
N	-3.48833300	0.17370100	-0.38908200
C	-3.83137600	-1.13321800	-0.88638900
C	-3.58839300	-1.41035500	-2.23563800
C	-4.41618600	-2.04829300	-0.00920200
C	-3.93527500	-2.67903300	-2.69379000
C	-4.74392500	-3.30227300	-0.52004900
C	-4.50456900	-3.63707500	-1.85333000
H	-3.75702200	-2.92339200	-3.73787400
H	-5.19471100	-4.03532300	0.14381000
H	-1.64036700	5.14555900	0.88754100
C	-1.09421100	3.64098400	-1.27422500
H	-0.94464400	2.76899800	-1.91362400
H	-1.89489800	4.26001900	-1.69326700
C	0.19908700	4.41841100	-1.16899900

C	1. 40217300	3. 73313000	-0. 95437500
C	0. 21812800	5. 81133800	-1. 25705300
C	2. 59957000	4. 43113400	-0. 84007600
H	1. 39804400	2. 64945700	-0. 88050200
C	1. 41820700	6. 51182600	-1. 13882100
H	-0. 71136200	6. 34978800	-1. 42910800
C	2. 61017200	5. 82304200	-0. 93204600
H	3. 51865500	3. 87277200	-0. 68791400
H	1. 42014400	7. 59487400	-1. 21381500
H	3. 54475600	6. 36863900	-0. 84564000
C	-4. 83257000	-5. 01132000	-2. 37440800
H	-5. 18161600	-4. 96727000	-3. 40866700
H	-3. 94355300	-5. 64959800	-2. 35325700
H	-5. 60343400	-5. 49201900	-1. 76862700
C	-2. 96647000	-0. 39651000	-3. 15886800
H	-3. 38747200	0. 60196000	-3. 00533200
H	-1. 88447500	-0. 33641800	-2. 99747700
H	-3. 13573600	-0. 67931900	-4. 19882900
C	-4. 66481700	-1. 69389300	1. 43057300
H	-5. 00433700	-2. 56829600	1. 98759200
H	-3. 74817900	-1. 31925700	1. 89467200
H	-5. 42037200	-0. 90770900	1. 51817200
C	0. 58295400	-1. 70438000	-0. 51402600
C	-0. 73492400	-1. 25069400	-0. 33158000
H	1. 22591100	-1. 04923100	-1. 09790900
C	0. 97012100	-3. 10929700	-0. 45570200
C	2. 10683100	-3. 53688100	-1. 15665900
C	0. 26363000	-4. 04293400	0. 31940100
C	2. 51076100	-4. 86554800	-1. 11463000
H	2. 68119800	-2. 80953800	-1. 72585700
C	0. 67457200	-5. 36936500	0. 36802800
H	-0. 59258200	-3. 71960200	0. 90237200
C	1. 79356300	-5. 78561500	-0. 35328500
H	3. 39384900	-5. 17813900	-1. 66259700
H	0. 12502800	-6. 08113700	0. 97570000
H	2. 11020300	-6. 82319100	-0. 31313600
C	-0. 90938800	0. 12949200	-0. 48105800
O	-0. 00434800	0. 96231600	-0. 71282300
H	-1. 54018500	-1. 90095800	-0. 01441700
C	4. 20472200	-1. 06705000	0. 35498400
C	5. 22146900	-2. 03294700	0. 36613800
H	6. 19183200	-1. 91761400	-0. 09333100
C	4. 75162300	-3. 13091200	1. 08308400
H	5. 27427500	-4. 05439900	1. 28151300

C	3.45317500	-2.83911200	1.49463900
H	2.72905100	-3.41974800	2.04389800
N	3.12389000	-1.59118100	1.07286500
C	4.25616800	0.26592500	-0.17865800
C	1.90285900	-0.91977500	1.25304800
H	1.90068600	0.09430400	0.89081500
C	0.97013800	-1.32990300	2.25262200
O	0.91464400	-2.45281400	2.77804700
C	-0.06187000	-0.30112400	2.63195900
C	0.21901000	1.06743500	2.64123900
C	-1.31108500	-0.74254900	3.07877300
C	-0.72760800	1.97577400	3.11222700
H	1.19073400	1.42661800	2.31441800
C	-2.26886000	0.16682500	3.51739600
H	-1.49998100	-1.81228000	3.09465700
C	-1.97739300	1.53127700	3.53805000
H	-0.47854500	3.03260100	3.15796000
H	-3.23267000	-0.18637300	3.87199900
H	-2.71124400	2.23981800	3.91269500
C	5.56834100	0.61334600	-0.92558500
F	6.63215000	0.53591300	-0.11167200
F	5.51733200	1.84919400	-1.41351500
F	5.78621000	-0.22716400	-1.94864200
O	3.41366400	1.14926700	-0.11140000

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C	3.99196200	0.84648100	0.14912400
C	5.33414500	1.53648600	0.38689800
H	3.72946200	0.16659900	0.96179500
H	5.35675300	2.01837200	1.37403100
N	2.99754100	1.94371800	0.16918400
O	5.56149700	2.49015800	-0.64255400
C	3.29821200	3.20928400	-0.25214000
C	4.71835100	3.61252300	-0.54413800
H	4.76971000	4.15709000	-1.48829000
H	5.04644800	4.28222600	0.26400900
N	2.24482600	3.97805300	-0.22692400
C	1.68913800	1.92649400	0.47604900
N	1.25321300	3.16407200	0.22815200
C	-0.09063300	3.64882100	0.40204900
C	-0.87924400	3.78740000	-0.74092700
C	-0.56229900	3.85235000	1.70030200
C	-2.22086100	4.11382000	-0.54900900
C	-1.90942600	4.17827800	1.83605400

C	-2.75404000	4.29178900	0.72932900
H	-2.86605400	4.21272100	-1.41775000
H	-2.31336700	4.33107700	2.83343400
H	6.14043900	0.80559400	0.32550500
C	3.93543000	0.13855500	-1.21543600
H	2.90802900	-0.19121400	-1.38197000
H	4.21858600	0.86282800	-1.98624000
C	4.86110300	-1.05318600	-1.23921300
C	4.40703400	-2.28610000	-0.76234800
C	6.17671900	-0.93982900	-1.69620200
C	5.26129200	-3.38482700	-0.73308900
H	3.37387500	-2.36813500	-0.43372000
C	7.03007700	-2.04069900	-1.67110600
H	6.52932300	0.01735900	-2.07535400
C	6.57406100	-3.26441300	-1.18571400
H	4.89667400	-4.33682600	-0.35956000
H	8.04885300	-1.94352300	-2.03292800
H	7.23844400	-4.12250200	-1.16621200
C	-4.22243500	4.56326500	0.92229800
H	-4.73167500	3.65013500	1.24816800
H	-4.38663500	5.32272200	1.69046300
H	-4.69113300	4.89886100	-0.00459500
C	-0.30179800	3.56145300	-2.11177000
H	0.46863900	4.30360000	-2.33904400
H	0.15917500	2.57021200	-2.18281100
H	-1.08344400	3.62505200	-2.86966200
C	0.33408300	3.68833400	2.89906600
H	1.30326500	4.16943400	2.73946300
H	-0.12879300	4.13442000	3.78034400
H	0.51579200	2.63018300	3.11608300
C	-1.10286900	-0.39530900	1.53603100
C	-0.40907400	0.64439100	0.96676800
H	-0.55463900	-1.03306200	2.22762000
C	-2.56613200	-0.50173500	1.57843300
C	-3.15247600	-1.53432700	2.32489800
C	-3.40301800	0.40405100	0.91200200
C	-4.53193300	-1.66840700	2.39703300
H	-2.50663900	-2.24628400	2.83287200
C	-4.78639000	0.26552600	0.98026900
H	-2.97632000	1.21729400	0.32975900
C	-5.35504200	-0.77181000	1.71676800
H	-4.96694600	-2.48082400	2.96952400
H	-5.42214600	0.96168900	0.44316600
H	-6.43386300	-0.88165000	1.75855200

C	0.97823300	0.80784200	1.23025300
O	1.68054500	0.26442800	2.08713800
H	-0.88067200	1.30178900	0.24739800
C	-2.83596300	-1.15568300	-1.77236700
C	-2.97004500	-0.19095000	-2.77471100
H	-3.88482600	0.03785200	-3.30001200
C	-1.71768600	0.39626900	-2.96308900
H	-1.45854700	1.16377000	-3.67716100
C	-0.83489300	-0.21050200	-2.07495500
H	0.22073400	-0.07868300	-1.90635000
N	-1.50159000	-1.16133500	-1.35961400
C	-3.85968800	-2.01327700	-1.23269400
C	-0.96303000	-1.99496900	-0.36388000
H	-1.65349000	-2.73132200	0.01005700
C	0.40954300	-2.06450400	-0.08603300
O	1.27134600	-1.23603500	-0.48824700
C	0.83194200	-3.15612900	0.85931300
C	0.23323700	-4.42050800	0.85213300
C	1.88636900	-2.90885700	1.74499000
C	0.67677700	-5.41578700	1.71909400
H	-0.56498200	-4.63560400	0.14816800
C	2.32839600	-3.90384500	2.61073000
H	2.32729100	-1.91667500	1.75330300
C	1.72507800	-5.16076400	2.60006000
H	0.20935500	-6.39527300	1.69825500
H	3.14140800	-3.69764400	3.30013800
H	2.07113600	-5.93803900	3.27416300
O	-3.73936700	-2.91667700	-0.42455400
C	-5.28085600	-1.77812500	-1.80506800
F	-5.66091100	-0.49097600	-1.75422600
F	-5.33039000	-2.14935100	-3.09487800
F	-6.17785600	-2.49197900	-1.13457300

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C	-3.86947500	0.35593400	-1.21498200
C	-5.18795300	0.99582700	-1.64646400
H	-3.42974400	-0.21788100	-2.03096400
H	-5.10239400	1.43093200	-2.65362700
N	-2.93455600	1.46965000	-0.93195800
O	-5.58820500	1.99248500	-0.72085300
C	-3.33682500	2.76433600	-0.75922500
C	-4.78837000	3.14096600	-0.84161000
H	-5.04103400	3.81836300	-0.02387000
H	-4.97726800	3.65539500	-1.79607200

N	-2.32213500	3.55232500	-0.55282000
C	-1.59356100	1.44301200	-0.77699000
N	-1.24300400	2.72244400	-0.58070300
C	0.07530500	3.29677600	-0.47149100
C	0.46638000	3.80869700	0.76535400
C	0.90400000	3.28946800	-1.59929100
C	1.77063100	4.29535300	0.86723700
C	2.19342300	3.78456600	-1.43942500
C	2.64765500	4.28023500	-0.21479200
H	2.10936600	4.68166900	1.82549700
H	2.87045400	3.76475100	-2.29048900
H	-5.96656200	0.23041000	-1.65576400
C	-4.00801600	-0.53466400	0.02122200
H	-3.00078400	-0.80036700	0.35247500
H	-4.50084300	0.03318600	0.81874300
C	-4.77559500	-1.78588800	-0.32125100
C	-4.18284300	-2.74312500	-1.15205300
C	-6.07451800	-1.99537800	0.14222700
C	-4.88164200	-3.89356100	-1.50458500
H	-3.16128600	-2.58237300	-1.49449800
C	-6.77380800	-3.14859100	-0.20935200
H	-6.53769500	-1.25266800	0.78830100
C	-6.17814300	-4.09849100	-1.03348800
H	-4.41198200	-4.63495100	-2.14422400
H	-7.78162300	-3.30399900	0.16359700
H	-6.72089700	-4.99818300	-1.30673700
C	4.05992800	4.78641200	-0.08495000
H	4.76710900	4.04415200	-0.46797200
H	4.19799100	5.70940200	-0.65842200
H	4.31245200	4.99562500	0.95761100
C	-0.47159100	3.83324900	1.94238200
H	-1.14777000	4.69235100	1.87514400
H	-1.08855000	2.93354200	1.98918200
H	0.08873600	3.90556400	2.87671500
C	0.45392200	2.72560400	-2.92035700
H	-0.59341600	2.96510900	-3.13033900
H	1.06307400	3.13134600	-3.73094700
H	0.56200500	1.63468100	-2.92987400
C	1.63997800	-0.46216100	-0.85323900
C	0.56947600	0.32129100	-0.41489700
H	1.44383900	-1.16299800	-1.66513900
C	3.01047000	0.06157200	-0.72204000
C	3.95683600	-0.19525900	-1.72125100
C	3.39286400	0.83076200	0.38753100

C	5.24700900	0.31653000	-1.62716800
H	3.67679500	-0.81235000	-2.57131800
C	4.68131400	1.34285800	0.47823700
H	2.68611500	0.99118700	1.19825800
C	5.61252100	1.09323200	-0.53028400
H	5.97192800	0.09457200	-2.40460700
H	4.96481800	1.92885800	1.34864800
H	6.62288700	1.48416600	-0.45031700
C	-0.73433200	0.19049100	-0.92323800
O	-1.26562700	-0.74538300	-1.54013300
H	0.78024200	1.15830500	0.23674300
C	-0.37309900	-1.85830800	1.69925000
C	-1.64787500	-2.44085300	1.65873100
H	-2.50526300	-2.12064200	2.23275300
C	-1.58374000	-3.52540900	0.78422400
H	-2.38739200	-4.20168500	0.53170700
C	-0.28610000	-3.59482600	0.29304100
H	0.17336900	-4.26406400	-0.41435600
N	0.45836700	-2.60907900	0.86036100
C	0.05962800	-0.70567400	2.43263700
C	1.81044700	-2.31765500	0.62484300
H	2.26517600	-1.73653100	1.40801400
C	2.60517000	-3.13213100	-0.25138900
O	2.13529000	-3.91222300	-1.09152700
C	4.09848000	-2.93582600	-0.20134700
C	4.77289400	-2.26542600	0.82434300
C	4.83620600	-3.44500900	-1.27499700
C	6.15067600	-2.08533000	0.75922000
H	4.23428700	-1.87415100	1.68115400
C	6.21299700	-3.26985800	-1.33771300
H	4.29613800	-3.97275600	-2.05438900
C	6.87434600	-2.58163900	-0.32192100
H	6.65939800	-1.55206000	1.55689500
H	6.77223500	-3.66726100	-2.18004600
H	7.95000500	-2.43761900	-0.36966300
O	1.19255000	-0.28187400	2.60476400
C	-1.08517400	0.14344500	3.04198400
F	-1.87529900	0.64971000	2.06045700
F	-1.88153900	-0.55103900	3.86270500
F	-0.59869400	1.17422900	3.72339000

TS4SR''

C	-2.84756800	2.49457700	-0.75234000
C	-3.66879900	3.69097200	-1.22528700

H	-2.82958800	1.70854600	-1.50623200
H	-3.39508200	3.97201200	-2.25365500
N	-1.45213900	2.98442400	-0.60929800
O	-3.48621700	4.79632300	-0.35479100
C	-1.15039100	4.31188100	-0.48152900
C	-2.21700400	5.36969400	-0.52792700
H	-2.05745300	6.09299600	0.27404600
H	-2.15056400	5.89686600	-1.49205300
N	0.13259400	4.50089100	-0.37729500
C	-0.28390200	2.29955800	-0.56028000
N	0.65991600	3.24729300	-0.43661100
C	2.08675200	3.08721500	-0.34570600
C	2.66127200	3.12564700	0.92582200
C	2.81092300	2.85361900	-1.51442000
C	4.02473500	2.86256200	1.01350500
C	4.17198000	2.58825100	-1.37130600
C	4.78638800	2.56483000	-0.11890800
H	4.49901100	2.86523800	1.99094600
H	4.75833600	2.36726000	-2.25998400
H	-4.72794600	3.43033900	-1.19895000
C	-3.34924300	1.91530400	0.57726300
H	-2.62568900	1.16783700	0.91641200
H	-3.41345400	2.72304500	1.31518800
C	-4.69296300	1.26301500	0.36549300
C	-4.74984000	0.00897900	-0.24619800
C	-5.88101600	1.90993100	0.71205400
C	-5.97898700	-0.58962300	-0.50521400
H	-3.81911300	-0.49522700	-0.49991400
C	-7.11171100	1.31247300	0.45072600
H	-5.83733900	2.88603500	1.19191900
C	-7.16087200	0.06236500	-0.16075000
H	-6.00871500	-1.57437400	-0.96033200
H	-8.02982100	1.82131900	0.72884300
H	-8.11944000	-0.40738700	-0.35947200
C	6.23430300	2.17773300	0.02598200
H	6.30883100	1.15073600	0.40284200
H	6.76034100	2.22609700	-0.93056400
H	6.75118700	2.82689700	0.73861100
C	1.82195100	3.42711000	2.13723400
H	1.36013900	4.41619500	2.05474600
H	1.02126500	2.68714500	2.24796600
H	2.43156900	3.39748500	3.04220000
C	2.13449600	2.79996700	-2.85662700
H	1.42960000	3.62743900	-2.98496700

H	2.87212100	2.84880600	-3.66012500
H	1.58079200	1.85853700	-2.95941900
C	1.19365000	-1.13446300	-1.12095100
C	1.07323700	0.20640200	-0.72367200
H	0.27832300	-1.59676700	-1.48913700
C	2.44469400	-1.71873600	-1.59910400
C	2.40219600	-2.88776700	-2.37217900
C	3.69814200	-1.15740400	-1.30227200
C	3.57284400	-3.47959100	-2.83478200
H	1.43700700	-3.32523800	-2.61424900
C	4.86410200	-1.74852300	-1.76787000
H	3.75958400	-0.26009500	-0.69146200
C	4.80731900	-2.91167500	-2.53556500
H	3.51996700	-4.38387600	-3.43357000
H	5.82573900	-1.30269000	-1.52827900
H	5.72213000	-3.37133000	-2.89709700
C	-0.20082700	0.79019700	-0.71360800
O	-1.29724400	0.22439400	-0.89690200
H	1.95000000	0.77514800	-0.45724200
C	-1.20996900	-3.77227000	0.11192000
C	-1.44316400	-4.97640800	-0.56139400
H	-2.41632600	-5.37620800	-0.80399700
C	-0.20339300	-5.55699100	-0.83426700
H	-0.02098500	-6.49750000	-1.33314600
C	0.77673600	-4.71316000	-0.32500300
H	1.85180800	-4.78873900	-0.30539500
N	0.17578400	-3.62887100	0.24039000
C	-2.17465400	-2.86560000	0.67852900
C	0.80627900	-2.50157900	0.78629500
H	0.11106300	-1.79031400	1.19617000
C	2.17794200	-2.53236600	1.19233500
O	2.99145700	-3.40287300	0.85988300
C	2.66487900	-1.36006300	2.00463600
C	1.82584800	-0.51622900	2.73924000
C	4.05017900	-1.17217000	2.07661200
C	2.36788000	0.47754400	3.55131700
H	0.74956800	-0.65934800	2.72520300
C	4.58870200	-0.16481600	2.86835000
H	4.67927600	-1.85340500	1.51145600
C	3.74671800	0.65732300	3.61760700
H	1.70966400	1.09904600	4.15192000
H	5.66637200	-0.03517600	2.92506500
H	4.16561200	1.42358400	4.26549400
O	-1.98129900	-1.81174200	1.26162500

C	-3.65217300	-3.30605200	0.51684400
F	-4.03241000	-3.20339400	-0.77170900
F	-3.85583500	-4.57648900	0.89281500
F	-4.45439700	-2.53936900	1.24392500

TS4SR'''

C	-3.89788700	-0.82311600	-1.30825900
C	-5.32897700	-0.85908600	-1.83794200
H	-3.20523400	-1.26744500	-2.02067600
H	-5.36120000	-0.56630000	-2.89689600
N	-3.52363900	0.60539800	-1.16949800
O	-6.17600400	-0.01436000	-1.07403500
C	-4.44276200	1.61410100	-1.10696800
C	-5.90125700	1.34159700	-1.33209800
H	-6.49792000	1.95007600	-0.65134300
H	-6.16386500	1.60703700	-2.36650800
N	-3.87452400	2.75695700	-0.84926400
C	-2.31293800	1.14684100	-0.90530900
N	-2.55190100	2.45436900	-0.73643300
C	-1.62722600	3.49861700	-0.38466600
C	-1.61666100	3.92151500	0.94657500
C	-0.77624200	4.00974700	-1.36572700
C	-0.67714100	4.88842300	1.29736100
C	0.14416200	4.97445800	-0.96190900
C	0.21453300	5.41600900	0.36075300
H	-0.63656700	5.23161700	2.32790900
H	0.83175900	5.38249900	-1.69799300
H	-5.71297700	-1.87668600	-1.74092100
C	-3.74292400	-1.48740500	0.06314500
H	-2.78681200	-1.16721000	0.48684200
H	-4.54276300	-1.12671700	0.72059600
C	-3.75407800	-2.99056100	-0.03654700
C	-2.63634100	-3.64525700	-0.56728000
C	-4.84332900	-3.74403000	0.40043900
C	-2.61394500	-5.03282100	-0.65361000
H	-1.78409000	-3.04888400	-0.88884300
C	-4.82007500	-5.13584300	0.31491800
H	-5.70985900	-3.23830300	0.82057100
C	-3.70546400	-5.78134300	-0.21131100
H	-1.74045900	-5.53321600	-1.05971600
H	-5.67114500	-5.71328400	0.66224900
H	-3.68390900	-6.86462000	-0.27519700
C	1.25556700	6.42051700	0.77872600
H	2.14502400	5.90899100	1.16071200

H	1. 56586400	7. 04255400	-0. 06333800
H	0. 88266300	7. 07081000	1. 57321900
C	-2. 58820100	3. 36081500	1. 95102800
H	-3. 58028900	3. 80222200	1. 81514400
H	-2. 69334700	2. 27648000	1. 84389000
H	-2. 25216100	3. 57295500	2. 96759400
C	-0. 81261600	3. 49832300	-2. 77942600
H	-1. 83848600	3. 40557700	-3. 14703300
H	-0. 26736800	4. 17115400	-3. 44281700
H	-0. 34085000	2. 51069600	-2. 83360200
C	1. 37444100	0. 33370900	-0. 67971400
C	0. 13903400	0. 97061000	-0. 45639500
H	1. 35212100	-0. 55527000	-1. 30600800
C	2. 61987800	1. 10439900	-0. 67625500
C	3. 71086300	0. 65119100	-1. 43176000
C	2. 76723400	2. 28091200	0. 07829700
C	4. 91220500	1. 34880400	-1. 44117300
H	3. 60596400	-0. 25815700	-2. 01866800
C	3. 96799900	2. 98114200	0. 06032800
H	1. 95067000	2. 63061900	0. 70225800
C	5. 04346800	2. 51890800	-0. 69651000
H	5. 74741400	0. 97303600	-2. 02424500
H	4. 07143200	3. 88561500	0. 65207200
H	5. 98079800	3. 06641500	-0. 70208900
C	-1. 02261800	0. 34612800	-0. 92178200
O	-1. 12977900	-0. 79516000	-1. 41824900
H	0. 09503600	1. 93487600	0. 02596000
C	4. 30682500	-1. 73698900	0. 43872600
C	5. 60948400	-1. 35541400	0. 78054300
H	6. 51209500	-1. 78875900	0. 37696000
C	5. 51177600	-0. 31118000	1. 69811900
H	6. 32301000	0. 22550800	2. 16657800
C	4. 15887500	-0. 06530600	1. 90981500
H	3. 65711000	0. 65537600	2. 53307200
N	3. 42369500	-0. 93571100	1. 17005800
C	3. 89531400	-2. 64514100	-0. 59102300
C	2. 02014700	-1. 03694200	1. 10747200
H	1. 67036900	-1. 96386100	0. 68541900
C	1. 19915600	-0. 29065500	2. 01258800
O	1. 53790300	0. 77332800	2. 55410400
C	-0. 19036700	-0. 80727400	2. 27446800
C	-0. 54276400	-2. 15649800	2. 17854600
C	-1. 12650000	0. 10547000	2. 77414800
C	-1. 79555600	-2. 58981400	2. 60952900

H	0.17125600	-2.88470300	1.80774300
C	-2.38056800	-0.32367200	3.19502400
H	-0.82083000	1.14367900	2.86150100
C	-2.71233200	-1.67750700	3.12596800
H	-2.05553500	-3.64149300	2.53828800
H	-3.09324500	0.39194500	3.59595000
H	-3.68584200	-2.02043900	3.46394000
O	2.76068400	-2.91372400	-0.95644400
C	5.05681500	-3.29093700	-1.38497200
F	5.73995300	-2.35144600	-2.06194300
F	5.92914100	-3.92148900	-0.58434200
F	4.59694900	-4.17404400	-2.26391000

TS4SS

C	3.08678200	2.32241300	0.49516100
C	3.95280900	3.52644100	0.85798100
H	3.02191200	1.62659500	1.33078800
H	3.67603800	3.93145900	1.84198100
N	1.71575700	2.85186500	0.26936700
O	3.83729300	4.52951300	-0.13834800
C	1.47850600	4.17208000	0.01333000
C	2.59219900	5.17740900	-0.06818000
H	2.47346000	5.78676800	-0.96584200
H	2.53501500	5.83405600	0.81199300
N	0.20194100	4.41336000	-0.07903700
C	0.51263300	2.23187000	0.31557900
N	-0.38652600	3.20381200	0.11589400
C	-1.82747100	3.16256200	0.17629300
C	-2.54581500	3.18467100	-1.01776000
C	-2.42321800	3.14615300	1.44186000
C	-3.93775100	3.14108300	-0.91174100
C	-3.81239000	3.08440400	1.48767200
C	-4.58285200	3.06171800	0.32079300
H	-4.52889300	3.14513800	-1.82474900
H	-4.30483600	3.04771200	2.45623400
H	4.99766100	3.21184800	0.88342100
C	3.60181200	1.59607600	-0.75078500
H	2.81689600	0.92610100	-1.11203500
H	3.82119500	2.34027000	-1.52390900
C	4.83186800	0.79177900	-0.40480900
C	4.69851200	-0.35748100	0.38307000
C	6.10287100	1.18074900	-0.82983200
C	5.81865300	-1.10771600	0.72692300
H	3.70575400	-0.66799900	0.70136300

C	7.22655400	0.43206500	-0.48101500
H	6.21165000	2.07374700	-1.44134700
C	7.08539000	-0.71360500	0.29621400
H	5.69755500	-2.00758900	1.32196600
H	8.20927300	0.74360200	-0.82064100
H	7.95840000	-1.30037600	0.56383700
C	-6.07919600	2.91610400	0.39971700
H	-6.34452500	1.85967400	0.51927100
H	-6.48875200	3.46027700	1.25403900
H	-6.56230800	3.27998500	-0.50979900
C	-1.85684700	3.19244000	-2.35341500
H	-1.06282200	3.94308700	-2.38850000
H	-1.42445500	2.20191500	-2.53581300
H	-2.57436500	3.41046700	-3.14650400
C	-1.59326100	3.14037300	2.69730400
H	-1.10686700	2.16716100	2.83028200
H	-0.81463700	3.90872000	2.66511100
H	-2.22087300	3.32540200	3.56998300
C	-1.11344700	-1.10760600	1.06744300
C	-0.94936800	0.22962300	0.80418500
H	-0.22302500	-1.70887100	1.23330100
C	-2.39862000	-1.71677000	1.42711800
C	-2.45389100	-3.09071000	1.69982600
C	-3.58140700	-0.96487700	1.51865800
C	-3.65725700	-3.69807600	2.04294600
H	-1.54339400	-3.67667100	1.62332300
C	-4.78144700	-1.57502000	1.85573100
H	-3.56928100	0.10308300	1.31906300
C	-4.82529600	-2.94394500	2.11937800
H	-3.68207400	-4.76350900	2.24929600
H	-5.68935900	-0.98146800	1.90572000
H	-5.76611200	-3.41855000	2.38085800
C	0.36035700	0.74441200	0.61237900
O	1.42528200	0.13039400	0.72959800
H	-1.80233600	0.85729600	0.59475500
C	1.65953900	-2.73185700	-0.85594800
C	2.89804300	-2.33497000	-1.37306300
H	3.85799500	-2.72988100	-1.07617500
C	2.65486200	-1.35073300	-2.32994300
H	3.38865000	-0.82935100	-2.92741900
C	1.27935600	-1.15357500	-2.37812500
H	0.68172700	-0.47868700	-2.96662600
N	0.66893600	-1.98888600	-1.49840100
C	1.41574200	-3.70412100	0.16297100

O	0.34032500	-4.12515500	0.56296100
C	2.68941500	-4.26848600	0.84314000
F	2.36794900	-5.12919100	1.80191100
F	3.42382200	-3.28830200	1.39972300
F	3.47803100	-4.90466900	-0.03614300
C	-0.72816100	-2.08968600	-1.29702400
H	-1.06953600	-3.06328300	-0.98538800
C	-1.57215000	-1.05476200	-1.71832200
O	-1.15917600	0.09835200	-2.02426700
C	-3.05660800	-1.28896100	-1.66262100
C	-3.65931900	-2.54107900	-1.49454800
C	-3.87608500	-0.16244800	-1.76533700
C	-5.04200900	-2.65011600	-1.39792800
H	-3.05463000	-3.44025600	-1.43653500
C	-5.25988600	-0.26842300	-1.67350600
H	-3.39322800	0.79545800	-1.91633000
C	-5.84917200	-1.51589100	-1.48298300
H	-5.49287000	-3.62711500	-1.25243400
H	-5.87660000	0.62365000	-1.75382400
H	-6.92853400	-1.60857200	-1.40793800

TS4SS'

C	-2.71341500	-2.61807700	-0.80950500
C	-3.84753500	-3.42761000	-1.43664800
H	-1.83870400	-2.56733400	-1.46124400
H	-4.07819300	-3.06112500	-2.44654000
N	-3.25056700	-1.24126500	-0.70884900
O	-4.99466600	-3.35304400	-0.60052400
C	-4.58209000	-0.98340200	-0.53331500
C	-5.60410700	-2.08468900	-0.61879700
H	-6.29126100	-2.02898500	0.22710700
H	-6.17740600	-1.93536600	-1.54508400
N	-4.80426600	0.29685900	-0.42375000
C	-2.61407500	-0.05796500	-0.70814000
N	-3.56704500	0.85818000	-0.53294000
C	-3.41998600	2.29065200	-0.56683400
C	-3.47353800	2.98655400	0.64125700
C	-3.21523700	2.90180300	-1.80520600
C	-3.30177400	4.36763600	0.58513700
C	-3.04895400	4.28507000	-1.80495000
C	-3.08788900	5.03030800	-0.62516500
H	-3.32833900	4.93744800	1.51019100
H	-2.88147100	4.79196100	-2.75155300
H	-3.56345300	-4.47839600	-1.49228600

C	-2.34063900	-3.12467900	0.59351500
H	-1.63270500	-2.41736200	1.03230700
H	-3.25374800	-3.15559800	1.19708800
C	-1.70935500	-4.49388800	0.52037100
C	-0.33461000	-4.61353400	0.29476100
C	-2.48365400	-5.65083100	0.64422500
C	0.25039600	-5.87255600	0.18736300
H	0.26518500	-3.70840100	0.22922100
C	-1.89734700	-6.90976800	0.53876500
H	-3.55246400	-5.55894200	0.82712200
C	-0.52841700	-7.02206800	0.30704500
H	1.31917600	-5.95540600	0.01666600
H	-2.50794000	-7.80132900	0.64140400
H	-0.06918500	-8.00217700	0.22661400
C	-2.92784700	6.52743500	-0.66188500
H	-2.25324400	6.83159000	-1.46494700
H	-3.89358700	7.01208800	-0.83754700
H	-2.53294600	6.90532000	0.28330600
C	-3.67490200	2.25909900	1.94279700
H	-4.62922300	1.72493100	1.95321800
H	-2.87915800	1.52290200	2.10247700
H	-3.65721200	2.95842700	2.77992600
C	-3.16549600	2.09810700	-3.07790100
H	-2.25506600	1.49197200	-3.13531000
H	-4.02153700	1.41961100	-3.14776900
H	-3.18320800	2.75999400	-3.94459200
C	0.85797900	1.43306900	-0.65435900
C	-0.47607900	1.18718000	-0.40828900
H	1.28622300	0.95846500	-1.53585500
C	1.61372000	2.55087800	-0.07572100
C	2.85175500	2.89246600	-0.63935400
C	1.16032100	3.26990000	1.03905500
C	3.61185800	3.92854100	-0.11487300
H	3.21809500	2.32135600	-1.48950900
C	1.92349300	4.30693700	1.56453200
H	0.22249900	3.00104100	1.51847100
C	3.14723000	4.64257000	0.98943900
H	4.57021400	4.17465900	-0.56008600
H	1.56505600	4.84694700	2.43526100
H	3.74169400	5.44970700	1.40518000
C	-1.16211400	0.16228000	-1.10628400
O	-0.79935200	-0.53085600	-2.06305100
H	-1.00267200	1.69528100	0.39157800
C	4.02965100	-0.91581900	-1.19890600

C	4.09885300	-1.72183100	-2.34153000
H	4.98391400	-1.88117200	-2.93878500
C	2.82895400	-2.26037400	-2.55449200
H	2.52475900	-2.91746800	-3.35508100
C	1.99895800	-1.77994300	-1.54737000
H	0.94331800	-1.90801100	-1.37081200
N	2.71900500	-0.97971200	-0.71995000
C	5.09466200	-0.16552900	-0.58671000
O	5.06025500	0.53637300	0.41025500
C	6.45656900	-0.26950500	-1.31969400
F	7.38035300	0.45152400	-0.69527600
F	6.36370100	0.18040700	-2.58133300
F	6.89012800	-1.53742300	-1.37879300
C	2.24183000	-0.28122900	0.40783900
H	2.97799400	0.37840300	0.82986400
C	1.09767900	-0.64654900	1.12654100
O	0.19484200	-1.42284700	0.71780700
C	0.85281500	0.13431800	2.38845900
C	1.85767000	0.79362300	3.10638500
C	-0.46734200	0.22878000	2.84170100
C	1.54274800	1.54639200	4.23381000
H	2.89525600	0.71688400	2.79650500
C	-0.78386400	0.98179100	3.96849200
H	-1.23334300	-0.30543900	2.28596900
C	0.22216100	1.64914600	4.66534100
H	2.33375800	2.05325200	4.77726900
H	-1.81345800	1.04427800	4.30956800
H	-0.02014300	2.23540500	5.54617000

TS4SS''

C	3.20634300	-1.86845000	-0.97473800
C	4.23127800	-2.85062500	-1.53506900
H	3.06088600	-1.02283100	-1.64551000
H	4.02944700	-3.06839500	-2.59457300
N	1.91582100	-2.59926400	-0.90351400
O	4.23568300	-4.05433100	-0.78359800
C	1.85077300	-3.96441400	-0.85728900
C	3.07951800	-4.81146200	-1.03062500
H	3.05769400	-5.64221300	-0.32281700
H	3.08876400	-5.22183200	-2.05222200
N	0.62769900	-4.37785400	-0.69532300
C	0.65449600	-2.13032300	-0.74532000
N	-0.10557600	-3.23272400	-0.63596500
C	-1.51630300	-3.31469000	-0.36734600
C	-1.90460600	-3.41248100	0.97010900

C	-2.41275100	-3.22119500	-1.43006500
C	-3.26873700	-3.36325400	1.23792900
C	-3.76873600	-3.17138800	-1.10826400
C	-4.20915500	-3.21694900	0.21489500
H	-3.60435900	-3.41214000	2.27053200
H	-4.49476900	-3.06366800	-1.91031900
H	5.22633200	-2.41127300	-1.44359000
C	3.57839200	-1.36746300	0.42601400
H	2.71947800	-0.81750700	0.82243300
H	3.77597200	-2.23393700	1.06779400
C	4.77664500	-0.45455900	0.36152100
C	4.62773600	0.81692800	-0.19668800
C	6.03090600	-0.85594200	0.82366800
C	5.70972700	1.68663600	-0.26921500
H	3.65460400	1.13166200	-0.56440900
C	7.11942200	0.00992100	0.74173700
H	6.15205100	-1.84680900	1.25681400
C	6.95893900	1.28285700	0.19920800
H	5.55741500	2.67970900	-0.67992900
H	8.09061900	-0.30843100	1.10879800
H	7.80603500	1.96025800	0.14698200
C	-5.66936000	-3.06631200	0.55203300
H	-5.84483900	-2.09305800	1.02508500
H	-6.29557600	-3.12583700	-0.34127800
H	-5.99739900	-3.83695600	1.25590500
C	-0.87466500	-3.54678900	2.05855900
H	-0.26870400	-4.44708200	1.91249000
H	-0.20232400	-2.68133300	2.06637200
H	-1.35562500	-3.60248500	3.03687600
C	-1.92431400	-3.08151100	-2.84553700
H	-1.15417400	-3.82399400	-3.07726500
H	-2.74740000	-3.20461400	-3.55198100
H	-1.49324500	-2.08388700	-2.99510300
C	-1.44007100	0.97054600	-1.20741700
C	-1.06356500	-0.31594200	-0.79137500
H	-0.66568700	1.55168800	-1.70828000
C	-2.81849800	1.33989100	-1.51348400
C	-3.06045900	2.45031000	-2.33488000
C	-3.91856300	0.63239800	-0.99988000
C	-4.35996900	2.84145900	-2.63864100
H	-2.21521700	3.00195700	-2.73856100
C	-5.21403700	1.02469400	-1.30603700
H	-3.75727400	-0.22048300	-0.34495300
C	-5.44048200	2.12952200	-2.12663700

H	-4.52827800	3.70249500	-3.27853300
H	-6.05476500	0.47032500	-0.89773000
H	-6.45576200	2.43376100	-2.36235600
C	0.29546500	-0.65793800	-0.81940400
O	1.26141600	0.11543800	-0.99530400
H	-1.81339800	-1.02228700	-0.47253400
C	0.65372600	3.91340900	-0.67279600
C	0.54184500	4.99797800	-1.53757900
H	1.37813000	5.44192800	-2.05869600
C	-0.79299900	5.42587900	-1.50998300
H	-1.22144100	6.26581000	-2.03733600
C	-1.48282900	4.58020100	-0.65476500
H	-2.52370900	4.52415700	-0.37891800
N	-0.60922600	3.66207400	-0.13880100
C	1.93021800	3.34218700	-0.28138800
C	-0.94577000	2.49174700	0.55555900
H	-0.10360900	1.87495700	0.81567200
C	-2.20475200	2.31919900	1.20686100
O	-3.19800000	3.03262300	1.01670400
C	-2.33502900	1.10803400	2.09200600
C	-1.24900100	0.45565200	2.68452200
C	-3.63209900	0.66378000	2.37102900
C	-1.46313100	-0.61435500	3.55046500
H	-0.23550200	0.80757400	2.51566400
C	-3.84309700	-0.41824500	3.21742300
H	-4.45696800	1.20499600	1.91720700
C	-2.75647900	-1.05692800	3.81517000
H	-0.61603200	-1.09247300	4.03462000
H	-4.85512400	-0.75098400	3.43324600
H	-2.91921600	-1.88362500	4.50258000
C	2.16582800	2.84225100	1.17404400
O	2.91262000	3.37854900	-0.99726900
F	3.42385300	3.08429200	1.52517900
F	1.96068400	1.51640400	1.31087600
F	1.36405800	3.45901800	2.04936900

TS4SS'''

C	-3.66904700	-0.12794000	-1.51261100
C	-4.82223500	0.24383000	-2.44852200
H	-2.95138000	-0.77696700	-2.01084700
H	-4.44453300	0.59057200	-3.42311400
N	-2.95960600	1.14999700	-1.21062800
O	-5.65280900	1.24238200	-1.85407000
C	-3.59596400	2.36278900	-1.26478100

C	-5.00615900	2.49506000	-1.77659400
H	-5.59300400	3.12954500	-1.10732500
H	-4.97231800	2.98380200	-2.76454500
N	-2.80320300	3.34157000	-0.92154100
C	-1.66974600	1.38476600	-0.82069100
N	-1.60409600	2.72409700	-0.64410200
C	-0.52021700	3.53683200	-0.14740800
C	-0.39523500	3.69294400	1.24189600
C	0.31167900	4.18596400	-1.06974000
C	0.64887100	4.49778300	1.70048300
C	1.33926000	4.98131700	-0.55295100
C	1.53137700	5.13958200	0.82297400
H	0.77151200	4.63028700	2.77253200
H	2.00413700	5.49008400	-1.24643700
H	-5.45333800	-0.63148600	-2.60817300
C	-4.14716200	-0.79416000	-0.20126200
H	-3.32127400	-0.76544200	0.50987100
H	-4.96930200	-0.19701500	0.20918000
C	-4.58598000	-2.22730400	-0.41928300
C	-3.63751100	-3.26151600	-0.40337000
C	-5.93183800	-2.54521700	-0.64770800
C	-4.03307800	-4.58133000	-0.62170900
H	-2.59502500	-3.03083600	-0.20135700
C	-6.32625300	-3.86664400	-0.86737600
H	-6.67929900	-1.75406000	-0.63680600
C	-5.37537300	-4.88775900	-0.85801700
H	-3.28975400	-5.37364200	-0.59759800
H	-7.37489500	-4.09692200	-1.03704500
H	-5.67947700	-5.91792000	-1.02389400
C	2.66736300	5.97762400	1.35947900
H	3.44061800	5.34396500	1.81185000
H	3.14129000	6.56547400	0.56801100
H	2.32155500	6.66875500	2.13654000
C	-1.36934200	3.04956600	2.19790500
H	-2.39632600	3.36902600	1.98357800
H	-1.34169300	1.95628100	2.14507700
H	-1.13650300	3.33127200	3.22763600
C	0.11740600	4.03004600	-2.55864800
H	0.28009600	2.99310900	-2.87778000
H	-0.89723000	4.31348400	-2.86061900
H	0.82287200	4.66000100	-3.10667100
C	1.65757200	-0.30429600	-1.31070000
C	0.74324900	0.66057300	-0.91664600
H	1.26255000	-1.29404500	-1.51668000

C	2.97132600	0.01620000	-1.85772600
C	3.54596600	-0.84779200	-2.81190900
C	3.67143000	1.19312000	-1.52079900
C	4.74896400	-0.53004500	-3.43468200
H	3.03268500	-1.77070000	-3.06697000
C	4.87716000	1.50501800	-2.14032000
H	3.27634100	1.85200000	-0.75408800
C	5.41727200	0.65174900	-3.10605500
H	5.16873300	-1.20810500	-4.17268200
H	5.40597400	2.41219700	-1.86000100
H	6.35944100	0.89913300	-3.58790300
C	-0.62915500	0.29553100	-0.78501500
O	-1.08181500	-0.86987400	-0.80779200
H	1.03776100	1.69705900	-0.83024400
C	0.58189600	-0.70526100	2.65576500
C	0.44444100	0.30939200	3.62123800
H	-0.40709400	0.43439600	4.27240800
C	1.59829500	1.09589100	3.58406900
H	1.82268300	1.95389400	4.20337200
C	2.43896800	0.56792900	2.60806800
H	3.42817600	0.84116800	2.27975900
N	1.84775000	-0.53566900	2.05127100
C	-0.34189300	-1.75161200	2.32467900
O	-0.18804200	-2.68039600	1.53611600
C	-1.72306100	-1.66358900	3.03817400
F	-2.52655300	-2.65670100	2.65254100
F	-2.35538100	-0.49033000	2.73633900
F	-1.61694400	-1.71255700	4.38432300
C	2.42042900	-1.39008900	1.10615100
H	1.81898100	-2.26551800	0.93752700
C	3.80341800	-1.35345300	0.77022200
O	4.57546600	-0.41269900	1.06791200
C	4.36007000	-2.53383300	0.00864900
C	3.59397200	-3.59357400	-0.50648800
C	5.74995600	-2.56209200	-0.18405000
C	4.20336800	-4.64421300	-1.19275800
H	2.51553500	-3.61217600	-0.38598500
C	6.35960700	-3.61475600	-0.86168600
H	6.32838000	-1.73396500	0.21079000
C	5.58820800	-4.66198200	-1.37106900
H	3.59293600	-5.45408100	-1.58465500
H	7.43884600	-3.61902100	-0.99462500
H	6.06090500	-5.48531000	-1.90083700

M4RR

C	3.30761000	0.53774500	-0.38318100
C	4.56984900	0.95165200	0.37086300
H	2.84519100	-0.33761900	0.07678500
H	4.39932100	0.95290400	1.45418500
N	2.34820200	1.65778900	-0.22835000
O	5.00055700	2.23718900	-0.05781600
C	2.72412000	2.92522200	0.12327000
C	4.15639100	3.24494000	0.44097100
H	4.43958300	4.19106700	-0.02262600
H	4.25790300	3.34146900	1.53215600
N	1.70025900	3.72486100	0.19146300
C	1.00531200	1.66526500	-0.37294200
N	0.63651400	2.92798100	-0.12304000
C	-0.67295700	3.50957500	-0.25040900
C	-1.15497000	3.76532900	-1.53489800
C	-1.40981200	3.75624400	0.90968200
C	-2.44333900	4.28578300	-1.64030500
C	-2.69173000	4.27881300	0.75012200
C	-3.22670700	4.53815300	-0.51356400
H	-2.84697400	4.48996400	-2.62860900
H	-3.29103800	4.47592600	1.63554900
H	5.36891300	0.24653200	0.13330800
C	3.59617500	0.28059300	-1.86856200
H	2.64494100	0.32157500	-2.40215600
H	4.25991800	1.06863700	-2.24035600
C	4.21879900	-1.08287100	-2.05555200
C	3.46328400	-2.22793200	-1.77055700
C	5.53425000	-1.23119100	-2.49544000
C	4.01647400	-3.49317200	-1.93517200
H	2.44167000	-2.10356600	-1.41706000
C	6.08880700	-2.50023400	-2.66090400
H	6.12702600	-0.34646500	-2.71502500
C	5.33046100	-3.63317200	-2.38325000
H	3.41918400	-4.37262800	-1.71310100
H	7.11282300	-2.60091100	-3.00676400
H	5.76039500	-4.62140600	-2.51214000
C	-4.63796100	5.04397400	-0.65853100
H	-5.33464800	4.20282100	-0.73628300
H	-4.93506800	5.64388200	0.20439100
H	-4.75094100	5.65123100	-1.55916600
C	-0.33040000	3.44605900	-2.75216400
H	0.69634900	3.80806600	-2.64553400
H	-0.29074600	2.36254300	-2.91058700
H	-0.76687000	3.90241100	-3.64162900

C	-0.86684900	3.39266900	2.26431500
H	-0.79372100	2.30273500	2.36116000
H	0.13427700	3.80240700	2.42029200
H	-1.52573200	3.76156300	3.05185100
C	-1.91303700	-0.78532900	-0.47097400
C	-1.11901800	0.46982500	-0.29883400
H	-1.66755900	-1.20853300	-1.45340900
C	-3.41739100	-0.62289800	-0.39218100
C	-4.23586800	-1.57004900	-1.01778800
C	-4.03055400	0.42548300	0.30147400
C	-5.62266700	-1.48095100	-0.94937900
H	-3.77626300	-2.38699300	-1.57045200
C	-5.41879900	0.52048800	0.36887800
H	-3.42918400	1.17352900	0.80933300
C	-6.22007500	-0.43218700	-0.25406200
H	-6.23570000	-2.22774700	-1.44360800
H	-5.87340700	1.34213900	0.91407900
H	-7.30143800	-0.35739100	-0.20078000
C	0.18349400	0.45586500	-0.71212300
O	0.81249600	-0.49786800	-1.27901600
H	-1.54020800	1.32056400	0.21133500
C	-0.59792500	-0.72429000	2.69321700
C	-1.24962600	-0.23162600	3.82882600
H	-0.78389200	0.31339300	4.63424900
C	-2.59153600	-0.61798600	3.74761500
H	-3.37173400	-0.42150700	4.46693400
C	-2.74094300	-1.32938200	2.56599400
H	-3.61574500	-1.78449400	2.13087900
N	-1.54507300	-1.40674800	1.93267100
C	0.80651100	-0.69565500	2.36839000
O	1.38461900	-1.36219100	1.52596700
C	1.70130400	0.32099300	3.12231000
F	2.98198300	-0.02737900	3.00120500
F	1.43730100	0.43749200	4.42588100
F	1.56717800	1.54539700	2.57120600
C	-1.35339100	-1.85001300	0.55684900
H	-0.27962300	-1.87723900	0.37804300
C	-1.91436100	-3.24366300	0.31390400
O	-2.77008000	-3.72887600	1.02861400
C	-1.37780400	-3.99563400	-0.86695800
C	-0.33118000	-3.51377300	-1.66465600
C	-1.94933700	-5.24235500	-1.14764200
C	0.13874700	-4.28764500	-2.72369500
H	0.11559600	-2.53611800	-1.48754500

C	-1.47838500	-6.00611800	-2.20705200
H	-2.75782600	-5.59391700	-0.51540600
C	-0.42915500	-5.53000300	-2.99432400
H	0.95317300	-3.91206700	-3.33560500
H	-1.92378500	-6.97243400	-2.41981400
H	-0.05751000	-6.12815300	-3.82050900

M4RS

C	4.26148600	1.01013800	-0.04059300
C	5.61566100	1.66559300	0.21641200
H	4.00582400	0.29325500	0.73956300
H	5.72512700	1.93126000	1.27762900
N	3.25344700	2.08911300	0.04277900
O	5.77630200	2.82124100	-0.59339300
C	3.54668600	3.42359700	-0.02039800
C	4.97206200	3.88196200	-0.13339400
H	5.04230100	4.69962800	-0.85221000
H	5.31743300	4.24260000	0.84629600
N	2.46880900	4.14943900	0.04809800
C	1.91067600	1.97540700	0.11859600
N	1.45824800	3.23191800	0.14151600
C	0.10527000	3.67287200	0.33503600
C	-0.59830400	4.15950900	-0.76884900
C	-0.43491900	3.58646400	1.61743700
C	-1.91219900	4.56531100	-0.55558000
C	-1.75167800	4.01688500	1.78026100
C	-2.50462900	4.49568300	0.70870200
H	-2.49100300	4.93658000	-1.39774800
H	-2.20184000	3.96012300	2.76878200
H	6.40782000	0.96485300	-0.05572700
C	4.17972000	0.31949200	-1.40878300
H	3.12419600	0.17144100	-1.65614300
H	4.62364200	0.97772700	-2.16390700
C	4.87946900	-1.01746100	-1.36437600
C	4.27497700	-2.08412600	-0.68667800
C	6.13065000	-1.20395600	-1.95405200
C	4.91809700	-3.31495000	-0.61082300
H	3.30037100	-1.93053500	-0.22226900
C	6.77358600	-2.43847500	-1.87568900
H	6.60118100	-0.37870200	-2.48386000
C	6.16766400	-3.49590800	-1.20408700
H	4.43660200	-4.13522800	-0.08714000
H	7.74516300	-2.57229900	-2.34104300
H	6.66559300	-4.45864600	-1.14358700

C	-3.94399400	4.89786400	0.89254200
H	-4.60621300	4.14122600	0.45833500
H	-4.19647600	4.99965200	1.95039000
H	-4.15675500	5.84709500	0.39415500
C	0.04213000	4.19871300	-2.13017700
H	0.91900200	4.85244800	-2.13392400
H	0.37556800	3.19827900	-2.42806200
H	-0.66527100	4.55958500	-2.87788200
C	0.35754700	3.00753800	2.75923300
H	0.48129200	1.92289700	2.63960000
H	1.35640900	3.45112800	2.81535700
H	-0.15146400	3.18468100	3.70783700
C	-0.63980400	-0.75552700	-0.65898900
C	-0.02719800	0.59738800	-0.45811000
H	0.18284700	-1.46462200	-0.83190800
C	-1.60400100	-0.82732800	-1.82373800
C	-1.57952900	-1.93159100	-2.67818300
C	-2.59117100	0.14512000	-2.01279600
C	-2.52207900	-2.07243000	-3.69230300
H	-0.81888800	-2.69558600	-2.53572100
C	-3.54179700	0.00250200	-3.02033100
H	-2.63907200	1.00486700	-1.34591100
C	-3.51212100	-1.10784400	-3.86102800
H	-2.49018300	-2.94063100	-4.34286100
H	-4.31593700	0.75400800	-3.13950100
H	-4.25730400	-1.22100700	-4.64189500
C	1.20157400	0.65246900	0.14031500
O	1.88100700	-0.30759200	0.62672500
H	-0.51483400	1.48155400	-0.84655600
C	-3.83700000	-0.78781800	0.62883500
C	-4.61319500	0.30470900	1.01321100
H	-5.68200100	0.38657300	0.88311300
C	-3.75719400	1.24812900	1.59342100
H	-4.02895200	2.20236400	2.01958500
C	-2.47519200	0.71728000	1.55047100
H	-1.53785400	1.11335200	1.90216200
N	-2.52108000	-0.51392600	0.98624200
C	-4.27240600	-1.96495100	-0.08774000
C	-1.36622500	-1.32167100	0.61970500
H	-1.76819300	-2.29581800	0.35343600
C	-0.37722700	-1.50658300	1.76786200
O	-0.33634000	-0.74409500	2.71227900
C	0.54178400	-2.68854700	1.68043200
C	0.30953700	-3.77726900	0.83680300

C	1.68014700	-2.67907200	2.49387300
C	1.20374000	-4.84617200	0.81066100
H	-0.56834500	-3.81893900	0.19918100
C	2.57153100	-3.74108500	2.46475000
H	1.85291900	-1.81042200	3.11944500
C	2.33112100	-4.83109900	1.62486100
H	1.01216000	-5.69125600	0.15776400
H	3.45807900	-3.72409000	3.09063900
H	3.02463700	-5.66674800	1.60688600
C	-5.75743600	-1.94377100	-0.52816500
F	-6.57290200	-1.87806200	0.53741900
F	-6.05852000	-3.04196100	-1.20979900
F	-6.02916800	-0.88391400	-1.30276300
O	-3.62214500	-2.95169000	-0.38128700

M4SR

C	4.09508000	0.90707500	0.33908200
C	5.45286400	1.57479400	0.52190400
H	3.87938000	0.19782600	1.13888900
H	5.55078700	1.96565800	1.54473400
N	3.10136500	1.99861800	0.45754000
O	5.61455300	2.62428600	-0.42274600
C	3.39300200	3.30179400	0.15580900
C	4.80838400	3.73518600	-0.10472600
H	4.83546600	4.42808800	-0.94689000
H	5.18970600	4.25157100	0.78841700
N	2.32506200	4.04467100	0.18664500
C	1.77152700	1.91904600	0.66557700
N	1.32461100	3.17238800	0.51060400
C	-0.02938300	3.63810500	0.64004100
C	-0.77199800	3.81766000	-0.52726300
C	-0.55592600	3.80427200	1.92129000
C	-2.11137800	4.17523600	-0.38160700
C	-1.89932600	4.15863900	2.01375000
C	-2.69218600	4.33383400	0.87792300
H	-2.71933100	4.31045100	-1.27272700
H	-2.34313900	4.28253100	2.99835400
H	6.24883100	0.85220400	0.34304900
C	3.89305800	0.24758100	-1.03781700
H	2.88435400	-0.18146100	-1.04681400
H	3.94767500	1.03465900	-1.79877900
C	4.90922200	-0.82727500	-1.33695100
C	4.61052300	-2.17097800	-1.10110300
C	6.16638600	-0.49171100	-1.85108400

C	5.56077000	-3.15837500	-1.35332300
H	3.61644400	-2.43703000	-0.75190100
C	7.11550500	-1.47772700	-2.10355400
H	6.39526800	0.55237600	-2.05645800
C	6.81564000	-2.81472300	-1.84900300
H	5.31519300	-4.19955400	-1.16855600
H	8.08645800	-1.20322700	-2.50399200
H	7.55434600	-3.58523900	-2.04571100
C	-4.15828400	4.64665500	1.01911200
H	-4.70567000	3.74478800	1.31291400
H	-4.32904700	5.40286900	1.78946900
H	-4.58082500	5.00791800	0.07926300
C	-0.15808400	3.55348100	-1.87600000
H	0.70171100	4.20438200	-2.05812100
H	0.19179900	2.51537700	-1.93714900
H	-0.89052200	3.70972100	-2.66923500
C	0.28289900	3.54739900	3.14281700
H	1.26284100	4.02662200	3.06188400
H	-0.21468300	3.92494500	4.03724800
H	0.44406600	2.47105500	3.27121400
C	-1.08488300	-0.60936200	1.05674800
C	-0.26048100	0.58457500	0.70404900
H	-0.67416800	-1.05350800	1.97272400
C	-2.55282300	-0.29659300	1.27175600
C	-3.26751800	-0.97616700	2.26080700
C	-3.24143900	0.59019700	0.43870500
C	-4.63563700	-0.77780600	2.42004800
H	-2.74291300	-1.68014000	2.90292700
C	-4.61285000	0.78488600	0.58922000
H	-2.71531200	1.11078900	-0.35878600
C	-5.31435900	0.10208000	1.58068200
H	-5.17289100	-1.31691900	3.19383300
H	-5.13564900	1.45950500	-0.08254000
H	-6.38343900	0.25123300	1.69450700
C	1.05871300	0.64795300	1.06128100
O	1.78072100	-0.20716800	1.65995500
H	-0.73020700	1.40335100	0.18212700
C	-2.72225800	-1.45886800	-1.83476900
C	-2.81889500	-0.70507100	-3.00285800
H	-3.69226300	-0.64606100	-3.63523300
C	-1.58599600	-0.06998400	-3.19987200
H	-1.30552700	0.57367400	-4.02007700
C	-0.76224300	-0.44370600	-2.14775000
H	0.25704900	-0.18013200	-1.92149400

N	-1.43687900	-1.29325900	-1.33122700
C	-3.76010700	-2.24220200	-1.20299400
C	-0.98455500	-1.75425100	-0.02519400
H	-1.67022000	-2.54134800	0.27722100
C	0.43284700	-2.30186300	-0.02371600
O	1.27117600	-1.95202200	-0.83159400
C	0.76339000	-3.26139400	1.07560500
C	-0.14795400	-4.21641400	1.53668600
C	2.04700300	-3.20096700	1.62715800
C	0.23251300	-5.11357300	2.53218400
H	-1.14410300	-4.29049400	1.10964500
C	2.41742000	-4.08961300	2.62676300
H	2.71050500	-2.41274500	1.28959200
C	1.51122400	-5.04987000	3.07775800
H	-0.47174000	-5.86222200	2.87968600
H	3.40885900	-4.02953200	3.06389600
H	1.80168600	-5.74486300	3.85950400
O	-3.65837000	-2.99238300	-0.24960500
C	-5.16385000	-2.09879600	-1.84230000
F	-5.55128500	-0.81825200	-1.91775300
F	-5.16608300	-2.58951900	-3.09298000
F	-6.06929600	-2.76378500	-1.13623100

M4SS

C	-3.52436500	-1.90417900	0.77641000
C	-4.59413100	-2.91011500	1.18924400
H	-3.36116900	-1.15023900	1.54381600
H	-4.43249100	-3.25654600	2.22010400
N	-2.25800900	-2.66410900	0.63879000
O	-4.61126800	-4.01727200	0.29933700
C	-2.22866000	-4.01491300	0.42445800
C	-3.48351100	-4.83725600	0.48765600
H	-3.47052100	-5.58974900	-0.30223800
H	-3.52794400	-5.34862700	1.46062500
N	-1.01707700	-4.43594900	0.20969200
C	-0.98715500	-2.20803300	0.53866600
N	-0.25575200	-3.30587000	0.28788000
C	1.15424600	-3.38930700	0.02120000
C	1.57644800	-3.18138800	-1.29083100
C	2.02777800	-3.56900900	1.09461200
C	2.95133200	-3.14778400	-1.51984700
C	3.39129900	-3.53568900	0.81461700
C	3.86792600	-3.30852100	-0.48051000
H	3.30927400	-2.96688700	-2.53028600

H	4.09972300	-3.65685500	1.63087200
H	-5.57269900	-2.42983100	1.12569800
C	-3.84156300	-1.22149200	-0.56040200
H	-2.92359500	-0.73866100	-0.90727900
H	-4.14689700	-1.98821200	-1.28162000
C	-4.91296300	-0.17402400	-0.39219800
C	-4.58935700	1.03435900	0.23684100
C	-6.22034700	-0.38721500	-0.83127800
C	-5.56343200	2.01335100	0.41096400
H	-3.56470100	1.18956400	0.57149600
C	-7.19608800	0.59267900	-0.65282600
H	-6.47305700	-1.32441500	-1.32229400
C	-6.86774200	1.79440300	-0.03247600
H	-5.30104200	2.95209800	0.88803400
H	-8.20896700	0.41748800	-1.00204400
H	-7.62467000	2.56044400	0.10379000
C	5.34925900	-3.19267900	-0.72879300
H	5.73246500	-2.26230500	-0.29476600
H	5.89426900	-4.02153400	-0.26930000
H	5.57385300	-3.18183900	-1.79801200
C	0.57553400	-2.91582800	-2.37940700
H	-0.13635400	-3.74111000	-2.47695800
H	0.01315700	-2.00671800	-2.13923300
H	1.07588200	-2.76069000	-3.33574000
C	1.50187200	-3.68504600	2.49832500
H	1.08903700	-2.71954000	2.81422900
H	0.70619900	-4.43185700	2.56855500
H	2.29987100	-3.95795300	3.19026800
C	1.16300500	0.97290200	0.70194500
C	0.72194800	-0.44071900	0.56237400
H	0.35686600	1.53053200	1.19064500
C	2.44368900	1.18722000	1.49288400
C	2.66511000	2.43039900	2.09286100
C	3.44108200	0.21331400	1.58602600
C	3.86029800	2.70159000	2.75339500
H	1.89409900	3.19347200	2.01963400
C	4.64166100	0.48598100	2.23610800
H	3.29274900	-0.76363800	1.13321300
C	4.85733900	1.73144700	2.82090200
H	4.01277500	3.67311800	3.21385100
H	5.41091500	-0.27953200	2.28632900
H	5.79337900	1.94228300	3.32874500
C	-0.60634000	-0.74953900	0.71279900
O	-1.57455600	0.02011000	0.99282400

H	1.44552600	-1.17748200	0.25921600
C	-0.99935400	2.67703300	-0.92986400
C	-2.18642300	2.37314800	-1.59671500
H	-3.11636000	2.91387200	-1.50077900
C	-1.94270000	1.25715200	-2.39910100
H	-2.64048900	0.76211100	-3.05819100
C	-0.61803700	0.89085600	-2.19968400
H	-0.04300600	0.09429300	-2.63710800
N	-0.03535000	1.75540600	-1.33372700
C	-0.77316700	3.74328800	0.00584500
O	0.27624400	4.06533900	0.54026100
C	-2.03290100	4.56184700	0.38210700
F	-1.72622300	5.52455300	1.24250700
F	-2.96321100	3.77772700	0.94947100
F	-2.59147200	5.13228000	-0.69629400
C	1.29155400	1.66383400	-0.72382600
H	1.62671100	2.68520100	-0.55820500
C	2.31704000	0.89876200	-1.54749100
O	2.01381100	-0.05984700	-2.23767000
C	3.76258000	1.25327200	-1.37633400
C	4.21352100	2.48484500	-0.89290300
C	4.69270800	0.25506600	-1.69046300
C	5.57578400	2.70592200	-0.71512200
H	3.51733100	3.27713500	-0.64073200
C	6.05077400	0.47622800	-1.50794800
H	4.32124100	-0.69755500	-2.05582100
C	6.49383400	1.70358100	-1.01538600
H	5.91846600	3.66160500	-0.33280600
H	6.76509700	-0.30650600	-1.74497500
H	7.55470600	1.87821200	-0.86598700

TS4^{Rot}RS

C	-4.17173100	0.88166500	1.20554700
C	-5.54814200	1.53538500	1.31997500
H	-4.08924300	0.27115000	0.30383200
H	-5.89372900	1.89038900	0.33900400
N	-3.20694700	1.98113800	1.03426000
O	-5.51194300	2.61472300	2.24301500
C	-3.46136800	3.30477400	1.26042700
C	-4.82846200	3.72844200	1.71356800
H	-4.74487600	4.48060300	2.49919500
H	-5.37744600	4.16184500	0.86515300
N	-2.40917100	4.03412400	1.02217700
C	-1.91594400	1.87464600	0.67475300

N	-1.45424900	3.12367400	0.65076000
C	-0.19493400	3.55952800	0.11179200
C	0.76367500	4.08412500	0.97657500
C	-0.01508600	3.45113000	-1.27201800
C	1.96404600	4.51277600	0.40907500
C	1.20351200	3.88653500	-1.78507100
C	2.20183300	4.41501500	-0.96218400
H	2.73404000	4.92083200	1.05917600
H	1.38241200	3.79896700	-2.85355600
H	-6.26241900	0.80397600	1.70353600
C	-3.79817500	0.03691500	2.43170700
H	-2.70827500	-0.07556600	2.45862400
H	-4.10583800	0.57080100	3.33752300
C	-4.44145400	-1.32531600	2.34338600
C	-3.98230200	-2.22492300	1.37342600
C	-5.49366000	-1.69910300	3.17869100
C	-4.56761500	-3.48026800	1.25197900
H	-3.16897000	-1.91850000	0.71438500
C	-6.07953800	-2.95874700	3.05590600
H	-5.85214700	-1.00354000	3.93380900
C	-5.61686300	-3.85062500	2.09331400
H	-4.20313400	-4.17338900	0.50015400
H	-6.89613200	-3.24113800	3.71289900
H	-6.07106000	-4.83178000	1.99735600
C	3.52487800	4.82595800	-1.55256800
H	4.11815000	5.40256500	-0.83941400
H	4.10077800	3.93854600	-1.83506900
H	3.38440000	5.42901200	-2.45342700
C	0.50400700	4.17759500	2.45615200
H	-0.28627200	4.90386500	2.66809400
H	0.17713400	3.21434600	2.86172800
H	1.40732400	4.48314000	2.98587600
C	-1.09349300	2.88589100	-2.15728200
H	-1.26704600	1.82568800	-1.94382800
H	-2.03572900	3.42601700	-2.01322400
H	-0.80278500	2.97083800	-3.20515200
C	0.58864900	-1.00105300	0.85318000
C	-0.07304800	0.33617900	0.99519800
H	-0.19525700	-1.72600600	0.59460400
C	1.29772800	-1.47329900	2.10646000
C	1.12847700	-2.78699600	2.54684400
C	2.16800300	-0.63520900	2.81104200
C	1.80290800	-3.25654000	3.67072900
H	0.45665600	-3.44669500	2.00242000

C	2.84470300	-1.10321700	3.93261900
H	2.33243900	0.38526300	2.46975000
C	2.66323300	-2.41383000	4.36742600
H	1.65487300	-4.27997000	4.00124600
H	3.52152700	-0.44257800	4.46599200
H	3.19218300	-2.77623700	5.24340400
C	-1.25393900	0.56564600	0.35111300
O	-1.93757400	-0.19143300	-0.41430100
H	0.37796900	1.10832300	1.60881500
C	3.99279700	-0.60565800	0.20743000
C	4.78362000	0.49563800	0.44053800
H	5.82547200	0.47097500	0.72518100
C	3.96466800	1.63571200	0.23783100
H	4.25536300	2.67112500	0.34084700
C	2.71310500	1.18904400	-0.12641300
H	1.80919300	1.71499800	-0.38404700
N	2.73452000	-0.18048600	-0.15520800
C	4.34317700	-2.04815300	0.31754700
C	1.59779700	-1.06249600	-0.35316600
H	1.98657700	-2.08315200	-0.38429200
C	0.83551200	-0.77613500	-1.64395500
O	0.73870700	0.35198800	-2.08094200
C	0.14138100	-1.92978800	-2.29757700
C	0.71385100	-3.20270900	-2.36772500
C	-1.10299800	-1.69349500	-2.89133700
C	0.04736200	-4.23055900	-3.03116900
H	1.69696800	-3.39272900	-1.94967000
C	-1.77078400	-2.72476300	-3.53765100
H	-1.54263300	-0.70812500	-2.78699700
C	-1.19550800	-3.99388300	-3.61012800
H	0.50253000	-5.21321500	-3.09815300
H	-2.74398000	-2.54467900	-3.98293900
H	-1.71746400	-4.79811700	-4.11927000
C	4.93745400	-2.66615000	-0.96353300
F	4.01377000	-2.59751700	-1.94082000
F	5.27453100	-3.93840000	-0.79618600
F	6.01247900	-1.98660200	-1.36768200
O	4.18453800	-2.74589500	1.28397400

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C	4.57472400	-2.82789400	-2.64422300
C	6.07148500	-2.79016300	-2.93094000
H	4.26596700	-3.77967800	-2.20952100
H	6.63717600	-3.13624400	-2.05417300

N	4. 34739700	-1. 79702500	-1. 60795000
O	6. 46981100	-1. 47213400	-3. 28323300
C	5. 16827500	-0. 71701900	-1. 42669700
C	6. 47356400	-0. 61548400	-2. 16449000
H	6. 62417300	0. 40563400	-2. 51781400
H	7. 29130400	-0. 87459000	-1. 47604500
N	4. 68063600	0. 10295400	-0. 54117900
C	3. 27543200	-1. 62957200	-0. 81022200
N	3. 50368400	-0. 48071400	-0. 16151200
C	2. 67854500	0. 13403900	0. 84471100
C	1. 86275400	1. 19981100	0. 46497900
C	2. 67942000	-0. 41353800	2. 12889900
C	1. 00803600	1. 72561300	1. 43313200
C	1. 80589200	0. 14490800	3. 05798800
C	0. 95770400	1. 20331100	2. 72563200
H	0. 35322500	2. 55009800	1. 16248500
H	1. 77448300	-0. 26781800	4. 06331800
H	6. 30335700	-3. 43561200	-3. 77818300
C	3. 69583500	-2. 48079500	-3. 85849800
H	2. 65336200	-2. 46580400	-3. 51946000
H	3. 97038300	-1. 47571300	-4. 19857600
C	3. 84906500	-3. 47584400	-4. 98212100
C	2. 99339500	-4. 57696900	-5. 06268900
C	4. 85348700	-3. 32429100	-5. 94342800
C	3. 15091800	-5. 51851500	-6. 07668900
H	2. 18341900	-4. 66776200	-4. 34421200
C	5. 01084600	-4. 26497900	-6. 95782300
H	5. 51094200	-2. 45823700	-5. 89596600
C	4. 16167700	-5. 36767000	-7. 02307200
H	2. 47642500	-6. 36749500	-6. 13007400
H	5. 79155800	-4. 13363800	-7. 70042500
H	4. 28211300	-6. 10084100	-7. 81425000
C	-0. 01745900	1. 73693900	3. 74138400
H	-0. 45952600	2. 67953900	3. 41187100
H	-0. 82788000	1. 01619200	3. 89354600
H	0. 46754800	1. 90041300	4. 70734200
C	1. 85309400	1. 69845500	-0. 95521800
H	2. 86118900	1. 94001700	-1. 30205400
H	1. 44434700	0. 93096700	-1. 62441200
H	1. 22870500	2. 58863600	-1. 04513600
C	3. 55070800	-1. 59171900	2. 46971800
H	4. 57755800	-1. 44185600	2. 12329300
H	3. 57050300	-1. 75382400	3. 54837700
H	3. 16598100	-2. 50191300	1. 99600100

C	-0.25662900	-2.94149500	-0.11150900
C	0.94295200	-2.08766100	-0.36796000
H	0.08969600	-3.92954200	0.22020100
C	-1.16025000	-2.34698000	0.95152400
C	-1.68110100	-3.15502100	1.96280600
C	-1.50961800	-0.99215200	0.92674400
C	-2.52166000	-2.62534100	2.93870300
H	-1.41856600	-4.21002300	1.98793000
C	-2.34995900	-0.46115700	1.89980300
H	-1.13421200	-0.34623700	0.13502200
C	-2.85617800	-1.27467100	2.91125800
H	-2.91299700	-3.26889300	3.72049700
H	-2.61453500	0.59199000	1.86338900
H	-3.51341300	-0.85935800	3.66909600
C	2.15637500	-2.63298200	-0.67778400
O	2.49138900	-3.84224500	-0.87439400
H	0.84334600	-1.01986900	-0.24569300
C	-2.92015200	-1.57065500	-1.86541800
C	-3.03520100	-0.31517300	-2.41559500
H	-3.94590800	0.26279200	-2.47393700
C	-1.74569300	0.04567200	-2.88322400
H	-1.47226900	0.96299200	-3.38336900
C	-0.89838100	-1.00584700	-2.61506100
H	0.14719500	-1.15608000	-2.82365900
N	-1.61802300	-1.99884200	-2.00051000
C	-3.97117900	-2.41622000	-1.23402100
C	-1.09787200	-3.22132100	-1.41359500
H	-1.95645900	-3.82905500	-1.11520400
C	-0.22453600	-4.02810000	-2.36636200
O	0.47736600	-3.48620400	-3.19553500
C	-0.20496800	-5.51093400	-2.17050600
C	-1.38703500	-6.24268500	-2.02720100
C	1.02977400	-6.16790000	-2.18333600
C	-1.33423600	-7.62976900	-1.91560300
H	-2.35055300	-5.74252500	-2.04710800
C	1.07568700	-7.55056400	-2.05337800
H	1.93054600	-5.56531400	-2.23465500
C	-0.10461700	-8.28235900	-1.92464800
H	-2.25383500	-8.19832400	-1.82408500
H	2.03369600	-8.06044400	-2.04487900
H	-0.06495800	-9.36280700	-1.82742900
O	-4.23734800	-2.46959100	-0.06272800
C	-4.76119200	-3.29704000	-2.22288100
F	-5.39793600	-2.54123300	-3.12023300

F	-3.89974000	-4.08991100	-2.88672200
F	-5.64736800	-4.06726400	-1.60589000

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C	1.10285100	-2.04914600	-3.54936400
C	1.93442300	-2.77990900	-4.60026500
H	0.99352100	-2.64136200	-2.64137500
H	2.80718600	-3.26508200	-4.13998600
N	1.87753400	-0.84633800	-3.16728300
O	2.35564600	-1.88360900	-5.61754800
C	2.92440500	-0.34645600	-3.89257800
C	3.37373300	-1.02971200	-5.15188100
H	3.57499700	-0.28568200	-5.92384600
H	4.29822800	-1.59030200	-4.95120000
N	3.42256200	0.71818800	-3.33421700
C	1.68888700	-0.02267000	-2.11454900
N	2.64756000	0.90245800	-2.22281300
C	2.97646800	1.94665500	-1.29248400
C	2.60705900	3.25628900	-1.61078500
C	3.64484900	1.59688000	-0.12026200
C	2.92732900	4.24818000	-0.68931600
C	3.95178300	2.63079900	0.76631700
C	3.59485400	3.95243000	0.50360300
H	2.64516800	5.27623900	-0.90310000
H	4.47003700	2.38857800	1.69114800
H	1.31524900	-3.54421400	-5.07468900
C	-0.28614900	-1.64548200	-4.06019400
H	-0.68456800	-0.87377300	-3.39583100
H	-0.18462900	-1.22269500	-5.06580700
C	-1.21255700	-2.83825200	-4.05740100
C	-1.68782500	-3.33489300	-2.83653000
C	-1.57988400	-3.47483000	-5.24330000
C	-2.52219800	-4.44768000	-2.81478600
H	-1.39505800	-2.83426700	-1.91346800
C	-2.41645200	-4.58999200	-5.21894500
H	-1.21439400	-3.08967300	-6.19258500
C	-2.88878900	-5.07762200	-4.00413700
H	-2.88833400	-4.82031500	-1.86268100
H	-2.69933500	-5.07415300	-6.14844600
H	-3.54128600	-5.94486400	-3.98367800
C	3.89716400	5.04932400	1.49048500
H	4.39100300	5.89323100	1.00149300
H	2.97146500	5.42505600	1.93846700
H	4.54357900	4.69314700	2.29549900

C	1. 85783200	3. 55354400	-2. 88182900
H	2. 44595800	3. 27453600	-3. 76071400
H	0. 92120700	2. 98579800	-2. 91679400
H	1. 61624000	4. 61520000	-2. 94654400
C	3. 96699200	0. 16165200	0. 19965400
H	4. 66665500	0. 10484800	1. 03489900
H	3. 05900600	-0. 38666000	0. 48430700
H	4. 41305900	-0. 34750400	-0. 65992200
C	-1. 09419100	0. 76140900	0. 38169000
C	0. 11471800	0. 91528000	-0. 48615000
H	-1. 73418700	-0. 00586200	-0. 07938500
C	-1. 90234200	2. 02807400	0. 58361300
C	-3. 28586900	1. 93261600	0. 75701800
C	-1. 29652100	3. 28003300	0. 72132200
C	-4. 04986300	3. 05588800	1. 06054100
H	-3. 76663900	0. 96145100	0. 65917200
C	-2. 05784300	4. 40503800	1. 02719300
H	-0. 21725200	3. 37703500	0. 62899600
C	-3. 43524900	4. 29784300	1. 19847600
H	-5. 12300700	2. 95980300	1. 19226100
H	-1. 56975100	5. 36756400	1. 14481900
H	-4. 02514500	5. 17490600	1. 44411400
C	0. 58836700	-0. 20628400	-1. 11006600
O	0. 15329100	-1. 39749800	-1. 00637500
H	0. 54479900	1. 89025300	-0. 66490600
C	-0. 65935000	1. 93998000	3. 63508900
C	0. 26687300	2. 92303000	3. 96089700
H	0. 10851300	3. 67284300	4. 72217600
C	1. 40984400	2. 70705600	3. 17742900
H	2. 33302500	3. 26744700	3. 19446500
C	1. 14837500	1. 60757800	2. 37647700
H	1. 74011600	1. 13600700	1. 61009200
N	-0. 09265700	1. 12858500	2. 65919400
C	-1. 93046200	1. 81414000	4. 33138700
C	-0. 80327200	0. 17646800	1. 81680600
H	-1. 78273800	0. 03465300	2. 25683900
C	-0. 08521900	-1. 17073600	1. 74907800
O	1. 12142800	-1. 23378200	1. 87567600
C	-0. 91029500	-2. 39724400	1. 50968700
C	-2. 28507200	-2. 45888800	1. 74539100
C	-0. 24308400	-3. 52974000	1. 02940500
C	-2. 98445000	-3. 63955000	1. 49648400
H	-2. 82776300	-1. 60954200	2. 14603500
C	-0. 93956700	-4. 70159000	0. 77861200

H	0.82053900	-3.45024300	0.83645200
C	-2.31584700	-4.75855600	1.01349000
H	-4.05147400	-3.68195000	1.68839700
H	-0.41809900	-5.57283800	0.39499800
H	-2.86209000	-5.67721900	0.82101900
O	-2.44864600	2.73972700	4.92320100
C	-2.63902100	0.44464500	4.48313800
F	-1.77809000	-0.58332900	4.44852800
F	-3.29326000	0.39455000	5.63549100
F	-3.53889000	0.25030500	3.49695800

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C	-4.11401900	0.62361200	-0.86455600
C	-5.41773300	1.37502400	-1.11562500
H	-3.77772400	0.09596300	-1.75550700
H	-5.37926200	1.92321700	-2.06801400
N	-3.08608700	1.64947900	-0.56864300
O	-5.69370300	2.26954200	-0.04823600
C	-3.39906000	2.91785600	-0.16632500
C	-4.82641500	3.37654500	-0.07612300
H	-4.97220100	3.94815700	0.84154500
H	-5.04618700	4.02762700	-0.93504300
N	-2.32853300	3.62028000	0.06087500
C	-1.73769700	1.54160000	-0.56589700
N	-1.30368700	2.75883600	-0.20031600
C	0.04586000	3.24334800	-0.07885900
C	0.57572500	3.38934200	1.20586400
C	0.76881700	3.50825700	-1.24349900
C	1.90679200	3.79133900	1.30099200
C	2.09453900	3.91064300	-1.09171200
C	2.67996900	4.04875900	0.16678300
H	2.35209900	3.89522200	2.28748400
H	2.68912500	4.09879200	-1.98182200
H	-6.23735000	0.65475200	-1.15417600
C	-4.21123500	-0.35502100	0.30974300
H	-3.19284000	-0.62025200	0.60290400
H	-4.69259900	0.15112000	1.15379500
C	-4.96851800	-1.59555700	-0.09147600
C	-4.36196800	-2.50827300	-0.96385600
C	-6.26218800	-1.84729200	0.36727700
C	-5.04294100	-3.65509700	-1.35965900
H	-3.34854400	-2.30386400	-1.30554400
C	-6.94419300	-2.99648900	-0.03126200

H	-6.73489400	-1.14103300	1.04586600
C	-6.33508500	-3.90216100	-0.89483400
H	-4.56372600	-4.36104200	-2.03137300
H	-7.94869300	-3.18347200	0.33527600
H	-6.86340700	-4.79852400	-1.20409000
C	4.11814500	4.47599900	0.30517400
H	4.65232500	4.37332900	-0.64179600
H	4.18454200	5.52307600	0.61715500
H	4.63395900	3.87642400	1.06021600
C	-0.25253300	3.10884400	2.42972500
H	-0.99114200	3.90180000	2.58231700
H	-0.79930300	2.16495600	2.34336300
H	0.38375900	3.05234100	3.31435000
C	0.17280300	3.29067900	-2.60646000
H	0.16072100	2.21936600	-2.83663700
H	-0.85432200	3.66213100	-2.66216300
H	0.76592600	3.79841400	-3.36843200
C	1.23928300	-0.84587900	-1.13977600
C	0.34896100	0.26551100	-0.68908000
H	0.72075700	-1.44487900	-1.89774400
C	2.54740900	-0.31776100	-1.70459300
C	3.03332400	-0.78332100	-2.92752700
C	3.32819700	0.58170900	-0.96961600
C	4.27295400	-0.36495400	-3.40731900
H	2.43992500	-1.49316600	-3.49746700
C	4.56974400	0.99455700	-1.44194800
H	2.97230200	0.95091500	-0.00951800
C	5.04723600	0.52078500	-2.66297300
H	4.63561100	-0.73752400	-4.36035200
H	5.16895300	1.68098700	-0.85090600
H	6.01742300	0.83969700	-3.03053400
C	-0.99316200	0.27855500	-0.97258300
O	-1.70876900	-0.61020400	-1.51611500
H	0.81423900	1.09677800	-0.18478500
C	-0.63464700	-1.94736000	1.27030100
C	-1.76294700	-2.75303700	1.20718700
H	-2.67628000	-2.57293200	1.75665000
C	-1.46158500	-3.83633300	0.36673800
H	-2.11072700	-4.65964400	0.10852500
C	-0.17298400	-3.64889600	-0.09071200
H	0.41159200	-4.22064300	-0.79148700
N	0.35261300	-2.52563200	0.48204300
C	-0.57838700	-0.72805200	2.05589000
C	1.56069000	-1.83869700	0.03904300

H	1. 93523100	-1. 24177000	0. 86402500
C	2. 67506900	-2. 78212700	-0. 42006700
O	2. 46441400	-3. 64724500	-1. 24868900
C	4. 06668100	-2. 49876500	0. 04771500
C	4. 35169200	-1. 92945900	1. 29256100
C	5. 11070500	-2. 81197800	-0. 82844300
C	5. 67187900	-1. 68151300	1. 65524300
H	3. 55533300	-1. 69368400	1. 99074000
C	6. 42546900	-2. 54191200	-0. 47218400
H	4. 86600100	-3. 24568400	-1. 79237800
C	6. 70687800	-1. 97771300	0. 77149400
H	5. 89173500	-1. 25291500	2. 62733400
H	7. 23160500	-2. 76815800	-1. 16222600
H	7. 73439300	-1. 76893900	1. 05197600
C	0. 71703600	-0. 30987300	2. 80513400
O	-1. 56984600	-0. 06930400	2. 32057900
F	0. 39625400	0. 26700800	3. 95849800
F	1. 47417000	0. 56531700	2. 12096500
F	1. 48808900	-1. 37648400	3. 07822100

TS5RR

C	3. 54795300	0. 76185400	-0. 32305700
C	4. 71941000	1. 49593200	0. 32575700
H	3. 07794100	0. 05641100	0. 37433100
H	4. 45263700	1. 84266400	1. 33361400
N	2. 53453100	1. 81428700	-0. 57534900
O	5. 10389800	2. 59234200	-0. 49624100
C	2. 78579100	3. 15577700	-0. 58032300
C	4. 19226700	3. 66173100	-0. 42824900
H	4. 43415200	4. 36217900	-1. 22980000
H	4. 26498200	4. 18934300	0. 53334500
N	1. 67705200	3. 84560200	-0. 62848100
C	1. 20369500	1. 67299500	-0. 58250200
N	0. 69648000	2. 90004000	-0. 62584100
C	-0. 70150300	3. 24402100	-0. 58266100
C	-1. 54789400	2. 77694500	-1. 59044300
C	-1. 15875300	3. 94132000	0. 54507800
C	-2. 91439800	3. 02233900	-1. 43821000
C	-2. 52885500	4. 15831800	0. 63959700
C	-3. 42164800	3. 70202000	-0. 33529200
H	-3. 59742800	2. 65205100	-2. 19812200
H	-2. 91376500	4. 68371800	1. 51014100
H	5. 57750000	0. 82458300	0. 38922600
C	3. 95818200	0. 05981600	-1. 62170700

H	3.05642800	-0.13315900	-2.20619100
H	4.61302000	0.72513800	-2.19410100
C	4.65297900	-1.24376400	-1.30441800
C	3.95443500	-2.25103800	-0.62613100
C	5.98426900	-1.45688500	-1.66153300
C	4.58643900	-3.45282400	-0.32333000
H	2.92062900	-2.08208600	-0.32386300
C	6.61432900	-2.66314900	-1.35979800
H	6.52944400	-0.67366200	-2.18268100
C	5.91505800	-3.66321500	-0.69123900
H	4.03976800	-4.22740200	0.20502600
H	7.65006300	-2.81865500	-1.64529400
H	6.40381600	-4.60280600	-0.45360900
C	-4.89681900	3.96808900	-0.19679000
H	-5.23617200	3.74945200	0.81927300
H	-5.11913200	5.01971600	-0.40465900
H	-5.47377200	3.34930000	-0.88650300
C	-1.05867000	2.00423600	-2.78822400
H	-0.01724700	2.22505900	-3.03356300
H	-1.14338300	0.92457300	-2.61813300
H	-1.67058500	2.24530400	-3.65951300
C	-0.22228300	4.41701500	1.62497700
H	0.50328100	3.64604800	1.89484000
H	0.33614900	5.29813500	1.29746400
H	-0.78885700	4.67759600	2.52007800
C	-1.59897600	-0.85852900	-0.16054800
C	-0.58495700	0.15894500	0.38102600
H	-1.39870500	-0.98397700	-1.23009000
C	-3.02156600	-0.36788800	-0.01218200
C	-3.88135200	-0.41088200	-1.11185200
C	-3.49124400	0.16176300	1.19518900
C	-5.18292600	0.07760400	-1.01940300
H	-3.52311700	-0.82620100	-2.05203400
C	-4.79155700	0.64716900	1.28879100
H	-2.83343400	0.19932400	2.06195500
C	-5.63942600	0.61028300	0.18278000
H	-5.83702600	0.04193300	-1.88522700
H	-5.14567200	1.05474900	2.23086000
H	-6.65179500	0.99533200	0.25995500
C	0.48927800	0.34968200	-0.54761700
O	0.97346700	-0.53387400	-1.24864300
H	-1.03991300	1.07258700	0.75690900
C	-0.75299000	-1.28382300	2.57053700
C	-1.20827900	-1.19722400	3.87004100

H	-0.77579900	-0.59148800	4.65216800
C	-2.32688800	-2.06357600	3.97632400
H	-2.91555100	-2.25661600	4.86134200
C	-2.53042800	-2.64080600	2.74438400
H	-3.27572100	-3.33469400	2.40018300
N	-1.55427600	-2.17521500	1.89695300
C	0.37678700	-0.60298600	1.83594400
O	1.36539100	-1.28542000	1.40636800
C	0.77985800	0.65732800	2.63579700
F	1.70588000	1.40168900	1.97932500
F	1.34126600	0.31528600	3.80162300
F	-0.23756000	1.49239300	2.91578900
C	-1.37589000	-2.27440100	0.46251400
H	-0.32271800	-2.52251000	0.29649000
C	-2.24978500	-3.28502100	-0.25547200
O	-3.27316300	-3.72941900	0.22486300
C	-1.83363900	-3.67860000	-1.64431500
C	-0.60699200	-3.31588300	-2.21329800
C	-2.73634600	-4.45104200	-2.38397700
C	-0.29446800	-3.72731300	-3.50624200
H	0.10760800	-2.70291500	-1.67196900
C	-2.42055500	-4.85803500	-3.67328200
H	-3.68074900	-4.72113800	-1.92347000
C	-1.19657100	-4.49667400	-4.23582700
H	0.65880200	-3.44481200	-3.94076900
H	-3.12527200	-5.45670300	-4.24117500
H	-0.94700600	-4.81498300	-5.24320500

TS5RS

C	3.89708000	0.01296200	-0.03868100
C	4.97845600	0.19255500	1.02127500
H	3.16996900	-0.73779700	0.28017800
H	4.51946400	0.27556200	2.01572200
N	3.16369600	1.29512100	-0.05644000
O	5.75081200	1.34964800	0.71941400
C	3.65428700	2.46703200	0.43886600
C	5.05246500	2.54191700	0.98529900
H	5.60022300	3.36364300	0.52017000
H	4.98324200	2.73157500	2.06582700
N	2.73607400	3.39557700	0.45767500
C	1.86392800	1.49510800	-0.31108700
N	1.62482500	2.76827600	-0.01679600
C	0.36112400	3.45139900	-0.08795600
C	-0.20243200	3.70036900	-1.34091800

C	-0.27400400	3.74700500	1.12180600
C	-1.46202000	4.29551500	-1.35965300
C	-1.53249300	4.34102300	1.04331600
C	-2.13641100	4.62463500	-0.18326000
H	-1.93434500	4.49095400	-2.31890700
H	-2.05945000	4.57254500	1.96556000
H	5.65819300	-0.66105600	1.00009800
C	4.47238000	-0.32071900	-1.41899000
H	3.69289700	-0.14444000	-2.16349100
H	5.31821800	0.34378700	-1.62358300
C	4.89686700	-1.76935100	-1.45136400
C	3.91745100	-2.76882400	-1.42729100
C	6.24308100	-2.13592600	-1.45991700
C	4.28388800	-4.11035500	-1.41725400
H	2.86625300	-2.48650200	-1.41051200
C	6.61028000	-3.48076300	-1.45273900
H	7.00747400	-1.36235200	-1.47469200
C	5.63135500	-4.46961100	-1.43145400
H	3.51362500	-4.87528100	-1.40064000
H	7.66090700	-3.75375600	-1.46285400
H	5.91623600	-5.51700900	-1.42562600
C	-3.48951900	5.28307600	-0.24045600
H	-3.38567800	6.37168800	-0.29478500
H	-4.04625800	4.95726100	-1.12236000
H	-4.07988200	5.05088000	0.64926500
C	0.49565200	3.30793900	-2.61664200
H	1.56055500	3.55468400	-2.58479800
H	0.40635300	2.23116000	-2.80030100
H	0.04826200	3.82523400	-3.46657100
C	0.35548100	3.39093200	2.44189600
H	0.82106200	2.39868400	2.41157300
H	1.13450800	4.11343500	2.70460800
H	-0.39782600	3.39227000	3.23153100
C	-1.36818200	-0.55231400	-0.72565900
C	-0.32824100	0.34158800	-0.07814600
H	-0.89940700	-1.03287900	-1.59277300
C	-2.60051700	0.19498800	-1.20779000
C	-3.17375300	-0.16138500	-2.43270600
C	-3.21987200	1.19189700	-0.44797700
C	-4.34213000	0.44682600	-2.88206100
H	-2.70259400	-0.93731400	-3.03077100
C	-4.39047900	1.80010300	-0.89489600
H	-2.79345900	1.50309400	0.50026100
C	-4.95830600	1.42854600	-2.11065300

H	-4.77073500	0.15110900	-3.83451600
H	-4.86154700	2.56578500	-0.28520500
H	-5.87294200	1.90084600	-2.45507600
C	0.91279100	0.41303700	-0.77221600
O	1.37692500	-0.39433300	-1.57881400
H	-0.68536100	1.28042300	0.32581100
C	0.50835800	-1.85513000	1.17571500
C	1.55532900	-2.74503700	1.27156700
H	2.50140200	-2.53240500	1.74920400
C	1.12669000	-3.95763500	0.67540300
H	1.68794500	-4.87704700	0.59286200
C	-0.15873400	-3.76536200	0.22290200
H	-0.82070200	-4.43003400	-0.30480700
N	-0.54047800	-2.48426000	0.53694700
C	0.47898400	-0.43905500	1.63424400
C	-1.75463400	-1.75468800	0.19531000
H	-2.18937100	-1.38082100	1.11883000
C	-2.78830200	-2.61050900	-0.53372100
O	-2.44512100	-3.30812700	-1.46922300
C	-4.22947700	-2.51073500	-0.14299900
C	-4.71141900	-1.63113000	0.83287900
C	-5.12981000	-3.33438100	-0.82970200
C	-6.07422000	-1.57909700	1.11069900
H	-4.04602600	-0.96660000	1.37317900
C	-6.48645100	-3.28762700	-0.54329200
H	-4.73847900	-4.00537700	-1.58660300
C	-6.96085200	-2.40660400	0.42867500
H	-6.44223300	-0.88990400	1.86327400
H	-7.17597800	-3.93337200	-1.07703800
H	-8.02213500	-2.36552900	0.65271000
O	1.57105000	0.12324100	1.92714100
C	-0.66440300	-0.13105400	2.68555900
F	-1.71070700	0.60218000	2.23829600
F	-1.19842400	-1.26521600	3.17460900
F	-0.16013000	0.54145500	3.71834900

TS5SR

C	-3.97387400	-0.23953400	-0.80701200
C	-5.42621700	0.10420700	-1.13007700
H	-3.46408700	-0.63364500	-1.68573500
H	-5.50190000	0.63319400	-2.09095500
N	-3.30778200	1.04386200	-0.47576200
O	-5.99403500	0.88901300	-0.09338700
C	-3.98844300	2.17868900	-0.14135200

C	-5.48937700	2.20187000	-0.10928200
H	-5.83014500	2.70878600	0.79484200
H	-5.85606500	2.75730900	-0.98494200
N	-3.17335700	3.17156400	0.08156300
C	-1.99466900	1.34014800	-0.41463500
N	-1.93783400	2.63466400	-0.09979700
C	-0.77231700	3.47430300	0.00970500
C	-0.41238500	3.91353800	1.28500900
C	-0.03366200	3.74991100	-1.14496800
C	0.76066100	4.65982400	1.38419200
C	1.13450300	4.49027500	-0.98500000
C	1.54506500	4.95058100	0.26706000
H	1.08014200	5.00146900	2.36555300
H	1.75105600	4.69077500	-1.85770600
H	-6.00148500	-0.82195900	-1.18900700
C	-3.83995700	-1.21897700	0.36357800
H	-2.82092000	-1.14826700	0.75551200
H	-4.52423800	-0.90418600	1.15934900
C	-4.13572100	-2.62665700	-0.08935500
C	-3.19678000	-3.29830100	-0.88078200
C	-5.32732500	-3.27194700	0.24536900
C	-3.44614300	-4.59439400	-1.31904700
H	-2.26394500	-2.79615600	-1.12997900
C	-5.57879800	-4.57026500	-0.19607100
H	-6.05870700	-2.75622400	0.86355500
C	-4.63791800	-5.23371500	-0.97795000
H	-2.70540000	-5.10935600	-1.92322500
H	-6.50738100	-5.06306500	0.07478600
H	-4.83016300	-6.24629500	-1.31868000
C	2.80724000	5.76045400	0.40471900
H	3.49702600	5.54811200	-0.41535800
H	2.58212200	6.83189700	0.38925200
H	3.31369500	5.54324500	1.34869000
C	-1.22919800	3.54379900	2.49392000
H	-2.19958900	4.04824400	2.47764000
H	-1.40662300	2.46242500	2.52223500
H	-0.70215100	3.83076900	3.40517400
C	-0.42999200	3.21789300	-2.49632900
H	-0.13644100	2.16625400	-2.59979800
H	-1.50932300	3.28731300	-2.66139300
H	0.07496900	3.77892200	-3.28439100
C	1.54617800	-0.06705400	-0.91757000
C	0.39694900	0.60021700	-0.18673000
H	1.15332700	-0.50466300	-1.84151700

C	2. 59294800	0. 97515400	-1. 26392300
C	2. 86031700	1. 30280900	-2. 59423000
C	3. 26255900	1. 67241400	-0. 25204200
C	3. 76651100	2. 31262500	-2. 91045500
H	2. 35604500	0. 75317400	-3. 38433800
C	4. 17831000	2. 67207200	-0. 56507000
H	3. 04454200	1. 45142000	0. 79068000
C	4. 43058800	2. 99920500	-1. 89631700
H	3. 96141500	2. 55561600	-3. 95059600
H	4. 69000200	3. 20264000	0. 23259900
H	5. 14342400	3. 78110900	-2. 14081100
C	-0. 87476300	0. 37896400	-0. 75791700
O	-1. 21592300	-0. 57831500	-1. 46717300
H	0. 59669900	1. 57959100	0. 22498900
C	0. 09046800	-1. 68974200	1. 22054400
C	-0. 75173200	-2. 76532000	1. 41583400
H	-1. 65399500	-2. 73338200	2. 00968900
C	-0. 20258900	-3. 87077200	0. 72639800
H	-0. 60651800	-4. 87089600	0. 67106800
C	0. 95028500	-3. 43402500	0. 11753600
H	1. 64996300	-3. 96932600	-0. 50670700
N	1. 14611100	-2. 11080600	0. 42782700
C	-0. 16737600	-0. 30461700	1. 68570900
C	2. 17364600	-1. 23745600	-0. 13527100
H	2. 77722300	-0. 83160600	0. 67665800
C	3. 13207500	-2. 04672300	-1. 02333100
O	3. 07732700	-1. 95863500	-2. 23210100
C	4. 15406400	-2. 90806100	-0. 35182800
C	4. 18596300	-3. 08568900	1. 03567300
C	5. 09605700	-3. 55458800	-1. 15785800
C	5. 15750500	-3. 90155000	1. 60670600
H	3. 45041400	-2. 60142800	1. 67198700
C	6. 06762100	-4. 36367200	-0. 58417000
H	5. 04830300	-3. 40309700	-2. 23109100
C	6. 09791800	-4. 53729200	0. 79940300
H	5. 17922400	-4. 04183100	2. 68209700
H	6. 80085300	-4. 86011000	-1. 21121700
H	6. 85565900	-5. 17135200	1. 24890400
C	0. 89505700	0. 33014800	2. 62241400
O	-1. 32816600	0. 05315000	1. 98886700
F	0. 50225200	0. 14134900	3. 88671200
F	1. 03555200	1. 65395600	2. 45222600
F	2. 13132500	-0. 20261800	2. 52743400

TS5SS

C	3. 58724900	-0. 87448900	-0. 98514200
C	4. 76147500	-1. 54009300	-1. 69937200
H	3. 31454800	0. 05620400	-1. 48230500
H	4. 62582800	-1. 50443600	-2. 78978500
N	2. 43478900	-1. 79708900	-1. 15439400
O	4. 91003700	-2. 88451800	-1. 27100500
C	2. 55298700	-3. 11136600	-1. 50838600
C	3. 89981000	-3. 70589300	-1. 80370700
H	3. 97828000	-4. 68967100	-1. 33876000
H	4. 01232400	-3. 81858900	-2. 89181800
N	1. 38671600	-3. 69284600	-1. 56548500
C	1. 12736200	-1. 56796600	-0. 94198500
N	0. 50715900	-2. 71618700	-1. 21492500
C	-0. 90677700	-2. 98709600	-1. 15394700
C	-1. 35196700	-3. 90399500	-0. 19400100
C	-1. 76520700	-2. 28157300	-2. 00163600
C	-2. 72835600	-4. 07604800	-0. 08028100
C	-3. 13456000	-2. 48032100	-1. 82822100
C	-3. 63179500	-3. 36618100	-0. 87460300
H	-3. 10629600	-4. 77374500	0. 66292200
H	-3. 82661100	-1. 90885200	-2. 44185400
H	5. 67900200	-1. 00917800	-1. 44052100
C	3. 84049000	-0. 61266700	0. 50665400
H	2. 88710900	-0. 40716500	1. 00358100
H	4. 28568000	-1. 51182100	0. 94716800
C	4. 72692200	0. 59494200	0. 68111000
C	4. 13064300	1. 86037800	0. 70626200
C	6. 11419300	0. 49020100	0. 79370800
C	4. 91731100	3. 00131600	0. 82793900
H	3. 04464900	1. 92222600	0. 65961300
C	6. 90144100	1. 63380700	0. 91628300
H	6. 57928400	-0. 49350900	0. 80346200
C	6. 30383400	2. 89090500	0. 92817600
H	4. 44766800	3. 97976700	0. 85702900
H	7. 97907600	1. 54123400	1. 00941500
H	6. 91511700	3. 78258200	1. 02641700
C	-5. 11324700	-3. 56938300	-0. 70112600
H	-5. 40788800	-3. 39324000	0. 33743700
H	-5. 68222500	-2. 88836100	-1. 33673600
H	-5. 39476600	-4. 59646400	-0. 95326700
C	-0. 39808200	-4. 67351900	0. 68058500
H	0. 08483200	-5. 47451200	0. 11404500
H	0. 38577800	-4. 02870800	1. 08289500

H	-0.93675600	-5.11692100	1.51932600
C	-1.26425700	-1.31212300	-3.04004000
H	-1.08798400	-0.32014400	-2.60845700
H	-0.33205500	-1.65239500	-3.49937300
H	-2.01083300	-1.19338400	-3.82715600
C	-1.46291100	1.11268000	-0.17506900
C	-0.64888500	-0.13185900	0.20905200
H	-1.05335500	1.49492700	-1.11634900
C	-2.92136800	0.78045500	-0.40800700
C	-3.53700500	1.18361700	-1.59538800
C	-3.67046900	0.06261800	0.53156900
C	-4.87142600	0.87307100	-1.85040700
H	-2.96301700	1.74818300	-2.32763400
C	-5.00521800	-0.23984400	0.28145500
H	-3.20487900	-0.26751100	1.45873100
C	-5.60883900	0.15827400	-0.91073800
H	-5.33259300	1.19308800	-2.77974900
H	-5.57709100	-0.79033500	1.02235400
H	-6.65018500	-0.08258900	-1.10233200
C	0.54972000	-0.22434200	-0.56866500
O	1.22574700	0.74580500	-0.90941400
H	-1.24471100	-1.03649800	0.27951800
C	-1.12337900	0.68525400	2.65798100
C	-1.81763800	0.29296600	3.78279500
H	-1.57412400	-0.54964500	4.41280200
C	-2.87945000	1.21914800	3.95623300
H	-3.61040900	1.22541200	4.75170000
C	-2.81150900	2.13434400	2.93086000
H	-3.43412400	2.97681300	2.68919200
N	-1.72493900	1.81302900	2.15332100
C	0.09011500	0.13034700	1.95835200
O	1.15334700	0.82332300	1.88821800
C	0.30638700	-1.33270400	2.40158300
F	1.28894900	-1.93119200	1.68457700
F	-0.77889800	-2.12045000	2.28106700
F	0.68742800	-1.38530800	3.68311800
C	-1.27183800	2.27392900	0.85598000
H	-0.19265400	2.43123100	0.94482600
C	-1.91825100	3.53815100	0.32578600
O	-2.97808200	3.96220300	0.74148200
C	-1.21071100	4.23627000	-0.80106000
C	0.06912800	3.87798000	-1.24175500
C	-1.88148000	5.29769600	-1.41971300
C	0.66397000	4.57851700	-2.28722700

H	0.60786100	3.04761500	-0.79471000
C	-1.28430000	5.99275800	-2.46294600
H	-2.87172700	5.56060000	-1.06292400
C	-0.00837600	5.63403600	-2.89732300
H	1.65655100	4.29652400	-2.62269200
H	-1.80988400	6.81427000	-2.93871800
H	0.46081600	6.17739400	-3.71160500

M5RR

C	3.80104300	0.83546900	0.05522300
C	5.00855100	1.71575500	0.37362200
H	3.48347700	0.28888500	0.94465300
H	4.87480000	2.21900400	1.34184100
N	2.70026300	1.75411200	-0.30108600
O	5.21237200	2.67479500	-0.65239600
C	2.86795900	3.07502800	-0.63574600
C	4.23700200	3.69014400	-0.60870500
H	4.37355300	4.33126100	-1.48080400
H	4.34402400	4.30077200	0.29966800
N	1.73085000	3.63638700	-0.93069700
C	1.39196700	1.48242600	-0.41596900
N	0.82267900	2.62571100	-0.78980000
C	-0.58891700	2.80765700	-1.00840700
C	-1.12026800	2.46784500	-2.25462900
C	-1.36629000	3.24873600	0.06716900
C	-2.50994900	2.50032700	-2.37751500
C	-2.74788100	3.25895300	-0.10762800
C	-3.33454700	2.87089100	-1.31451100
H	-2.95688800	2.21586400	-3.32718600
H	-3.38153300	3.55878700	0.72317600
H	5.90317800	1.09191200	0.41830800
C	4.04763500	-0.14459000	-1.09928000
H	3.08044400	-0.54205600	-1.42787800
H	4.49112000	0.40920900	-1.93415400
C	4.95511100	-1.26515300	-0.65205400
C	4.46985100	-2.23589200	0.23198100
C	6.28370600	-1.33460600	-1.07391000
C	5.30186500	-3.25742100	0.67814100
H	3.43325000	-2.18170500	0.55838800
C	7.11695500	-2.35903800	-0.62762800
H	6.66568200	-0.58409000	-1.76196400
C	6.62703400	-3.32216000	0.24930900
H	4.91356700	-4.00795400	1.35943700
H	8.14679900	-2.40426800	-0.96771400

H	7.27371500	-4.12179200	0.59626600
C	-4.83240400	2.88165900	-1.47214500
H	-5.32359900	2.67966800	-0.51707300
H	-5.17801400	3.85734000	-1.82875500
H	-5.15655100	2.12873300	-2.19558600
C	-0.23145300	2.09448400	-3.40773700
H	0.55216600	2.84567700	-3.54794500
H	0.24498600	1.13091600	-3.20415600
H	-0.81275100	2.03157600	-4.32961600
C	-0.73318300	3.70725800	1.35523200
H	0.02219300	3.00604300	1.72346900
H	-0.23292600	4.66986800	1.20951500
H	-1.49084400	3.82794100	2.13097100
C	-1.77341200	-0.50011300	0.21244800
C	-0.47908400	0.10277900	0.73329800
H	-1.96045400	0.00380300	-0.74205300
C	-2.97695500	-0.27974200	1.10448400
C	-4.19776800	0.07091400	0.51919400
C	-2.91647000	-0.43111300	2.49202500
C	-5.33350500	0.26775800	1.29856600
H	-4.25029700	0.19242700	-0.56121300
C	-4.05196200	-0.23117100	3.27407500
H	-1.97873400	-0.70086600	2.96951900
C	-5.26221200	0.11820400	2.68175300
H	-6.27330800	0.53622600	0.82483900
H	-3.98857000	-0.35171800	4.35097600
H	-6.14542700	0.27238900	3.29364200
C	0.65165400	0.12582100	-0.37218300
O	0.44122800	-0.27260300	-1.56994300
H	-0.68480400	1.05373700	1.22654500
C	-0.07352100	-2.15957900	1.86070300
C	0.23976200	-3.06464600	2.85190700
H	0.98126100	-2.92135600	3.62364000
C	-0.59770600	-4.19008600	2.66486600
H	-0.62656300	-5.08551900	3.26781200
C	-1.39251800	-3.94010700	1.56935100
H	-2.16225100	-4.53557400	1.11226400
N	-1.08329400	-2.69632100	1.08490700
C	0.46695200	-0.81600600	1.52700600
O	1.46113600	-0.79942200	0.49089900
C	1.08355100	-0.13605100	2.73753200
F	1.52549500	1.10242500	2.40991200
F	2.15226700	-0.80469300	3.19162100
F	0.22364600	0.01123000	3.75021600

C	-1.54979600	-2.00883600	-0.11612100
H	-0.75366900	-2.04774400	-0.86752800
C	-2.83033100	-2.56425300	-0.72287900
O	-3.56270900	-3.32571500	-0.12528200
C	-3.20307500	-2.06457500	-2.09072000
C	-2.35079000	-1.29627400	-2.89554500
C	-4.48685400	-2.38491700	-2.54610800
C	-2.79420200	-0.86108100	-4.14293700
H	-1.35084600	-1.02015300	-2.56179600
C	-4.92229400	-1.94428900	-3.78872400
H	-5.12804000	-2.97910100	-1.90383600
C	-4.07403300	-1.17948400	-4.58969900
H	-2.13071900	-0.27149500	-4.76829000
H	-5.91986600	-2.19487100	-4.13452900
H	-4.41156200	-0.83423500	-5.56208600

M5RS

C	4.08364300	0.07157800	0.11125600
C	5.41502200	0.57295400	0.66472600
H	3.67540600	-0.70809100	0.75546300
H	5.35597800	0.70812900	1.75435000
N	3.14578700	1.21399400	0.17544200
O	5.79186300	1.79197400	0.04337800
C	3.54206500	2.51546600	0.33683800
C	4.99475400	2.85926700	0.49871400
H	5.23391800	3.74186200	-0.09614800
H	5.19916500	3.08041700	1.55640600
N	2.52352400	3.32250800	0.34595300
C	1.80395700	1.21928700	0.05944400
N	1.44473400	2.49469300	0.17372500
C	0.12881400	3.08078800	0.12632600
C	-0.40176000	3.41602800	-1.12330400
C	-0.50137800	3.38514000	1.33604200
C	-1.63063700	4.07156500	-1.13261900
C	-1.72926700	4.04119300	1.26733000
C	-2.30134700	4.39627100	0.04644800
H	-2.07628700	4.33229200	-2.08921000
H	-2.24367000	4.28909500	2.19265800
H	6.19137400	-0.16151500	0.44137700
C	4.18026000	-0.44018500	-1.33314300
H	3.16537700	-0.51089400	-1.74028500
H	4.73586700	0.29821000	-1.92222400
C	4.85823600	-1.78763700	-1.37255800
C	4.14070100	-2.92895300	-0.99622200

C	6.19718200	-1.92040800	-1.74479600
C	4.75503700	-4.17680300	-0.99673400
H	3.09734600	-2.82166400	-0.70643500
C	6.81308600	-3.17065700	-1.74446300
H	6.75825700	-1.03794600	-2.04446100
C	6.09287800	-4.30117400	-1.37004000
H	4.18646500	-5.05604800	-0.70991600
H	7.85354800	-3.26029300	-2.04093200
H	6.56993900	-5.27619900	-1.37263400
C	-3.60872400	5.14194600	-0.00261200
H	-3.43552200	6.22189300	-0.05324700
H	-4.18706900	4.85470500	-0.88444700
H	-4.21177600	4.94300800	0.88679500
C	0.33666600	3.09725000	-2.39346200
H	1.30129800	3.61639200	-2.41618800
H	0.52777800	2.02054900	-2.46126300
H	-0.24569600	3.41657400	-3.25960700
C	0.10795900	3.02112800	2.66460900
H	-0.04138400	1.96266800	2.89948400
H	1.18506700	3.20654500	2.67580800
H	-0.35080100	3.60823500	3.46202400
C	-1.48400700	-0.75789700	-0.35869300
C	-0.34631100	-0.23453900	0.50801500
H	-1.02737300	-1.26667900	-1.21476100
C	-2.38881800	0.33325100	-0.89185400
C	-2.44403100	0.57423400	-2.26632800
C	-3.26292000	1.02470600	-0.04894100
C	-3.39173500	1.44931100	-2.79284500
H	-1.73934200	0.06165900	-2.91478700
C	-4.22918200	1.87621400	-0.57467100
H	-3.22248400	0.86393400	1.02680400
C	-4.30270700	2.08249700	-1.95042600
H	-3.43030100	1.62014900	-3.86442300
H	-4.92689000	2.37665300	0.09065500
H	-5.06289400	2.73967900	-2.36288800
C	0.92487700	0.03137600	-0.39826700
O	0.86226300	0.01708000	-1.66580000
H	-0.67173700	0.57735500	1.16640700
C	-0.11776200	-2.70611200	1.20729100
C	0.40712300	-3.92180000	1.58939900
H	1.40946500	-4.08112200	1.95825000
C	-0.60409900	-4.89537400	1.39255000
H	-0.52971600	-5.95658800	1.57789300
C	-1.71095100	-4.24336200	0.90050100

H	-2.67572000	-4.62095300	0.59872200
N	-1.40877800	-2.91431700	0.78050900
C	0.48771300	-1.34225600	1.17374000
C	-2.30428100	-1.84219700	0.38530400
H	-2.77520200	-1.40974500	1.27497100
C	-3.36768800	-2.33037100	-0.60935500
O	-3.04686800	-3.04665100	-1.53319300
C	-4.75011000	-1.78020000	-0.48769000
C	-5.34946800	-1.50877900	0.74525400
C	-5.43863300	-1.50672700	-1.67254200
C	-6.62753500	-0.96208000	0.78970000
H	-4.83202700	-1.73842900	1.67210100
C	-6.70252900	-0.93256800	-1.62510700
H	-4.95189500	-1.71900200	-2.61898000
C	-7.29768700	-0.66086900	-0.39410000
H	-7.09828500	-0.76625700	1.74750500
H	-7.22489700	-0.69528700	-2.54604000
H	-8.28708500	-0.21595500	-0.35635700
O	1.56974500	-1.19521000	0.26133100
C	0.96869700	-0.94733800	2.56358300
F	-0.05055500	-0.85651600	3.42912000
F	1.86431600	-1.80892000	3.05850700
F	1.57699600	0.26126000	2.54850300

M5SR

C	-4.13431000	0.39148600	-0.44465900
C	-5.35757600	1.04809700	-1.08189800
H	-3.60279300	-0.24623400	-1.15641800
H	-5.09694500	1.51651400	-2.04112900
N	-3.22330800	1.50650600	-0.12345800
O	-5.89759100	2.01047300	-0.18533600
C	-3.64318200	2.79191900	0.08541600
C	-5.09237000	3.16099600	-0.07278600
H	-5.43796100	3.72800500	0.79341400
H	-5.18491500	3.79574300	-0.96584500
N	-2.63663400	3.58710400	0.29950500
C	-1.88084200	1.50492900	-0.04871200
N	-1.54148500	2.76291300	0.21657300
C	-0.22469500	3.34617300	0.26178100
C	0.39018700	3.56981900	1.49577200
C	0.33995200	3.73358100	-0.95886000
C	1.64669400	4.17536900	1.47830200
C	1.58489100	4.35294200	-0.91526000
C	2.25516800	4.57138500	0.28838000

H	2. 15398900	4. 35132000	2. 42420700
H	2. 05015100	4. 65731800	-1. 84854600
H	-6. 13224700	0. 29747000	-1. 24686900
C	-4. 51199400	-0. 38619400	0. 82508200
H	-3. 60170700	-0. 58197500	1. 39139100
H	-5. 17328700	0. 24310500	1. 42916600
C	-5. 18592900	-1. 68924100	0. 47165800
C	-4. 41672400	-2. 75828700	-0. 00129900
C	-6. 56887800	-1. 84325400	0. 58123100
C	-5. 02475900	-3. 96005500	-0. 35004600
H	-3. 33970500	-2. 63140000	-0. 09325500
C	-7. 17812500	-3. 04693100	0. 23147500
H	-7. 17021500	-1. 01425700	0. 94789500
C	-6. 40649100	-4. 10753800	-0. 23385400
H	-4. 41849200	-4. 78463300	-0. 71193600
H	-8. 25422200	-3. 15545800	0. 32510900
H	-6. 87900800	-5. 04647900	-0. 50461700
C	3. 59849500	5. 25161700	0. 30132200
H	4. 11132800	5. 11652700	-0. 65397200
H	3. 48659200	6. 32679000	0. 47569900
H	4. 23526600	4. 85213200	1. 09490200
C	-0. 24410600	3. 16809900	2. 80140000
H	-1. 33355800	3. 14723700	2. 73612600
H	0. 08697800	2. 17229900	3. 11197000
H	0. 04130000	3. 87224900	3. 58567000
C	-0. 38458600	3. 50650700	-2. 25740100
H	-0. 61591100	2. 44321600	-2. 38942000
H	-1. 32588100	4. 06728400	-2. 27382700
H	0. 23121400	3. 84008200	-3. 09475800
C	1. 42090000	-0. 46411900	-0. 58508800
C	0. 29233200	0. 05158400	0. 30519500
H	0. 96256600	-0. 97896900	-1. 43546200
C	2. 29429300	0. 64705500	-1. 13645700
C	2. 09166200	1. 09249700	-2. 44579700
C	3. 34337400	1. 19667600	-0. 39427500
C	2. 94556100	2. 03315600	-3. 01385600
H	1. 25618800	0. 68373500	-3. 00713500
C	4. 20651300	2. 12936200	-0. 96624100
H	3. 51087200	0. 88848700	0. 63498600
C	4. 01709600	2. 54184400	-2. 28157800
H	2. 78269600	2. 35798200	-4. 03742700
H	5. 02990200	2. 52974500	-0. 38188100
H	4. 69641500	3. 26050000	-2. 73093600
C	-1. 01064600	0. 32525600	-0. 54352000

O	-1.02225900	0.32891100	-1.81204800
H	0.63584600	0.85925200	0.96029500
C	0.08969300	-2.42411000	0.99766500
C	-0.42956400	-3.65423300	1.34061700
H	-1.43176300	-3.82910200	1.70372500
C	0.58756200	-4.61496700	1.11842100
H	0.52044800	-5.68131200	1.27468000
C	1.69438400	-3.94160100	0.65343400
H	2.66851400	-4.30566800	0.36170900
N	1.38386300	-2.60938600	0.57640000
C	-0.51758100	-1.06105300	0.99635500
C	2.25377000	-1.51073600	0.16985000
H	2.69453700	-1.06137500	1.06696600
C	3.37004400	-2.05473000	-0.74452400
O	3.15721000	-2.19698300	-1.92864300
C	4.69716400	-2.38231300	-0.14461600
C	4.87344700	-2.55261100	1.23239000
C	5.78272200	-2.55176300	-1.01050400
C	6.12673600	-2.88710400	1.73634000
H	4.03279600	-2.45663500	1.91383400
C	7.03510100	-2.86980700	-0.50351300
H	5.61929900	-2.42387000	-2.07544000
C	7.20715100	-3.03805600	0.87085100
H	6.25907600	-3.03034900	2.80349300
H	7.87792500	-2.98985300	-1.17607400
H	8.18554500	-3.29085400	1.26707500
C	-0.93630000	-0.67839800	2.40926000
O	-1.63451400	-0.90791100	0.13126100
F	-1.78661000	-1.56196900	2.94607500
F	-1.57086400	0.51458000	2.42590900
F	0.12279200	-0.56897500	3.22503000

M5SS

C	3.73016300	-0.50118700	-0.94506900
C	4.77219100	-1.01187400	-1.93902500
H	3.26847700	0.42810300	-1.29028400
H	4.37032100	-1.01413600	-2.96174200
N	2.66664900	-1.52532100	-0.94151900
O	5.18276900	-2.31909100	-1.56150700
C	2.85503600	-2.82914600	-1.32122700
C	4.19512100	-3.28932400	-1.82372500
H	4.49173900	-4.21334300	-1.32450000
H	4.11082800	-3.48427600	-2.90242300
N	1.74097100	-3.50052200	-1.27169000

C	1.36585300	-1.38050700	-0.64604600
N	0.82111200	-2.57916500	-0.84688600
C	-0.58194900	-2.89485700	-0.75670000
C	-1.07045800	-3.43297600	0.43807800
C	-1.39299500	-2.60760100	-1.85747000
C	-2.44695000	-3.60821000	0.54292400
C	-2.76724800	-2.79641700	-1.69679100
C	-3.30988500	-3.27579400	-0.50488700
H	-2.85745000	-4.00188600	1.46927900
H	-3.42636500	-2.55555500	-2.52757400
H	5.65684700	-0.37421600	-1.90297200
C	4.31713800	-0.33064300	0.46298400
H	3.49226700	-0.23753300	1.16864200
H	4.88674500	-1.23288100	0.70783600
C	5.19019100	0.89734400	0.53542700
C	4.59595700	2.15762300	0.66051100
C	6.58051800	0.80512700	0.45111200
C	5.38417500	3.30360300	0.69955600
H	3.51186400	2.22407000	0.72755700
C	7.36999400	1.95282000	0.49044700
H	7.04594000	-0.17392900	0.35982600
C	6.77220600	3.20385500	0.61393900
H	4.91463300	4.27696300	0.80105100
H	8.45036900	1.86822600	0.42752500
H	7.38516600	4.09897200	0.64564300
C	-4.79558800	-3.46420100	-0.34996900
H	-5.12436400	-3.13653800	0.63943800
H	-5.34634400	-2.89334700	-1.10146000
H	-5.06537000	-4.51926400	-0.46286800
C	-0.13960400	-3.78473400	1.56766900
H	0.66103100	-4.44421800	1.22044700
H	0.33331900	-2.89378100	1.99121800
H	-0.68394700	-4.29074600	2.36605500
C	-0.80770500	-2.13238900	-3.15912300
H	-0.31640100	-1.16380400	-3.01836900
H	-0.06417300	-2.84797300	-3.52532900
H	-1.59171700	-2.03638200	-3.91250800
C	-1.79972800	0.54595600	0.16023500
C	-0.47809600	-0.03782400	0.63521300
H	-2.00628400	0.04892500	-0.79350900
C	-2.97089700	0.29513600	1.08590500
C	-4.19014500	-0.12083700	0.54260100
C	-2.88174800	0.49264000	2.46682200
C	-5.29851400	-0.33361600	1.35764200

H	-4.26546600	-0.27923800	-0.53185200
C	-3.98813500	0.27368300	3.28352000
H	-1.94370300	0.81481900	2.91005800
C	-5.19892800	-0.13830300	2.73281300
H	-6.23809700	-0.65495200	0.91772700
H	-3.90293200	0.42971000	4.35432000
H	-6.06026700	-0.30571900	3.37182100
C	0.60957600	-0.04102300	-0.50489900
O	0.36095400	0.37289500	-1.69286900
H	-0.64855400	-0.99490500	1.13163800
C	-0.05860700	2.23312900	1.74673000
C	0.28115800	3.14419100	2.72422300
H	1.05645900	3.01390300	3.46417500
C	-0.58334800	4.25465300	2.57478700
H	-0.60158500	5.14922100	3.17942100
C	-1.42141400	3.99014600	1.51552300
H	-2.22055000	4.57196100	1.09240700
N	-1.11140700	2.75205000	1.01762200
C	0.48239000	0.89212400	1.39989300
O	1.45075200	0.87226400	0.33793600
C	1.12265900	0.22154700	2.60296800
F	1.57604700	-1.01037400	2.27006100
F	0.27321200	0.06165700	3.62266200
F	2.18591000	0.90384900	3.04882800
C	-1.61477800	2.06083400	-0.16491600
H	-0.84972000	2.11765600	-0.94640300
C	-2.92919500	2.59702200	-0.71459900
O	-3.65767500	3.32824100	-0.07590300
C	-3.33616100	2.11612700	-2.07819400
C	-2.48470300	1.40097300	-2.93067900
C	-4.64395400	2.40393800	-2.48395800
C	-2.95101700	0.98482400	-4.17565300
H	-1.46568300	1.15450700	-2.63569100
C	-5.10219900	1.98410300	-3.72572000
H	-5.28456600	2.95736700	-1.80550000
C	-4.25407400	1.27267900	-4.57408000
H	-2.28764100	0.43698300	-4.83760100
H	-6.11810900	2.20940500	-4.03353300
H	-4.60979300	0.94357900	-5.54552600

TS6RR

C	3.97128300	1.21496900	0.17040800
C	5.14010300	2.17272700	0.39778000
H	3.68877800	0.72591800	1.10771100

H	4.96659500	2.78592500	1.29405400
N	2.83608600	2.03728000	-0.25291500
O	5.31626500	3.00565100	-0.73847200
C	2.95005600	3.29793800	-0.78450700
C	4.28992200	3.97097300	-0.84518900
H	4.41392700	4.48599500	-1.79887600
H	4.36765100	4.70934800	-0.03363900
N	1.78759300	3.75344900	-1.14757200
C	1.54067300	1.64087900	-0.28956200
N	0.94296300	2.71259200	-0.82787200
C	-0.45883500	2.75174500	-1.12855500
C	-0.85882000	2.44731500	-2.43544900
C	-1.36992400	2.98760300	-0.09755500
C	-2.22377500	2.34642600	-2.68421900
C	-2.73041000	2.85934900	-0.39306300
C	-3.17197900	2.52460100	-1.67192500
H	-2.56036300	2.10042200	-3.68842400
H	-3.45708500	3.00604700	0.40227300
H	6.06454100	1.60685200	0.52916500
C	4.27114900	0.15332900	-0.89928300
H	3.32364200	-0.31932000	-1.18023900
H	4.67471900	0.66131400	-1.78198200
C	5.23430600	-0.88438900	-0.37981400
C	4.77084500	-1.88191200	0.48421400
C	6.59140600	-0.84799900	-0.70589600
C	5.64964400	-2.82306100	1.01096400
H	3.71260500	-1.91595100	0.73245900
C	7.47277500	-1.79090900	-0.17963000
H	6.95720600	-0.07830100	-1.38174200
C	7.00339300	-2.77923000	0.68075900
H	5.27695100	-3.59457700	1.67746000
H	8.52476800	-1.75410300	-0.44487100
H	7.68862500	-3.51479400	1.08983000
C	-4.63619400	2.33477800	-1.97302200
H	-5.24866800	2.48745500	-1.08092500
H	-4.97386800	3.03484100	-2.74316400
H	-4.82087800	1.32183400	-2.35184800
C	0.16433000	2.21549100	-3.51277200
H	0.80232700	3.09452000	-3.64143300
H	0.80071300	1.36779600	-3.24292200
H	-0.32394800	1.99632500	-4.46457300
C	-0.91614400	3.37671700	1.28662100
H	-0.02336400	2.82633400	1.59662500
H	-0.66347700	4.44151300	1.31937800

H	-1.70888500	3.19156500	2.01469100
C	-1.91513900	-0.61513700	0.24340700
C	-0.51879100	-0.17525700	0.65374500
H	-2.15342200	-0.01971800	-0.64714000
C	-2.99012800	-0.35587600	1.27888900
C	-4.24328400	0.09616500	0.85286400
C	-2.78079600	-0.56671200	2.64323400
C	-5.26306700	0.34135600	1.76620800
H	-4.41524500	0.25961900	-0.20866300
C	-3.80063000	-0.31977900	3.55992100
H	-1.82053700	-0.92420800	3.00065800
C	-5.04232100	0.13514200	3.12622900
H	-6.22761400	0.69482700	1.41496300
H	-3.62130100	-0.48724100	4.61710100
H	-5.83387300	0.32638000	3.84366100
C	0.49238900	-0.31660500	-0.49191100
O	0.36226800	-0.36217300	-1.69363100
H	-0.53543900	0.79936800	1.13485400
C	-0.21912300	-2.52855500	1.60291300
C	0.11891600	-3.55005600	2.46283400
H	0.93965200	-3.53325500	3.16431300
C	-0.81083700	-4.59552700	2.25295400
H	-0.84826800	-5.54418500	2.76710500
C	-1.68514100	-4.18369400	1.27332300
H	-2.53581100	-4.67956800	0.84032400
N	-1.33759100	-2.91722500	0.88508600
C	0.40066800	-1.20116000	1.35897600
O	1.33096500	-1.17316600	0.23230600
C	1.15382300	-0.68375200	2.57628300
F	1.59585900	0.57027100	2.39288600
F	2.22850800	-1.44435300	2.83039600
F	0.38843600	-0.67516500	3.67397600
C	-1.86429200	-2.10581300	-0.20545200
H	-1.17081500	-2.17864000	-1.05104500
C	-3.25251500	-2.49837500	-0.69386700
O	-3.99617900	-3.20047600	-0.04260400
C	-3.70054200	-1.90465300	-1.99901200
C	-2.85045200	-1.21937200	-2.87648300
C	-5.05253800	-2.06100200	-2.32737100
C	-3.35416300	-0.71930700	-4.07527100
H	-1.79976100	-1.05726800	-2.64618000
C	-5.55164500	-1.54874000	-3.51730400
H	-5.69329500	-2.59066300	-1.63035500
C	-4.69914500	-0.88127900	-4.39741300

H	-2.68714900	-0.20416400	-4.75925600
H	-6.60115200	-1.67266500	-3.76294200
H	-5.08410200	-0.48748800	-5.33277200

TS6RS

C	4.11316400	0.17946300	0.20032700
C	5.38542800	0.63541300	0.91212900
H	3.62747400	-0.61616200	0.77128500
H	5.19052300	0.78825800	1.98370000
N	3.20484000	1.33299400	0.18804400
O	5.87332100	1.83389800	0.32905700
C	3.62154500	2.62604200	0.37996000
C	5.06159400	2.93722000	0.66805200
H	5.39009500	3.79091900	0.07339200
H	5.17325700	3.18817100	1.73316200
N	2.62084200	3.44983900	0.31023100
C	1.86418900	1.31480200	-0.03686400
N	1.55290100	2.61406700	0.05297600
C	0.24188500	3.18906200	-0.03983400
C	-0.34504200	3.35597700	-1.29770500
C	-0.37722700	3.60157700	1.14373000
C	-1.58935500	3.98269800	-1.34670300
C	-1.61903900	4.22701600	1.04205500
C	-2.22837400	4.44093500	-0.19436300
H	-2.06928900	4.11986900	-2.31268900
H	-2.11520300	4.56283700	1.94973500
H	6.16439400	-0.12039400	0.79872200
C	4.36745600	-0.29398000	-1.23867800
H	3.39744800	-0.42147000	-1.73115000
H	4.91245900	0.49793200	-1.76403100
C	5.14404000	-1.58686900	-1.26845300
C	4.48776300	-2.80090600	-1.04004200
C	6.52376800	-1.59516100	-1.48691400
C	5.19962200	-3.99672100	-1.03313200
H	3.41299300	-2.79591000	-0.87414800
C	7.23777400	-2.79159000	-1.47957600
H	7.03885300	-0.65434500	-1.66800600
C	6.57629900	-3.99537200	-1.25236700
H	4.67792200	-4.93317900	-0.86165400
H	8.30889000	-2.78276300	-1.65523900
H	7.12965600	-4.92900900	-1.24970000
C	-3.53849200	5.17864400	-0.28936500
H	-3.36707800	6.24704800	-0.45673000
H	-4.13950200	4.80441400	-1.12176900

H	-4.11965900	5.07816800	0.63092500
C	0.34955800	2.88851600	-2.54773200
H	1.37278400	3.27476700	-2.58981700
H	0.40977900	1.79629900	-2.57820700
H	-0.18782700	3.23508400	-3.43235000
C	0.29075000	3.38478500	2.47594300
H	0.59630600	2.34091300	2.59680000
H	1.19336600	3.99692400	2.56081100
H	-0.38431600	3.64709300	3.29237800
C	-1.67374100	-0.96834300	-0.59478900
C	-0.40215900	-0.49770500	0.10863500
H	-1.38905000	-1.51890000	-1.49859300
C	-2.59819900	0.16179800	-0.99362300
C	-2.96123200	0.32015700	-2.33164000
C	-3.19943800	0.97171100	-0.02578400
C	-3.93553800	1.24758700	-2.69491300
H	-2.48972800	-0.30270000	-3.08668300
C	-4.18799500	1.88088600	-0.38352500
H	-2.91902000	0.87190800	1.02102900
C	-4.56561100	2.01407100	-1.71863000
H	-4.21402100	1.35563200	-3.73835400
H	-4.66555100	2.48618500	0.38105700
H	-5.34650800	2.71574700	-1.99595400
C	0.82028100	-0.45672600	-0.82636800
O	0.92499500	-0.35002200	-2.02251200
H	-0.55698300	0.41046900	0.69356400
C	-0.18257900	-2.95590200	0.80454700
C	0.36571400	-4.19521900	1.04744400
H	1.40136300	-4.38404900	1.28951600
C	-0.67708500	-5.14455200	0.90814800
H	-0.59766700	-6.21609800	1.01394600
C	-1.82570900	-4.45464500	0.59279600
H	-2.82336200	-4.80647300	0.38284600
N	-1.52017800	-3.12299300	0.52364900
C	0.41492700	-1.59134100	0.83487000
C	-2.41483700	-2.00310600	0.29269100
H	-2.67818600	-1.53877400	1.24912200
C	-3.67556300	-2.41055900	-0.48153600
O	-3.57636800	-3.12239800	-1.45826400
C	-4.97181400	-1.78822300	-0.08667400
C	-5.29497900	-1.49894800	1.24227100
C	-5.87405800	-1.47618200	-1.10780800
C	-6.51504200	-0.90356100	1.54519400
H	-4.61138400	-1.75595600	2.04574200

C	-7.07939700	-0.85610100	-0.80428200
H	-5.60067400	-1.70553200	-2.13255500
C	-7.40081400	-0.57139900	0.52234000
H	-6.77221600	-0.69442200	2.57810600
H	-7.76932400	-0.59430200	-1.59953600
H	-8.34465800	-0.09117000	0.75972000
O	1.52862700	-1.42509700	-0.06737200
C	0.84820200	-1.23689600	2.24947900
F	-0.20819400	-1.26920400	3.07357700
F	1.76812600	-2.09453900	2.70468300
F	1.38634800	-0.01017200	2.33828800

TS6SR

C	-4.07217100	0.30654600	-0.78450200
C	-5.34694400	0.82388700	-1.44901400
H	-3.49928800	-0.30538600	-1.48789000
H	-5.12150000	1.24484900	-2.43917900
N	-3.26151200	1.48745000	-0.46530100
O	-5.96085000	1.80500600	-0.62576700
C	-3.78301500	2.75005600	-0.34300400
C	-5.23339200	3.01443600	-0.62712500
H	-5.65953700	3.66239500	0.14031400
H	-5.32211700	3.51918800	-1.60027200
N	-2.85770100	3.60476900	-0.02732100
C	-1.92734500	1.51776200	-0.20330500
N	-1.72733000	2.81646700	0.04846200
C	-0.46975300	3.43187700	0.35685600
C	-0.16687100	3.69600600	1.69542900
C	0.38531300	3.76989700	-0.69500500
C	1.04697800	4.32254500	1.97109700
C	1.58057000	4.40885000	-0.36977100
C	1.92560000	4.69230600	0.95113600
H	1.30646000	4.53559700	3.00562100
H	2.26366700	4.68015700	-1.16981600
H	-6.06240200	0.00768500	-1.56372400
C	-4.36380700	-0.48396400	0.49939200
H	-3.41399200	-0.64398800	1.01508800
H	-5.00066400	0.13479000	1.14063200
C	-5.02830300	-1.80634500	0.20752000
C	-4.27583400	-2.86778900	-0.30732800
C	-6.39743300	-1.98719400	0.41455000
C	-4.88227500	-4.08514200	-0.60118200
H	-3.21173000	-2.72481400	-0.47866800
C	-7.00596500	-3.20622900	0.12162200

H	-6.98830700	-1.16478900	0.81122800
C	-6.24879600	-4.25844700	-0.38563600
H	-4.28695400	-4.90144700	-0.99864800
H	-8.07048400	-3.33312300	0.29164000
H	-6.72033800	-5.20916900	-0.61281100
C	3.21190000	5.40835300	1.27273000
H	3.68650400	4.98771900	2.16363600
H	3.91704800	5.33975400	0.44105100
H	3.02671800	6.46920700	1.47004000
C	-1.13050300	3.31495400	2.78748000
H	-2.09728700	3.80468700	2.63889000
H	-1.30892300	2.23606500	2.79047300
H	-0.74026000	3.60494300	3.76447000
C	0.01687300	3.46689100	-2.12239400
H	-0.07268700	2.38871300	-2.29095400
H	-0.94809400	3.91777300	-2.37633700
H	0.77601000	3.86092000	-2.80096600
C	1.79381700	-0.44108900	-0.90835100
C	0.48086300	-0.16670400	-0.16596200
H	1.55932000	-0.78153900	-1.92181400
C	2.67964600	0.78614100	-1.00949500
C	2.94106200	1.36054000	-2.25452300
C	3.30943400	1.31308200	0.12243800
C	3.83738500	2.41982100	-2.37249800
H	2.45126400	0.95663900	-3.13608200
C	4.22052100	2.35853700	0.00445500
H	3.09754300	0.90297500	1.10741900
C	4.49439700	2.90839300	-1.24545800
H	4.03621900	2.85000200	-3.34908000
H	4.71397900	2.74590700	0.89057200
H	5.21050000	3.71928800	-1.33969900
C	-0.75134200	-0.07573500	-1.08920200
O	-0.87467700	0.17422100	-2.26359800
H	0.56522600	0.66109900	0.54016000
C	0.38063900	-2.70968900	0.18012200
C	-0.11737000	-3.99293800	0.22526200
H	-1.13778800	-4.26032000	0.45897900
C	0.95209200	-4.86420600	-0.09664600
H	0.91472400	-5.94101800	-0.16512100
C	2.06592300	-4.08653500	-0.31940500
H	3.07382900	-4.36449100	-0.58936000
N	1.71168400	-2.77310800	-0.15449000
C	-0.27144400	-1.39160900	0.40737600
C	2.56299900	-1.59130200	-0.23283300

H	2.84814100	-1.29174300	0.78200800
C	3.82911100	-1.92376500	-1.04942900
O	3.80794700	-1.80691100	-2.25550700
C	5.05296800	-2.37168200	-0.32553900
C	5.01732500	-2.80389600	1.00443300
C	6.26293500	-2.38052500	-1.02838600
C	6.18471600	-3.23789800	1.62482800
H	4.07983900	-2.83249900	1.55231600
C	7.42829900	-2.79990600	-0.40184500
H	6.26467100	-2.04908900	-2.06128200
C	7.38903000	-3.22884100	0.92534000
H	6.15365700	-3.58248900	2.65272500
H	8.36767500	-2.79605300	-0.94429800
H	8.29973800	-3.55977300	1.41401300
C	-0.70047600	-1.25195700	1.85855800
O	-1.40175800	-1.16649000	-0.45667500
F	-1.60097900	-2.18603700	2.18753500
F	-1.25953000	-0.06063800	2.11881900
F	0.36075000	-1.38134100	2.66646000

TS6SS

C	3.81148000	-0.72819300	-1.06976300
C	4.89104800	-1.17338700	-2.05478000
H	3.36158400	0.21625900	-1.39503200
H	4.53068100	-1.07312400	-3.08874600
N	2.76336000	-1.74882200	-1.11707600
O	5.26333000	-2.51884200	-1.79336200
C	2.94019200	-3.02446100	-1.58961900
C	4.25642900	-3.42927600	-2.18681300
H	4.54765900	-4.42015400	-1.83487200
H	4.16739400	-3.45796500	-3.28268400
N	1.84740600	-3.71904800	-1.46542300
C	1.50236400	-1.60434000	-0.64150500
N	0.98201200	-2.81402500	-0.88732700
C	-0.36494700	-3.15149100	-0.53188500
C	-0.59201600	-3.75426500	0.70913000
C	-1.40252900	-2.73468400	-1.37012700
C	-1.91359800	-3.89355300	1.12752300
C	-2.70869000	-2.88634100	-0.90279000
C	-2.98066300	-3.44117000	0.34799100
H	-2.11384300	-4.34677200	2.09562200
H	-3.53369600	-2.54907300	-1.52635400
H	5.78617100	-0.56096700	-1.93048400
C	4.32807100	-0.59377900	0.37076000

H	3.45581100	-0.50533000	1.02580500
H	4.85595000	-1.51834500	0.62953600
C	5.22405200	0.60700000	0.53733100
C	4.65812900	1.87451500	0.70970600
C	6.61449800	0.48668400	0.48946800
C	5.47009800	2.99805800	0.82968100
H	3.57511600	1.96761900	0.75436500
C	7.42853600	1.61099000	0.60979600
H	7.06009700	-0.49763200	0.36313600
C	6.85710100	2.86924400	0.77908800
H	5.01973900	3.97618400	0.96689000
H	8.50805000	1.50264700	0.57458200
H	7.48962700	3.74617700	0.87407100
C	-4.38994200	-3.52403100	0.87025100
H	-4.55711200	-2.74549900	1.62205400
H	-5.12004200	-3.37340600	0.07200500
H	-4.58101100	-4.49298200	1.33939700
C	0.56309400	-4.20132500	1.56478800
H	1.20279700	-4.90183300	1.02083000
H	1.18327100	-3.34766100	1.85300400
H	0.20363500	-4.68817100	2.47286400
C	-1.11605300	-2.11920800	-2.71464800
H	-0.60269900	-1.15736000	-2.61149600
H	-0.46875300	-2.77201800	-3.30813400
H	-2.04584400	-1.95954100	-3.26534800
C	-1.96032900	0.73474800	-0.10282300
C	-0.63775800	0.14218900	0.36764600
H	-2.12652600	0.31687900	-1.10289000
C	-3.16325200	0.38755800	0.75069500
C	-4.38549800	0.12252300	0.12312600
C	-3.10284800	0.35870500	2.14497700
C	-5.52783600	-0.14289800	0.87109000
H	-4.44065300	0.13419000	-0.96373700
C	-4.24445400	0.08310900	2.89531300
H	-2.16595000	0.55450500	2.65676400
C	-5.46019900	-0.15994700	2.26273600
H	-6.46856600	-0.34195000	0.36744700
H	-4.18107200	0.06622300	3.97856500
H	-6.34912300	-0.36906200	2.84930800
C	0.50225500	0.42481300	-0.62221300
O	0.53230800	0.65477000	-1.81045100
H	-0.74395100	-0.90234600	0.66021400
C	-0.35706100	2.28712400	1.74123400
C	-0.08608500	3.12044700	2.80439400

H	0.64338800	2.93459900	3.57857300
C	-0.94661700	4.23691600	2.68636700
H	-1.00928500	5.08119200	3.35632900
C	-1.71398600	4.05438800	1.55884600
H	-2.48941500	4.66649000	1.13357800
N	-1.36679600	2.85869600	0.98785500
C	0.23243400	0.98803000	1.33244300
O	1.27584100	1.10765500	0.31319500
C	0.83802100	0.24373500	2.51365800
F	1.23903400	-0.98817800	2.17219800
F	-0.03279400	0.11293300	3.52192200
F	1.91404400	0.89348800	2.97724600
C	-1.78816200	2.27610400	-0.27975700
H	-0.98947200	2.44112800	-1.01212500
C	-3.07755100	2.84740800	-0.85652200
O	-3.86405900	3.48098700	-0.18566900
C	-3.37593400	2.52201700	-2.29084100
C	-2.45434600	1.92821700	-3.16329300
C	-4.66217800	2.82939900	-2.74833000
C	-2.82563400	1.65085600	-4.47629600
H	-1.44885000	1.66897900	-2.84083200
C	-5.02749500	2.54936600	-4.05815000
H	-5.36010900	3.28469200	-2.05384600
C	-4.10744500	1.95942900	-4.92424700
H	-2.10808300	1.19387300	-5.14961300
H	-6.02713600	2.78877300	-4.40536200
H	-4.39005500	1.73913300	-5.94883700

M6RR

C	-1.81925500	-0.92970900	0.09670300
C	-0.43571000	-0.41664700	0.49343600
H	-2.03392400	-0.49144500	-0.88392500
C	-2.93547600	-0.53146500	1.04054000
C	-4.15865400	-0.12650500	0.49922400
C	-2.79440800	-0.58821100	2.42942100
C	-5.22327700	0.21499700	1.32703300
H	-4.27680900	-0.08049100	-0.58132500
C	-3.85919300	-0.24266000	3.25737200
H	-1.85470900	-0.90024900	2.87550400
C	-5.07491500	0.15736000	2.71010800
H	-6.16589300	0.53001200	0.89125300
H	-3.73571200	-0.28963300	4.33442400
H	-5.90285000	0.42545100	3.35828100
C	0.61823500	-0.70446800	-0.56627700

O	0.78703500	-0.43953800	-1.71584500
H	-0.46540600	0.62208200	0.82847600
C	-0.20413100	-2.60362500	1.81877700
C	0.05812200	-3.44190100	2.88016600
H	0.84164800	-3.30793000	3.61032900
C	-0.89580300	-4.48430200	2.82659300
H	-0.98867000	-5.31261300	3.51250000
C	-1.70713800	-4.25524500	1.73855300
H	-2.55080200	-4.80903900	1.36712800
N	-1.29613100	-3.09979800	1.12915500
C	0.44010300	-1.35916100	1.35588900
O	1.35656200	-1.54160500	0.21392500
C	1.21942300	-0.63406100	2.44124900
F	1.77529600	0.47914700	1.94771500
F	2.19879800	-1.39155000	2.93925100
F	0.41218800	-0.27644000	3.44636000
C	-1.74591200	-2.47595600	-0.10632400
H	-1.00146700	-2.68969600	-0.88449100
C	-3.10517800	-2.95331300	-0.61210900
O	-3.89452500	-3.51911200	0.11233500
C	-3.45978300	-2.61301100	-2.02768900
C	-2.54890400	-2.09463000	-2.95720800
C	-4.78850100	-2.82818800	-2.41184700
C	-2.96695300	-1.80214600	-4.25166500
H	-1.51122600	-1.90867900	-2.69561000
C	-5.20227600	-2.53287900	-3.70355100
H	-5.48000300	-3.22690800	-1.67743900
C	-4.29037300	-2.02025800	-4.62570800
H	-2.25600100	-1.40291500	-4.96674400
H	-6.23420300	-2.70083900	-3.99315900
H	-4.61177700	-1.78869400	-5.63607600

M6RS

C	-1.83656000	-0.90458000	-0.38069000
C	-0.74256100	-0.26733000	0.48202500
H	-1.38562000	-1.32604500	-1.28691100
C	-2.92546300	0.06424800	-0.78769600
C	-3.26417100	0.19662900	-2.13417500
C	-3.67622800	0.74761900	0.17306400
C	-4.33840300	0.99597000	-2.51714500
H	-2.69084100	-0.34076300	-2.88454100
C	-4.75353900	1.54049300	-0.20701700
H	-3.43575100	0.64719600	1.22963200
C	-5.08812200	1.66452000	-1.55403700

H	-4.59050900	1.09124800	-3.56829500
H	-5.33510700	2.05738300	0.54929400
H	-5.93071800	2.28085200	-1.84979800
C	0.50753900	0.15447100	-0.28225700
O	0.79409700	0.93577000	-1.12953100
H	-1.13415300	0.50270300	1.15013100
C	-0.08867600	-2.69433800	1.00231500
C	0.65670100	-3.83017200	1.22651200
H	1.69092700	-3.84907700	1.53724400
C	-0.18507000	-4.93644900	0.95812300
H	0.07935100	-5.98150900	1.01624500
C	-1.41608500	-4.44138000	0.58962000
H	-2.31814600	-4.95168900	0.29081700
N	-1.35394300	-3.07622300	0.60871400
C	0.23481500	-1.25695200	1.15104000
C	-2.42527700	-2.12334900	0.37696300
H	-2.83510900	-1.78429400	1.33462900
C	-3.52744700	-2.69759200	-0.52586900
O	-3.21419500	-3.29217800	-1.53548700
C	-4.94617600	-2.37814000	-0.20308600
C	-5.40667900	-2.21444900	1.10674700
C	-5.83012600	-2.23077100	-1.27678000
C	-6.74408900	-1.90908500	1.33731700
H	-4.73767900	-2.34937700	1.95097700
C	-7.15869100	-1.90193800	-1.04388500
H	-5.44909600	-2.35911800	-2.28459700
C	-7.61593700	-1.74284500	0.26395100
H	-7.10523800	-1.79808700	2.35414000
H	-7.83950800	-1.76953400	-1.87805200
H	-8.65541900	-1.49026900	0.44728100
O	1.32385000	-0.77265300	0.31055400
C	0.55064400	-0.87902100	2.58999000
F	-0.52073700	-1.11522400	3.35950600
F	1.58103100	-1.57091700	3.07523200
F	0.84569400	0.42377900	2.69039600

M6SR

C	-0.89738300	-1.08207200	-1.11723800
C	0.39855200	-1.42913100	-1.86439100
H	-0.76143000	-0.15648300	-0.54877100
C	-2.06146900	-0.90060800	-2.07078300
C	-2.76350100	0.30430500	-2.10308900
C	-2.46255300	-1.94270500	-2.91159900
C	-3.84111500	0.46988300	-2.96871000

H	-2.46473000	1.11105000	-1.44045400
C	-3.54358000	-1.78134500	-3.77255300
H	-1.92682900	-2.89006400	-2.90289800
C	-4.23356400	-0.57191000	-3.80468600
H	-4.37518900	1.41428800	-2.98820000
H	-3.84426300	-2.59900500	-4.41940100
H	-5.07331300	-0.44259400	-4.47963600
C	1.37583600	-0.27529800	-2.05739800
O	1.38674200	0.78239700	-2.59707700
H	0.20530400	-1.98031800	-2.78724300
C	1.25590700	-2.25615300	0.40134900
C	2.07394400	-2.46844400	1.48863300
H	3.15373200	-2.47287000	1.46768000
C	1.23148200	-2.65991800	2.60922500
H	1.53786100	-2.84062400	3.62845300
C	-0.07015300	-2.56756400	2.16913800
H	-1.00068500	-2.65352600	2.71026200
N	-0.05376700	-2.31634100	0.82357700
C	1.55476900	-2.01269400	-1.02739800
C	-1.19362300	-2.17989100	-0.07973400
H	-1.36128700	-3.13108500	-0.59866200
C	-2.44661800	-1.79668100	0.73597700
O	-2.66629500	-0.62679600	0.96534200
C	-3.35435600	-2.87758900	1.21065600
C	-2.98143700	-4.22606000	1.19801500
C	-4.60936200	-2.50655200	1.70635000
C	-3.86078200	-5.19382500	1.67299600
H	-1.99928900	-4.52747800	0.84515000
C	-5.48917700	-3.47597100	2.16688300
H	-4.87362600	-1.45441700	1.71422400
C	-5.11492500	-4.82002200	2.14951200
H	-3.56709700	-6.23793200	1.67056800
H	-6.46581900	-3.18789300	2.54095900
H	-5.80262700	-5.57719200	2.51224700
C	2.21406000	-3.20931400	-1.69375000
O	2.36872800	-0.83424500	-1.29419400
F	3.35836400	-3.54631400	-1.09905400
F	2.47765200	-2.96027700	-2.98263300
F	1.38184700	-4.25925400	-1.64177300

M6SS

C	-1.88309700	0.89378300	-0.01222700
C	-0.52236600	0.32025400	0.38105800
H	-2.11325800	0.47672600	-0.99869900

C	-3.01687500	0.53054200	0.92463700
C	-4.25198500	0.17518100	0.37591900
C	-2.87920000	0.57204600	2.31444300
C	-5.33182000	-0.13293200	1.19720800
H	-4.36762400	0.14133400	-0.70532300
C	-3.95938400	0.26003300	3.13576300
H	-1.92996000	0.84366500	2.76672700
C	-5.18682500	-0.09102000	2.58117500
H	-6.28370800	-0.40921900	0.75534900
H	-3.83833000	0.29410600	4.21356000
H	-6.02642700	-0.33354900	3.22443300
C	0.54373000	0.57563100	-0.67484700
O	0.70370400	0.31431900	-1.82648900
H	-0.59472100	-0.71965300	0.70595900
C	-0.20354900	2.48123700	1.73132600
C	0.09015400	3.29674000	2.80242700
H	0.86782600	3.12454100	3.53095500
C	-0.82248600	4.37608100	2.76028300
H	-0.88360100	5.19978400	3.45524400
C	-1.64102000	4.19126500	1.66917000
H	-2.46212600	4.78178100	1.30341100
N	-1.27440700	3.02822700	1.04704600
C	0.39001400	1.21763700	1.25373600
O	1.31334500	1.37592900	0.11356500
C	1.13974800	0.44992500	2.33049800
F	1.65078400	-0.67913200	1.82446500
F	0.31900900	0.11381100	3.33203400
F	2.14830000	1.16257700	2.83606400
C	-1.74681700	2.43795400	-0.19627900
H	-0.99268800	2.63125000	-0.97037200
C	-3.08477000	2.97612600	-0.69864000
O	-3.85247200	3.56472600	0.03094500
C	-3.44854100	2.66864500	-2.11909900
C	-2.55379800	2.13246700	-3.05396900
C	-4.76792900	2.93621000	-2.50326800
C	-2.97742300	1.87493400	-4.35392300
H	-1.52437600	1.90583700	-2.79207800
C	-5.18758000	2.67492400	-3.80029000
H	-5.44763400	3.34762700	-1.76480400
C	-4.29126900	2.14507600	-4.72801400
H	-2.27832100	1.46267100	-5.07324400
H	-6.21214900	2.88339700	-4.08975200
H	-4.61764600	1.94094100	-5.74271000

TS7RR

C	-1.80841900	-0.91132600	0.15537800
C	-0.41208700	-0.48388900	0.58833300
H	-1.94948400	-0.45954400	-0.83066600
C	-2.95100300	-0.48097000	1.05685000
C	-4.19400600	-0.20808600	0.47453700
C	-2.81970800	-0.34683200	2.44144200
C	-5.28164200	0.17059500	1.25364700
H	-4.30695400	-0.28646900	-0.60451800
C	-3.90749100	0.03607800	3.22314300
H	-1.86461700	-0.52115600	2.92718500
C	-5.14172500	0.29055600	2.63387200
H	-6.23583500	0.37900500	0.78069300
H	-3.78419700	0.13971800	4.29639600
H	-5.98730400	0.58915900	3.24475200
C	0.65689300	-0.78839500	-0.54233300
O	0.33768900	-0.62810300	-1.71679800
H	-0.37905000	0.57752000	0.84828700
C	-0.29672900	-2.57465100	1.91784800
C	0.01844600	-3.53273100	2.92336700
H	0.77483800	-3.39760100	3.68247400
C	-0.82435600	-4.60240200	2.74741500
H	-0.87974000	-5.50420900	3.33737600
C	-1.64121500	-4.31802600	1.62542600
H	-2.41312200	-4.92253000	1.17600000
N	-1.33963300	-3.11568900	1.14522500
C	0.18803500	-1.32245400	1.65282500
O	1.70566200	-1.25166600	-0.01838800
C	1.20593000	-0.72939300	2.60326200
F	1.66886400	0.44056400	2.18563000
F	2.22971700	-1.54972200	2.82647600
F	0.59461200	-0.52046300	3.78985800
C	-1.77778400	-2.44884000	-0.08662900
H	-1.01248300	-2.64751900	-0.84536300
C	-3.12200500	-2.95342500	-0.60055700
O	-3.87523800	-3.57929900	0.11736500
C	-3.47792300	-2.60564400	-2.00698100
C	-2.57992300	-2.00667100	-2.90099900
C	-4.78116500	-2.90670000	-2.42195200
C	-2.99308100	-1.72105000	-4.19920500
H	-1.56528500	-1.74277000	-2.60876700
C	-5.18587800	-2.61559000	-3.71669100
H	-5.45892600	-3.36587500	-1.71009400
C	-4.28957800	-2.02367400	-4.60704900

H	-2.29695800	-1.25908500	-4.89069000
H	-6.19677800	-2.84819300	-4.03427600
H	-4.60405600	-1.79549700	-5.62050000

TS7SR

C	-1.72507600	-1.83900200	-1.01204000
C	-0.58922000	-0.82665400	-1.12097400
H	-2.61188900	-1.25031500	-0.75124000
C	-2.00773900	-2.61930100	-2.28351300
C	-3.32351000	-3.00877700	-2.55334600
C	-1.00244900	-2.99163400	-3.17894000
C	-3.62942800	-3.75962500	-3.68376200
H	-4.11821400	-2.70101000	-1.87710300
C	-1.30681400	-3.74238400	-4.31262000
H	0.02705000	-2.68738500	-3.01209500
C	-2.61831000	-4.13169300	-4.56655300
H	-4.65819700	-4.04338100	-3.88122300
H	-0.51394200	-4.01796700	-5.00045200
H	-2.85401000	-4.71261400	-5.45211000
C	-0.56633900	0.22484000	0.09297900
O	-1.64121200	0.62086700	0.52043800
H	-0.66636500	-0.25160800	-2.04764100
C	0.97452700	-2.56698900	-0.31066700
C	2.14176300	-3.33175000	-0.03455400
H	3.14920400	-3.02614400	-0.27594700
C	1.73454000	-4.50304700	0.56382700
H	2.35168400	-5.32212500	0.89896300
C	0.32622600	-4.44996500	0.66386900
H	-0.35991800	-5.17039700	1.08961800
N	-0.11864000	-3.31962100	0.12846200
C	0.76908300	-1.36303200	-0.93524900
C	-1.48097800	-2.80655100	0.17571500
H	-2.14986800	-3.66667300	0.07792100
C	-1.70802600	-2.13632000	1.55091000
O	-0.76581700	-1.94964600	2.28597700
C	-3.10062400	-1.75314300	1.91425900
C	-4.22508800	-2.33988300	1.32753500
C	-3.25866700	-0.77781800	2.90307700
C	-5.50035900	-1.95859900	1.73453700
H	-4.12323100	-3.10615500	0.56436700
C	-4.53155700	-0.39396800	3.30090400
H	-2.36968100	-0.32236800	3.32518000
C	-5.65273900	-0.98561100	2.71871200
H	-6.37222000	-2.42092000	1.28409200

H	-4.65372700	0.37112800	4.06000800
H	-6.64756300	-0.68440100	3.03081000
C	1.95047500	-0.69271900	-1.60367400
O	0.62113900	0.44196700	0.44294500
F	2.99823200	-0.57900300	-0.79249200
F	1.65050700	0.49766000	-2.10243800
F	2.33019500	-1.47636500	-2.63883600

TS7SS

C	-1.87212300	0.87990800	0.04160700
C	-0.49453600	0.39162500	0.46958400
H	-2.02937000	0.44941100	-0.95143100
C	-3.03219000	0.48129100	0.93562300
C	-4.28469200	0.26768300	0.34836500
C	-2.90804100	0.32087800	2.31810500
C	-5.38780500	-0.07781900	1.12119800
H	-4.39307800	0.36629000	-0.72950600
C	-4.01136300	-0.02961500	3.09326700
H	-1.94746100	0.45021600	2.80718400
C	-5.25434900	-0.22449900	2.49943800
H	-6.34925500	-0.24047600	0.64505300
H	-3.89361100	-0.15457500	4.16487000
H	-6.11188900	-0.49832100	3.10523800
C	0.58914100	0.67334300	-0.65294600
O	0.26700300	0.54988100	-1.83101700
H	-0.50240200	-0.67441500	0.71215800
C	-0.30131800	2.45413000	1.83398200
C	0.04687400	3.38255100	2.85627400
H	0.79520200	3.20748900	3.61528200
C	-0.75415600	4.48628000	2.69614800
H	-0.77710500	5.37933800	3.30132300
C	-1.57772600	4.25248300	1.56757700
H	-2.32478200	4.89374700	1.12685000
N	-1.32032400	3.04781700	1.06795200
C	0.13543200	1.18865800	1.54877300
O	1.65461400	1.08239400	-0.11752700
C	1.12874800	0.54197000	2.48994300
F	1.54186900	-0.64077900	2.05589100
F	0.51085400	0.34286300	3.67485800
F	2.18540200	1.31648700	2.72191300
C	-1.78028900	2.41866300	-0.17580000
H	-1.00512900	2.59939600	-0.92910800
C	-3.10069000	2.98469000	-0.68773000
O	-3.82908000	3.63551500	0.03376900

C	-3.46620100	2.66560800	-2.09849400
C	-2.58871100	2.04274700	-2.99648300
C	-4.75680500	3.01785700	-2.51315900
C	-3.00910700	1.78380700	-4.29781200
H	-1.58492300	1.73964100	-2.70478700
C	-5.16913100	2.75261400	-3.81101000
H	-5.41917900	3.49540400	-1.79878800
C	-4.29326600	2.13611500	-4.70496800
H	-2.32865800	1.30310200	-4.99214200
H	-6.17031800	3.02434600	-4.12821200
H	-4.61420100	1.92801200	-5.72073300

TS7RS

C	-2.81743600	-0.31823600	-0.31802200
C	-1.36548700	-0.44997800	-0.77895100
H	-3.38388100	-0.03718200	-1.21335300
C	-3.04518600	0.72935900	0.75810400
C	-4.27584300	1.39169800	0.80185300
C	-2.08740000	1.02998600	1.72872600
C	-4.55021100	2.32362500	1.79724000
H	-5.02138200	1.19168000	0.03550600
C	-2.35938200	1.96488500	2.72525300
H	-1.11287200	0.55111500	1.71785900
C	-3.59115300	2.60983200	2.76585600
H	-5.50784500	2.83353500	1.81011600
H	-1.60194800	2.18846800	3.46920300
H	-3.79934600	3.33897900	3.54160100
C	-1.19543800	-1.28255000	-2.06307300
O	-1.92413500	-1.18236300	-3.04412500
H	-0.92379700	0.54120300	-0.91958100
C	-1.03785000	-2.17580500	0.98978200
C	-0.47789600	-3.01511500	1.99278300
H	0.58009300	-3.13810200	2.17330100
C	-1.52268700	-3.59465900	2.67608200
H	-1.46829500	-4.27549700	3.51135600
C	-2.71736000	-3.12553600	2.08527400
H	-3.74445800	-3.36277800	2.33150900
N	-2.42979300	-2.27830500	1.10426900
C	-0.48106900	-1.31995600	0.07336700
C	-3.35895300	-1.69737000	0.14563100
H	-4.31130000	-1.54915900	0.66296500
C	-3.55596400	-2.70357700	-1.01415900
O	-2.81558400	-3.65844000	-1.09632800
C	-4.65553100	-2.46405400	-1.98971000

C	-5.64712800	-1.49646300	-1.80275400
C	-4.69233000	-3.28181000	-3.12444500
C	-6.65696200	-1.34247000	-2.74821400
H	-5.65562500	-0.86698500	-0.91782700
C	-5.69509400	-3.12049000	-4.07098900
H	-3.92361200	-4.04031700	-3.23720500
C	-6.67662400	-2.14648900	-3.88501300
H	-7.42796700	-0.59447200	-2.59717600
H	-5.72130000	-3.75555100	-4.95090800
H	-7.45737900	-2.01489000	-4.62674600
O	-0.23565200	-2.10622200	-1.87043100
C	1.00111300	-1.01870500	0.16472300
F	1.23287100	-0.36193100	1.31581700
F	1.73461800	-2.12835800	0.17724100
F	1.41563600	-0.23883900	-0.82976900
C	-2.32056500	-2.44745500	-5.84076000
C	-3.05233900	-3.12470500	-6.99815900
H	-2.86995500	-2.55011100	-4.90191700
H	-3.33141300	-4.15544200	-6.73365800
N	-1.04937300	-3.19340000	-5.69880100
O	-2.22419200	-3.11240700	-8.15013100
C	-0.46101200	-3.88210300	-6.72874200
C	-1.15972200	-4.02872700	-8.05219100
H	-0.46337500	-3.82834200	-8.86775500
H	-1.51896500	-5.06386700	-8.14228700
N	0.67302700	-4.40607000	-6.35486600
C	-0.23354000	-3.31051900	-4.64502400
N	0.79583100	-4.03902800	-5.05038300
C	1.93787400	-4.42081000	-4.26185000
C	2.74412000	-3.41259100	-3.72146100
C	2.17361400	-5.78429100	-4.06837400
C	3.83183900	-3.82134100	-2.95378300
C	3.27968000	-6.13303300	-3.29524600
C	4.11612900	-5.16995300	-2.73191800
H	4.47968100	-3.06248600	-2.52230900
H	3.48597200	-7.18626000	-3.12479400
H	-3.95252300	-2.55911300	-7.24163100
C	-2.02673500	-0.96736600	-6.11722100
H	-1.42952800	-0.58387700	-5.28569400
H	-1.44171400	-0.89634000	-7.03944200
C	-3.31316300	-0.18744900	-6.25152800
C	-4.11677600	0.05124100	-5.13199700
C	-3.73666200	0.26550500	-7.50346700
C	-5.31348800	0.75001500	-5.26804800

H	-3.79158400	-0.30699300	-4.15636900
C	-4.93538100	0.96166200	-7.63785800
H	-3.12049000	0.06775300	-8.37725900
C	-5.72492100	1.20814300	-6.51797300
H	-5.92618000	0.93884200	-4.39186100
H	-5.25030200	1.31255900	-8.61528800
H	-6.65700200	1.75491400	-6.61855700
C	5.30513400	-5.56437400	-1.89587900
H	6.22831500	-5.15913100	-2.31941800
H	5.21153400	-5.17002300	-0.87998200
H	5.40567900	-6.64922700	-1.83349200
C	2.46397700	-1.94746700	-3.93547300
H	2.13920500	-1.74087300	-4.95954900
H	1.68592400	-1.59915300	-3.24792700
H	3.36645900	-1.36488800	-3.74387300
C	1.27414900	-6.83909600	-4.65649600
H	0.21886900	-6.58222800	-4.52295300
H	1.45002300	-6.95142000	-5.72958600
H	1.45608700	-7.80036400	-4.17426700
H	-0.36959700	-2.90659500	-3.64056900

TS7RS'

C	-2.76633900	-0.70655000	-0.21543200
C	-1.30546500	-0.87261200	-0.62185100
H	-3.33555000	-0.73817700	-1.15163400
C	-3.08454900	0.58991000	0.50835300
C	-4.36692500	1.13241600	0.37266800
C	-2.16329900	1.24465300	1.32798700
C	-4.72445700	2.29644800	1.04416600
H	-5.08451700	0.64184200	-0.28196800
C	-2.51884000	2.41217000	2.00048500
H	-1.15428600	0.85913900	1.44198700
C	-3.79923500	2.93915400	1.86404000
H	-5.72069100	2.70828500	0.91882600
H	-1.78862100	2.91079100	2.62961100
H	-4.07256000	3.85001700	2.38641900
C	-1.07157600	-2.05123700	-1.68618900
O	-1.92128300	-2.21039700	-2.55117800
H	-0.91782800	0.04747000	-1.06753000
C	-0.89630000	-2.04553800	1.51883900
C	-0.28079900	-2.60223900	2.67414200
H	0.78287000	-2.60715700	2.86143600
C	-1.28369700	-3.09759300	3.47677000
H	-1.18318800	-3.58006100	4.43663300

C	-2.50573500	-2.85550400	2.81017700
H	-3.51398400	-3.10971400	3.10966300
N	-2.27564300	-2.21881300	1.66845900
C	-0.40366800	-1.38059500	0.42543400
C	-3.24384300	-1.92203900	0.62123200
H	-4.18294800	-1.66088900	1.11761700
C	-3.45548300	-3.18760900	-0.24025200
O	-2.71623400	-4.13507600	-0.10771500
C	-4.58233100	-3.17056000	-1.21487700
C	-5.74711200	-2.42767200	-1.00374900
C	-4.45181200	-3.95366700	-2.36545800
C	-6.78129300	-2.47787000	-1.93414800
H	-5.87380900	-1.82511400	-0.10873800
C	-5.48013000	-3.99072500	-3.29687200
H	-3.52248300	-4.49024200	-2.52145700
C	-6.64624600	-3.25645600	-3.08015600
H	-7.69064900	-1.91176300	-1.76238100
H	-5.37296300	-4.58625400	-4.19727500
H	-7.44998200	-3.28928300	-3.80883800
O	-0.01324300	-2.66950500	-1.40921500
C	1.06418700	-1.01021000	0.41080700
F	1.26331800	-0.09746500	1.38920900
F	1.85550100	-2.04634100	0.67330000
F	1.43864000	-0.44969100	-0.72996100

TS7RS''

C	-2.63121900	-0.63354600	-0.37444700
C	-1.19774600	-0.27782100	-0.78124900
H	-3.21900900	-0.56204400	-1.29596700
C	-3.23605800	0.29333300	0.66464300
C	-4.59889300	0.59364100	0.58354000
C	-2.49013200	0.83143800	1.71610100
C	-5.20968800	1.40026000	1.53833600
H	-5.18345000	0.21129400	-0.25019200
C	-3.09952400	1.64234800	2.67060500
H	-1.42386700	0.64090800	1.79660200
C	-4.45993600	1.92348000	2.58858600
H	-6.26697100	1.62894000	1.45494600
H	-2.50536000	2.05786100	3.47777100
H	-4.93101400	2.55692900	3.33266900
C	-0.74011700	-1.00278900	-2.05304500
O	-1.46433200	-1.08209000	-3.05453500
H	-1.10122300	0.80555200	-0.90120100
C	-0.38998500	-1.80787800	1.01905600

C	0.37683900	-2.40575400	2.05896800
H	1.41197100	-2.17892200	2.26933700
C	-0.45077400	-3.27285800	2.73449000
H	-0.20894600	-3.88170000	3.59185700
C	-1.71381200	-3.22039800	2.10224200
H	-2.61882600	-3.76698700	2.33277200
N	-1.67943800	-2.34673900	1.10333600
C	-0.11061200	-0.82801000	0.10305700
C	-2.71243400	-2.11076700	0.10455600
H	-3.67847600	-2.27172400	0.59185600
C	-2.53927500	-3.15119700	-1.02992300
O	-1.50584300	-3.78267100	-1.09693300
C	-3.66039800	-3.35973200	-1.98541100
C	-4.88562300	-2.69396800	-1.87904700
C	-3.46193700	-4.28416900	-3.01764500
C	-5.89137100	-2.93233100	-2.80990500
H	-5.07353900	-1.99257700	-1.07177900
C	-4.46593500	-4.51816800	-3.94667700
H	-2.51568200	-4.81485700	-3.06891600
C	-5.67997800	-3.83821800	-3.84630800
H	-6.83963700	-2.41314500	-2.72500100
H	-4.30553200	-5.23368800	-4.74673900
H	-6.46534200	-4.02008500	-4.57251600
O	0.38628000	-1.54406700	-1.84382600
C	1.19618600	-0.07133700	0.22139000
F	1.15448300	0.66270800	1.34823800
F	2.23883800	-0.89328200	0.31013200
F	1.38405100	0.76133500	-0.79428900
C	-1.29483200	-3.69986600	-5.46227500
C	-1.08095900	-4.96045000	-5.95098200
C	-0.19358800	-5.84227900	-5.26782300
C	0.42528000	-5.34136100	-4.08780100
C	0.16279400	-4.06499600	-3.66417100
H	-1.97172200	-3.00041500	-5.93824300
H	-1.59182800	-5.26081400	-6.85460300
H	1.10737000	-5.94659500	-3.50806300
H	0.59322500	-3.62425000	-2.77156100
C	0.95595700	-7.96237200	-4.99260400
C	-0.61910900	-7.56649300	-6.92323800
H	0.59521300	-8.15509400	-3.97721200
H	1.02522100	-8.91145800	-5.51918700
H	1.95701400	-7.52370600	-4.93826600
H	-1.70744600	-7.55923100	-6.80508300
H	-0.35025700	-6.95345000	-7.78906100

H	-0.30246600	-8.58917800	-7.11520000
N	0.04149900	-7.08580900	-5.71535200
N	-0.68023600	-3.26556300	-4.34641500
H	-0.92097100	-2.32072200	-3.93980100

TS7RS'''

C	4.16233000	-0.36017000	0.36587200
C	5.28144700	0.11736700	1.28528100
H	3.55906100	-1.10965900	0.87258800
H	4.88303300	0.31257600	2.29128300
N	3.29853800	0.81481500	0.11795200
O	5.89761600	1.28445000	0.76396300
C	3.71020900	2.10534700	0.30518000
C	5.05610600	2.40487400	0.89973900
H	5.51437200	3.24348400	0.37385000
H	4.92946000	2.67660200	1.95786300
N	2.79566600	2.95011300	-0.07460400
C	2.05938200	0.86932900	-0.41150000
N	1.77839700	2.16602100	-0.53116000
C	0.57043900	2.79790600	-0.99091200
C	0.36412300	2.92948800	-2.36790100
C	-0.26609800	3.36505700	-0.02849000
C	-0.77944000	3.61419900	-2.76899900
C	-1.39006100	4.05030300	-0.48679200
C	-1.66324400	4.17873000	-1.84625100
H	-0.97308500	3.72947500	-3.83274700
H	-2.07147300	4.48369400	0.24028300
H	6.04834500	-0.65683700	1.34938600
C	4.66550300	-0.92734900	-0.96743900
H	3.81425700	-1.00429000	-1.65279800
H	5.39327400	-0.23271200	-1.40016400
C	5.26610200	-2.29444800	-0.75105800
C	4.41883600	-3.37747700	-0.49127600
C	6.64694700	-2.49265000	-0.75606600
C	4.95062500	-4.63898800	-0.24615100
H	3.34215700	-3.21406400	-0.48696600
C	7.17928400	-3.75702600	-0.50920800
H	7.30778800	-1.65286000	-0.95835400
C	6.33199500	-4.83115900	-0.25426800
H	4.28623500	-5.47515900	-0.05147800
H	8.25492800	-3.90176300	-0.51910700
H	6.74571400	-5.81659800	-0.06513500
C	-2.86664900	4.94927400	-2.32228600
H	-2.57335600	5.94373200	-2.67441900

H	-3.35583000	4.43600100	-3.15464800
H	-3.59662800	5.07158700	-1.51934500
C	1.35909000	2.41027900	-3.37032700
H	2.37153900	2.74376700	-3.11960400
H	1.35374200	1.31835800	-3.38750000
H	1.11783600	2.78147200	-4.36767700
C	0.05578400	3.31633800	1.44162000
H	0.61904800	2.42109200	1.71401900
H	0.65902600	4.18522800	1.72455000
H	-0.86688600	3.33506300	2.02592200
C	-1.68539800	-0.38991100	-0.00881300
C	-0.41339900	-0.21742400	0.76815200
H	-1.46037700	-0.61812400	-1.06513600
C	-2.60365100	0.81257400	0.03990800
C	-3.28644100	1.22429600	-1.10595800
C	-2.90223500	1.43615500	1.25552800
C	-4.26994400	2.20769900	-1.03570200
H	-3.06440100	0.74279500	-2.05545200
C	-3.87186400	2.43245100	1.32794500
H	-2.38652800	1.11524100	2.15794800
C	-4.56812700	2.81377500	0.18188600
H	-4.80753200	2.49798600	-1.93357400
H	-4.09596300	2.90002100	2.28260700
H	-5.33895300	3.57673100	0.23940600
C	1.26705100	-0.34390500	-0.87166700
O	0.74382800	-0.30449800	-1.96357100
H	-0.34435500	0.59342600	1.48036700
C	-0.27783100	-2.70278500	0.87560700
C	0.20286700	-3.99146500	1.01417500
H	1.22878200	-4.25252600	1.22774200
C	-0.88190600	-4.87083100	0.80005600
H	-0.86051500	-5.95028400	0.82071200
C	-1.98963700	-4.09388000	0.53517800
H	-3.00491500	-4.37412400	0.30017200
N	-1.61826200	-2.78195300	0.57099500
C	0.37273900	-1.38755400	1.01329600
C	-2.50550700	-1.63054300	0.49348400
H	-2.88194800	-1.40988800	1.49706100
C	-3.63981700	-1.89780200	-0.49455500
O	-3.39251000	-2.47238800	-1.53718900
C	-5.01631000	-1.36747400	-0.22909100
C	-5.41550200	-0.80512700	0.98655900
C	-5.92762300	-1.42214500	-1.29074200
C	-6.70167100	-0.29175200	1.12963000

H	-4.73325100	-0.74804900	1.82639800
C	-7.20998600	-0.91254200	-1.14586100
H	-5.59918500	-1.86151700	-2.22662400
C	-7.59764700	-0.34102500	0.06615000
H	-7.00133700	0.15004600	2.07439100
H	-7.90741600	-0.95463400	-1.97617200
H	-8.59787000	0.06483900	0.18084800
O	1.57547400	-1.45724700	-0.18546300
C	1.25033100	-1.29649800	2.24526600
F	0.52933000	-1.42953200	3.36192200
F	2.21915300	-2.22762400	2.28481000
F	1.87797900	-0.09886200	2.32387400

TS7RS'''

C	4.22864500	-0.38511700	0.00937000
C	5.50450700	0.12427000	0.67818300
H	3.69931800	-1.05545000	0.68362300
H	5.31214800	0.36916100	1.73208400
N	3.35282600	0.79319500	-0.19842300
O	6.01608100	1.25523300	-0.00408500
C	3.79437000	2.08574900	-0.12485500
C	5.21945600	2.39145000	0.23487800
H	5.58797700	3.20648600	-0.38909700
H	5.27304100	2.69865800	1.28894500
N	2.84063800	2.92485600	-0.40930200
C	2.05507000	0.84382400	-0.56824900
N	1.76541600	2.13603800	-0.68894000
C	0.51645100	2.77575500	-1.01485500
C	0.16379800	2.89803100	-2.36287400
C	-0.18947200	3.38141400	0.02599700
C	-0.98656000	3.62806000	-2.64726100
C	-1.32932400	4.10737600	-0.31755400
C	-1.73612300	4.24530900	-1.64245100
H	-1.28876000	3.74408900	-3.68518100
H	-1.90961000	4.57637800	0.47302400
H	6.26323500	-0.65969200	0.62885800
C	4.48940700	-1.06981100	-1.33707200
H	3.55167400	-1.08684500	-1.90506800
H	5.20267300	-0.46336300	-1.90588600
C	5.00390100	-2.48333100	-1.17649400
C	4.30657400	-3.41323600	-0.39437600
C	6.16315200	-2.89460000	-1.83673700
C	4.75747600	-4.72704300	-0.29025200
H	3.40197600	-3.10804500	0.12726300

C	6.61203900	-4.20960600	-1.73633900
H	6.71558300	-2.17985600	-2.44068200
C	5.90854800	-5.13083600	-0.96512700
H	4.20754400	-5.43599400	0.32221300
H	7.51375300	-4.51179500	-2.25901900
H	6.26122000	-6.15374300	-0.88119400
C	-2.93675800	5.08269100	-1.99647700
H	-2.62506800	6.08705600	-2.30098500
H	-3.49146500	4.64238000	-2.82904900
H	-3.61249500	5.18050300	-1.14425600
C	1.02608000	2.32645200	-3.45560000
H	2.05993200	2.67204100	-3.34922400
H	1.02616800	1.23455700	-3.41823200
H	0.66150600	2.64859400	-4.43200100
C	0.27707800	3.33121200	1.45747000
H	0.92589000	2.47615300	1.66335000
H	0.84343800	4.23579000	1.70007200
H	-0.58396100	3.28104400	2.12872700
C	-1.62614100	-0.28747200	-0.06219100
C	-0.32803100	-0.17506200	0.68682000
H	-1.41839100	-0.38404000	-1.14200700
C	-2.55420000	0.89484800	0.13093700
C	-3.31749300	1.36234900	-0.93909200
C	-2.76786500	1.43945200	1.40150500
C	-4.29560000	2.33437600	-0.74315700
H	-3.15805400	0.94298100	-1.92996100
C	-3.73163100	2.42531300	1.59729100
H	-2.18546300	1.07285300	2.24392400
C	-4.50539600	2.86873500	0.52500900
H	-4.89335500	2.67465600	-1.58317000
H	-3.88765500	2.83887700	2.58908700
H	-5.26724100	3.62674500	0.67851800
C	1.21525000	-0.38892600	-0.86771100
O	0.64996600	-0.45833600	-1.95924900
H	-0.15243900	0.71883800	1.27121500
C	-0.25227600	-2.64777500	0.88991400
C	0.21020700	-3.94327200	1.05547900
H	1.20659500	-4.21632000	1.37008100
C	-0.84542500	-4.81250000	0.71092800
H	-0.83194400	-5.89216900	0.72377900
C	-1.91900000	-4.02534500	0.34208600
H	-2.91497500	-4.30089200	0.02708800
N	-1.54944100	-2.71666100	0.43172000
C	0.39241700	-1.34781000	1.04041200

C	-2.43661800	-1.56364200	0.31810300
H	-2.92580100	-1.41258500	1.28490000
C	-3.44810200	-1.83714900	-0.80207400
O	-3.01466900	-2.24556400	-1.86729700
C	-4.90210200	-1.59848700	-0.60438100
C	-5.41982400	-0.87930300	0.47917800
C	-5.77190300	-2.10339600	-1.57985200
C	-6.79086800	-0.66952400	0.57940800
H	-4.76356300	-0.44362000	1.22564600
C	-7.14060900	-1.90647500	-1.46710200
H	-5.35139300	-2.64742300	-2.41882000
C	-7.65078700	-1.18735500	-0.38634200
H	-7.18700900	-0.09810000	1.41198200
H	-7.81147500	-2.30685500	-2.21961100
H	-8.72068100	-1.02724700	-0.29919400
O	1.66540800	-1.47444300	-0.20687900
C	1.33001600	-1.21910300	2.22124300
F	0.64883500	-1.25646400	3.36798800
F	2.25812100	-2.18699000	2.27077400
F	1.99817800	-0.04653600	2.18945000
C	-0.84707700	-4.20857800	-2.75531000
C	-0.50880700	-5.50282400	-3.04728500
C	0.83419500	-5.94532100	-2.88580100
C	1.77362200	-4.98516000	-2.41776800
C	1.36593100	-3.70799500	-2.15173400
H	-1.85326900	-3.82127600	-2.84812600
H	-1.28419600	-6.17063900	-3.39403000
H	2.81509300	-5.22853400	-2.25502100
H	2.02644900	-2.94233000	-1.76667200
C	2.58806300	-7.61806500	-2.98208400
C	0.21467600	-8.16760800	-3.64308300
H	2.90475800	-7.49110500	-1.94160700
H	2.68219800	-8.66931700	-3.24531700
H	3.25417400	-7.03625100	-3.62697300
H	-0.58640600	-8.30928000	-2.91074500
H	-0.22298900	-7.83706200	-4.59037700
H	0.70400000	-9.12524000	-3.80603200
N	1.19987000	-7.20821300	-3.15921100
N	0.08277400	-3.33201500	-2.32552300
H	-0.15969600	-2.35929500	-2.11332000

PRR

C	-1.74242300	-0.95728400	0.17796400
C	-0.51106700	-0.42506000	0.86219900

H	-1.78425400	-0.54062700	-0.83325000
C	-3.01498000	-0.52949000	0.89749800
C	-4.05760800	0.04915300	0.17085300
C	-3.17950200	-0.74881300	2.26821900
C	-5.24856000	0.40377600	0.79996000
H	-3.93716400	0.21710700	-0.89706200
C	-4.37066100	-0.39819100	2.89503800
H	-2.37386000	-1.19394900	2.84538100
C	-5.40732400	0.17862600	2.16385000
H	-6.04924600	0.85660600	0.22384500
H	-4.48964200	-0.57564400	3.95903000
H	-6.33419100	0.45258600	2.65752800
H	-0.22893900	0.60596700	0.68016900
C	-0.21122000	-2.55276300	2.00459600
C	0.20178900	-3.47339900	2.94549700
H	0.94268300	-3.29741200	3.71143500
C	-0.54219800	-4.65774600	2.72005600
H	-0.48490100	-5.57656200	3.28421800
C	-1.38244200	-4.42633700	1.65497400
H	-2.10990800	-5.06513200	1.18372500
N	-1.19894900	-3.13378900	1.23434900
C	0.17577000	-1.18335700	1.72364200
C	1.36674900	-0.64883900	2.45932400
F	1.65196500	0.61337100	2.11590600
F	2.46272400	-1.38705300	2.22462000
F	1.16826800	-0.66825300	3.78885800
C	-1.65525400	-2.50634800	0.00471800
H	-0.91412700	-2.71214400	-0.77885900
C	-3.02332800	-3.01410600	-0.45187600
O	-3.74594600	-3.64584100	0.28763400
C	-3.48135300	-2.61868600	-1.82189200
C	-2.61604400	-2.18664400	-2.83215000
C	-4.85720300	-2.67637200	-2.06929500
C	-3.12407800	-1.81605700	-4.07385000
H	-1.54354100	-2.14655100	-2.66976500
C	-5.36249500	-2.29861900	-3.30588600
H	-5.51088100	-3.00892200	-1.26990100
C	-4.49544200	-1.86742400	-4.30970600
H	-2.44821400	-1.48805700	-4.85637400
H	-6.43107000	-2.33654800	-3.48939100
H	-4.88918400	-1.57093900	-5.27662900

PRS

C	-1.87489600	-0.57429100	-0.29901700
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C	-0.76755000	-0.24543000	0.66975800
H	-1.42596700	-0.95277600	-1.22733700
C	-2.73680000	0.62970800	-0.62817100
C	-3.13204800	0.88867000	-1.94159700
C	-3.17554200	1.47847200	0.39216400
C	-3.94554200	1.98152000	-2.23081800
H	-2.80270000	0.22415100	-2.73531200
C	-3.98992800	2.56967300	0.10489900
H	-2.86970500	1.28562100	1.41832600
C	-4.37559200	2.82409800	-1.20921000
H	-4.24141200	2.17542200	-3.25691000
H	-4.32017500	3.22269200	0.90640900
H	-5.00715700	3.67685200	-1.43649200
H	-0.36671700	0.76277900	0.66973100
C	-0.77789400	-2.53774600	1.47784100
C	-0.34379600	-3.72708600	2.02913400
H	0.56324400	-3.85737400	2.60050300
C	-1.28690800	-4.72161100	1.67144900
H	-1.24864300	-5.77135700	1.92102900
C	-2.26605300	-4.11250100	0.91894800
H	-3.15258300	-4.52117800	0.45674500
N	-1.94436400	-2.78658700	0.78953800
C	-0.25910300	-1.18166600	1.47876500
C	-2.76591200	-1.70549100	0.25115700
H	-3.38544500	-1.29128200	1.05661900
C	-3.66410300	-2.25484700	-0.87639700
O	-3.23100100	-2.30450500	-2.00868700
C	-5.04714400	-2.70712800	-0.55232900
C	-5.49388100	-2.88073800	0.76189300
C	-5.90798900	-2.98369300	-1.62090000
C	-6.79049200	-3.32469500	1.00173000
H	-4.83102100	-2.69595200	1.60192000
C	-7.20417100	-3.41522200	-1.37835200
H	-5.53735600	-2.84879500	-2.63139000
C	-7.64575700	-3.58550100	-0.06581800
H	-7.13262100	-3.46603300	2.02122400
H	-7.87201100	-3.62168600	-2.20797000
H	-8.65884500	-3.92538500	0.12431700
C	0.86215400	-0.87569800	2.42366100
F	0.49182200	-1.05737800	3.70121100
F	1.91707800	-1.68135400	2.21252300
F	1.29309100	0.38672600	2.30781100

PSR

C	-0.97119800	-1.29146900	-1.17726600
C	0.33307900	-1.65242900	-1.84208300
H	-0.85281000	-0.31461400	-0.68864700
C	-2.12756600	-1.20774800	-2.15476500
C	-3.05103300	-0.16387900	-2.07296900
C	-2.30393300	-2.19423300	-3.12952300
C	-4.12839000	-0.10354300	-2.95280300
H	-2.92304300	0.59848600	-1.30996800
C	-3.38086800	-2.13553000	-4.00927500
H	-1.58727400	-3.00932200	-3.20419600
C	-4.29561700	-1.08867400	-3.92265300
H	-4.83701500	0.71530900	-2.88096000
H	-3.50416400	-2.90573200	-4.76387000
H	-5.13452500	-1.04077100	-4.60936900
H	0.47840600	-1.37220900	-2.88022200
C	1.13052100	-2.62338800	0.23843900
C	1.98933700	-3.04891000	1.23257300
H	3.05598700	-3.17850000	1.12409000
C	1.21197500	-3.24303300	2.40061400
H	1.56650000	-3.55805100	3.37048200
C	-0.09284200	-2.93461500	2.08599500
H	-0.98457700	-2.94778000	2.69542300
N	-0.13545900	-2.54222500	0.77353800
C	1.30885300	-2.25680200	-1.15505500
C	-1.30948800	-2.29986700	-0.06101600
H	-1.61636400	-3.24221600	-0.53205300
C	-2.45397600	-1.74832600	0.81303100
O	-2.51020500	-0.55688100	1.03469200
C	-3.46921700	-2.69163800	1.36173100
C	-3.28331100	-4.07813700	1.36230700
C	-4.63222000	-2.14621600	1.91733600
C	-4.25406500	-4.90884000	1.91324100
H	-2.37408600	-4.51588800	0.96118800
C	-5.60517800	-2.97826300	2.45303300
H	-4.75194500	-1.06805300	1.91311900
C	-5.41554700	-4.36058700	2.45134700
H	-4.10316500	-5.98285900	1.92148500
H	-6.51072500	-2.55425300	2.87374000
H	-6.17448100	-5.01199200	2.87274700
C	2.62753200	-2.58339100	-1.78532300
F	3.64505200	-2.01801200	-1.11286300
F	2.70437500	-2.16264500	-3.05385600

F	2.85808000	-3.90648400	-1.78631800
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PSS

C	-1.80788300	0.92302300	0.06461000
C	-0.59525700	0.33302000	0.73449100
H	-1.86845100	0.52745800	-0.95399100
C	-3.09476400	0.53208100	0.77956300
C	-4.15954500	0.00588200	0.04535000
C	-3.24921900	0.73317300	2.15430100
C	-5.36198000	-0.31517100	0.67068100
H	-4.04704100	-0.14918300	-1.02541100
C	-4.45153600	0.41582700	2.77746300
H	-2.42659000	1.13560300	2.73865000
C	-5.51027300	-0.10854500	2.03863700
H	-6.17978600	-0.72720400	0.08802000
H	-4.56180200	0.57820700	3.84481500
H	-6.44595900	-0.35639100	2.52943200
H	-0.34776500	-0.70250700	0.52911100
C	-0.22045700	2.42458000	1.92116500
C	0.22073700	3.30887100	2.88389200
H	0.95241000	3.08994400	3.64763600
C	-0.48235000	4.52244800	2.68407200
H	-0.39601900	5.42590500	3.26899700
C	-1.32701500	4.34405300	1.61225900
H	-2.03064100	5.01856200	1.15504900
N	-1.18623900	3.05619100	1.16248900
C	0.11911800	1.04892700	1.60999500
C	1.29650100	0.45936400	2.32508700
F	1.52550500	-0.80972300	1.96549200
F	1.11627300	0.47270100	3.65727800
F	2.41837200	1.15519500	2.08279700
C	-1.66040100	2.47010600	-0.08043900
H	-0.90745400	2.66053500	-0.85654500
C	-3.00529800	3.03744600	-0.53516100
O	-3.70844300	3.68341100	0.21084500
C	-3.47000300	2.68206500	-1.91387200
C	-2.61568800	2.23596700	-2.92737400
C	-4.84161900	2.79312100	-2.16663300
C	-3.13036500	1.90380800	-4.17710800
H	-1.54610200	2.15499400	-2.76117100
C	-5.35387500	2.45356900	-3.41137400
H	-5.48690200	3.13562200	-1.36465300
C	-4.49778800	2.00798600	-4.41830900
H	-2.46255000	1.56500500	-4.96191900

H	-6.41952100	2.53293100	-3.59884200
H	-4.89707300	1.74226000	-5.39191000