

Supporting Information

**Mechanisms, Regio- and Stereoselectivities for NHC-Catalyzed [3+3]
Annulations for the Synthesis of Axially and Centrally Chiral
Dihydropyridinones**

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1. Computational Details:

(1) 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:

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

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

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

2. Test calculations of stereoselective transition states.

Table S1 Different computational levels.

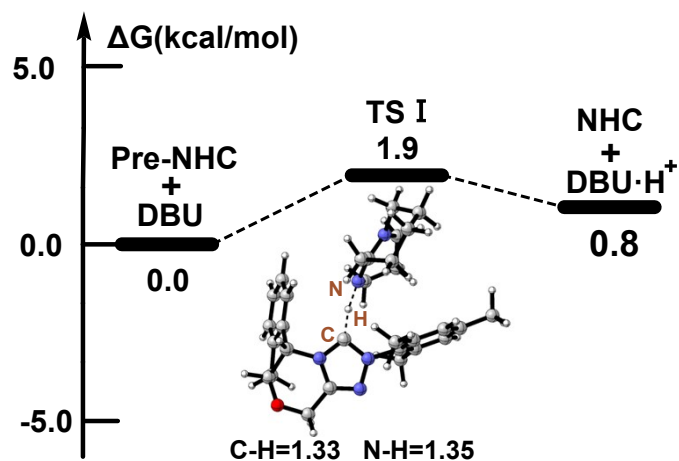
Level	Functional	Basis set	Solvent model
L1	M06-2X-D3	6-311++G(2df,2pd)	IEFPCM
L2	M06-2X-D3	6-311++G(d, p)	IEFPCM
L3	M06-2X-D3	6-31G(d, p)	IEFPCM
L4	ω B97X-D	6-311++G(2df,2pd)	IEFPCM
L5	B3LYP-D3	6-311++G(2df,2pd)	IEFPCM
L6	M06-2X-D3	6-311++G(2df,2pd)	SMD

Table S2 Comparison of relative energies for stereoselective transition states at different levels. Energies are given in kcal/mol.

species	L1	L2	L3	L4	L5	L6
TS5(RR)	1.7	2.0	1.9	1.4	0.9	0.6
TS5(RS)	4.5	8.5	8.6	8.1	6.8	4.0
TS5(SR)	1.4	1.5	1.1	1.8	0.8	0.8
TS5(SS)	0.0	0.0	0.0	0.0	0.0	0.0

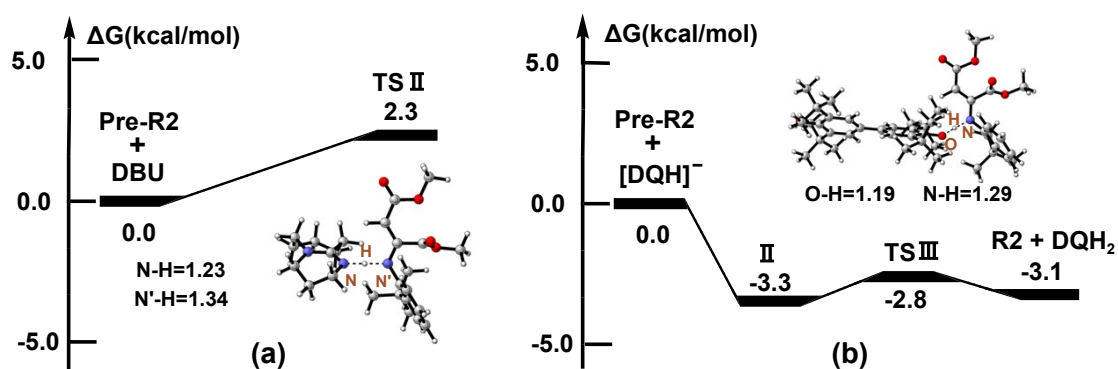
3. List of Figures

Fig. S1 The deprotonation of Pre-NHC by base (DBU) generating NHC (distance in Å and energies in kcal/mol).



It is noteworthy that Pre-NHC was first deprotonated by the base (DBU) to generate the active catalyst NHC. As shown in Fig. S1, the proton H is transferred from the C atom of Pre-NHC to the N atom of DBU via the transition state TSI with an energy barrier of 1.9 kcal/mol, which occurs readily under experimental conditions.

Fig. S2 The deprotonation of Pre-R2 by base generating R2 (distance in Å and energies in kcal/mol).



Pre-R2 is deprotonated by DBU/[DQH]⁻ to form R2, as depicted in Fig. S2. This process proceeds via transition state TSII/TSIII with an energy barrier of 2.3/0.5 kcal/mol. Clearly, the [DQH]⁻ mediated deprotonation pathway is energetically more favorable.

Fig. S3 Optimized geometries of transition states and intermediates (distance in Å).

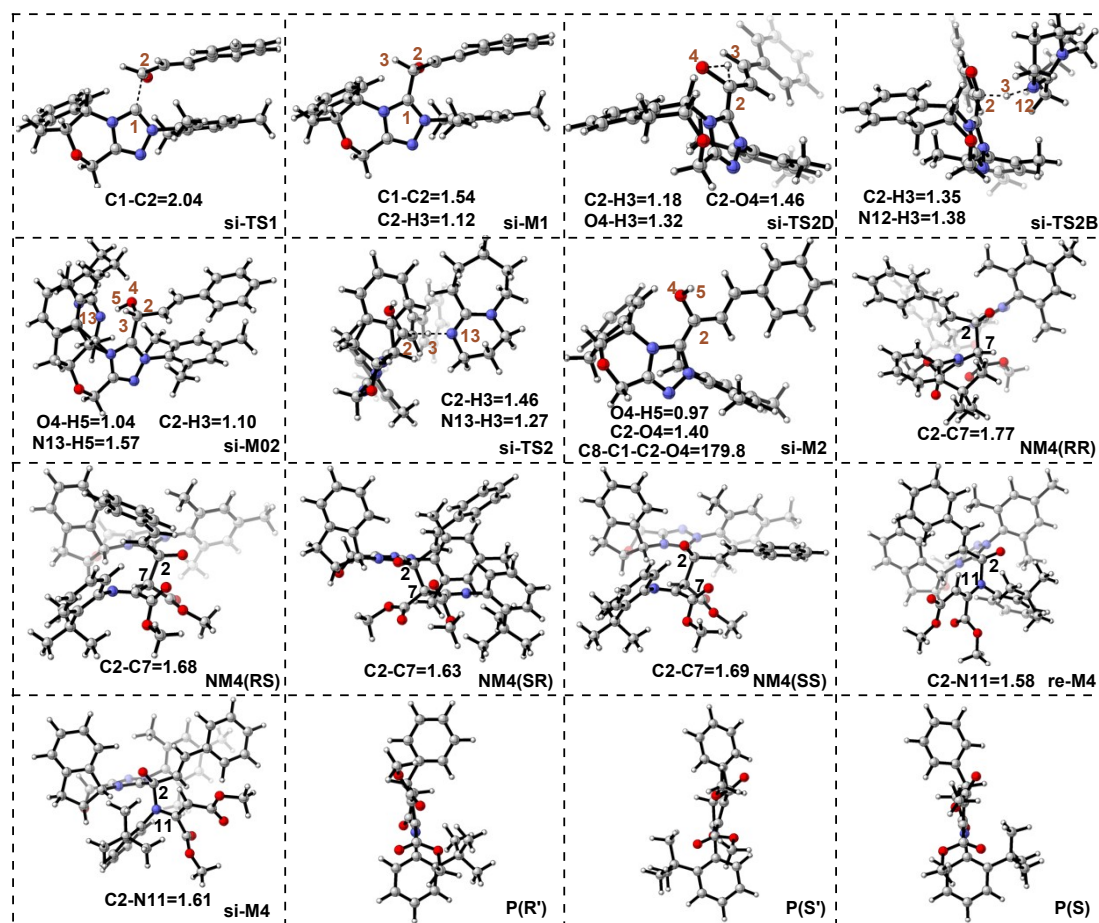
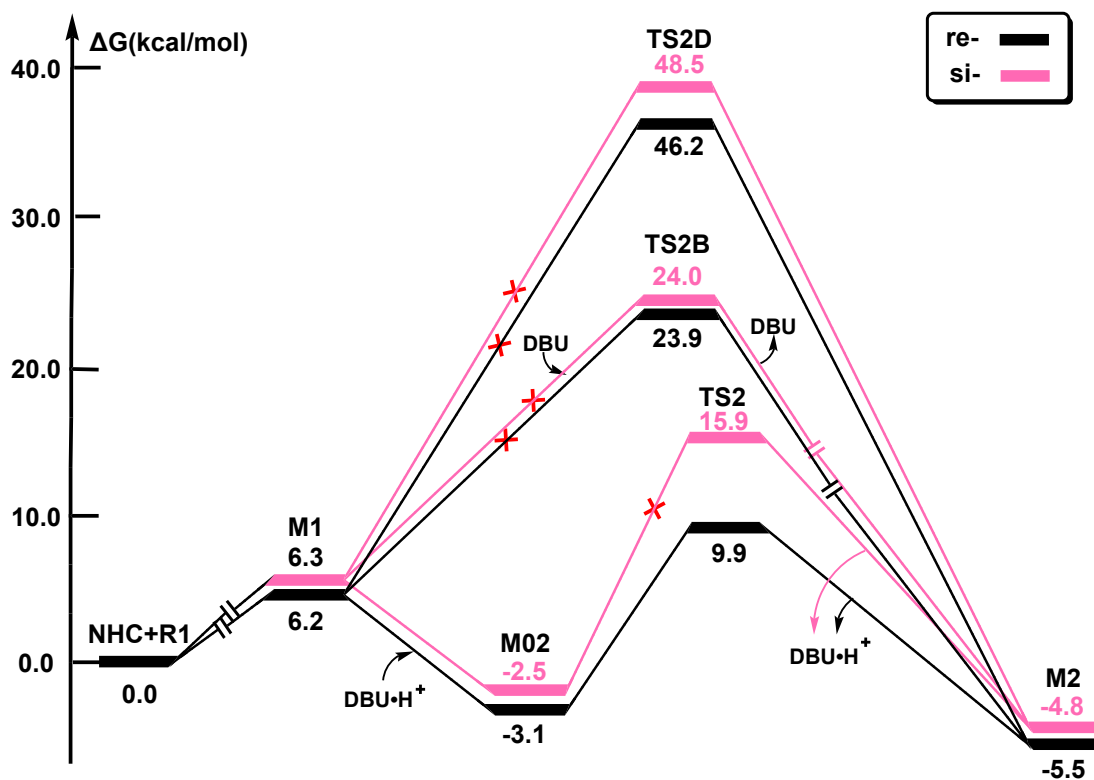
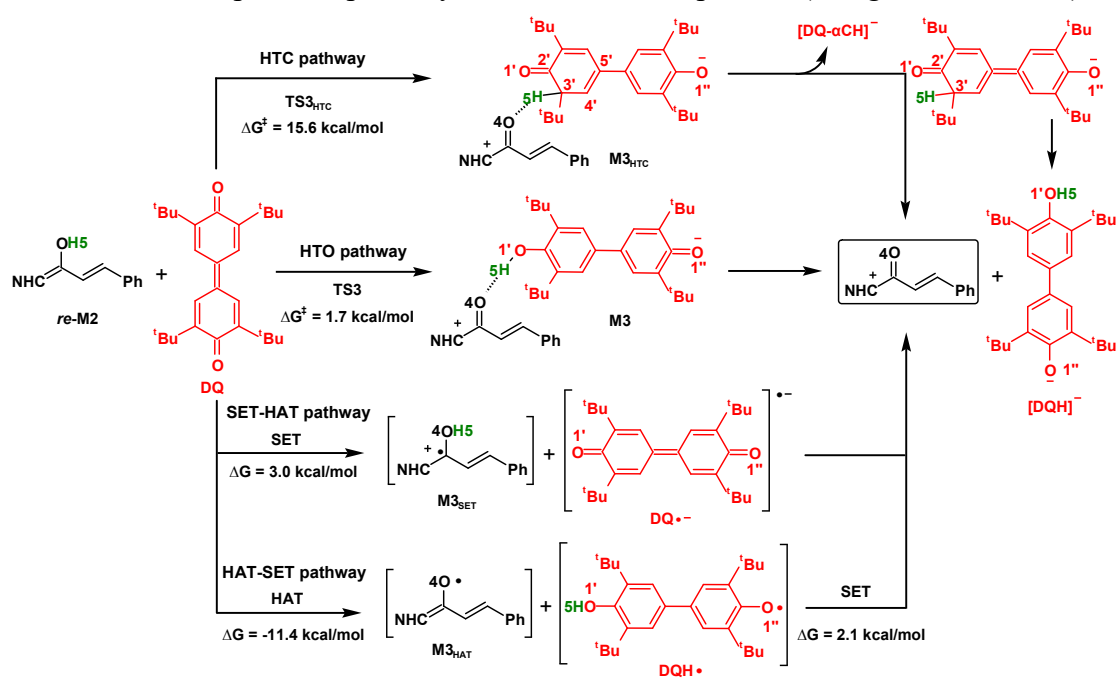


Fig. S4 Free energy profiles of possible mechanisms for M1→M2 conversion (energies in kcal/mol).



Scheme S1 Four possible pathways for the oxidation process (energies in kcal/mol).



Scheme S2 The other possible HTC pathways for the oxidation process (energies in kcal/mol).

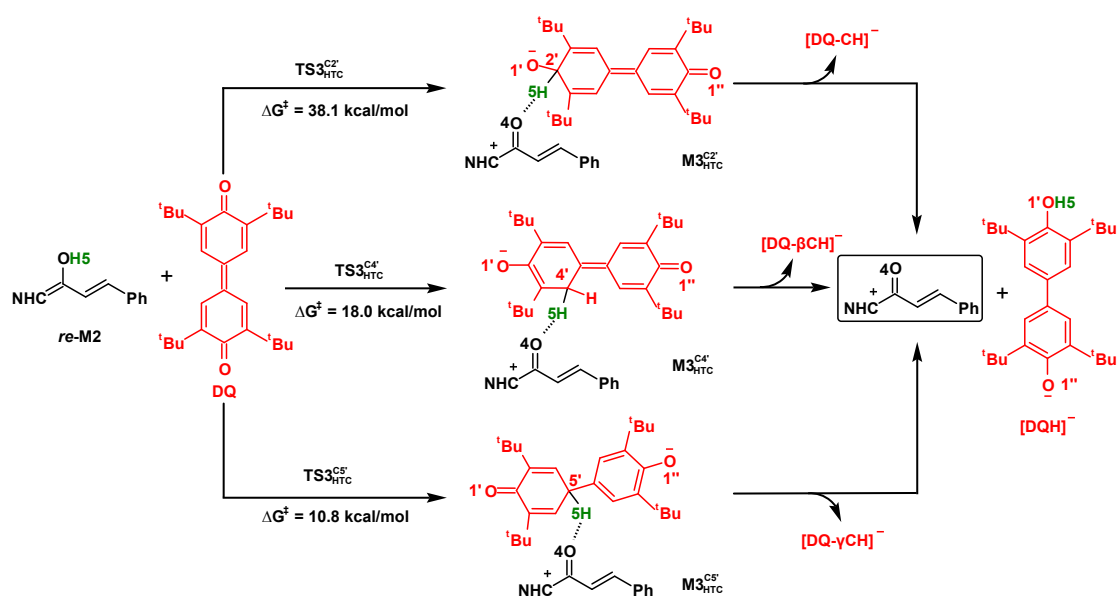


Fig. S5 Conformational search for TS4.

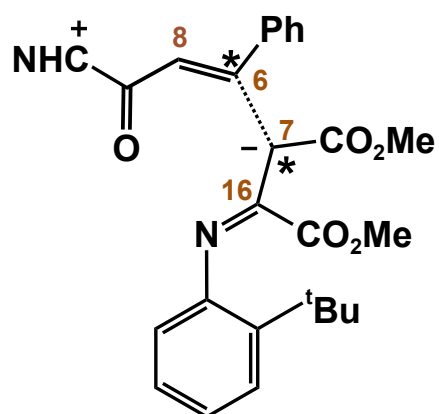


Table S3 Energies of different conformations.

species	Dihedral angle C8-C6-C7-C16	Free energies (a.u.)	relative energies (kcal/mol)
TS4(RR)	-53.57	-1474.758704	1.7
TS4(RR)'	-8.66	-1474.746191	9.5
TS4(RR)"	55.41	-1474.745815	9.8
TS4(RR)'''	-175.20	-1474.752899	5.3
TS4(RS)	-172.97	-1474.748809	7.9
TS4(RS)'	77.08	-1474.746922	9.3
TS4(RS)"	-49.97	-1474.74092	12.8
TS4(RS)'''	-101.49	-1474.741748	12.3
TS4(SR)	-70.89	-1474.759131	1.4
TS4(SR)'	46.14	-1474.753252	5.1
TS4(SR)"	106.03	-1474.749968	7.2
TS4(SR)'''	171.90	-1474.750319	6.9
TS4(SS)	15.29	-1474.761367	0.0
TS4(SS)'	53.35	-1474.757052	2.7
TS4(SS)"	-84.54	-1474.746867	9.1
TS4(SS)'''	-179.54	-1474.750314	6.9

Fig. S6 Free energy profiles for transformation from intermediate M04 to product P (energies in kcal/mol).

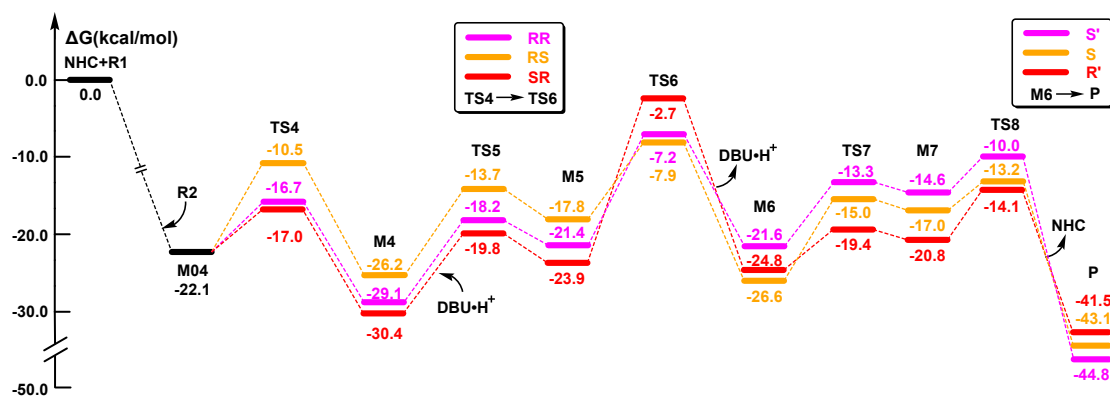


Fig. S7 Free energy profiles of possible mechanisms for **M4** → **M6** conversion (energies in kcal/mol).

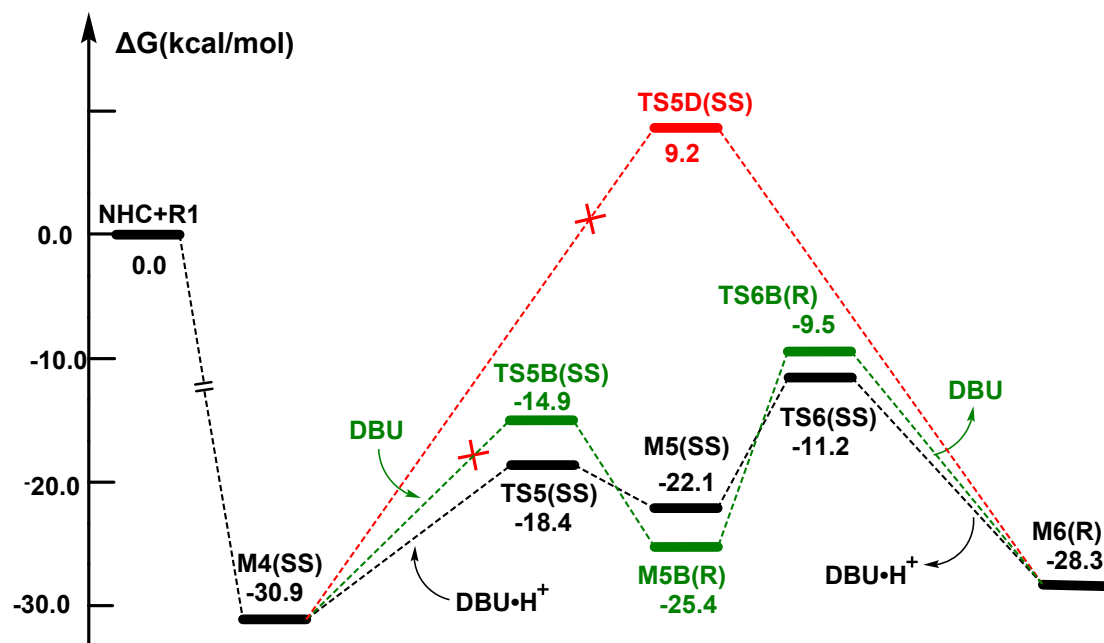


Fig. S8 Free energy profile for the C2-C7 bond formation pathway in the **R2** and **M3** addition reaction (distance in Å and energies in kcal/mol).

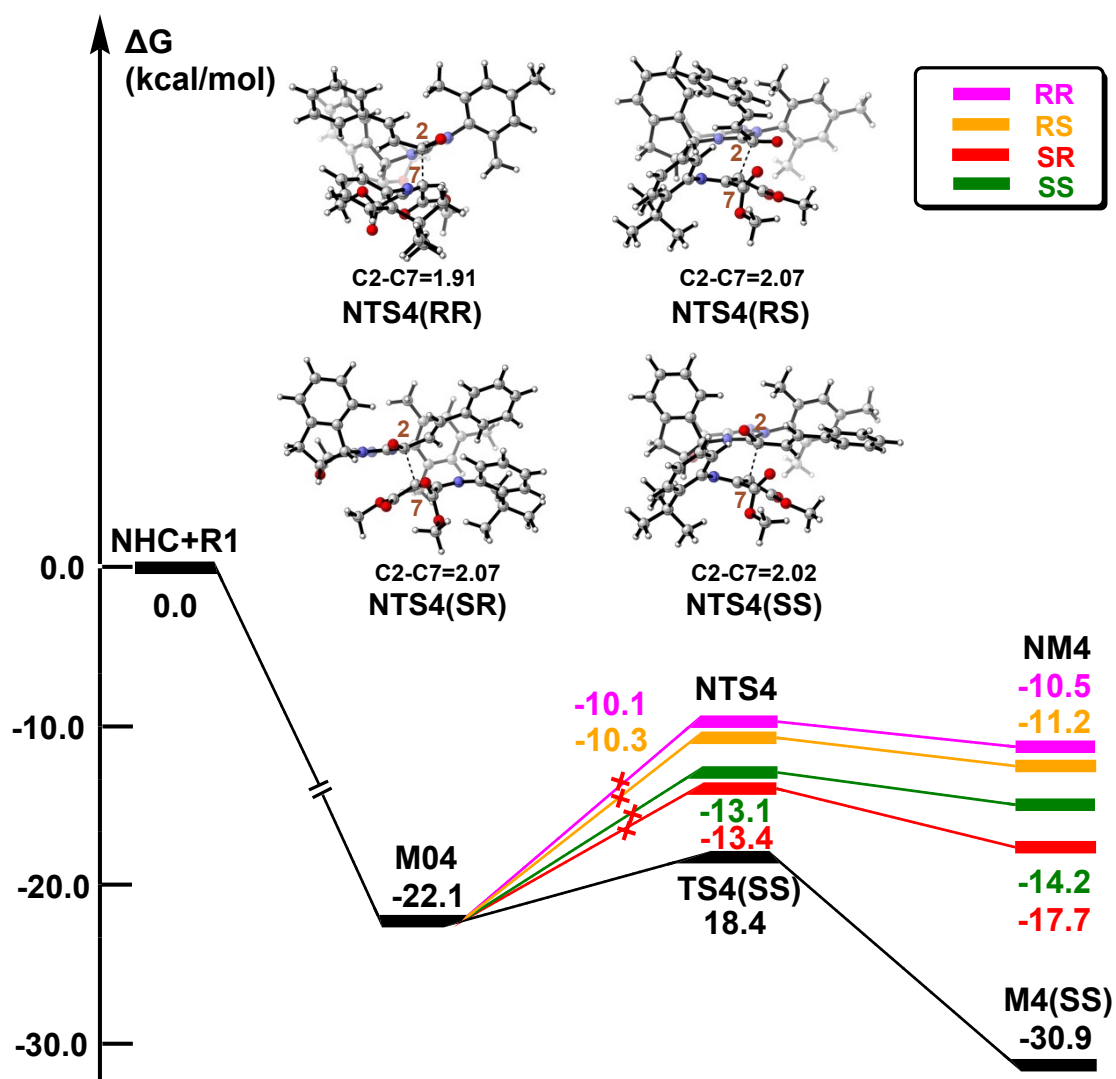


Fig. S9 Free energy profile for the C2-N11 bond formation pathway (distance in Å and energies in kcal/mol).

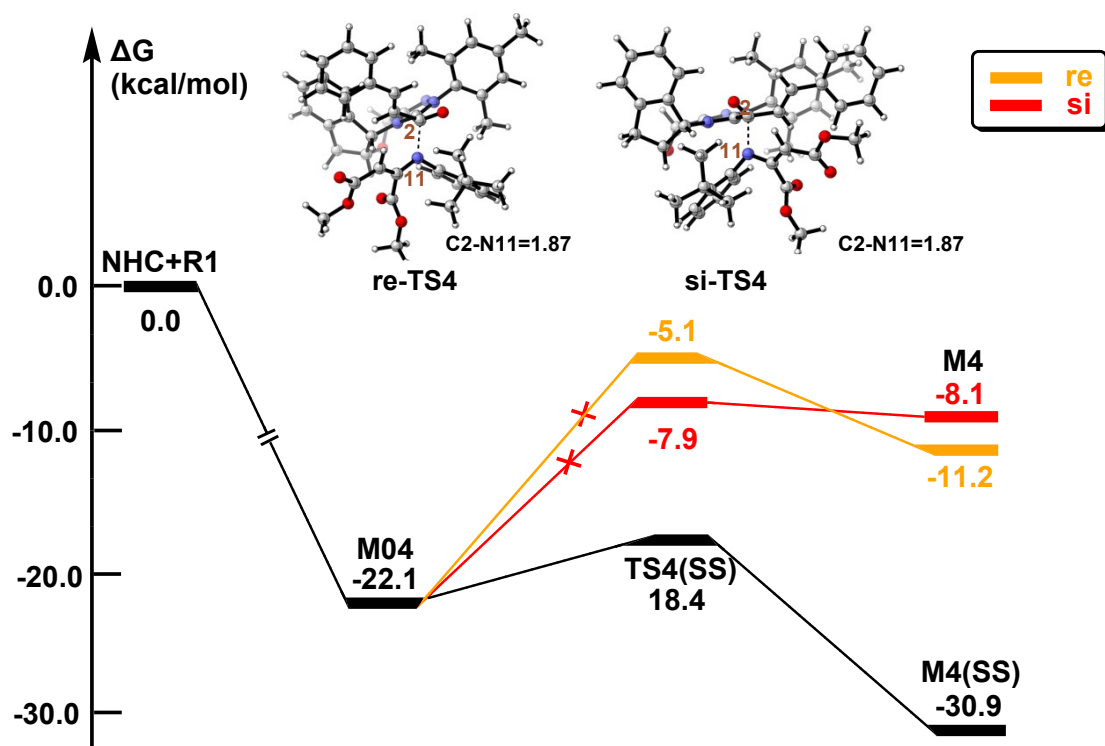
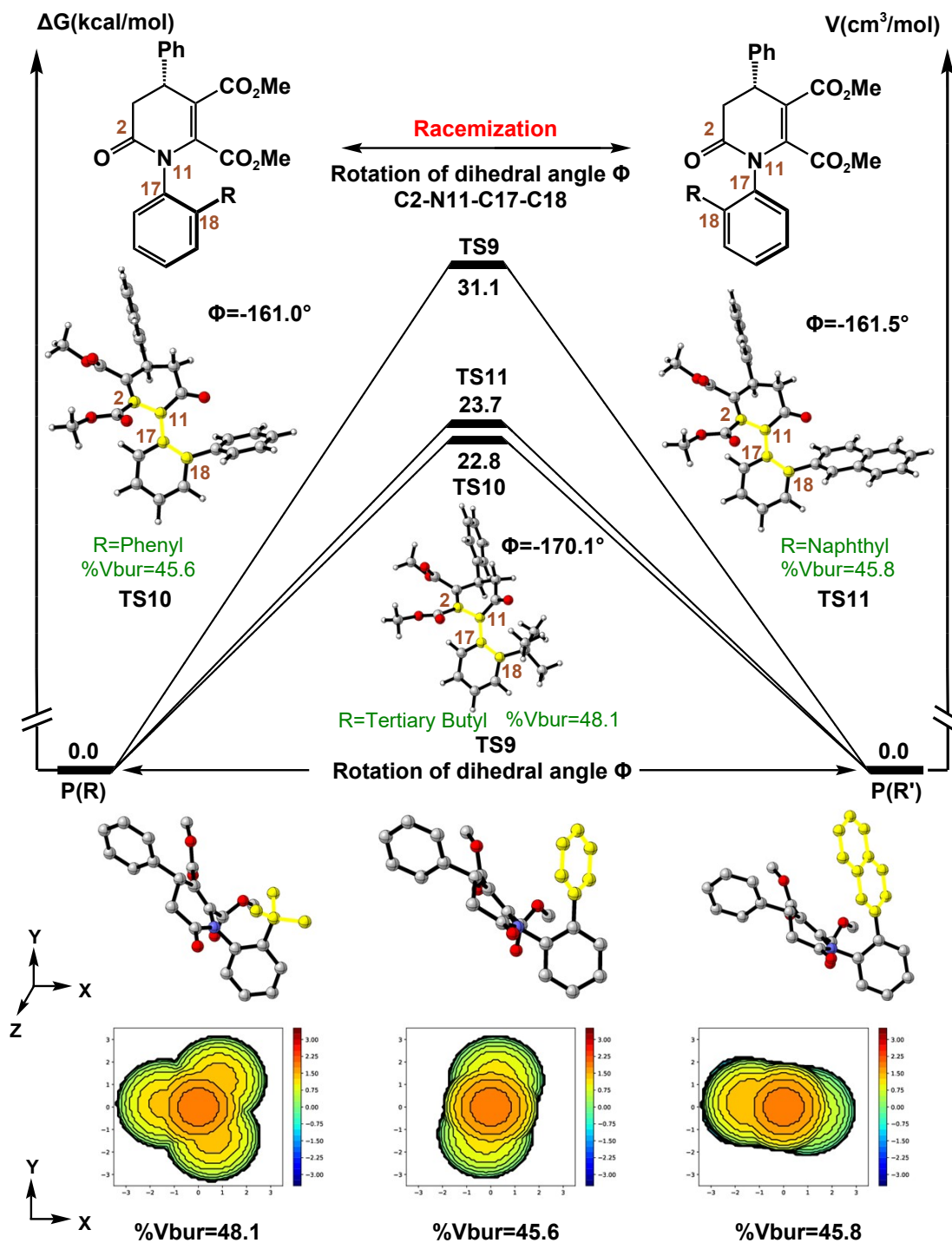


Fig. S10 Energy profiles and buried volume plot models involved in the racemization process.



4. Cartesian coordinates of all the stationary points

Pre-NHC

C	0.08290000	-0.09682100	0.73605500
C	-0.56171600	-1.78316300	-0.46205000
C	-2.36341100	-0.74840200	0.98885600
H	-2.32475500	-1.07365000	2.02935800
N	0.70306500	-1.62414800	-0.74387700
N	1.08692700	-0.56534800	0.01550500
N	-0.98176300	-0.85037400	0.44827000
C	-1.51394700	-2.78864000	-1.03464400
H	-1.04397600	-3.77308400	-1.03769100
H	-1.74868700	-2.51612300	-2.07054800
C	-3.26548800	-1.64112700	0.10126100
O	-2.67051400	-2.87589800	-0.23355500
C	-3.70187500	0.63314400	-0.40829300
C	-2.93898700	0.62510600	0.76364300
C	-2.79670300	1.76318300	1.54894700
C	-3.42650700	2.93521500	1.13264000
C	-4.18484200	2.95165200	-0.03962100
C	-4.33351200	1.80211900	-0.81532100
C	-3.70823300	-0.72677600	-1.06162800
H	-2.22423500	1.74078500	2.47173800
H	-4.67461300	3.87039300	-0.34572200
H	-4.93642000	1.81944600	-1.71761000
H	-2.99514400	-0.75097400	-1.89428700
H	-4.68292100	-1.01782500	-1.45721700
C	2.43968300	-0.07017900	-0.02484800
C	2.69151600	1.10627500	-0.73167800
C	3.42462600	-0.80916900	0.63680100
C	4.01134100	1.55766100	-0.75134500
C	4.72411400	-0.31379700	0.58287200
C	5.03402400	0.86372900	-0.10406800
H	4.24363600	2.47070600	-1.29262900
H	5.51461100	-0.85941200	1.09137400
C	3.08855300	-2.07944700	1.37112100
H	2.74655200	-2.85340700	0.67801600
H	2.28991700	-1.91747200	2.10167400
H	3.96510500	-2.45431900	1.90053400
C	1.59401800	1.85593500	-1.44088100
H	0.95999900	2.40157100	-0.73462400
H	0.95141400	1.17878000	-2.01058400
H	2.02108200	2.58342300	-2.13192900
H	-4.13969600	-1.89753500	0.70269000

C	6.45666000	1.35424100	-0.16410000
H	6.95511000	1.22854900	0.79990800
H	7.02545500	0.78435900	-0.90555300
H	6.50061700	2.40798200	-0.44552000
H	0.12646900	0.73255300	1.42704000
H	-3.33628400	3.83709300	1.72842500
TSI			
C	0.99360300	-0.60773300	-0.57362100
C	2.64697400	-2.06218900	-0.70248600
C	3.22642200	0.31448900	-1.31305500
H	2.97618600	0.58903300	-2.33920900
N	1.62775100	-2.75909700	-0.28461300
N	0.62342500	-1.83585700	-0.21594100
N	2.29666700	-0.75075900	-0.88800900
C	4.05663000	-2.52814200	-0.90774100
H	4.06281700	-3.44449400	-1.49960800
H	4.50957300	-2.74691900	0.06724500
C	4.66486900	-0.23538900	-1.16628700
O	4.79925900	-1.56460000	-1.62406500
C	4.24657300	1.29664800	0.59844100
C	3.21103300	1.45331500	-0.32737800
C	2.32786900	2.52377900	-0.26104700
C	2.49111600	3.45175900	0.76750300
C	3.52202500	3.30155700	1.69719900
C	4.40903700	2.22718000	1.61877600
C	5.05002700	0.05251700	0.30257000
H	1.52812300	2.63370500	-0.98763600
H	3.63979600	4.03569300	2.48767300
H	5.21219900	2.12224300	2.34146300
H	4.74184900	-0.76331500	0.96782900
H	6.12669700	0.18564300	0.42424300
C	-0.68738200	-2.18094500	0.25756400
C	-0.88815300	-2.30808500	1.63227600
C	-1.70858200	-2.34138900	-0.68507300
C	-2.18786600	-2.58368600	2.06475900
C	-2.98670200	-2.61077800	-0.20298100
C	-3.24533000	-2.72463700	1.16705200
H	-2.37441000	-2.68239300	3.13125000
H	-3.79975600	-2.74037700	-0.91349500
C	-1.41944100	-2.24993700	-2.16018700
H	-0.63889200	-2.96147500	-2.44656300
H	-1.06511100	-1.25254000	-2.43979400
H	-2.31766000	-2.46600500	-2.74065100

C	0.24654000	-2.18702900	2.61529500
H	1.00608200	-1.47541000	2.28127100
H	0.74381700	-3.15349800	2.74410700
H	-0.12574600	-1.86552200	3.58973700
H	5.30450300	0.35974300	-1.82150200
C	-4.64766700	-2.97609500	1.65590900
H	-5.23124700	-2.05010700	1.63394200
H	-5.16079600	-3.70173900	1.02029800
H	-4.64931100	-3.34910700	2.68175700
H	0.16959600	0.42171700	-0.43511700
H	1.81787400	4.29974100	0.84032800
C	-3.18088400	0.70602900	-2.32465100
C	-4.51802500	1.44753200	-2.35740500
C	-4.94664900	2.04842500	-1.01967000
C	-1.96803600	1.58628600	-1.96943500
C	-3.92209100	3.03127500	-0.45151900
C	-1.79919400	1.77530200	-0.48357000
H	-3.23481500	-0.12845300	-1.61299600
H	-4.45407500	2.25367400	-3.10041900
H	-5.11986500	1.25681500	-0.27937000
H	-3.55567100	3.69946800	-1.23812300
H	-2.05220300	2.56206700	-2.46268000
H	-3.00127700	0.26678600	-3.31094300
H	-5.29414100	0.76022300	-2.70889500
H	-5.89659000	2.57613300	-1.15261100
H	-1.04290100	1.13176800	-2.33367700
H	-4.38365700	3.66759300	0.30704000
C	-2.83750800	2.32871000	1.67301200
H	-3.86916200	2.09994100	1.95926100
H	-2.59041300	3.31885100	2.07451600
C	-1.88651400	1.27228100	2.21116800
H	-1.78720000	1.38245600	3.29318700
H	-2.27952900	0.27067900	2.00213500
C	-0.54535800	1.43544400	1.50860600
H	0.17446300	0.67120200	1.82745100
H	-0.10239500	2.41148400	1.74704200
N	-0.71612300	1.30766000	0.06976400
N	-2.78669700	2.37841800	0.20592800

NHC

C	0.10187200	0.00957900	0.80591000
C	-0.53694200	-1.74056900	-0.47081000
C	-2.30472000	-0.72550100	0.98187400
H	-2.26385800	-1.00141800	2.03812800

N	0.72178200	-1.59105900	-0.75145200
N	1.07841300	-0.51646600	0.03976500
N	-0.94265900	-0.80257000	0.44237800
C	-1.48526900	-2.75286800	-1.03545300
H	-1.00248100	-3.73049400	-1.08093900
H	-1.77298500	-2.47008500	-2.05608900
C	-3.22812700	-1.66715300	0.16646800
O	-2.61667000	-2.88770100	-0.19760000
C	-3.78042400	0.57708400	-0.37106200
C	-2.93339800	0.62521900	0.73900200
C	-2.75214100	1.80122400	1.45711800
C	-3.44229400	2.94265000	1.05167500
C	-4.29587700	2.89763800	-0.05297300
C	-4.47118400	1.71590500	-0.77225500
C	-3.78261200	-0.80031700	-0.98529500
H	-2.08486900	1.82629500	2.31261900
H	-4.83172400	3.79278200	-0.35263900
H	-5.13694900	1.68625400	-1.62955400
H	-3.12118300	-0.82247800	-1.85940700
H	-4.76902800	-1.13640000	-1.31185300
C	2.43118700	-0.05182000	-0.00923000
C	2.70695400	1.14890700	-0.66860400
C	3.42987300	-0.82323300	0.59218000
C	4.03366700	1.57891500	-0.70764400
C	4.74212000	-0.35758300	0.52272800
C	5.06127100	0.84093200	-0.11876900
H	4.26981800	2.50926600	-1.21866000
H	5.53347400	-0.94341700	0.98480300
C	3.08665900	-2.10987600	1.29449900
H	2.75001300	-2.86797500	0.58159000
H	2.27081400	-1.95582800	2.00752800
H	3.95289400	-2.49829800	1.83274400
C	1.60390800	1.94193800	-1.31808600
H	0.88703400	2.29559900	-0.57182000
H	1.04563600	1.32207100	-2.02676700
H	2.01092300	2.80200200	-1.85244600
H	-4.05838400	-1.94843700	0.81879300
C	6.48392600	1.33780900	-0.15038200
H	6.72096500	1.89093300	0.76426900
H	7.19049500	0.50762400	-0.22362400
H	6.64957300	2.00962800	-0.99555700
H	-3.32026800	3.87136700	1.59950500

R1

C	2.42552800	1.22364200	-0.00002300
C	1.04014100	1.13834900	-0.00003100
C	0.40442000	-0.11298300	-0.00001000
C	1.19505900	-1.27040500	0.00001300
C	2.58352400	-1.18489800	0.00002400
C	3.20154900	0.06274000	0.00000700
H	2.90526100	2.19691900	-0.00004200
H	0.44979900	2.04898600	-0.00006100
H	0.71057200	-2.24296500	0.00002700
H	3.18136900	-2.09020300	0.00004300
H	4.28433500	0.13395600	0.00001300
C	-1.05271100	-0.25985900	-0.00001400
H	-1.42952400	-1.28266200	-0.00006600
C	-1.97248300	0.71941200	0.00004800
C	-3.40810600	0.38509100	0.00003100
H	-4.09819500	1.24916300	0.00009800
O	-3.84911800	-0.74914000	-0.00004900
H	-1.71220200	1.77339000	0.00011500

Pre-R2

C	2.47657500	-0.07488200	0.18106300
C	1.31230900	0.32924000	0.87146600
C	1.18441200	1.62072500	1.38832600
C	2.19358800	2.56088200	1.21961000
C	3.35144200	2.18642500	0.55194200
C	3.48211400	0.89152500	0.05418400
H	0.27908200	1.87465200	1.93000100
H	2.07832500	3.56151700	1.62191400
H	4.16035900	2.89647800	0.41466300
H	4.39973800	0.64120900	-0.46217900
C	2.65540900	-1.48018400	-0.42141600
C	2.65466300	-2.55512300	0.68192400
C	1.54751300	-1.77324700	-1.44980800
C	3.99800800	-1.60616100	-1.15734600
H	3.38584300	-2.31651800	1.45993400
H	1.67854200	-2.68727300	1.15296700
H	2.92437000	-3.52281500	0.24670900
H	1.56044100	-1.02489600	-2.24838000
H	1.72295900	-2.75668000	-1.89845700
H	0.55288300	-1.77314300	-1.00328000
H	4.07156900	-2.60899000	-1.58676300
H	4.08148600	-0.88543200	-1.97628000
H	4.84918700	-1.46994700	-0.48311700
N	0.21595200	-0.56264400	1.07365000

H	0.36875800	-1.37517300	1.65517700
C	-1.07316500	-0.30120300	0.72623800
C	-2.12533800	-1.04687300	1.14690000
H	-1.96819300	-1.83028500	1.87968200
C	-3.49710100	-0.91655300	0.67142300
O	-4.45198900	-1.47310000	1.18017700
O	-3.61926000	-0.13275100	-0.42002600
C	-4.95450700	0.08285300	-0.87651000
H	-4.87285500	0.75852700	-1.72585100
H	-5.40887800	-0.86145200	-1.18262300
H	-5.56093000	0.53315100	-0.08826100
C	-1.24159800	0.89415700	-0.19250400
O	-0.77571000	0.61803100	-1.40441200
O	-1.68320200	1.95897100	0.15878600
C	-0.81604300	1.70831900	-2.33500600
H	-0.20955000	2.53583700	-1.96187100
H	-0.40747200	1.31882600	-3.26430800
H	-1.84572300	2.04231700	-2.47433200

TSII

C	-1.62393600	-2.41882900	0.25235300
C	-1.53189400	-1.34368200	-0.66828900
C	-2.23414100	-1.40314300	-1.88057600
C	-3.04684300	-2.48251900	-2.20645800
C	-3.15397700	-3.53635900	-1.30951900
C	-2.44708500	-3.49265400	-0.10961800
H	-2.13028800	-0.56896900	-2.56789200
H	-3.58108000	-2.49703400	-3.15117700
H	-3.77966900	-4.39395400	-1.53534700
H	-2.55523100	-4.33075900	0.56776700
C	-0.85410900	-2.44963800	1.58355900
C	0.65277000	-2.54248100	1.29434000
C	-1.14676500	-1.20603200	2.44172400
C	-1.22693200	-3.67373800	2.43349200
H	0.88329100	-3.45811700	0.73931400
H	1.00169600	-1.69219200	0.70712700
H	1.21165600	-2.56395600	2.23701600
H	-2.21791300	-1.12516400	2.65136300
H	-0.61533500	-1.29592600	3.39600900
H	-0.82967400	-0.28444200	1.95370600
H	-0.66357100	-3.63708900	3.37057200
H	-2.29263100	-3.68668800	2.68326700
H	-0.97464900	-4.61392700	1.93401800
N	-0.72352700	-0.19836400	-0.43109100

H	0.58004100	-0.21088200	-0.73386100
C	-1.28260800	1.01693800	-0.37700000
C	-0.56143100	2.19448300	-0.36808500
H	0.50572700	2.15949900	-0.54984500
C	-1.08015300	3.50755300	-0.09169000
O	-0.44884800	4.55141700	-0.19659000
O	-2.36895600	3.51550200	0.34907100
C	-2.92858100	4.80298900	0.58016400
H	-3.95821300	4.63054600	0.89130700
H	-2.38050600	5.32841800	1.36542700
H	-2.90599400	5.40747200	-0.32937200
C	-2.80129600	1.06547900	-0.34808400
O	-3.27538200	0.63697600	0.82079100
O	-3.49035700	1.37656300	-1.28976700
C	-4.70071300	0.54405600	0.89928500
H	-5.07402000	-0.13708500	0.13145000
H	-4.91950400	0.15874500	1.89296100
H	-5.15136700	1.52879300	0.76011800
C	3.17308300	-0.10048500	2.04518400
C	4.59953000	0.38066800	2.31332100
C	5.53766600	0.27697900	1.11168900
C	2.40831400	0.72403000	0.99192000
C	5.04010700	1.05690700	-0.10484500
C	2.72079900	0.29566000	-0.42023000
H	3.18818300	-1.15272500	1.73644400
H	4.56243400	1.42764400	2.64256100
H	5.67890600	-0.77188200	0.82229400
H	4.68313900	2.04782900	0.19561200
H	2.62788200	1.79177300	1.11360100
H	2.60215200	-0.05806200	2.97800400
H	5.01752900	-0.19393900	3.14609200
H	6.52144800	0.66820800	1.39059700
H	1.33027700	0.60498300	1.12914900
H	5.85517200	1.22015500	-0.81301000
C	4.39032300	-0.24632400	-2.12994000
H	5.36420500	-0.71901600	-1.97109500
H	4.51743200	0.53968700	-2.88360200
C	3.36558500	-1.27342400	-2.58346800
H	3.59182400	-1.59040100	-3.60332700
H	3.40911300	-2.15345300	-1.93378700
C	1.97731900	-0.65505600	-2.49649300
H	1.19537600	-1.38111300	-2.73464100
H	1.88551600	0.17704000	-3.20565100
N	1.73903400	-0.17825900	-1.14041700

N	3.98660700	0.36720000	-0.85815300
II			
C	-1.92358000	-2.38077200	0.10183400
C	-1.85257100	-1.27823500	-0.78203900
C	-2.72309200	-1.17769600	-1.87166300
C	-3.69268700	-2.14373300	-2.11415700
C	-3.77653800	-3.23510200	-1.26084000
C	-2.90113300	-3.34238400	-0.18269100
H	-2.62626100	-0.31834400	-2.52791400
H	-4.36152400	-2.04489700	-2.96258200
H	-4.52020100	-4.00800600	-1.42600200
H	-3.00077100	-4.20629400	0.46211000
C	-0.98956700	-2.55816000	1.31107700
C	0.45095100	-2.78582900	0.82216900
C	-1.05115900	-1.34186300	2.25294700
C	-1.37579200	-3.78500900	2.15136600
H	0.49916400	-3.67376700	0.18283300
H	0.84868600	-1.93970900	0.25707100
H	1.10602200	-2.95315300	1.68482300
H	-2.06815600	-1.20199100	2.63273300
H	-0.38693800	-1.51714300	3.10656900
H	-0.74835000	-0.41560300	1.76517500
H	-0.70042000	-3.84857000	3.00942500
H	-2.39838300	-3.71104800	2.53426400
H	-1.28002800	-4.71741700	1.58702000
N	-0.91295100	-0.21692700	-0.60298300
H	0.10202700	-0.36374900	-0.81533100
C	-1.28900600	1.07655000	-0.44864400
C	-0.42075900	2.12563700	-0.51647100
H	0.60278000	1.94059200	-0.81984200
C	-0.73300900	3.50283700	-0.17911400
O	0.00252700	4.45007100	-0.39805400
O	-1.92431900	3.65803000	0.44392300
C	-2.29840800	5.00446700	0.72803300
H	-3.28621100	4.94970300	1.18240700
H	-1.58701600	5.46073800	1.41937800
H	-2.33320100	5.59658100	-0.18867600
C	-2.76845900	1.28919700	-0.18921200
O	-3.10042300	0.88026900	1.03118500
O	-3.54301600	1.71785100	-1.00848000
C	-4.49602700	0.97112000	1.34189100
H	-5.07471000	0.37546400	0.63308000
H	-4.60125000	0.57813700	2.35048500

H	-4.82204400	2.01188100	1.29607400
C	3.03311400	-0.53344000	2.01445700
C	4.42667100	-0.08802200	2.45963400
C	5.46346200	-0.03379200	1.33829100
C	2.35725200	0.40737500	1.00038500
C	5.05275000	0.88528800	0.18547900
C	2.77231600	0.13253600	-0.42610300
H	3.08374100	-1.54220300	1.58551200
H	4.34667700	0.90982500	2.91199500
H	5.64567400	-1.03822600	0.93519800
H	4.65561400	1.82810500	0.57830000
H	2.56076900	1.45318500	1.26386400
H	2.38730200	-0.60209600	2.89648000
H	4.78260100	-0.76023700	3.24745500
H	6.41397000	0.32480200	1.74760000
H	1.27287400	0.27849000	1.03401400
H	5.92705200	1.14674000	-0.41608400
C	4.63748000	-0.22918300	-1.99221400
H	5.58224700	-0.73652500	-1.76586900
H	4.86580500	0.60821400	-2.66442400
C	3.65989900	-1.19105000	-2.64740100
H	3.98149700	-1.40699900	-3.66897300
H	3.63878200	-2.13440900	-2.09101500
C	2.26910600	-0.56720600	-2.61599900
H	1.52834800	-1.23680800	-3.06280400
H	2.26748000	0.35737900	-3.21116700
N	1.85724900	-0.27530600	-1.24859300
N	4.08869300	0.28743400	-0.73668900

TSIII

C	5.22152700	1.15196900	-1.56048100
C	4.60493500	-0.07891800	-1.22812500
C	4.91647000	-1.23845800	-1.95929800
C	5.81800000	-1.22184000	-3.01379200
C	6.41039000	-0.01612700	-3.36969200
C	6.10487000	1.13509600	-2.65058800
H	4.41207800	-2.15944900	-1.68324400
H	6.03751200	-2.13461300	-3.55872500
H	7.10743600	0.03577400	-4.20002800
H	6.58769800	2.05719900	-2.95228100
C	4.96033100	2.49287200	-0.84477400
C	3.81202100	3.21759600	-1.56931100
C	4.58872200	2.33952400	0.64222700
C	6.21245100	3.38941100	-0.89905500

H	4.06121900	3.38351100	-2.62332400
H	2.88952100	2.63294100	-1.50413300
H	3.63378800	4.19388200	-1.10171100
H	5.27025900	1.65541000	1.15807700
H	4.65363600	3.32287500	1.12174600
H	3.57107600	1.97132800	0.76457900
H	6.03168500	4.28833700	-0.30230600
H	7.08792000	2.87607800	-0.48755500
H	6.45268900	3.72402800	-1.91103800
N	3.61971100	-0.19193800	-0.22106000
H	2.49432000	0.42146600	-0.31998500
C	3.73782800	-1.05790100	0.78576900
C	2.68922000	-1.37339500	1.62761500
H	1.70466800	-0.98486500	1.39086500
C	2.78082000	-2.08986900	2.86939000
O	1.82926000	-2.42924300	3.56224200
O	4.05835800	-2.35846700	3.26505600
C	4.17886600	-3.13940700	4.44751000
H	5.24757600	-3.26793100	4.61520700
H	3.72156300	-2.62915600	5.29814000
H	3.69841500	-4.11282700	4.32265600
C	5.08886500	-1.72784400	0.96211300
O	6.00375000	-0.85663800	1.39135100
O	5.32685200	-2.87975700	0.68832200
C	7.32938600	-1.38134000	1.51255100
H	7.67950400	-1.74256300	0.54334200
H	7.94645200	-0.55554800	1.85971000
H	7.34459600	-2.20265400	2.23193700
H	-8.58491500	0.08648600	0.25613900
C	-4.51727000	-1.13204000	-0.52850900
H	-3.82142800	-1.91456300	-0.80766400
C	-3.99169700	0.11452700	-0.17855900
C	-4.88622700	1.11267200	0.20901700
H	-4.48169200	2.08773800	0.45303200
C	-6.26648300	0.90804100	0.26398400
C	-6.74702600	-0.36773900	-0.09763700
C	-5.88401800	-1.40737800	-0.50377700
C	-7.21576800	2.04264600	0.69262700
C	-6.42254900	-2.79494400	-0.89006900
C	-6.44922300	3.33523900	1.00976300
H	-5.73917200	3.19516900	1.82997000
H	-5.90515300	3.70613300	0.13637000
H	-7.16396200	4.10612400	1.31229600
C	-8.19468000	2.39893600	-0.44755800

H	-8.81894500	1.57060700	-0.79238700
H	-8.86374600	3.20192400	-0.12289700
H	-7.63188800	2.75296700	-1.31633100
C	-7.96422500	1.66473100	1.98992700
H	-8.64460600	2.47337200	2.27418500
H	-8.55511500	0.74631700	1.93230800
H	-7.24331000	1.52247700	2.80016100
C	-7.15504100	-3.43782800	0.30252800
H	-8.01261200	-2.84411300	0.61822600
H	-7.50781500	-4.43632200	0.02163700
H	-6.47284600	-3.54720200	1.15202000
C	-7.37131300	-2.68284900	-2.09810500
H	-7.72672600	-3.68013100	-2.38004500
H	-8.23587000	-2.05743300	-1.87690900
H	-6.84237300	-2.25757900	-2.95747600
C	-5.29001300	-3.74875900	-1.29323200
H	-4.58610300	-3.91803700	-0.47250200
H	-5.72269400	-4.71586100	-1.56623000
H	-4.73194100	-3.37592400	-2.15803800
O	-8.08560100	-0.66445000	-0.07640200
C	-2.53124200	0.37129100	-0.21921300
C	-1.72586500	-0.19037900	-1.20959800
H	-2.21528500	-0.79394000	-1.96546100
C	-1.91634800	1.19750000	0.72424900
H	-2.53800500	1.62524100	1.50319600
C	-0.34926400	0.03010900	-1.29023300
C	-0.54962700	1.46196500	0.70919900
C	0.26356700	0.85618300	-0.29975000
C	0.45545100	-0.63849500	-2.42193000
C	0.07120900	2.39866300	1.76110300
C	-0.98299800	2.95571100	2.72885700
H	-1.75267400	3.53460500	2.20753500
H	-1.47570200	2.16125400	3.29885100
H	-0.49128900	3.62190400	3.44475400
C	1.11011100	1.64770400	2.61037400
H	0.64094500	0.80877700	3.13790000
H	1.91587600	1.25427100	1.99186700
H	1.53655700	2.32409300	3.36117500
C	0.73552700	3.60726500	1.07504400
H	1.52861900	3.28648500	0.39958900
H	-0.00770200	4.17592800	0.50474400
H	1.16175700	4.27582000	1.83270300
C	1.22654100	-1.84056300	-1.85082600
H	1.89512000	-1.54138400	-1.04271000

H	0.52675100	-2.58818400	-1.46189800
H	1.83081200	-2.31182900	-2.63603300
C	-0.46142700	-1.17709500	-3.53312900
H	-1.11104600	-1.98433200	-3.18258300
H	-1.08991100	-0.38732000	-3.95817300
H	0.15846700	-1.58665300	-4.33657000
C	1.43195000	0.33846000	-3.10414000
H	0.90342900	1.23871300	-3.43801800
H	2.24342500	0.64496300	-2.44743100
H	1.86908200	-0.14370000	-3.98613600
O	1.55882600	1.15153400	-0.31212700

R2

C	-2.48081500	-0.10133500	-0.13136800
C	-1.29702900	0.30717400	-0.81266800
C	-1.23102600	1.61562000	-1.32773100
C	-2.26686000	2.52841500	-1.16210500
C	-3.41327200	2.14211000	-0.48122800
C	-3.50228800	0.84101500	0.01581600
H	-0.34249700	1.89821600	-1.88292200
H	-2.17671900	3.52908500	-1.57511500
H	-4.23695700	2.83465900	-0.33995100
H	-4.40905400	0.56345100	0.54067900
C	-2.63609700	-1.52112000	0.43712700
C	-2.58675600	-2.55383500	-0.70315800
C	-1.52185300	-1.81572400	1.45752900
C	-3.97538200	-1.70744800	1.16406700
H	-3.41005800	-2.38447500	-1.40573700
H	-1.64248500	-2.48654200	-1.24353100
H	-2.69414000	-3.56473000	-0.29324600
H	-1.55041400	-1.08699400	2.27505400
H	-1.66947200	-2.81383500	1.88599300
H	-0.53607000	-1.77439200	0.99431500
H	-4.03171100	-2.73050100	1.54874300
H	-4.07710400	-1.02476700	2.01412000
H	-4.82896300	-1.55682700	0.49529700
N	-0.25882100	-0.59490200	-1.05403500
C	0.98458800	-0.30917000	-0.73759500
C	2.06624300	-1.12648100	-1.09541200
H	1.86143800	-1.95004700	-1.76963300
C	3.40062200	-1.04954900	-0.61290800
O	4.35543500	-1.72770800	-0.99648500
O	3.58387800	-0.13245100	0.39653000
C	4.92496100	0.04038000	0.82472400

H	4.89811500	0.80496200	1.60150100
H	5.33283800	-0.88935400	1.22927000
H	5.56447900	0.36891200	0.00093000
C	1.26771200	0.96341100	0.04911800
O	0.84601600	0.85319400	1.31432100
O	1.74169000	1.97735000	-0.40940200
C	1.00481800	2.03167200	2.10546500
H	0.44210900	2.85882600	1.66670600
H	0.61705000	1.78652900	3.09232700
H	2.05981400	2.30824900	2.16570000

DBU

C	-1.90188500	-1.24944800	0.61414700
C	-2.75230500	0.00204900	0.38882300
C	-1.96352000	1.30822700	0.29701100
C	-0.89094800	-1.54782900	-0.50762100
C	-0.90557100	1.29023600	-0.80985800
C	0.40214300	-0.77739000	-0.36493400
H	-1.36199000	-1.17086700	1.56667100
H	-3.31863300	-0.12740400	-0.54392700
H	-1.46562900	1.52359100	1.25146100
H	-1.32800900	0.85674200	-1.72386700
H	-1.35352100	-1.35611600	-1.48412300
H	-2.57371300	-2.10893200	0.70711500
H	-3.49206200	0.08271500	1.19262700
H	-2.66048300	2.13180800	0.10648600
H	-0.60589300	-2.60054700	-0.48641100
H	-0.61218700	2.31285200	-1.06378800
C	1.42083300	1.44032000	0.01058400
H	1.00440700	2.23002200	0.64813700
H	1.89086900	1.93146400	-0.85248200
C	2.44478500	0.62185500	0.77950600
H	3.36139500	1.20221900	0.91230100
H	2.05253300	0.37569700	1.77242400
C	2.69863000	-0.67492200	0.01613400
H	3.44230600	-1.28898100	0.53362100
H	3.11978900	-0.43435500	-0.97242900
N	1.47665400	-1.45342900	-0.13977400
N	0.32161000	0.59078600	-0.44687900

DBUH⁺

C	1.93923600	1.27328100	0.57395900
C	2.79030400	0.01697700	0.38864600

C	2.00438300	-1.29404900	0.36023400
C	0.91508400	1.51169500	-0.55286600
C	0.95556800	-1.34720700	-0.74941300
C	-0.33181600	0.69443800	-0.37286300
H	1.41410500	1.24224000	1.53577900
H	3.35078700	0.10962600	-0.55067300
H	1.50904000	-1.47200400	1.32230000
H	1.35466700	-0.94905200	-1.68735200
H	1.35749700	1.28003800	-1.52780200
H	2.59831000	2.14467600	0.60305500
H	3.53148900	-0.02843100	1.19211400
H	2.70178900	-2.12206100	0.20182100
H	0.62388800	2.56328500	-0.58017600
H	0.65214900	-2.37624900	-0.94615500
C	-1.46064500	-1.45279400	-0.09005700
H	-1.09825200	-2.32566600	0.45733300
H	-1.90613900	-1.79792000	-1.02882900
C	-2.46192700	-0.67770600	0.75032300
H	-3.38363200	-1.25428700	0.83896200
H	-2.05768900	-0.51838800	1.75392400
C	-2.74404600	0.66585000	0.09752800
H	-3.34470100	1.30792500	0.74137900
H	-3.26716800	0.54058100	-0.85559000
N	-1.46551600	1.33480000	-0.13560600
N	-0.28347900	-0.62489800	-0.40799900
H	-1.43001900	2.34346400	-0.09779600

DQ

C	-1.45912800	1.23534600	0.03397400
H	-0.91772300	2.16751000	0.09138600
C	-0.69350300	-0.00000200	0.01197400
C	-1.45913000	-1.23534900	0.03394500
H	-0.91772700	-2.16751600	0.09132600
C	-2.80833800	-1.28188700	-0.00285500
C	-3.56891400	0.00000200	-0.09127500
C	-2.80833600	1.28188800	-0.00282000
C	-3.58505800	-2.59808200	0.02960800
C	-3.58505400	2.59808200	0.02968800
C	-2.64748200	-3.80126700	0.18510200
H	-1.95476400	-3.89116900	-0.65807100
H	-2.06539300	-3.74599400	1.11086100
H	-3.24632400	-4.71553800	0.22068100
C	-4.55609300	-2.60327100	1.22600300
H	-5.29528300	-1.80669300	1.14323300

H	-5.08048300	-3.56379500	1.26222600
H	-4.00807300	-2.48159000	2.16602700
C	-4.36815300	-2.77895900	-1.28468300
H	-4.89749900	-3.73735700	-1.26096100
H	-5.09668000	-1.98141300	-1.42699800
H	-3.68417100	-2.79073200	-2.13933500
C	-4.36815100	2.77900400	-1.28459600
H	-5.09667100	1.98145700	-1.42694300
H	-4.89750600	3.73739700	-1.26083500
H	-3.68416900	2.79081700	-2.13924800
C	-4.55608700	2.60323100	1.22608400
H	-5.08046900	3.56375800	1.26234700
H	-5.29528400	1.80666300	1.14328500
H	-4.00806600	2.48150800	2.16610300
C	-2.64747700	3.80126100	0.18522200
H	-1.95475900	3.89119100	-0.65794800
H	-3.24631800	4.71553000	0.22083200
H	-2.06538800	3.74595500	1.11097900
O	-4.78940400	0.00000400	-0.22711600
C	0.69350300	-0.00000200	-0.01196100
C	1.45912800	1.23534600	-0.03396100
H	0.91772200	2.16751100	-0.09136200
C	1.45913000	-1.23534900	-0.03393300
H	0.91772600	-2.16751600	-0.09130200
C	2.80833600	1.28188800	0.00281900
C	2.80833800	-1.28188800	0.00285400
C	3.56891600	0.00000200	0.09125400
C	3.58505400	2.59808200	-0.02968500
C	3.58505700	-2.59808300	-0.02960500
C	2.64747700	-3.80127000	-0.18506000
H	1.95477700	-3.89115600	0.65813000
H	2.06536900	-3.74601400	-1.11080700
H	3.24631800	-4.71554200	-0.22063400
C	4.55606600	-2.60329000	-1.22602100
H	4.00802500	-2.48163400	-2.16603600
H	5.29525200	-1.80670400	-1.14328400
H	5.08046300	-3.56381100	-1.26223500
C	4.36818100	-2.77894000	1.28467200
H	5.09672300	-1.98140200	1.42695000
H	3.68422000	-2.79068200	2.13934100
H	4.89751200	-3.73734700	1.26095900
C	4.55606200	2.60325000	-1.22610100
H	5.29525500	1.80667400	-1.14333300
H	4.00802100	2.48155000	-2.16611100

H	5.08045000	3.56377400	-1.26235600
C	2.64747300	3.80126400	-0.18518100
H	2.06536700	3.74597500	-1.11092800
H	1.95477100	3.89117800	0.65800400
H	3.24631200	4.71553400	-0.22078600
C	4.36817800	2.77898600	1.28458600
H	3.68421500	2.79077500	2.13925300
H	5.09670800	1.98144300	1.42690000
H	4.89752200	3.73738400	1.26083200
O	4.78941000	0.00000400	0.22706300

[DQH]⁻

H	-5.27896200	-0.77828200	0.19391100
C	-1.44823900	1.15467800	-0.32316800
H	-0.89063800	2.03976300	-0.60386600
C	-0.72083800	0.00432900	0.00549100
C	-1.45371900	-1.14065600	0.33161100
H	-0.90191800	-2.02706300	0.61883900
C	-2.85011100	-1.17803700	0.32494800
C	-3.53137000	0.01090100	-0.00774600
C	-2.84194100	1.19858300	-0.32879000
C	-3.60384300	-2.47266400	0.68342100
C	-3.59268600	2.49263100	-0.68517700
C	-2.63924600	-3.62152100	1.01412100
H	-1.98687300	-3.85847300	0.16860800
H	-2.01494800	-3.38812700	1.88129800
H	-3.22111200	-4.51714200	1.25099400
C	-4.47131700	-2.27306400	1.94518900
H	-5.21733100	-1.47727800	1.87062100
H	-5.00434800	-3.20002600	2.17889300
H	-3.82988700	-2.02363700	2.79544900
C	-4.44713700	-2.95985300	-0.51550400
H	-4.99901300	-3.86381800	-0.23930400
H	-5.17274600	-2.23367800	-0.89158300
H	-3.78674700	-3.20458600	-1.35255600
C	-4.46031100	2.28621800	-1.94009200
H	-5.22109800	1.52185600	-1.78461200
H	-4.95999300	3.22603000	-2.20042800
H	-3.83543800	1.98989600	-2.78902500
C	-4.47025600	2.94218500	0.49820100
H	-4.98305600	3.87616800	0.24261800
H	-5.22044500	2.19330600	0.75182500
H	-3.84946100	3.12872300	1.38083000
C	-2.62472800	3.64442100	-0.99100900

H	-1.98882100	3.42441300	-1.85418700
H	-3.20507700	4.54213500	-1.22462900
H	-1.98095100	3.87496100	-0.13619400
O	-4.90432700	0.07559800	-0.03796000
C	0.75858000	0.00092300	0.00620600
C	1.49505200	1.15116000	0.32399200
H	0.94076200	2.04297300	0.60276300
C	1.48970000	-1.15196400	-0.31421100
H	0.93111800	-2.04143400	-0.59203100
C	2.88301100	1.18827000	0.32979500
C	2.87747800	-1.19409100	-0.32540900
C	3.64311100	-0.00419100	0.00039300
C	3.63655000	2.47545100	0.68963200
C	3.62482800	-2.48310000	-0.69137900
C	2.67706000	-3.64610600	-1.00966400
H	2.03299500	-3.89226700	-0.15835500
H	2.03629100	-3.42625300	-1.87040500
H	3.26655600	-4.53703100	-1.25181900
C	4.50134400	-2.24778900	-1.93412500
H	3.87579000	-1.99114000	-2.79664900
H	5.19700100	-1.43036100	-1.74543000
H	5.06434900	-3.15595000	-2.18294300
C	4.51407700	-2.92135700	0.48642300
H	5.19904300	-2.11544600	0.75028500
H	3.89587100	-3.16491500	1.35805300
H	5.08899100	-3.81671900	0.21895400
C	4.51815400	2.91005200	-0.49531700
H	5.19847900	2.10169400	-0.76374200
H	3.89411100	3.15496900	-1.36239300
H	5.09798400	3.80373200	-0.23286400
C	2.69433400	3.64134300	1.01391400
H	2.04531500	3.88917400	0.16688100
H	2.05866500	3.42363800	1.87899500
H	3.28804300	4.53062800	1.25180800
C	4.52199200	2.23897800	1.92578400
H	3.90261200	1.98313900	2.79299100
H	5.21515100	1.42064300	1.73178800
H	5.08792100	3.14648200	2.17032400
O	4.92365600	-0.00623300	-0.00315200
DQH₂			
H	5.28538600	-0.76395800	-0.20964100
H	-5.28542500	0.76396400	-0.20925500
C	-1.45463400	-1.14609800	0.35895500

H	-0.89110300	-2.01941600	0.66455800
C	-0.74223500	-0.00340500	-0.01124500
C	-1.46562700	1.13133400	-0.37641000
H	-0.91230500	2.00816400	-0.68999200
C	-2.86138300	1.16417600	-0.37521700
C	-3.53645700	-0.01426700	0.00809800
C	-2.84752600	-1.19004400	0.37545800
C	-3.61967400	2.43982700	-0.78663300
C	-3.59647000	-2.46727600	0.78989400
C	-2.65608100	3.57249700	-1.17154900
H	-2.00484900	3.85049600	-0.33773100
H	-2.03184700	3.29943000	-2.02721800
H	-3.23907000	4.45498000	-1.45018100
C	-4.49153100	2.18166800	-2.03456800
H	-5.23787600	1.39125500	-1.92011700
H	-5.02502200	3.09735700	-2.30722000
H	-3.85404200	1.89373800	-2.87542400
C	-4.45837100	2.97832500	0.39313600
H	-5.00976900	3.86977900	0.07877100
H	-5.18495800	2.27118000	0.80237500
H	-3.79593000	3.25838100	1.21724100
C	-4.45332600	-2.20667800	2.04231200
H	-5.21777400	-1.45158700	1.86137200
H	-4.94826100	-3.13539900	2.34665900
H	-3.82171800	-1.87330200	2.87224200
C	-4.48241300	-2.96681300	-0.36664200
H	-4.98829200	-3.89126900	-0.06742900
H	-5.23889900	-2.23290500	-0.64387200
H	-3.86917200	-3.18727500	-1.24651500
C	-2.62350400	-3.60326200	1.13657400
H	-1.98072200	-3.34561000	1.98415600
H	-3.20023700	-4.49050500	1.41383600
H	-1.98774100	-3.87016900	0.28631100
O	-4.90323000	-0.08079200	0.04461300
C	0.74227000	0.00358300	-0.01129600
C	1.46560700	-1.13117400	-0.37651800
H	0.91222500	-2.00794700	-0.69014100
C	1.45471500	1.14625000	0.35887700
H	0.89122300	2.01960400	0.66444900
C	2.86136400	-1.16412000	-0.37530000
C	2.84761100	1.19010900	0.37539300
C	3.53648100	0.01427600	0.00810800
C	3.61950500	-2.43990600	-0.78664900
C	3.59662500	2.46731000	0.78980400

C	2.62371900	3.60338600	1.13635800
H	1.98796700	3.87022700	0.28606700
H	1.98092800	3.34586100	1.98397200
H	3.20049800	4.49063100	1.41351600
C	4.45339900	2.20673200	2.04228200
H	3.82176700	1.87318600	2.87212400
H	5.21799000	1.45178600	1.86134900
H	4.94815900	3.13550500	2.34675600
C	4.48266100	2.96669000	-0.36672600
H	5.23900300	2.23263100	-0.64395200
H	3.86946200	3.18727800	-1.24659600
H	4.98872600	3.89104400	-0.06750900
C	4.45787800	-2.97869600	0.39319600
H	5.18439000	-2.27161500	0.80264000
H	3.79524100	-3.25885600	1.21711000
H	5.00926500	-3.87014300	0.07878100
C	2.65573100	-3.57230400	-1.17193600
H	2.00431300	-3.85033200	-0.33827700
H	2.03168300	-3.29894500	-2.02765200
H	3.23858000	-4.45485700	-1.45062400
C	4.49169400	-2.18181500	-2.03438100
H	3.85472600	-1.89127800	-2.87473300
H	5.23987100	-1.39326500	-1.91897100
H	5.02318400	-3.09825500	-2.30840700
O	4.90326400	0.08061300	0.04500400

DQ•--

C	-1.46834100	-1.19559800	-0.18475700
H	-0.91943500	-2.11084500	-0.36890200
C	-0.71877300	0.00000300	-0.00000100
C	-1.46834400	1.19560100	0.18475500
H	-0.91944200	2.11085100	0.36890100
C	-2.83947800	1.23826500	0.19534400
C	-3.60161500	-0.00000300	0.00001100
C	-2.83947400	-1.23826500	-0.19534900
C	-3.59889700	2.55064900	0.41590800
C	-3.59889200	-2.55064800	-0.41591900
C	-2.65332200	3.74100200	0.61699300
H	-2.02040200	3.61429000	1.50169200
H	-2.00481800	3.89913300	-0.25134600
H	-3.24692400	4.64962700	0.75962400
C	-4.47459000	2.85745300	-0.81312700
H	-5.18935000	2.05326900	-0.98590600
H	-5.02081000	3.79495400	-0.65720800

H	-3.84998400	2.97459300	-1.70550400
C	-4.48496000	2.44632500	1.67077300
H	-5.02010200	3.38985300	1.82854100
H	-5.20976000	1.63963200	1.56477200
H	-3.86896100	2.25536600	2.55636500
C	-4.47453700	-2.85748800	0.81314100
H	-5.18930500	-2.05331700	0.98595500
H	-5.02074700	-3.79499600	0.65722700
H	-3.84989900	-2.97463000	1.70549500
C	-4.48499900	-2.44629900	-1.67074900
H	-5.02015200	-3.38982300	-1.82851300
H	-5.20979100	-1.63960400	-1.56471000
H	-3.86903200	-2.25533100	-2.55636200
C	-2.65331500	-3.74099000	-0.61707200
H	-2.00479600	-3.89915800	0.25124900
H	-3.24691600	-4.64961000	-0.75973400
H	-2.02041000	-3.61423300	-1.50177500
O	-4.86043100	-0.00000800	0.00003700
C	0.71877300	0.00000300	0.00000100
C	1.46834100	-1.19559800	0.18475700
H	0.91943500	-2.11084500	0.36890200
C	1.46834400	1.19560100	-0.18475500
H	0.91944200	2.11085100	-0.36890100
C	2.83947400	-1.23826500	0.19534900
C	2.83947800	1.23826500	-0.19534400
C	3.60161500	-0.00000300	-0.00001100
C	3.59889200	-2.55064800	0.41591900
C	3.59889700	2.55064900	-0.41590800
C	2.65332200	3.74100200	-0.61699300
H	2.02040200	3.61429000	-1.50169200
H	2.00481800	3.89913300	0.25134600
H	3.24692400	4.64962700	-0.75962500
C	4.47459000	2.85745300	0.81312700
H	3.84998400	2.97459300	1.70550400
H	5.18935000	2.05326900	0.98590600
H	5.02081000	3.79495400	0.65720800
C	4.48496000	2.44632500	-1.67077300
H	5.20976000	1.63963200	-1.56477200
H	3.86896100	2.25536600	-2.55636500
H	5.02010200	3.38985300	-1.82854100
C	4.48499900	-2.44629900	1.67074900
H	5.20979100	-1.63960400	1.56471000
H	3.86903200	-2.25533100	2.55636200
H	5.02015200	-3.38982300	1.82851400

C	2.65331500	-3.74099000	0.61707200
H	2.02041000	-3.61423300	1.50177500
H	2.00479600	-3.89915800	-0.25124900
H	3.24691600	-4.64961000	0.75973400
C	4.47453700	-2.85748800	-0.81314100
H	3.84989900	-2.97463000	-1.70549500
H	5.18930600	-2.05331800	-0.98595500
H	5.02074700	-3.79499600	-0.65722600
O	4.86043100	-0.00000800	-0.00003700

[DQH]•

H	-5.24531700	-0.77722500	0.19277900
C	-1.42753200	1.16829100	-0.29987700
H	-0.87352500	2.05964900	-0.56383400
C	-0.70816600	0.00297900	0.00030500
C	-1.43174700	-1.15748000	0.29938500
H	-0.88253900	-2.05054200	0.56705200
C	-2.82309500	-1.19038800	0.30877600
C	-3.50139100	0.00972500	-0.00639200
C	-2.81642200	1.20810500	-0.31489200
C	-3.58027000	-2.48516100	0.65579300
C	-3.57141300	2.50255500	-0.65757200
C	-2.61507400	-3.63868000	0.96723100
H	-1.97184600	-3.87204300	0.11357700
H	-1.98397000	-3.41601200	1.83246900
H	-3.19789000	-4.53397100	1.20076100
C	-4.43843500	-2.29432200	1.92530600
H	-5.18660000	-1.49935200	1.86404800
H	-4.96939700	-3.22363300	2.15223100
H	-3.79165700	-2.05332900	2.77370400
C	-4.43162000	-2.95404000	-0.54488100
H	-4.97727900	-3.86344100	-0.27605500
H	-5.16524800	-2.22697600	-0.90342600
H	-3.77823500	-3.18398900	-1.39128800
C	-4.43815900	2.30412200	-1.91458900
H	-5.20179700	1.54114000	-1.76680600
H	-4.93565900	3.24695800	-2.16597200
H	-3.81358000	2.01434700	-2.76570000
C	-4.44793700	2.93822300	0.53202800
H	-4.95473700	3.87754000	0.28625000
H	-5.20399100	2.19190600	0.77499500
H	-3.82790000	3.11062700	1.41778000
C	-2.60309300	3.65664200	-0.95294700

H	-1.96549300	3.44398600	-1.81687800
H	-3.18445300	4.55418200	-1.18239300
H	-1.96338400	3.88484900	-0.09430600
O	-4.86047400	0.07580100	-0.03034600
C	0.75905900	0.00021400	0.00166900
C	1.48143300	1.17958900	0.30551000
H	0.91429400	2.06299800	0.57133900
C	1.47864200	-1.18085500	-0.30224600
H	0.90948600	-2.06302400	-0.56813500
C	2.85312900	1.22540300	0.31679600
C	2.85025900	-1.22939600	-0.31489500
C	3.60285800	-0.00268800	0.00035400
C	3.61598700	2.50468700	0.65795900
C	3.61035000	-2.50977100	-0.65811400
C	2.65644800	-3.67291400	-0.95843500
H	2.01565500	-3.90700400	-0.10206000
H	2.01927500	-3.46419300	-1.82382000
H	3.24627300	-4.56513900	-1.18735600
C	4.48289200	-2.28629000	-1.90777400
H	3.86259800	-1.99295200	-2.76095900
H	5.23142900	-1.51395500	-1.73422700
H	4.99330400	-3.22033200	-2.16582700
C	4.49562900	-2.92623700	0.53274000
H	5.23335900	-2.15780000	0.76208700
H	3.88200000	-3.10600300	1.42163200
H	5.01850100	-3.85710900	0.28855900
C	4.49882300	2.91933200	-0.53536200
H	5.23469800	2.14962500	-0.76644400
H	3.88309300	3.09981000	-1.42265400
H	5.02383200	3.84944300	-0.29287400
C	2.66457900	3.66942800	0.96013300
H	2.02235400	3.90447000	0.10509700
H	2.02886400	3.46188100	1.82687700
H	3.25634000	4.56073400	1.18766400
C	4.49131900	2.28042300	1.90548900
H	3.87272400	1.98850300	2.76039300
H	5.23818400	1.50680500	1.73043800
H	5.00384000	3.21379100	2.16177600
O	4.85323200	-0.00382400	-0.00083900
re-TS1			
C	0.87828900	-0.11416600	-0.04914900
C	1.86695600	-1.99638300	-0.70006600
C	3.17193800	0.10350900	-1.13860500

H	2.84339200	0.63369500	-2.03259200
N	0.72366100	-2.38280800	-0.22003200
N	0.13433300	-1.20524500	0.17220600
N	2.00324200	-0.63311700	-0.60952300
C	2.94527600	-2.87336200	-1.25782000
H	2.50466900	-3.61691400	-1.92362700
H	3.44977900	-3.40409400	-0.44060100
C	4.29663600	-0.92955800	-1.39162900
O	3.85568300	-2.11252100	-2.02159600
C	4.85401400	0.30954000	0.53830700
C	3.81851100	0.99597700	-0.10582200
C	3.55316800	2.33142700	0.17461100
C	4.31396400	2.96520800	1.15764000
C	5.32546200	2.27494600	1.82786900
C	5.61159500	0.94519600	1.51511500
C	5.00085200	-1.08266500	-0.02433600
H	2.78239300	2.85234100	-0.38521100
H	5.91065500	2.78473400	2.58669100
H	6.42158800	0.42296100	2.01517500
H	4.48775400	-1.81170800	0.61437900
H	6.03838800	-1.40623500	-0.12837000
C	-1.18603500	-1.24179300	0.73282600
C	-1.34519200	-0.99673000	2.09884900
C	-2.26127200	-1.48151400	-0.12609600
C	-2.64586900	-0.98697600	2.60190700
C	-3.54199700	-1.46414900	0.42393700
C	-3.75249200	-1.21517300	1.78014800
H	-2.79808400	-0.78850600	3.66024900
H	-4.39752200	-1.60310700	-0.23336100
C	-2.03963700	-1.69539400	-1.59814000
H	-1.46222200	-2.60512100	-1.78505500
H	-1.47637200	-0.85528800	-2.02144500
H	-2.99464000	-1.76755700	-2.12124900
C	-0.15707100	-0.71607400	2.98119100
H	0.28492000	0.25814900	2.74607100
H	0.62576000	-1.46714200	2.84107600
H	-0.45230200	-0.71259500	4.03154600
H	4.99691200	-0.47208200	-2.09445500
C	-5.14681700	-1.18957600	2.35028400
H	-5.27158200	-0.35206600	3.04207600
H	-5.89061400	-1.09217100	1.55644100
H	-5.35850300	-2.10885000	2.90592000
C	-5.41124000	1.59099400	0.20213400
C	-4.05475900	1.87083300	0.08631600

C	-3.36465900	1.58876800	-1.10087300
C	-4.08113000	1.05412600	-2.17919600
C	-5.43801300	0.76431600	-2.06177000
C	-6.10684500	1.02649000	-0.86764900
H	-5.92982600	1.81360200	1.12972000
H	-3.52170400	2.31333100	0.92291200
H	-3.55906000	0.84304000	-3.10904300
H	-5.97333400	0.33634100	-2.90351800
H	-7.16531500	0.80528800	-0.77425300
C	-1.91041300	1.77944600	-1.22334700
H	-1.50069000	1.91727400	-2.22332800
C	-1.05023300	1.70493000	-0.20458900
C	0.43214100	1.83652600	-0.39633900
H	0.93939200	2.17436800	0.52798600
O	0.92582400	2.11021500	-1.51389700
H	-1.39192300	1.51523800	0.81195300
H	4.12663100	4.00738800	1.39506400

re-M1

C	0.88792500	-0.36285800	-0.18703500
C	2.25314500	-2.06426400	-0.39598200
C	3.25639300	0.17110000	-0.97512300
H	2.90537000	0.51687100	-1.94686100
N	1.10218800	-2.59769600	-0.11279300
N	0.26384900	-1.52242100	0.01684700
N	2.17140800	-0.69755200	-0.44773100
C	3.54061800	-2.78347200	-0.64890800
H	3.33600000	-3.71184300	-1.18312400
H	4.02007500	-3.03453100	0.30518100
C	4.55617400	-0.67230700	-1.01230000
O	4.37836500	-1.99683600	-1.46575800
C	4.76505900	0.91955100	0.71490000
C	3.65904800	1.29645900	-0.05257300
C	3.13269700	2.58314900	0.01172400
C	3.71498000	3.48745100	0.89905400
C	4.80443500	3.10952400	1.68777900
C	5.34363900	1.82629100	1.59656800
C	5.18997700	-0.48936900	0.38411600
H	2.28802000	2.83646000	-0.62628100
H	5.24785600	3.82907000	2.36888500
H	6.20775700	1.54662900	2.19137300
H	4.77721300	-1.19670700	1.11338300
H	6.27259600	-0.62846900	0.36434600
C	-1.14516900	-1.75858600	0.18331600

C	-1.62361000	-2.09695900	1.44730500
C	-1.95718700	-1.64859600	-0.94980300
C	-2.99611500	-2.32510800	1.56821400
C	-3.31871600	-1.87802000	-0.77490400
C	-3.85335500	-2.21272400	0.47322000
H	-3.40122800	-2.58732100	2.54203500
H	-3.98157100	-1.78798100	-1.63195700
C	-1.36943100	-1.28696000	-2.28779300
H	-0.64122500	-2.04185300	-2.60424100
H	-0.85090800	-0.32068000	-2.24845300
H	-2.15420300	-1.23142300	-3.04390500
C	-0.69291300	-2.19346600	2.62639600
H	-0.18237100	-1.24060200	2.80139800
H	0.07967800	-2.94846200	2.45551700
H	-1.24381900	-2.45781600	3.52982000
H	5.20783400	-0.20166300	-1.75207200
C	-5.33903000	-2.40148700	0.62822000
H	-5.58761300	-2.83615700	1.59817800
H	-5.84863300	-1.43530900	0.54649100
H	-5.73821400	-3.04900300	-0.15673200
C	-5.40350500	1.49214300	0.94140500
C	-4.05789000	1.27083900	0.66953200
C	-3.40315500	1.98740300	-0.34453100
C	-4.14872900	2.90885900	-1.09136100
C	-5.49741500	3.12874300	-0.82309400
C	-6.13001700	2.42359900	0.19759100
H	-5.89065600	0.93138100	1.73375000
H	-3.51125800	0.51959600	1.23339800
H	-3.65777100	3.46170700	-1.88794900
H	-6.05393000	3.85092400	-1.41220400
H	-7.18109400	2.59130600	0.40894300
C	-1.97776300	1.78998300	-0.65295600
H	-1.61380800	2.16350400	-1.60880000
C	-1.07686300	1.19619500	0.13070700
C	0.37963400	1.08912800	-0.29991100
H	0.93873000	1.58411000	0.53983900
O	0.69008200	1.52607200	-1.52249700
H	-1.33453900	0.83323000	1.12631900
H	3.32485100	4.49739300	0.97288200

si-TS1

C	-0.71738700	0.41270100	0.28576600
C	-2.19313000	-0.47825300	1.69425600
C	-3.10026100	1.28671000	0.24356900

H	-2.68143000	2.20816100	-0.16821400
N	-1.11043000	-1.16616100	1.89316100
N	-0.21967100	-0.60155800	1.00451400
N	-1.99062800	0.48612500	0.74299800
C	-3.52607000	-0.49916000	2.36818600
H	-3.46118700	-0.98369600	3.34221000
H	-4.26592300	-1.02968800	1.75272900
C	-4.12138200	1.60947600	1.39509600
O	-3.89330400	0.85481500	2.57794500
C	-5.26876500	0.55859200	-0.46996200
C	-3.91164800	0.52013500	-0.77883900
C	-3.43029400	-0.17255900	-1.88703400
C	-4.35405100	-0.82597800	-2.70087700
C	-5.71950200	-0.78450900	-2.40536400
C	-6.18684300	-0.09509400	-1.28834800
C	-5.52065800	1.35099600	0.78795300
H	-2.36298900	-0.22256100	-2.10613600
H	-6.42300300	-1.30315200	-3.04909000
H	-7.24717800	-0.07657400	-1.05467800
H	-6.15059400	0.82322900	1.51073300
H	-6.01552800	2.30073800	0.56101300
C	1.09500500	-1.16094600	0.86822800
C	1.24134500	-2.31064800	0.09209100
C	2.17071400	-0.51696500	1.48556000
C	2.53326200	-2.81539900	-0.06969900
C	3.43915600	-1.05813300	1.29630300
C	3.63890600	-2.20119300	0.51842700
H	2.67657800	-3.70620300	-0.67674500
H	4.29636200	-0.56227300	1.74721700
C	1.96627600	0.74716100	2.27366300
H	1.16531400	0.63472300	3.01037200
H	1.68384200	1.56758300	1.60447400
H	2.88386300	1.03019500	2.79246000
C	0.04811300	-2.95303700	-0.56312700
H	-0.42873300	-2.23389200	-1.23755200
H	-0.68944000	-3.26580000	0.18210400
H	0.35230400	-3.82990100	-1.13776000
H	-4.00801900	2.64565000	1.71433300
C	5.02961600	-2.74777500	0.32627300
H	5.71161100	-1.95450000	0.00433000
H	5.42214400	-3.15575700	1.26290300
H	5.04522600	-3.54259700	-0.42240400
C	5.30097300	2.79853500	0.12236900
C	4.00776900	2.46496000	-0.26502700

C	3.76391000	1.31871600	-1.03493400
C	4.85673500	0.52206800	-1.40421300
C	6.15187100	0.85547600	-1.02021600
C	6.37869300	1.99550400	-0.25208400
H	5.47044000	3.68813400	0.72103700
H	3.17989800	3.09789900	0.04115900
H	4.67720100	-0.37855100	-1.98677000
H	6.98343800	0.22353400	-1.31714100
H	7.38644300	2.25763500	0.05346900
C	2.41510700	0.88828400	-1.42839500
H	2.34848200	-0.07046700	-1.94275800
C	1.25899700	1.50774700	-1.17707600
C	-0.04459400	0.88776100	-1.58492300
H	-0.85424500	1.63744500	-1.70417700
O	-0.08743700	-0.17307400	-2.24253900
H	1.19579700	2.46394100	-0.66018100
H	-4.01080000	-1.37705500	-3.57061900

si-M1

C	0.72622300	-0.40037300	0.08912600
C	2.12864800	-0.01004800	1.73298600
C	3.11025100	-1.27754500	-0.14610100
H	2.70934200	-2.05592000	-0.79802300
N	1.03367400	0.59117500	2.08787900
N	0.17163800	0.34223900	1.05151300
N	1.97733200	-0.63818300	0.52659500
C	3.43114200	-0.19415400	2.43861900
H	3.31650800	-0.01825500	3.50777800
H	4.18837200	0.49504100	2.03997000
C	4.10460400	-1.89753400	0.90770900
O	3.79765500	-1.54868100	2.24974500
C	5.27585500	-0.34168300	-0.54932300
C	3.93195700	-0.25828100	-0.90049100
C	3.46119600	0.67147500	-1.82509100
C	4.39139300	1.52958800	-2.40886700
C	5.74607200	1.45124100	-2.07132200
C	6.19867200	0.51818700	-1.14059300
C	5.51281400	-1.42133300	0.47545800
H	2.39445800	0.72644000	-2.06265600
H	6.45403400	2.13111500	-2.53494300
H	7.25049800	0.46825700	-0.87555900
H	6.07140800	-1.06976100	1.34877200
H	6.07823500	-2.25440400	0.04666800
C	-1.14095600	0.93297700	1.06115900

C	-1.28584100	2.20091800	0.49950700
C	-2.19717500	0.21696700	1.63025300
C	-2.57411400	2.73911200	0.47161600
C	-3.46061700	0.79559400	1.57558900
C	-3.66878500	2.04748400	0.98888800
H	-2.72152600	3.72129000	0.02940200
H	-4.30799100	0.24941600	1.98474100
C	-1.98530500	-1.14639800	2.22808400
H	-1.10145700	-1.17053900	2.87139600
H	-1.84113300	-1.89036900	1.43733100
H	-2.85355000	-1.44509400	2.81764800
C	-0.09835500	2.92745500	-0.06821500
H	0.32106100	2.31898700	-0.87880400
H	0.67248100	3.07332300	0.69570700
H	-0.39363600	3.90596000	-0.45142000
H	4.02556000	-2.98419200	0.88982500
C	-5.05975300	2.61907800	0.91081300
H	-5.69180700	1.98691600	0.27792600
H	-5.52520300	2.65882800	1.89976400
H	-5.05384600	3.62706800	0.49141100
C	-5.37578700	-2.69646400	-0.61935500
C	-4.04587600	-2.36184000	-0.84965800
C	-3.69642900	-1.08470400	-1.31197300
C	-4.72514300	-0.16165600	-1.54540700
C	-6.05714900	-0.49494700	-1.31810600
C	-6.38814700	-1.76476900	-0.85018100
H	-5.62523200	-3.69013900	-0.26012700
H	-3.27156700	-3.10234400	-0.67028600
H	-4.46661400	0.83546000	-1.89411700
H	-6.83642900	0.23810000	-1.50448600
H	-7.42514900	-2.02843900	-0.66901700
C	-2.30443500	-0.65616300	-1.51672600
H	-2.15097200	0.34014500	-1.93020100
C	-1.19822500	-1.31624500	-1.17391900
C	0.17468200	-0.66833400	-1.33888600
H	0.84663300	-1.48428900	-1.71258800
O	0.23123800	0.47505400	-2.01769400
H	-1.22209500	-2.31496400	-0.73639300
H	4.06146100	2.26914000	-3.13161300
re-TS2D			
C	0.86962500	-0.39767000	-0.29654200
C	2.34562000	-2.03169100	-0.28519700
C	3.27396800	0.20013700	-1.01251400

H	3.01907300	0.50507500	-2.02673600
N	1.24728000	-2.58812000	0.11658200
N	0.32911800	-1.56690200	0.10729200
N	2.18392500	-0.68884900	-0.53632600
C	3.64884100	-2.73429800	-0.51573400
H	3.45922200	-3.67034800	-1.04325600
H	4.12697400	-2.97314100	0.44163800
C	4.59498300	-0.60952300	-0.90897600
O	4.48062700	-1.94751200	-1.33722700
C	4.60757300	1.01481100	0.79747000
C	3.58423700	1.36648500	-0.08978000
C	3.09086600	2.66891900	-0.11717000
C	3.58116000	3.59283100	0.80584900
C	4.56734300	3.22691700	1.72185100
C	5.09977200	1.93847800	1.71221100
C	5.08669200	-0.38808200	0.53774700
H	2.35978200	2.96389500	-0.86434100
H	4.94362100	3.95893200	2.42928900
H	5.90059600	1.66611900	2.39294400
H	4.62326600	-1.08956100	1.24059800
H	6.16924100	-0.50079400	0.62462900
C	-1.06851300	-1.87763100	0.18663400
C	-1.61179100	-2.21635800	1.42523800
C	-1.82762200	-1.79628000	-0.98761900
C	-2.98398000	-2.46761000	1.47903600
C	-3.19345200	-2.04515600	-0.87899400
C	-3.78830100	-2.37156900	0.34296400
H	-3.43351400	-2.72808200	2.43396900
H	-3.81158900	-1.98101300	-1.77136600
C	-1.19496800	-1.43676300	-2.30731900
H	-0.29589600	-2.03570400	-2.48725700
H	-0.90226400	-0.37962400	-2.33792100
H	-1.89628400	-1.62086700	-3.12286600
C	-0.74415800	-2.27721000	2.65365300
H	-0.23931600	-1.31971700	2.81890600
H	0.03425600	-3.03781800	2.54714000
H	-1.34182500	-2.51024500	3.53590800
H	5.30389500	-0.14162500	-1.59572100
C	-5.27866200	-2.57083700	0.42784500
H	-5.56553800	-3.04131400	1.37035500
H	-5.79047100	-1.60443200	0.36116800
H	-5.64178600	-3.19050900	-0.39612100
C	-5.41612800	1.46853900	0.92713200
C	-4.08880800	1.23274600	0.58698600

C	-3.41286400	2.07661500	-0.31173000
C	-4.12998400	3.14313400	-0.87406700
C	-5.46094600	3.37517300	-0.53947100
C	-6.11115000	2.54176600	0.36754200
H	-5.91516000	0.80443600	1.62730000
H	-3.57648200	0.36971000	1.00509800
H	-3.62856400	3.79867900	-1.58162300
H	-5.99066100	4.20950700	-0.98927500
H	-7.14917700	2.71953900	0.62939000
C	-2.01367700	1.86005500	-0.70002300
H	-1.65570600	2.38205400	-1.58437000
C	-1.14467300	1.06555300	-0.05025700
C	0.23022800	0.86634800	-0.49114100
H	0.97843000	1.78448800	-0.46082000
O	0.66549700	1.55902900	-1.70128000
H	-1.44491700	0.56094400	0.86587700
H	3.20215300	4.60941500	0.79894100

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C	0.48644600	-1.54279000	-0.49821600
C	2.04514000	-2.67969300	0.58196100
C	2.85861100	-1.59156200	-1.52408800
H	2.35603200	-1.62261300	-2.48940800
N	0.98460400	-2.86372500	1.29652000
N	0.00145400	-2.15839000	0.62057700
N	1.81527200	-1.90505900	-0.52675800
C	3.38690400	-3.30227800	0.74875400
H	3.31844900	-4.18027400	1.39062900
H	4.09742700	-2.59241000	1.19252000
C	4.04290200	-2.63478700	-1.41557600
O	3.79473900	-3.72199100	-0.53883800
C	4.87950900	-0.40488100	-0.95209600
C	3.53840800	-0.25275000	-1.30121800
C	2.97873500	1.01349600	-1.46055800
C	3.76064000	2.12808100	-1.16382500
C	5.08628800	1.97785000	-0.74607100
C	5.66128900	0.71139900	-0.66156700
C	5.31376900	-1.84314100	-1.01825800
H	1.95548200	1.08316100	-1.82344900
H	5.68175000	2.85563400	-0.51368000
H	6.70505000	0.59627100	-0.38385000
H	5.72380800	-2.21343200	-0.07296100
H	6.09788900	-1.98037900	-1.76838000
C	-1.36603200	-2.42360300	0.94638000

C	-1.90210600	-1.84999100	2.10357000
C	-2.12674000	-3.21581100	0.08036700
C	-3.24437200	-2.09300400	2.39013200
C	-3.46906900	-3.42025300	0.40089200
C	-4.04303400	-2.87238800	1.54934100
H	-3.68148200	-1.64788900	3.28077100
H	-4.08097900	-4.02479000	-0.26436800
C	-1.53004500	-3.78855500	-1.17706800
H	-0.53512800	-4.20415900	-0.99091400
H	-1.42537600	-3.01062200	-1.94218400
H	-2.16770900	-4.57796000	-1.57850400
C	-1.06556400	-0.93428300	2.95524000
H	-0.75721300	-0.05910900	2.36815400
H	-0.15360500	-1.43149600	3.29958500
H	-1.62873000	-0.59038000	3.82445800
H	4.17072200	-3.09939800	-2.39366100
C	-5.49113200	-3.12286300	1.88218600
H	-5.92790300	-2.26847500	2.40494200
H	-6.07564500	-3.31333100	0.97932100
H	-5.59364600	-3.99619900	2.53472500
C	-5.80102300	0.74725600	-0.56920100
C	-4.48860300	0.31699700	-0.72571800
C	-3.70629000	0.76567000	-1.80383400
C	-4.30060800	1.63790100	-2.72813300
C	-5.61522500	2.06791200	-2.57256800
C	-6.37231200	1.62784600	-1.48924800
H	-6.38689300	0.38574000	0.27106600
H	-4.06978500	-0.39264000	-0.01555700
H	-3.71397300	1.98430400	-3.57539400
H	-6.04862500	2.74835600	-3.29932100
H	-7.39825100	1.95949800	-1.36620400
C	-2.30967600	0.35108800	-1.99309700
H	-1.85866800	0.52145000	-2.96857300
C	-1.52889800	-0.18847700	-1.04376800
C	-0.08852900	-0.47712100	-1.28958900
H	0.41029800	0.27852500	-0.29906600
O	0.42801600	-0.19938800	-2.47786600
H	-1.91598200	-0.30762900	-0.03491400
H	3.33930600	3.12481800	-1.26619300
C	-1.38233600	3.50573000	-0.12196200
C	-1.28602700	4.96790700	0.31834000
C	-0.30361700	5.24259800	1.45972800
C	-0.04251400	2.91478500	-0.59204600
C	1.13753600	4.82189600	1.15308600

C	0.81722400	2.45186400	0.55845900
H	-1.77769200	2.88228300	0.69109400
H	-0.98159800	5.56881400	-0.54936200
H	-0.62444000	4.73073100	2.37615600
H	1.41332000	5.11242600	0.13312300
H	0.50754400	3.65756000	-1.18277000
H	-2.10036900	3.42772000	-0.94514100
H	-2.27978100	5.32378000	0.60967800
H	-0.30965200	6.31627600	1.67531200
H	-0.21050500	2.05337700	-1.24158900
H	1.82942300	5.34241500	1.81876800
C	2.10585200	3.01844500	2.57271500
H	1.81758600	3.71942000	3.36227300
H	3.18286100	3.13605700	2.39894900
C	1.78202100	1.59179700	2.98975000
H	2.48189200	1.26789900	3.76363400
H	0.77037700	1.54951500	3.40866700
C	1.85468700	0.69092200	1.76316600
H	1.58197000	-0.33999500	2.01589800
H	2.88280000	0.67057800	1.36847200
N	0.95548300	1.17150000	0.72799300
N	1.38095000	3.39115100	1.35205400

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C	1.21899700	-0.77719700	-0.12169300
C	2.35173200	-0.40533600	-1.94959600
C	3.29153100	0.72549400	0.10944000
H	2.74795400	1.61639700	0.42543300
N	1.37104400	-1.18130400	-2.31144100
N	0.67448500	-1.40660300	-1.16356100
N	2.30961300	-0.14755300	-0.60381600
C	3.38439600	0.20892800	-2.84452200
H	2.89190800	0.59208300	-3.73990200
H	4.11714700	-0.54680500	-3.15019900
C	4.43992900	1.02159700	-0.88744700
O	3.98819600	1.30319600	-2.19402000
C	5.24058700	-0.49132900	0.73693900
C	4.02590100	0.00872600	1.21943500
C	3.68160800	-0.11150500	2.56299100
C	4.55446500	-0.78991200	3.41264500
C	5.75196600	-1.31797900	2.92727900
C	6.10958900	-1.16245500	1.58866300
C	5.42890700	-0.15097200	-0.71933200
H	2.76089800	0.32754600	2.93319100

H	6.42176000	-1.83830600	3.60442700
H	7.05618100	-1.54584100	1.22094200
H	5.16316500	-1.00802900	-1.34897600
H	6.45109300	0.13780100	-0.97061900
C	-0.44302000	-2.32334300	-1.19215700
C	-0.18243000	-3.66238100	-0.89485900
C	-1.71569500	-1.82951700	-1.48513500
C	-1.27508300	-4.52782500	-0.85858400
C	-2.77289600	-2.73411200	-1.42504000
C	-2.57366700	-4.07894000	-1.10734800
H	-1.10662500	-5.57375500	-0.61554300
H	-3.78292900	-2.36876100	-1.59607400
C	-1.94143000	-0.37823800	-1.80346100
H	-1.44666400	-0.10393700	-2.74146300
H	-1.54075700	0.26516100	-1.00954200
H	-3.00838700	-0.17153200	-1.90313800
C	1.21268100	-4.13537800	-0.58184000
H	1.56335800	-3.73693600	0.37726600
H	1.92367900	-3.81714900	-1.34998300
H	1.24015500	-5.22357400	-0.51735900
H	4.91929400	1.93995500	-0.54196800
C	-3.74191600	-5.02659700	-1.04261300
H	-3.55765200	-5.82974800	-0.32540100
H	-4.65186100	-4.49891100	-0.74716100
H	-3.91981300	-5.48688200	-2.01988500
C	-4.66096300	-2.94696800	1.80232700
C	-3.38869100	-2.40959300	1.95502400
C	-3.11347700	-1.10279600	1.53258800
C	-4.14947100	-0.34058400	0.98064000
C	-5.42298700	-0.88109700	0.81955800
C	-5.68080100	-2.18791300	1.22610000
H	-4.86024100	-3.96144700	2.13360200
H	-2.60275400	-3.00667900	2.40838900
H	-3.94442000	0.67529800	0.64976300
H	-6.21222600	-0.28133400	0.37768500
H	-6.67246400	-2.61171400	1.10472900
C	-1.75432400	-0.53768000	1.55706400
H	-1.67349500	0.54645600	1.53185500
C	-0.64263000	-1.26799200	1.47636800
C	0.73066700	-0.66099200	1.32007100
H	1.44429700	-1.24664000	1.91928000
O	0.83677400	0.67166000	1.71081300
H	-0.69338800	-2.35397000	1.45728600
H	4.30599000	-0.89679900	4.46324300

C	-1.40938300	4.59262600	1.94498400
C	-2.63090800	5.44903300	1.60736700
C	-2.93872600	5.57195400	0.11573500
C	-1.52128900	3.12078500	1.49967300
C	-3.14459300	4.21709800	-0.56522400
C	-1.11681800	2.94072400	0.05358800
H	-0.50401300	5.02822500	1.50403200
H	-3.50680500	5.01601700	2.10912700
H	-2.13065800	6.10293300	-0.40307900
H	-3.77600300	3.57176700	0.05481800
H	-2.54114100	2.75762500	1.67575700
H	-1.26619200	4.60527900	3.02943000
H	-2.49221600	6.44886000	2.03116300
H	-3.84883300	6.16711700	-0.01255200
H	-0.84733700	2.50490700	2.09768000
H	-3.67104700	4.34415800	-1.51355500
C	-1.44864600	3.59598500	-2.28167700
H	-1.79065800	4.54894000	-2.69528300
H	-1.92016100	2.79138000	-2.86104300
C	0.06384600	3.49763200	-2.34534800
H	0.39502800	3.42590900	-3.38358700
H	0.50395500	4.39999800	-1.90767700
C	0.51250800	2.28090500	-1.54964400
H	1.60732200	2.25907700	-1.50356300
H	0.19481600	1.36426300	-2.06926400
N	-0.00838900	2.29400200	-0.18406200
N	-1.89181100	3.52884200	-0.88685600
H	0.49959800	1.30393500	0.97377300

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C	0.81003400	-1.58629800	-0.41055000
C	2.31434400	-3.01925200	0.29746600
C	3.17882200	-1.38844900	-1.42741200
H	2.84174000	-1.55616700	-2.44937500
N	1.23668600	-3.32323700	0.95176300
N	0.30456300	-2.42702600	0.50354500
N	2.11921600	-1.94100200	-0.53269200
C	3.61262400	-3.76396000	0.34606700
H	3.40326100	-4.83397100	0.37506200
H	4.17254700	-3.49987300	1.25044100
C	4.50610200	-2.13282100	-1.10167300
O	4.34545000	-3.50589000	-0.82874400
C	4.72953700	0.09468300	-0.36462900
C	3.57272700	0.05283700	-1.15514700

C	3.03291400	1.22577100	-1.67619800
C	3.63392500	2.44254700	-1.35381400
C	4.76876000	2.48493600	-0.54334000
C	5.33251900	1.30670900	-0.05203800
C	5.19462200	-1.29086000	-0.00918400
H	2.16016900	1.19176700	-2.31731500
H	5.22881200	3.44013600	-0.31021700
H	6.23449000	1.33326000	0.55145800
H	4.85586900	-1.56121500	0.99744400
H	6.27995800	-1.40600800	-0.03294000
C	-1.05795100	-2.59151800	0.93920400
C	-1.46660700	-1.94869700	2.10664700
C	-1.90291600	-3.39407400	0.16751800
C	-2.78821500	-2.13612000	2.51305800
C	-3.21347200	-3.54850800	0.61229600
C	-3.67117600	-2.93069700	1.77965700
H	-3.13487700	-1.64258200	3.41716100
H	-3.89629000	-4.16307200	0.03097000
C	-1.42132300	-4.02033500	-1.11252900
H	-0.45062100	-4.50627800	-0.98136500
H	-1.31212700	-3.25639900	-1.89152100
H	-2.13601300	-4.76234700	-1.47054500
C	-0.53347200	-1.02217900	2.83671700
H	-0.34147800	-0.12963200	2.22523800
H	0.43124400	-1.49659300	3.03972500
H	-0.96886700	-0.69513300	3.78191300
H	5.11149300	-2.08577100	-2.00935900
C	-5.10440600	-3.10028600	2.20936500
H	-5.28806600	-2.63037500	3.17713500
H	-5.77816800	-2.64812200	1.47467800
H	-5.36702600	-4.15915100	2.28272100
C	-5.61873200	0.22105100	-0.37066500
C	-4.26673400	-0.06713600	-0.51387200
C	-3.58950000	0.24843100	-1.70241600
C	-4.31717400	0.83762100	-2.74476700
C	-5.67251000	1.12288100	-2.60261600
C	-6.32874500	0.81908300	-1.41280200
H	-6.12448100	-0.02659700	0.55774400
H	-3.73830800	-0.55797900	0.29947800
H	-3.80806100	1.07829800	-3.67445200
H	-6.21445100	1.58384500	-3.42238600
H	-7.38506900	1.03912200	-1.29802500
C	-2.15355100	-0.01524900	-1.89055500
H	-1.78334900	0.07373200	-2.91043300

C	-1.29100700	-0.30007500	-0.90413300
C	0.17034800	-0.45423100	-1.08464600
H	0.62516400	0.59638500	-0.36179500
O	0.61481500	-0.33996300	-2.41978600
H	-1.64267600	-0.30755100	0.12401700
H	3.21800200	3.36513800	-1.74691600
C	-1.92421000	3.27716700	-0.39998300
C	-2.21161000	4.71799400	0.02695200
C	-1.37093400	5.23096900	1.19786200
C	-0.46991000	3.04018100	-0.84241100
C	0.13776300	5.17267400	0.94299200
C	0.45659800	2.81069600	0.32440800
H	-2.16813700	2.57668600	0.41005300
H	-2.03772500	5.37437300	-0.83647100
H	-1.59175800	4.66227600	2.11008400
H	0.37030500	5.52116300	-0.06892400
H	-0.11206000	3.88961400	-1.43597800
H	-2.58121000	3.01700800	-1.23628600
H	-3.27265400	4.81153100	0.28004800
H	-1.64457000	6.27224800	1.39734900
H	-0.40986500	2.15802400	-1.48215400
H	0.66318200	5.84065200	1.62866900
C	1.45863000	3.64593400	2.40480900
H	0.95917200	4.22856600	3.18465000
H	2.47151900	4.04832300	2.28246700
C	1.50565400	2.17579700	2.79190100
H	2.22688500	2.03323500	3.59936400
H	0.52181900	1.85803600	3.15367900
C	1.88534900	1.36055900	1.56237300
H	1.88728000	0.28581900	1.77884300
H	2.89737700	1.62680600	1.22958100
N	0.94155300	1.61330700	0.48540000
N	0.71257800	3.84063200	1.15460100
H	0.18063800	-1.01977300	-2.95705700

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C	0.86524300	-0.18792800	-1.00172700
C	2.67701600	-1.46723600	-1.12621300
C	3.14170600	0.98160900	-1.03624200
H	2.99767800	1.70137200	-1.84069600
N	1.75694900	-2.28272800	-0.74389400
N	0.61348500	-1.50050400	-0.63756300
N	2.23286400	-0.16601800	-1.26718600
C	4.08603500	-1.82242300	-1.50429400

H	4.07290900	-2.45750700	-2.39306100
H	4.56800200	-2.38348600	-0.69553200
C	4.59420700	0.42794300	-0.97596600
O	4.80760400	-0.65920100	-1.85204500
C	3.94781800	1.08823900	1.21915500
C	2.96896400	1.57934500	0.34909900
C	2.01712700	2.49218100	0.80001700
C	2.04109500	2.87992100	2.13991800
C	3.00468200	2.37177100	3.01240100
C	3.97154300	1.47883300	2.55399600
C	4.89264100	0.15267600	0.51437300
H	1.27950700	2.89841700	0.11791000
H	3.01008800	2.68542200	4.05166700
H	4.73585000	1.09930200	3.22567700
H	4.67897100	-0.88581600	0.79074100
H	5.94182800	0.33883600	0.75572400
C	-0.49190300	-1.97650200	0.12409100
C	-0.64431300	-1.53704700	1.44353300
C	-1.41725300	-2.82770200	-0.49274000
C	-1.78331000	-1.94813400	2.13884200
C	-2.53203000	-3.22223700	0.24228600
C	-2.73741100	-2.78081100	1.55387200
H	-1.92544300	-1.60881600	3.16214200
H	-3.26607900	-3.87792700	-0.22062500
C	-1.21097700	-3.25515300	-1.92055600
H	-0.25340800	-3.76928600	-2.04078800
H	-1.19029100	-2.38177200	-2.58075000
H	-2.01215000	-3.91997700	-2.24733000
C	0.36312500	-0.61083400	2.06967900
H	0.22237700	0.41612500	1.71174100
H	1.38713400	-0.89817700	1.80811600
H	0.26507600	-0.61163000	3.15683200
H	5.25701200	1.22018200	-1.33091900
C	-3.97881500	-3.18847000	2.30486800
H	-3.91752700	-2.90422400	3.35716800
H	-4.86371800	-2.70728100	1.87570100
H	-4.13638700	-4.26886200	2.24702100
C	-5.68669500	0.79535300	0.11881100
C	-4.31989300	0.77326700	-0.12867800
C	-3.67799900	1.86216500	-0.74945700
C	-4.46874000	2.97208500	-1.09214800
C	-5.83691300	2.99434300	-0.84165700
C	-6.45729400	1.90369700	-0.23640100
H	-6.15574800	-0.05838800	0.59921900

H	-3.74570100	-0.09907200	0.17464800
H	-3.99386800	3.82677800	-1.56734800
H	-6.41991800	3.86681500	-1.12091700
H	-7.52412600	1.91664700	-0.03890700
C	-2.24445900	1.88885400	-1.04497400
H	-1.85027100	2.82837300	-1.42597700
C	-1.40191500	0.84263500	-0.88109000
C	-0.00380500	0.85921700	-1.18748500
O	0.54360200	2.02911500	-1.71592200
H	-1.80222600	-0.09728700	-0.51529900
H	1.30519500	3.58862600	2.50635100
H	0.23764800	2.11012500	-2.63014300

si-TS2D

C	0.72352800	-0.31776000	-0.72480100
C	2.36297600	-1.73390700	-0.32179800
C	3.13707100	0.47913600	-1.10508300
H	2.72514100	1.20060300	-1.81016800
N	1.29841600	-2.38308600	0.02491100
N	0.27566100	-1.48638500	-0.20525400
N	2.07517000	-0.47573600	-0.78100300
C	3.78687400	-2.17349000	-0.40102800
H	3.85023000	-3.26119600	-0.40849300
H	4.36356400	-1.78571100	0.45015900
C	4.38796500	-0.27441000	-1.69945200
O	4.28103500	-1.68937300	-1.63636200
C	5.03707300	1.00186800	0.26430600
C	3.65841600	1.15433800	0.14598200
C	2.91419200	1.84321700	1.09936000
C	3.58278000	2.36750100	2.20310500
C	4.96528800	2.20804700	2.33738500
C	5.70258400	1.53151900	1.36790900
C	5.61057300	0.25409600	-0.91164200
H	1.84600900	1.98063400	0.94491500
H	5.47035700	2.61976900	3.20560900
H	6.77722500	1.41537600	1.47324200
H	6.25672200	-0.58044200	-0.62095800
H	6.20998300	0.91835300	-1.54179500
C	-1.00499200	-1.71286000	0.39640300
C	-1.37420300	-0.90590700	1.48123200
C	-1.83396700	-2.70265900	-0.13197000
C	-2.64343900	-1.10240200	2.01909100
C	-3.09214500	-2.86806900	0.45088600
C	-3.51652700	-2.06964800	1.51349100

H	-2.96067700	-0.48294300	2.85464700
H	-3.75960700	-3.62793300	0.05247900
C	-1.38704600	-3.53703100	-1.30208200
H	-0.53364700	-4.16542300	-1.03237400
H	-1.06746400	-2.90086400	-2.13373200
H	-2.19798500	-4.17947700	-1.64803000
C	-0.45131500	0.15426100	2.02504600
H	-0.43779700	1.03407400	1.36877000
H	0.57616500	-0.21492300	2.11067700
H	-0.78424600	0.47386600	3.01396400
H	4.47216400	-0.05951100	-2.76464400
C	-4.90142800	-2.21148600	2.08836800
H	-4.87299800	-2.25051800	3.18048400
H	-5.51578300	-1.34927600	1.80795500
H	-5.39469700	-3.11356400	1.72134100
C	-5.84827400	0.80836600	-0.59913500
C	-4.46144700	0.74015100	-0.66752800
C	-3.68584300	1.90889000	-0.76166000
C	-4.35332800	3.14217700	-0.75412300
C	-5.74147000	3.21122200	-0.67868200
C	-6.49759300	2.04369400	-0.60573100
H	-6.42678600	-0.10860200	-0.53230400
H	-3.97269300	-0.23030500	-0.62559700
H	-3.76892400	4.05690100	-0.81248100
H	-6.23330400	4.17923400	-0.67754000
H	-7.58000600	2.09383300	-0.54634500
C	-2.21936400	1.88247800	-0.84113200
H	-1.69473800	2.81883300	-0.66589200
C	-1.47949800	0.79508100	-1.11462300
C	-0.01833400	0.82452300	-1.16935700
H	0.50040500	1.39447700	-2.06594300
O	0.64251500	2.10693600	-0.96455500
H	-1.96328400	-0.15220800	-1.34216400
H	3.02889300	2.90729000	2.96456700

si-TS2B

C	1.43988300	0.16842500	-0.48089900
C	3.21688500	0.59658200	-1.73215500
C	3.50729200	1.07978700	0.70406100
H	2.89713600	1.74500500	1.31098900
N	2.41352300	-0.01725100	-2.53771600
N	1.31422300	-0.30579700	-1.75460500
N	2.69019600	0.73661100	-0.47470400
C	4.57821000	1.13799400	-2.02923100

H	4.59029200	1.59156400	-3.02137900
H	5.31647800	0.32581800	-2.01693700
C	4.87314000	1.70313300	0.25432600
O	4.88739100	2.14732500	-1.09328300
C	5.27454700	-0.40401500	1.37753400
C	3.90438700	-0.16649800	1.46091800
C	3.05388300	-1.02605000	2.15307300
C	3.60757200	-2.15507100	2.75404300
C	4.98034600	-2.40597100	2.66882300
C	5.82348100	-1.52980300	1.98810000
C	5.98066300	0.67110000	0.59293200
H	1.99923100	-0.76306800	2.23517000
H	5.39593800	-3.28939200	3.14388300
H	6.89101000	-1.72304000	1.93419100
H	6.44703200	0.27299500	-0.31417100
H	6.78140600	1.14160200	1.16995900
C	0.27482700	-1.12361300	-2.28659600
C	0.21788000	-2.46787600	-1.89363700
C	-0.64782000	-0.55660200	-3.16896700
C	-0.84017200	-3.23672800	-2.37053600
C	-1.69276400	-1.36721100	-3.61946200
C	-1.81321900	-2.69768600	-3.21928000
H	-0.91098700	-4.28006900	-2.07110600
H	-2.43034100	-0.94436900	-4.29722100
C	-0.51036300	0.87603400	-3.61018800
H	0.38687800	1.00416800	-4.22342600
H	-0.41623900	1.54512600	-2.74769200
H	-1.37953300	1.18120600	-4.19628100
C	1.24179900	-3.03441800	-0.94714900
H	1.08735300	-2.64277500	0.06581800
H	2.25593700	-2.75692700	-1.25016500
H	1.17083000	-4.12265900	-0.90947800
H	5.02730100	2.61271900	0.83641900
C	-2.97224900	-3.54455300	-3.67694500
H	-3.69425900	-3.67806300	-2.86455700
H	-3.49396700	-3.08208100	-4.51709500
H	-2.63626300	-4.53906400	-3.98143200
C	-3.88402300	-3.52678600	1.40604600
C	-2.79991300	-2.69645300	1.14844600
C	-2.32284000	-1.80332700	2.12542300
C	-2.96901000	-1.79664100	3.37109700
C	-4.05240700	-2.63074700	3.63153300
C	-4.51997200	-3.49948000	2.64834000
H	-4.23305700	-4.20624800	0.63379500

H	-2.31099400	-2.74849000	0.17802700
H	-2.61264300	-1.11765100	4.14173300
H	-4.53355700	-2.59962100	4.60460500
H	-5.36484800	-4.15096400	2.84698800
C	-1.20236700	-0.88373100	1.89487300
H	-0.83719500	-0.31734900	2.74838800
C	-0.60570300	-0.65393900	0.71086400
C	0.45131900	0.38053600	0.57355800
H	-0.22883700	1.30291400	-0.14799800
O	0.86211600	0.99882700	1.67916400
H	-0.96854700	-1.15708000	-0.18180600
H	2.97068600	-2.84241900	3.30263600
C	-3.85543500	0.61517500	-0.04901000
C	-5.21985400	1.26186500	0.18816600
C	-5.15744800	2.62570300	0.87395900
C	-2.92855000	1.38320400	-1.00571500
C	-4.32945300	3.64638900	0.09263500
C	-2.17930800	2.52191300	-0.35961200
H	-3.33498000	0.46869700	0.90453300
H	-5.73301300	1.37655600	-0.77661000
H	-4.73492400	2.52875900	1.88204700
H	-4.58075000	3.60088000	-0.97312100
H	-3.49531900	1.75763900	-1.86925500
H	-4.00449400	-0.38645300	-0.46779800
H	-5.83361600	0.58391700	0.79064300
H	-6.17275200	3.01994200	0.98794600
H	-2.16913800	0.70588900	-1.40244800
H	-4.56554200	4.66038900	0.42541900
C	-2.24286100	4.42342200	1.19691400
H	-2.86424100	4.46212200	2.09871400
H	-2.23492500	5.42827300	0.75568800
C	-0.83189600	3.96905900	1.52898200
H	-0.30158000	4.77006900	2.04918500
H	-0.84138200	3.08126400	2.16911700
C	-0.13483600	3.57403000	0.23426000
H	0.87137400	3.20054300	0.43513600
H	-0.06963400	4.43267300	-0.44732500
N	-0.87463700	2.49408600	-0.41075500
N	-2.88320400	3.49448400	0.25807900

si-M02

C	-0.36145000	-1.54606900	-0.22795600
C	0.53531100	-3.17178800	0.91846200
C	1.54836800	-2.82537700	-1.37565100

H	0.92514300	-3.19736000	-2.19084800
N	-0.41641400	-2.70482800	1.67704600
N	-0.95769600	-1.68917700	0.95468500
N	0.61786400	-2.47245900	-0.25847100
C	1.42609900	-4.33932800	1.20814300
H	0.83737100	-5.12385800	1.68503500
H	2.22504900	-4.04256500	1.89754800
C	2.53204400	-3.90306000	-0.83995700
O	1.92809300	-4.86069500	-0.00083700
C	3.71231700	-1.86507600	-1.09289700
C	2.49238800	-1.70824400	-1.75883800
C	2.30996000	-0.68189500	-2.68099200
C	3.34604700	0.22616300	-2.88202100
C	4.54051800	0.10993000	-2.16927800
C	4.73858800	-0.94562500	-1.28089000
C	3.71757800	-3.11326500	-0.24886400
H	1.39193200	-0.58393600	-3.25053100
H	5.33322400	0.83451000	-2.32961200
H	5.68372500	-1.05918500	-0.75871500
H	3.56013700	-2.87260200	0.80865200
H	4.65021400	-3.67652500	-0.31668100
C	-2.16781700	-1.03674800	1.39200600
C	-2.10013400	0.24235100	1.93810500
C	-3.36712600	-1.71206900	1.13959000
C	-3.31424400	0.88915500	2.17335500
C	-4.54713400	-1.02618900	1.40544900
C	-4.53773600	0.28572300	1.88476400
H	-3.29777100	1.89975500	2.57317600
H	-5.49696700	-1.51201300	1.19662400
C	-3.37888200	-3.10870900	0.57722900
H	-2.95396500	-3.82279800	1.28847800
H	-2.78856000	-3.17861900	-0.34331700
H	-4.39959000	-3.41625300	0.34640900
C	-0.78579800	0.91073100	2.23387000
H	-0.22267300	1.09729100	1.31347300
H	-0.16911400	0.28470600	2.88718500
H	-0.95109800	1.86580500	2.73539400
H	2.87785400	-4.45959500	-1.71340300
C	-5.82701600	1.04736600	2.02117800
H	-6.10762900	1.45809500	1.04351300
H	-6.63990800	0.39774400	2.35430800
H	-5.72991100	1.87790400	2.72334400
C	-6.50351000	0.50060100	-1.77487500
C	-5.16251300	0.15531600	-1.65899300

C	-4.18556900	1.14049800	-1.45246900
C	-4.59688700	2.47482000	-1.34916800
C	-5.93969500	2.82398300	-1.47021800
C	-6.89793300	1.83710400	-1.68670300
H	-7.24665600	-0.27474900	-1.93159700
H	-4.87392400	-0.89059800	-1.71273700
H	-3.85023700	3.24547600	-1.17717600
H	-6.23621900	3.86516000	-1.39302800
H	-7.94597700	2.10305100	-1.77884600
C	-2.75104900	0.83649200	-1.31783100
H	-2.11433700	1.66776700	-1.02327200
C	-2.16361800	-0.34660800	-1.50418500
C	-0.67360800	-0.53819000	-1.32575500
H	-0.30283600	-1.02563700	-2.24347400
O	-0.03501700	0.66687700	-1.07765900
H	-2.71713200	-1.22800800	-1.82154600
H	3.22114800	1.03063200	-3.59927700
C	1.89487700	4.08581900	-0.41992800
C	2.98205300	5.11409400	-0.10028900
C	3.97093000	4.68977200	0.98576700
C	2.43376700	2.74234700	-0.94712100
C	4.68321800	3.37120000	0.67396500
C	2.83000000	1.81482200	0.17654700
H	1.27538000	3.89867600	0.46722500
H	3.54407100	5.31953900	-1.02150200
H	3.45819700	4.58609800	1.95097500
H	5.01028200	3.34784000	-0.37087900
H	3.28336500	2.91797300	-1.61701900
H	1.23051700	4.50819800	-1.17996900
H	2.50913400	6.05721500	0.19283400
H	4.72467000	5.47467700	1.10819100
H	1.67084900	2.22586300	-1.53110700
H	5.58649500	3.27600500	1.28206700
C	4.08931900	1.58153200	2.27944600
H	4.27497000	2.38780200	2.99738300
H	4.98809400	0.95297900	2.24558000
C	2.87836100	0.76530900	2.69816000
H	3.12590500	0.15108200	3.56663200
H	2.05416700	1.43365400	2.97215100
C	2.45732900	-0.08820700	1.50806900
H	1.59478300	-0.71657300	1.76055900
H	3.28617000	-0.75730700	1.24004600
N	2.11173800	0.74904800	0.36955400
N	3.87081200	2.19033400	0.96343400

H	0.84878800	0.58069500	-0.54336700
si-TS2			
C	-0.13536200	-1.69065800	0.11816400
C	-0.83850200	-3.62871700	0.88729200
C	-2.66525500	-1.94327800	0.59212600
H	-2.69596800	-1.30097900	1.47493200
N	0.45541400	-3.72380400	0.88285800
N	0.87993300	-2.52398500	0.39304500
N	-1.25507700	-2.40177700	0.43210500
C	-1.79307400	-4.71189900	1.27968500
H	-1.39860500	-5.24283500	2.14683900
H	-1.88919100	-5.42635900	0.45216500
C	-3.53764700	-3.21822800	0.73066900
O	-3.04043100	-4.16573400	1.64073300
C	-3.88284800	-2.32987200	-1.41341400
C	-3.28747800	-1.33013700	-0.63712100
C	-3.44165900	0.01662200	-0.95320600
C	-4.12109600	0.35016100	-2.12629600
C	-4.65618200	-0.65013300	-2.94057300
C	-4.55979600	-1.99410100	-2.58020700
C	-3.75737000	-3.66965800	-0.73214000
H	-3.04825400	0.78322200	-0.28942600
H	-5.18521100	-0.37493400	-3.84688800
H	-5.02757100	-2.76210100	-3.18809000
H	-2.89571600	-4.22865600	-1.11651300
H	-4.64292700	-4.29777800	-0.84223300
C	2.29509100	-2.32585500	0.21671000
C	2.81637600	-2.29596900	-1.07846200
C	3.08089600	-2.20158600	1.36554700
C	4.19135200	-2.10399600	-1.20317800
C	4.45226000	-2.02548700	1.18506600
C	5.01999600	-1.96059900	-0.08894800
H	4.62490300	-2.06396500	-2.19929100
H	5.08741600	-1.92048000	2.06103900
C	2.46745100	-2.23933600	2.73994700
H	2.09715500	-3.24042900	2.97820700
H	1.61579000	-1.55407400	2.81247300
H	3.20252900	-1.95324500	3.49337500
C	1.92919800	-2.44143400	-2.28410800
H	1.32900800	-1.53782500	-2.43672900
H	1.23726700	-3.28155500	-2.16807400
H	2.53065200	-2.61274500	-3.17821000
H	-4.49569600	-2.89268100	1.14230300

C	6.48923500	-1.68391700	-0.26374300
H	6.64758300	-0.61174400	-0.42502600
H	7.05889300	-1.97730200	0.62028700
H	6.89188000	-2.21071400	-1.13191000
C	5.21046900	2.10724100	0.10874700
C	4.01009300	1.42635000	-0.05585400
C	3.05475200	1.86256400	-0.98760900
C	3.35902100	2.98733600	-1.76707600
C	4.56302300	3.66819800	-1.60541100
C	5.49362000	3.23419300	-0.66405300
H	5.93382300	1.74938400	0.83589600
H	3.81943200	0.52834000	0.52502700
H	2.63710500	3.33227200	-2.50320300
H	4.77547300	4.53948100	-2.21734000
H	6.43419400	3.76084600	-0.53963100
C	1.77792900	1.15612000	-1.17639000
H	1.26534000	1.30658600	-2.12411100
C	1.21538900	0.34943200	-0.26265700
C	-0.09371700	-0.31145500	-0.40387700
H	-0.81122100	0.60643300	0.46945400
O	-0.54028700	-0.28558500	-1.75576300
H	1.68640100	0.23577300	0.71420000
H	-4.25101900	1.39268900	-2.39750600
C	-2.54106300	3.59289500	-1.23756300
C	-2.66585500	5.10997700	-1.09540600
C	-2.66167400	5.61585800	0.34664700
C	-1.22950900	3.00343600	-0.68376600
C	-1.40552800	5.21316600	1.11987500
C	-1.27516500	2.77498400	0.80630600
H	-3.39401500	3.10470500	-0.74685000
H	-1.83293900	5.58044200	-1.63438500
H	-3.54115200	5.24654000	0.88880700
H	-0.51239700	5.35857500	0.50320800
H	-0.38377500	3.65660000	-0.93054400
H	-2.59765600	3.33580600	-2.29989600
H	-3.58477500	5.43875700	-1.59069700
H	-2.72504200	6.70861400	0.34101800
H	-1.02201300	2.04094400	-1.15541700
H	-1.28280900	5.84435900	2.00233400
C	-1.71255800	3.66927300	3.04974100
H	-2.49592600	4.38489700	3.31742100
H	-0.81116900	3.93095600	3.61583400
C	-2.15841200	2.24948800	3.36086100
H	-2.16230400	2.09536300	4.44148600

H	-3.17453500	2.08706100	2.98787100
C	-1.21266000	1.27730000	2.66952700
H	-1.52002300	0.23964100	2.82924500
H	-0.19729800	1.38285500	3.07382100
N	-1.20314000	1.54168600	1.23722600
N	-1.43824900	3.83164500	1.61524500
H	-1.48449400	-0.08622100	-1.78349800

si-M2

C	0.86533700	-0.19122400	-1.00065900
C	2.67746900	-1.47022400	-1.12239000
C	3.14142800	0.97895500	-1.03861900
H	2.99658500	1.69671100	-1.84472500
N	1.75764000	-2.28519000	-0.73830900
N	0.61392800	-1.50316500	-0.63416500
N	2.23285800	-0.16950400	-1.26618300
C	4.08639000	-1.82591400	-1.50036400
H	4.07286800	-2.46331300	-2.38746500
H	4.56913900	-2.38467500	-0.69048500
C	4.59415000	0.42586900	-0.97811400
O	4.80719800	-0.66331400	-1.85171300
C	3.94939300	1.09145100	1.21584900
C	2.96966100	1.58010400	0.34541100
C	2.01826900	2.49418600	0.79475300
C	2.04356200	2.88562400	2.13355800
C	3.00805400	2.37993300	3.00647900
C	3.97447600	1.48577200	2.54957000
C	4.89387700	0.15438200	0.51266400
H	1.27997600	2.89852500	0.11225000
H	3.01452000	2.69651000	4.04484900
H	4.73952500	1.10816800	3.22149500
H	4.68077600	-0.88345700	0.79190800
H	5.94319900	0.34147900	0.75269300
C	-0.49246500	-1.97773600	0.12696300
C	-0.64381000	-1.53744300	1.44813700
C	-1.41735200	-2.82760700	-0.48820100
C	-1.78143600	-1.94639400	2.14312500
C	-2.53389300	-3.22101500	0.24836200
C	-2.73899500	-2.77766700	1.55737500
H	-1.92263700	-1.60855000	3.16728400
H	-3.26719900	-3.87753800	-0.21397100
C	-1.21241200	-3.25832600	-1.91524700
H	-0.25455900	-3.77185200	-2.03560600
H	-1.19358900	-2.38649300	-2.57755100

H	-2.01337000	-3.92464800	-2.23949400
C	0.36756400	-0.61433400	2.07262900
H	0.23564000	0.41113400	1.70723800
H	1.39055100	-0.91066800	1.81705000
H	0.26507000	-0.60736300	3.15931800
H	5.25642600	1.21746900	-1.33546200
C	-3.98499500	-3.16233200	2.31283700
H	-4.75945300	-2.39795300	2.18798600
H	-4.39220700	-4.10836800	1.94950500
H	-3.78609100	-3.25655500	3.38289500
C	-5.69142400	0.78777700	0.10250600
C	-4.32445400	0.76441400	-0.14406300
C	-3.67885400	1.85809800	-0.75250000
C	-4.46645100	2.97342600	-1.08477200
C	-5.83473800	2.99700100	-0.83504400
C	-6.45863000	1.90203900	-0.24141900
H	-6.16343200	-0.07005800	0.57259900
H	-3.75349200	-0.11352300	0.14906600
H	-3.98901800	3.83155200	-1.55114500
H	-6.41506800	3.87378800	-1.10622300
H	-7.52561400	1.91578800	-0.04481500
C	-2.24505200	1.88459100	-1.04659500
H	-1.85061800	2.82418800	-1.42715100
C	-1.40217600	0.83883300	-0.88127900
C	-0.00410600	0.85550600	-1.18767300
O	0.54267600	2.02451700	-1.71870500
H	-1.80194500	-0.10061700	-0.51379700
H	1.30801700	3.59533400	2.49875500
H	0.23570800	2.10392400	-2.63274000

TS3

C	-2.67494300	-0.86020500	-0.16640100
C	-4.32760500	-1.96241700	0.77136100
C	-4.90098200	0.38536700	0.29234300
H	-4.32533100	1.30445200	0.36308100
N	-3.38721000	-2.84650600	0.63632600
N	-2.36703100	-2.16345000	0.03586500
N	-3.94821400	-0.73897500	0.29559600
C	-5.64691800	-2.07311100	1.45766700
H	-5.65817700	-2.94709500	2.10776600
H	-6.46379500	-2.15634400	0.72783000
C	-5.90556000	0.27819500	1.50477300
O	-5.76843800	-0.91446900	2.25891400
C	-7.12381100	0.35410200	-0.60001200

C	-5.77407900	0.34004600	-0.93968000
C	-5.35675100	0.28113600	-2.26646600
C	-6.32792900	0.22969000	-3.26274000
C	-7.68590300	0.24150500	-2.92971300
C	-8.09300500	0.30694300	-1.59950800
C	-7.31882100	0.43397600	0.89185100
H	-4.29814300	0.28580700	-2.51037700
H	-8.43086300	0.19738300	-3.71782000
H	-9.14856300	0.31489700	-1.34515800
H	-7.98390600	-0.34450900	1.27961600
H	-7.75213700	1.39611400	1.18059500
C	-1.23672500	-2.92191100	-0.42950500
C	-1.19252800	-3.27045000	-1.78284500
C	-0.24223100	-3.27046200	0.48547600
C	-0.07955700	-3.98521100	-2.21985900
C	0.84052700	-4.00645200	0.00239200
C	0.94484800	-4.35699600	-1.34531300
H	-0.01301400	-4.26205200	-3.26894100
H	1.62168300	-4.31178300	0.69413200
C	-0.31426900	-2.79720700	1.91146300
H	-1.28176600	-3.02887500	2.36636800
H	-0.18587800	-1.70634900	1.94568100
H	0.47278500	-3.25225700	2.51543400
C	-2.28304400	-2.84649200	-2.72900400
H	-2.21178500	-1.77286400	-2.93931700
H	-3.27480000	-3.03688400	-2.30769200
H	-2.19942900	-3.38194900	-3.67544500
H	-5.68812500	1.07313000	2.21851000
C	2.15471200	-5.09205900	-1.85819900
H	1.87811500	-5.82509500	-2.61963200
H	2.85597300	-4.38787700	-2.31906100
H	2.67917100	-5.60677900	-1.05045900
C	3.55911900	-1.15049300	-2.06236900
C	2.27681400	-0.80225200	-1.66374500
C	1.65133800	0.35802200	-2.16958900
C	2.39388500	1.17630100	-3.05018000
C	3.67540900	0.82736200	-3.44173600
C	4.26390100	-0.34357800	-2.95093800
H	4.02390600	-2.04456600	-1.65783400
H	1.75934500	-1.44772100	-0.95966300
H	1.93408800	2.08326700	-3.43613800
H	4.22433000	1.46519200	-4.12826100
H	5.26562100	-0.62326300	-3.25941900
C	0.31502600	0.74356700	-1.80279400

H	-0.07200400	1.66867000	-2.22200100
C	-0.53245900	-0.05552600	-1.06138500
C	-1.87139700	0.20650600	-0.74873300
O	-2.52697800	1.32037800	-1.02506800
H	-0.13202700	-0.98874300	-0.69385300
H	-6.02984200	0.18191500	-4.30490200
H	-2.46538300	2.04088400	-0.12272900
C	3.99932700	1.56338500	0.06439400
H	3.78124000	2.55601800	-0.30801000
C	2.96025100	0.86890000	0.75373600
C	3.30070200	-0.39537900	1.33280500
H	2.51314000	-0.93316600	1.84894100
C	4.53308800	-0.96762400	1.22046500
C	5.58731800	-0.26187200	0.46220600
C	5.27098400	1.07948300	-0.06721400
C	4.84778500	-2.33288200	1.83532400
C	6.40622500	1.93588600	-0.64094900
C	3.66990800	-2.87348000	2.65313700
H	3.40650600	-2.20643400	3.48118900
H	2.78149500	-3.01066500	2.02898200
H	3.93659900	-3.84823300	3.07332200
C	5.14220700	-3.34906900	0.71724500
H	5.94202100	-2.99203700	0.06674400
H	5.43911400	-4.31112500	1.15047400
H	4.24048200	-3.51708100	0.11488100
C	6.05549900	-2.22772900	2.78569100
H	6.24667400	-3.20248100	3.24806500
H	6.94762100	-1.90660400	2.25002900
H	5.84671700	-1.50944800	3.58592500
C	7.45702000	2.15744300	0.46535900
H	7.88929600	1.20790300	0.78424600
H	8.25989700	2.80304500	0.09217900
H	7.00153900	2.64704100	1.33270100
C	7.08309000	1.27353400	-1.85472700
H	7.97987800	1.84269500	-2.12583500
H	7.36995700	0.24616700	-1.63231000
H	6.41012000	1.28116800	-2.71618600
C	5.90779100	3.31208300	-1.09792300
H	5.49552000	3.89654400	-0.26870400
H	6.74615600	3.87533300	-1.51992400
H	5.13958500	3.21987000	-1.87396100
O	6.71295200	-0.77449100	0.29951700
C	1.66024900	1.43078100	0.93782000
C	1.21041600	2.53895500	0.15569400

H	1.89668000	2.95267500	-0.57226100
C	0.77995400	0.98683300	1.96556600
H	1.16337500	0.29044400	2.70120900
C	-0.04318100	3.09830900	0.28792500
C	-0.50147500	1.46580300	2.10411700
C	-0.98108900	2.41964600	1.12319400
C	-0.43405000	4.39296200	-0.44424000
C	-1.36702900	1.12175000	3.32544300
C	-0.58127000	0.32995300	4.37834500
H	-0.26649600	-0.65188100	4.00940700
H	0.30711600	0.87454600	4.71282200
H	-1.22288300	0.16215800	5.24861300
C	-1.82994200	2.43835700	3.97803400
H	-0.96751300	3.04508800	4.27278800
H	-2.44789400	3.01905500	3.29022100
H	-2.41713300	2.21963800	4.87628200
C	-2.60288000	0.29848000	2.93784400
H	-3.20822200	0.85332000	2.22152600
H	-2.31068800	-0.66368800	2.49977500
H	-3.21128100	0.08979700	3.82469300
C	-0.90761900	5.40211000	0.61911800
H	-1.78036900	5.01666400	1.15125100
H	-0.11195800	5.60065700	1.34449900
H	-1.18052000	6.34957400	0.14151100
C	0.77608700	5.00155000	-1.16622700
H	1.61710800	5.16658500	-0.48505400
H	1.11851100	4.36708400	-1.99158800
H	0.49091600	5.96864000	-1.59092700
C	-1.55026700	4.22232700	-1.49119600
H	-1.30107600	3.45368900	-2.22795800
H	-2.50040600	3.95647200	-1.02950900
H	-1.68027600	5.17166100	-2.02263600
O	-2.26258500	2.64167700	0.95565900
M3			
C	-2.87098600	-0.81174100	-0.20197600
C	-4.28758100	-1.61747800	1.23242900
C	-5.00795100	0.53527600	0.24401500
H	-4.44830500	1.40467700	-0.10907000
N	-3.33121100	-2.50542500	1.16861100
N	-2.45992700	-1.99140700	0.26387800
N	-4.04566100	-0.56888600	0.39175600
C	-5.46898200	-1.50113900	2.13847400
H	-5.35751700	-2.16725100	2.99295600

H	-6.39655300	-1.74585100	1.60454800
C	-5.70920000	0.82615900	1.62880400
O	-5.45371400	-0.16731400	2.61027000
C	-7.37412900	0.36816800	-0.07238800
C	-6.14127100	0.13890800	-0.67860200
C	-6.04931300	-0.39262500	-1.96196900
C	-7.22826800	-0.69933000	-2.63600600
C	-8.46900700	-0.47105300	-2.03451700
C	-8.55125400	0.06572100	-0.75215800
C	-7.21289400	0.95631700	1.30378000
H	-5.08203700	-0.55464500	-2.42611300
H	-9.37829100	-0.71780100	-2.57288100
H	-9.51643600	0.23833800	-0.28622900
H	-7.80500600	0.44338100	2.06741600
H	-7.51093500	2.00918700	1.31476000
C	-1.31959000	-2.74231300	-0.20621700
C	-1.37509300	-3.27659600	-1.49396400
C	-0.19371500	-2.82322900	0.62028900
C	-0.21749200	-3.89063200	-1.97370200
C	0.93011900	-3.44934300	0.09229900
C	0.94364700	-3.96722700	-1.20674700
H	-0.22599900	-4.30730500	-2.97730400
H	1.82954800	-3.51561600	0.69850800
C	-0.18757500	-2.19477400	1.98550900
H	-1.04218700	-2.52063800	2.58561600
H	-0.23629100	-1.10199600	1.89928100
H	0.72937300	-2.44514200	2.52346000
C	-2.60017000	-3.16147700	-2.36222400
H	-2.58571800	-2.22711900	-2.93664400
H	-3.52464800	-3.18825500	-1.77916300
H	-2.62772500	-3.98120800	-3.08145800
H	-5.30357700	1.74087600	2.06100900
C	2.20860900	-4.55447400	-1.77090400
H	2.00523200	-5.17548600	-2.64523700
H	2.88331300	-3.74694800	-2.07765400
H	2.73218700	-5.15691800	-1.02459300
C	3.49237100	-0.72878100	-2.15136400
C	2.14541400	-0.56675800	-1.85596800
C	1.25668800	-0.08624900	-2.83155500
C	1.74411200	0.21591200	-4.11235000
C	3.09068200	0.04531400	-4.41056300
C	3.96327500	-0.43068700	-3.43207600
H	4.17074200	-1.06988600	-1.37299000
H	1.79007100	-0.82089200	-0.86207700

H	1.05775600	0.58423200	-4.87004100
H	3.45950800	0.27775700	-5.40397400
H	5.01273600	-0.57445500	-3.66862200
C	-0.16636900	0.08231600	-2.56639500
H	-0.80058500	0.29328500	-3.42804100
C	-0.76905500	-0.04539100	-1.36719000
C	-2.22082600	0.01139100	-1.29117300
O	-2.97582600	0.59520300	-2.04925400
H	-0.21790900	-0.26536100	-0.45624400
H	-7.18240500	-1.11728200	-3.63600100
H	-2.15007500	3.71589400	0.32929400
C	4.27557200	1.52969400	0.22775900
H	4.07565500	2.50197600	-0.21381900
C	3.21374000	0.87651400	0.87154700
C	3.50105400	-0.35221400	1.48483200
H	2.68287900	-0.87709100	1.97421600
C	4.76479400	-0.92866000	1.47377500
C	5.85383300	-0.27814300	0.76396000
C	5.55807900	1.00673400	0.15419400
C	5.03881500	-2.25754600	2.18780600
C	6.68487300	1.76853900	-0.55544700
C	3.82718000	-2.77037200	2.97410200
H	3.49204400	-2.04680700	3.72570400
H	2.97944900	-2.99360800	2.31942600
H	4.09458500	-3.69763400	3.49157900
C	5.41713500	-3.32867600	1.15069000
H	6.28405400	-2.99570900	0.57892800
H	5.64861300	-4.28202000	1.64180900
H	4.58062700	-3.49671300	0.46046500
C	6.18559900	-2.08757800	3.20180500
H	6.40864500	-3.04724200	3.68372600
H	7.07722700	-1.71547400	2.69888400
H	5.89463400	-1.37746000	3.98437700
C	7.82307500	2.06211000	0.43790300
H	8.18864900	1.12818300	0.86537100
H	8.64823800	2.57880800	-0.06753000
H	7.46424000	2.70882100	1.24662900
C	7.23040800	0.92846900	-1.72404300
H	8.07306600	1.44197700	-2.20376400
H	7.55827600	-0.04589300	-1.36053600
H	6.44935500	0.78648200	-2.47903500
C	6.21466700	3.10786300	-1.13488900
H	5.84562400	3.78361600	-0.35574900
H	7.05518700	3.60128700	-1.63450200

H	5.41769900	2.97102800	-1.87451600
O	7.01556000	-0.80635000	0.68880800
C	1.85516600	1.45763900	0.89991900
C	1.39046600	2.27652900	-0.13561800
H	2.04741900	2.43804600	-0.98126100
C	0.98717000	1.23972000	1.97759500
H	1.35542500	0.65933800	2.81600300
C	0.12571800	2.86892300	-0.13243000
C	-0.30140300	1.77322500	2.03559800
C	-0.72666900	2.57058600	0.95122800
C	-0.27753500	3.86279800	-1.24029800
C	-1.18952700	1.56628100	3.27539000
C	-0.48656900	0.73876000	4.36076800
H	-0.20900100	-0.26005100	4.01005300
H	0.41514400	1.23720700	4.72943900
H	-1.17065800	0.61438400	5.20554100
C	-1.53632700	2.92728100	3.90961200
H	-0.61993600	3.45853500	4.18593900
H	-2.11298800	3.55606900	3.23185500
H	-2.12297000	2.76670400	4.82073900
C	-2.47991400	0.82311800	2.89372700
H	-3.00100900	1.33815900	2.08514500
H	-2.25063900	-0.20288200	2.57693300
H	-3.15448500	0.75708300	3.75352200
C	-0.45859200	5.26463200	-0.61678100
H	-1.22339900	5.31368900	0.16475900
H	0.48085200	5.59241700	-0.16237800
H	-0.73654800	5.98521000	-1.39252800
C	0.82106000	3.99756600	-2.30539100
H	1.75612700	4.37525600	-1.88196900
H	1.02157400	3.03805200	-2.79430400
H	0.48859700	4.70454700	-3.07124200
C	-1.54658800	3.43382300	-2.00585800
H	-1.35110400	2.52449300	-2.57843300
H	-2.41927800	3.21909200	-1.38395100
H	-1.82980700	4.22387600	-2.70862700
O	-2.01347000	3.05544800	1.01500000

TS_{3HTC}

C	-2.02105300	-0.53043200	-0.91867200
C	-3.20837500	-2.29674200	-1.46239300
C	-4.31547900	-0.88703600	0.21857100
H	-3.96711700	-0.32189200	1.07704800
N	-2.23185300	-2.28857800	-2.31771600

N	-1.51352800	-1.17627600	-1.99093900
N	-3.13217900	-1.24890800	-0.58496800
C	-4.32691300	-3.27170700	-1.29222500
H	-4.02886900	-4.25320700	-1.66045000
H	-5.21464600	-2.93773400	-1.84736500
C	-5.09599800	-2.17921600	0.66352400
O	-4.57596700	-3.37036100	0.09442700
C	-6.56109100	-0.70040900	-0.59324000
C	-5.30301500	-0.10503500	-0.61591200
C	-5.06118800	1.06085400	-1.33761100
C	-6.11078400	1.62313200	-2.05868700
C	-7.37563200	1.02827100	-2.04514300
C	-7.61099900	-0.13218800	-1.31146200
C	-6.57433500	-1.92852200	0.27997300
H	-4.07910100	1.52619900	-1.33078400
H	-8.18431300	1.47823800	-2.61202600
H	-8.59620500	-0.58850900	-1.30223300
H	-6.98755100	-2.80964300	-0.22136000
H	-7.17450200	-1.76148900	1.17930700
C	-0.40669500	-0.75748300	-2.79802300
C	-0.60823500	0.30292700	-3.68850900
C	0.83659500	-1.34677300	-2.57121700
C	0.51696100	0.81947900	-4.32577600
C	1.93217300	-0.78553400	-3.22638400
C	1.79516400	0.30543000	-4.08644200
H	0.39655100	1.65530300	-5.01050300
H	2.91520000	-1.20788300	-3.04141300
C	0.98697700	-2.51831400	-1.64535300
H	0.57420300	-3.42502500	-2.09977200
H	0.45840200	-2.35027700	-0.70183400
H	2.03915600	-2.68600600	-1.40904100
C	-1.96942900	0.91658200	-3.88164500
H	-2.16463200	1.66123100	-3.10051600
H	-2.76444900	0.16710100	-3.83783700
H	-2.02460800	1.42551300	-4.84523500
H	-4.97818900	-2.32011800	1.73822000
C	3.00095800	0.94113300	-4.72646700
H	2.82806800	1.13480800	-5.78809700
H	3.21534100	1.90392600	-4.24826800
H	3.88634700	0.30904700	-4.62563400
C	3.11306900	3.77245800	-1.83607700
C	2.03348400	2.98190200	-1.46082000
C	0.83060100	3.56949000	-1.02604000
C	0.74867200	4.97016000	-1.00104600

C	1.83016700	5.76046400	-1.37650300
C	3.01924400	5.16498300	-1.79004200
H	4.03745400	3.30194100	-2.15896900
H	2.13020600	1.89887800	-1.49659400
H	-0.17812100	5.43905700	-0.68077200
H	1.74421300	6.84172800	-1.34369100
H	3.86783400	5.77740900	-2.07606600
C	-0.31881100	2.77825800	-0.59029100
H	-1.13122300	3.30945700	-0.09712200
C	-0.44526800	1.44891700	-0.79583800
C	-1.57678700	0.70528200	-0.29838200
O	-2.33376600	1.18296100	0.63607400
H	0.33311600	0.91129000	-1.32233200
H	-5.94691100	2.53059600	-2.63031600
H	-1.72834900	0.96716100	1.72233200
C	3.26269700	-0.36598700	0.27910900
H	3.25534400	0.67004800	-0.04129300
C	2.17488700	-0.81577500	1.07918400
C	2.15374700	-2.19882700	1.42405800
H	1.32917400	-2.54902800	2.03534000
C	3.14902100	-3.07332800	1.08387700
C	4.31942600	-2.57602000	0.33798300
C	4.28694100	-1.18053300	-0.12982500
C	3.10076900	-4.54863700	1.48914500
C	5.45636400	-0.64349900	-0.96159600
C	1.78552800	-4.90582300	2.19117000
H	1.66546400	-4.36538100	3.13601300
H	0.91856300	-4.68984600	1.55682900
H	1.77873800	-5.97631000	2.41832200
C	3.20670600	-5.43051300	0.23059800
H	4.13210200	-5.22650800	-0.30836700
H	3.18599200	-6.48865200	0.51507300
H	2.35813500	-5.24320200	-0.43720100
C	4.25419400	-4.87715000	2.45451400
H	4.21034500	-5.93420500	2.74106600
H	5.21809000	-4.67590400	1.98740100
H	4.17017100	-4.27607200	3.36636400
C	6.71178100	-0.59110700	-0.07003900
H	6.95656400	-1.58968700	0.29546200
H	7.56325400	-0.20186100	-0.63994500
H	6.54284200	0.06915700	0.78701800
C	5.75104700	-1.53180000	-2.18461100
H	6.61153700	-1.12633100	-2.72854100
H	5.97101500	-2.55457600	-1.88281300

H	4.90348400	-1.54554200	-2.87732700
C	5.17515900	0.77227700	-1.48083900
H	5.07792200	1.49990300	-0.66756700
H	6.00208400	1.09799600	-2.12015400
H	4.25447100	0.79822900	-2.07889000
O	5.30929800	-3.30927600	0.12188100
C	1.19123100	0.08350700	1.60240800
C	1.55390400	1.46965800	1.84572900
H	2.51390400	1.80187600	1.46768100
C	-0.07626100	-0.33784700	2.02181500
H	-0.36030700	-1.36465000	1.81891700
C	0.81530200	2.32462100	2.59083200
C	-0.98626300	0.49582700	2.73992900
C	-0.45797800	1.82184800	3.19724300
C	1.30496000	3.72530900	2.96318600
C	-2.04677000	-0.18962900	3.64869900
C	-2.37746900	-1.59679000	3.12625600
H	-2.58805200	-1.60563000	2.05078300
H	-1.55736500	-2.29928300	3.30334600
H	-3.25768000	-1.98163400	3.65063800
C	-1.47179900	-0.34835400	5.06696400
H	-0.53312000	-0.91180000	5.03721700
H	-1.28417500	0.62442200	5.52455100
H	-2.18050600	-0.89792200	5.69621700
C	-3.34868100	0.62677700	3.72355900
H	-3.17038000	1.59892700	4.18117900
H	-3.77750200	0.79955100	2.73102100
H	-4.08891200	0.08564100	4.32200200
C	1.62451700	3.77376300	4.47063500
H	0.73511100	3.58057500	5.07061500
H	2.39036200	3.03296100	4.72305000
H	2.01412500	4.76512400	4.72658600
C	2.58593500	4.09687100	2.20378200
H	3.42526400	3.45241600	2.48536300
H	2.45047600	4.04074400	1.11881000
H	2.86150300	5.12491600	2.45770300
C	0.23188100	4.77740200	2.63094000
H	-0.00027300	4.76159100	1.56271700
H	-0.68382000	4.60359100	3.19553500
H	0.61252500	5.77461100	2.87660200
O	-1.05823500	2.48936700	4.03635900
TS3_{HTC}^{C2'}			
C	2.06062700	1.36790800	-0.01193400

C	3.80677400	2.09824000	1.07267600
C	4.25720500	0.01313000	-0.26312900
H	3.81652200	-0.93176000	0.07756700
N	2.86123700	2.96265200	1.32622400
N	1.78593200	2.50871800	0.64572400
N	3.37370800	1.11748300	0.22922200
C	5.16816400	2.07364500	1.69374700
H	5.07107000	2.35087700	2.74478400
H	5.82702400	2.80120300	1.20652600
C	5.67892900	0.20140700	0.35025100
O	5.67715400	0.76322400	1.64556000
C	5.81763900	0.60701900	-1.98364600
C	4.53370800	0.09944100	-1.75464800
C	3.72930700	-0.28109100	-2.82927800
C	4.22004300	-0.13270500	-4.12509000
C	5.49838700	0.37877600	-4.34996100
C	6.30717800	0.74717600	-3.27795900
C	6.52446100	0.94359300	-0.70040000
H	2.74490000	-0.69877700	-2.66845100
H	5.86805200	0.48183500	-5.36510800
H	7.30704700	1.13558900	-3.44605200
H	6.52683500	2.02722700	-0.54216500
H	7.56500200	0.61297400	-0.68127200
C	0.57209800	3.29140300	0.68756600
C	0.49266100	4.40431000	-0.15301000
C	-0.44345800	2.91037000	1.56181200
C	-0.70724200	5.11206000	-0.14888500
C	-1.62537600	3.64800600	1.52389800
C	-1.78252900	4.73187600	0.65891100
H	-0.81081100	5.97025600	-0.80808700
H	-2.44246800	3.36654600	2.18369700
C	-0.25586800	1.74640600	2.48998000
H	0.66358000	1.86376600	3.07263700
H	-0.18188600	0.79977300	1.93855200
H	-1.09039200	1.66637500	3.18895200
C	1.64094700	4.79400600	-1.04493200
H	1.96018900	3.96039400	-1.68092400
H	2.50977600	5.09746500	-0.45341500
H	1.35600300	5.62429100	-1.69191500
H	6.07521200	-0.80813600	0.47967100
C	-3.10133800	5.44922600	0.56098300
H	-2.96200900	6.51240000	0.35316800
H	-3.68829200	5.02283300	-0.26080800
H	-3.68233900	5.34217800	1.47939200

C	-4.43332900	1.58033100	-1.92351100
C	-3.12938400	1.23051800	-1.59369900
C	-2.06301200	2.07882700	-1.92893700
C	-2.33295600	3.28189100	-2.59866400
C	-3.63749600	3.62921500	-2.93084400
C	-4.68981400	2.77914600	-2.59073100
H	-5.24525900	0.91682000	-1.64008600
H	-2.94899700	0.29694100	-1.06668300
H	-1.50954400	3.94542500	-2.85070300
H	-3.83411800	4.56220500	-3.44882000
H	-5.70980000	3.05136500	-2.84289200
C	-0.68010200	1.77238900	-1.57449900
H	0.04688800	2.53340200	-1.85082700
C	-0.24787300	0.65004900	-0.96756900
C	1.14123300	0.37697000	-0.64426700
O	1.62858300	-0.75845300	-0.79948100
H	-0.91303300	-0.19283200	-0.77542300
H	3.60231900	-0.42853200	-4.96656100
H	1.76232400	-1.73467000	0.33283400
C	-4.21067000	-2.22709800	-0.79874200
C	-2.91815800	-2.55488000	-0.49044600
C	-2.21305400	-2.03746100	0.63779300
C	-2.93064300	-1.11897400	1.46122000
C	-4.22730900	-0.74145600	1.22920300
C	-4.93394400	-1.27034400	0.05159300
H	-2.39793200	-3.24154100	-1.14455200
H	-2.42305100	-0.69826600	2.32023400
C	-0.86253400	-2.42071100	0.91955800
C	-0.14770200	-1.89885200	2.04737400
C	-0.14557500	-3.34070700	0.09574000
C	1.20313800	-2.05627100	2.21273500
H	-0.70751800	-1.39105500	2.82144500
C	1.21007700	-3.51974200	0.18323100
H	-0.69185500	-3.90310900	-0.64737500
C	2.01757300	-2.65565800	1.11076800
O	-6.10302500	-0.91044900	-0.22284000
O	3.31894500	-2.76831500	1.20449400
C	-4.97201100	0.21061300	2.17201800
C	-5.38165900	1.49434900	1.42849400
C	-6.22520000	-0.48733700	2.73291800
C	-4.10757600	0.62999800	3.36597900
H	-4.49639200	2.00542100	1.03174700
H	-6.04935700	1.26384000	0.59796700
H	-5.89210800	2.17690600	2.11824400

H	-5.94206400	-1.37736900	3.30510800
H	-6.75888500	0.19260000	3.40669100
H	-6.89520400	-0.78517700	1.92660300
H	-4.68727000	1.29228400	4.01620500
H	-3.78385800	-0.22955800	3.96250300
H	-3.21795800	1.17851900	3.03993600
C	-4.92496000	-2.83443200	-2.01139300
C	-6.16577500	-3.61665200	-1.54346500
C	-5.35425800	-1.72903300	-2.99264200
C	-4.02495500	-3.80974300	-2.78049800
H	-5.87118400	-4.44618900	-0.89172900
H	-6.84798100	-2.96439600	-0.99779000
H	-6.69063200	-4.03599200	-2.40959200
H	-4.48879300	-1.13292900	-3.30328100
H	-5.79824100	-2.17874300	-3.88819600
H	-6.08580400	-1.06666000	-2.53029700
H	-4.58497700	-4.22313300	-3.62495100
H	-3.13477900	-3.31344400	-3.18196300
H	-3.70035100	-4.64725500	-2.15394800
C	1.95501000	-4.45554200	-0.76317700
C	2.78464300	-5.45062800	0.06853200
C	1.00662000	-5.26028900	-1.65975800
C	2.87506500	-3.62112300	-1.67380100
H	3.46728800	-4.91124200	0.72471400
H	2.12652700	-6.08394100	0.67314800
H	3.35613100	-6.10083100	-0.60285100
H	0.42107400	-4.61565700	-2.32296000
H	1.60029900	-5.93179800	-2.28749200
H	0.31616600	-5.87338800	-1.07136800
H	3.44780800	-4.29028500	-2.32538700
H	2.27651800	-2.95739200	-2.30594300
H	3.56655500	-3.02123600	-1.07940000
C	1.91715200	-1.57399700	3.47262400
C	2.67242200	-2.76749700	4.08899800
C	2.90796000	-0.45500700	3.11060500
C	0.94834300	-1.04219000	4.53489400
H	1.96399600	-3.53886400	4.40948900
H	3.36441600	-3.19238100	3.36264200
H	3.22708400	-2.43049100	4.97146300
H	2.36270500	0.40799500	2.70654500
H	3.44037800	-0.12063900	4.00818900
H	3.63355500	-0.81014300	2.37732400
H	1.52127300	-0.75264800	5.42093500
H	0.39700300	-0.16057600	4.19603000

H	0.22460200	-1.80592700	4.83675600
TS3_{HTC}^{C4'}			
C	1.74889400	-0.82512000	0.82040200
C	3.70851300	-1.72520400	0.45798700
C	3.62571200	0.67520200	-0.13466600
H	2.85712700	1.27495200	-0.62215800
N	3.01478700	-2.66373200	1.03364000
N	1.80403800	-2.08993000	1.27101900
N	2.98108100	-0.57860200	0.30932600
C	5.08661200	-1.76536200	-0.11580400
H	5.36033400	-2.79262200	-0.35549300
H	5.81546400	-1.35550300	0.59645100
C	4.82004600	0.36278300	-1.12169500
O	5.04021600	-1.02353800	-1.31682400
C	5.63050700	1.60269100	0.80113400
C	4.27422100	1.38703500	1.03618100
C	3.67670300	1.79214200	2.22916400
C	4.46638700	2.41921400	3.18866000
C	5.82664600	2.63953100	2.95601600
C	6.41612200	2.23559600	1.76176200
C	6.05576200	1.09192100	-0.54796400
H	2.61799200	1.63366500	2.40294300
H	6.42817600	3.12993900	3.71456300
H	7.47315800	2.40560200	1.58156000
H	6.90869100	0.40745700	-0.49531900
H	6.34945600	1.91421700	-1.20650900
C	0.82381100	-2.80771900	2.04286300
C	0.60723700	-2.42376000	3.36804900
C	0.13355900	-3.84948200	1.41524700
C	-0.38618200	-3.10986800	4.06820600
C	-0.84640800	-4.50004600	2.16012900
C	-1.12366000	-4.13856400	3.48212700
H	-0.58612800	-2.83038600	5.09929000
H	-1.40786400	-5.30659800	1.69484500
C	0.42653200	-4.21333000	-0.01129100
H	1.46093900	-4.55076600	-0.12705200
H	0.29501900	-3.34656600	-0.66825100
H	-0.24151500	-5.00289500	-0.35559700
C	1.37189400	-1.29742700	4.01138200
H	0.92384000	-0.32940900	3.75766400
H	2.41826400	-1.27918400	3.69350400
H	1.34659400	-1.39766600	5.09739100
H	4.56658800	0.73834300	-2.11265200

C	-2.17965400	-4.87252100	4.26548600
H	-2.50925700	-4.28927900	5.12735900
H	-3.04797500	-5.09423200	3.64058500
H	-1.78813400	-5.82570500	4.63461100
C	-4.93630800	-1.02782700	1.97737000
C	-3.61360000	-0.78469600	1.62924800
C	-2.95610200	0.36919900	2.08846600
C	-3.65790600	1.25919200	2.91532600
C	-4.97940900	1.01043400	3.26953600
C	-5.62461200	-0.13101100	2.79663700
H	-5.43549700	-1.91820700	1.60724800
H	-3.08729800	-1.48023000	0.98003900
H	-3.15128200	2.14606400	3.28615800
H	-5.50749100	1.71004300	3.90943400
H	-6.65881400	-0.32294200	3.06278600
C	-1.57518000	0.66429000	1.72841700
H	-1.23852200	1.69324200	1.84946600
C	-0.67265500	-0.26424400	1.32009800
C	0.65092900	0.14650000	0.94906200
O	0.97139700	1.36416700	0.79112100
H	-0.93853700	-1.31310100	1.25171100
H	4.02064600	2.74244900	4.12350400
H	0.25383800	2.00308700	-0.25709100
C	-2.15345000	-0.89052500	-1.78712500
H	-3.10770200	-0.59284500	-1.37309300
C	-1.09620000	0.07699300	-1.80926900
C	0.14338000	-0.35811100	-2.37895200
H	0.94749300	0.36387000	-2.45069100
C	0.34856600	-1.61195100	-2.88732500
C	-0.73877400	-2.60302200	-2.82780900
C	-2.03465800	-2.15919700	-2.27494300
C	1.67302800	-2.01067000	-3.54520700
C	-3.21653000	-3.13386600	-2.28016400
C	2.65619800	-0.83901200	-3.57032200
H	2.27737700	0.00306900	-4.15933800
H	2.86149200	-0.49215700	-2.55418200
H	3.60787300	-1.16267200	-4.00292100
C	2.33442500	-3.15488000	-2.75788300
H	1.68017600	-4.02687500	-2.71621000
H	3.28173700	-3.43653200	-3.23159400
H	2.55617000	-2.83305300	-1.73254000
C	1.43284700	-2.45036400	-5.00072800
H	2.38933200	-2.70006000	-5.47337100
H	0.78032400	-3.32168100	-5.04290300

H	0.97434800	-1.63689300	-5.57299200
C	-3.50242600	-3.60379200	-3.71920100
H	-2.63362400	-4.10152000	-4.14811900
H	-4.34749400	-4.30111200	-3.71707400
H	-3.77041600	-2.75037400	-4.35115100
C	-2.89961200	-4.34807800	-1.39001300
H	-3.76243200	-5.02278800	-1.35780700
H	-2.03809100	-4.89148000	-1.77897300
H	-2.68111300	-4.02469800	-0.36429100
C	-4.50320100	-2.48508600	-1.75404800
H	-4.79365700	-1.61550400	-2.35317800
H	-5.31730200	-3.21449300	-1.80489400
H	-4.41134900	-2.16544400	-0.71137700
O	-0.57329100	-3.77270900	-3.22848600
C	-1.31702600	1.41649700	-1.38934100
C	-2.58391800	1.88406400	-0.94709300
H	-3.39798500	1.17665100	-0.88667100
C	-0.23665600	2.40142400	-1.31687700
H	0.61772800	2.21126800	-1.96440200
C	-2.86037500	3.20420800	-0.67421200
C	-0.49164400	3.78807700	-1.04812700
C	-1.80897500	4.24016300	-0.72145100
C	-4.29538700	3.63601300	-0.35564400
C	0.67470000	4.77382700	-1.02031300
C	2.02854800	4.10344100	-1.29133000
H	2.24499800	3.33439900	-0.54020000
H	2.08722800	3.65383500	-2.28843300
H	2.81830100	4.85825500	-1.22637800
C	0.45643500	5.86617800	-2.08345300
H	0.45299800	5.42629200	-3.08651100
H	-0.49472000	6.37063700	-1.91315900
H	1.26947300	6.59968200	-2.03632900
C	0.76342900	5.41323200	0.38004400
H	-0.17000200	5.91731600	0.62813600
H	0.96530500	4.64150500	1.13200300
H	1.58545700	6.13756500	0.40680200
C	-4.76911800	4.59953100	-1.46237400
H	-4.12094500	5.47466400	-1.50883400
H	-4.76309600	4.09605500	-2.43521200
H	-5.79604800	4.91942700	-1.25309300
C	-5.27375400	2.45464900	-0.31124500
H	-5.34746600	1.94794300	-1.27963300
H	-4.99147200	1.71697800	0.44884700
H	-6.27008800	2.83071200	-0.05837300

C	-4.35916800	4.34442500	1.00946000
H	-4.07736200	3.65175800	1.80761400
H	-3.69611500	5.20729000	1.02952600
H	-5.38715300	4.67353800	1.19889500
O	-2.08006200	5.45673900	-0.50110000

TS3_{HTC}^{C5'}

C	0.30205400	-1.69433500	-0.67593700
C	-0.39426600	-3.75349900	-0.39666200
C	-2.23211700	-2.16123200	-0.77699300
H	-2.40424300	-1.12338300	-0.49080100
N	0.90169200	-3.84746400	-0.40469800
N	1.32877000	-2.56211400	-0.59398800
N	-0.81037800	-2.46060000	-0.55042300
C	-1.44309100	-4.80149200	-0.22333400
H	-1.02884400	-5.67061800	0.28726400
H	-1.83559100	-5.11185500	-1.20142500
C	-3.14446300	-3.13296200	0.05838200
O	-2.44959000	-4.24747900	0.59946900
C	-3.75608200	-3.22823200	-2.28238100
C	-2.61676200	-2.42986500	-2.21761600
C	-1.96933600	-1.99455700	-3.37029400
C	-2.48550900	-2.37956400	-4.60509700
C	-3.62955100	-3.17881500	-4.67719800
C	-4.27368000	-3.60619800	-3.51843000
C	-4.27147000	-3.55991600	-0.90647500
H	-1.08942900	-1.36221800	-3.30713700
H	-4.01761700	-3.47307900	-5.64701400
H	-5.15967800	-4.23093700	-3.57624800
H	-4.49683200	-4.62134700	-0.76906200
H	-5.18735400	-3.00116700	-0.68814100
C	2.70506700	-2.32271100	-0.94145500
C	3.00623500	-2.02963000	-2.27745300
C	3.66764100	-2.38089900	0.06722900
C	4.33204300	-1.72259400	-2.57455200
C	4.98100300	-2.06676300	-0.28548200
C	5.32591200	-1.71912300	-1.59254700
H	4.59467000	-1.47734200	-3.60071300
H	5.74737400	-2.08769700	0.48527800
C	3.28557700	-2.74984000	1.47111600
H	2.92139800	-3.78099400	1.51633500
H	2.48110800	-2.10644000	1.84016100
H	4.13769900	-2.64934000	2.14459200
C	1.95251200	-2.01192400	-3.35352000

H	1.44808000	-1.03845000	-3.38716200
H	1.19409800	-2.78499300	-3.19710800
H	2.41068300	-2.17927000	-4.32947300
H	-3.53677200	-2.61477000	0.93647400
C	6.73455800	-1.32209600	-1.94597000
H	7.08130100	-1.85564400	-2.83471900
H	6.77899400	-0.25107300	-2.17030800
H	7.42433200	-1.52668700	-1.12536500
C	5.40899400	2.58528200	-1.45289300
C	4.25141200	1.82448700	-1.35349000
C	3.03938600	2.29102900	-1.89314800
C	3.03962200	3.52055500	-2.56709200
C	4.20091500	4.28036400	-2.66932000
C	5.38816300	3.81877400	-2.10663600
H	6.33383500	2.21350800	-1.02263200
H	4.29236200	0.85387800	-0.86494500
H	2.11670400	3.88010800	-3.01407700
H	4.17788000	5.23213000	-3.19006500
H	6.29506500	4.40959500	-2.18261200
C	1.79086700	1.53223200	-1.79048000
H	0.95653000	1.86999800	-2.40473900
C	1.60391800	0.44785400	-1.01151700
C	0.33962000	-0.26980100	-0.99747900
O	-0.73215300	0.21795800	-1.50277000
H	2.39098500	0.08371100	-0.35786800
H	-1.99597100	-2.05551900	-5.51748200
H	-1.28792600	0.93057200	-0.53272900
C	0.82259700	1.30662400	1.74004500
H	1.09755400	2.22931900	1.24806000
C	-0.44317700	0.73291700	1.42019900
C	-0.77975100	-0.46873600	2.11467600
H	-1.74179000	-0.92835200	1.91006800
C	0.02723300	-1.05395300	3.05616600
C	1.34681700	-0.46395600	3.34577800
C	1.70605900	0.77032100	2.63426800
C	-0.41534700	-2.28398300	3.85481800
C	3.05587200	1.43439100	2.92101300
C	-1.84277600	-2.71140800	3.50276000
H	-2.56633700	-1.90804100	3.68220500
H	-1.91538500	-3.03413800	2.46076900
H	-2.12720100	-3.56429300	4.12702900
C	0.51428600	-3.47335600	3.55651800
H	1.54487200	-3.23553600	3.82361500
H	0.19098200	-4.35293800	4.12483200

H	0.47758400	-3.72826100	2.48924100
C	-0.39078100	-1.96410100	5.36185500
H	-0.72410900	-2.84080800	5.92835800
H	0.61123100	-1.69024500	5.68952900
H	-1.07505700	-1.13827100	5.58471900
C	3.15967200	1.80242300	4.41249200
H	3.06652300	0.91460900	5.03797200
H	4.12698800	2.27786500	4.61050200
H	2.37162200	2.51263400	4.68510000
C	4.19767300	0.47210000	2.54733200
H	5.16632200	0.95597400	2.71750900
H	4.14297200	-0.43823900	3.14468500
H	4.14061900	0.19758000	1.48589300
C	3.24498100	2.72152100	2.10915100
H	2.49013600	3.47529700	2.35922600
H	4.22873800	3.14645800	2.33256200
H	3.20187500	2.53359100	1.03059500
O	2.13294200	-0.99920100	4.15702100
C	-1.43859200	1.47785700	0.61723600
C	-1.10143700	2.83074000	0.15537900
H	-0.05371100	3.02246400	-0.04027900
C	-2.86658100	1.26480100	0.88092200
H	-3.15207800	0.30657800	1.30031100
C	-2.00847900	3.78529500	-0.14374100
C	-3.83557500	2.16573900	0.60482600
C	-3.45077200	3.50036500	0.06825800
C	-1.59595300	5.15130600	-0.69966600
C	-5.31930400	1.87050000	0.84563300
C	-5.53455100	0.45539400	1.39483100
H	-5.18292900	-0.30611000	0.69007100
H	-5.02981400	0.30414200	2.35498900
H	-6.60469100	0.29239200	1.55192100
C	-5.89590400	2.86344000	1.87140100
H	-5.37191900	2.77017900	2.82836600
H	-5.80625000	3.89080800	1.51930700
H	-6.95486700	2.64159100	2.04218600
C	-6.09532800	1.97224500	-0.48106700
H	-6.02220200	2.97256100	-0.90634000
H	-5.70473700	1.25046600	-1.20631900
H	-7.15152400	1.73952100	-0.30697100
C	-2.06310300	6.27163600	0.24746100
H	-3.14806400	6.27565100	0.34884900
H	-1.61601100	6.14402500	1.23889400
H	-1.74167000	7.24196800	-0.14636000

C	-0.07301400	5.26490300	-0.83734400
H	0.43426700	5.15489300	0.12749400
H	0.32902200	4.51336900	-1.52492800
H	0.17830200	6.25126300	-1.23855400
C	-2.20934800	5.35406600	-2.09701100
H	-1.85641700	4.57761400	-2.78418900
H	-3.29793900	5.32014800	-2.05679300
H	-1.90135700	6.32617000	-2.49714400
O	-4.30926600	4.34684000	-0.19700800

M3_{SET}

C	0.73723800	-0.29318400	-0.61684200
C	2.41705800	-1.68354100	-0.40509600
C	3.13243900	0.59309000	-1.04205600
H	2.72651300	1.31657900	-1.74369000
N	1.37691300	-2.37100800	-0.03958400
N	0.33420500	-1.50510200	-0.17428800
N	2.08256700	-0.41390500	-0.78589500
C	3.84696900	-2.09686100	-0.51825900
H	3.91875400	-3.17935900	-0.61933200
H	4.40841500	-1.78257300	0.37253500
C	4.42597200	-0.08797200	-1.63302300
O	4.34387100	-1.50163800	-1.69790500
C	4.96062400	1.10407300	0.41951800
C	3.58350900	1.22330800	0.25521400
C	2.78723100	1.84589300	1.21266700
C	3.39864000	2.35280200	2.35571200
C	4.78115300	2.23731800	2.52723600
C	5.57043000	1.61567300	1.56300700
C	5.59950800	0.40428100	-0.75149000
H	1.71184500	1.93382600	1.07997500
H	5.24319400	2.63576300	3.42461700
H	6.64332200	1.52544900	1.70275000
H	6.22656900	-0.44247800	-0.45435200
H	6.23678900	1.08881700	-1.31862900
C	-0.99260100	-1.93428300	0.17010200
C	-1.34082900	-1.93498200	1.52537500
C	-1.87516700	-2.27230900	-0.85600100
C	-2.65304400	-2.27666400	1.84128500
C	-3.17846400	-2.60595800	-0.48526400
C	-3.58367800	-2.60823900	0.85017200
H	-2.96050900	-2.27486200	2.88389400
H	-3.89391000	-2.86293800	-1.26178600
C	-1.45071700	-2.22435000	-2.29859600

H	-0.46774400	-2.68103300	-2.44080000
H	-1.39184200	-1.18829900	-2.65133900
H	-2.17200800	-2.74992200	-2.92540000
C	-0.34014100	-1.54703700	2.58063700
H	0.08012400	-0.55433600	2.38388600
H	0.49459400	-2.25337400	2.60696900
H	-0.81015000	-1.52906300	3.56439000
H	4.54774100	0.22139600	-2.67048700
C	-4.99678300	-2.96421300	1.22959900
H	-5.39146100	-2.25700800	1.96378000
H	-5.65307400	-2.96331900	0.35755100
H	-5.03395400	-3.96013800	1.68169200
C	-5.63666300	1.40839200	0.60296800
C	-4.30251400	1.21971200	0.27537800
C	-3.62388500	2.16059700	-0.52319700
C	-4.33010500	3.28635800	-0.98154700
C	-5.66514600	3.47396900	-0.64730100
C	-6.32290500	2.53578500	0.14593600
H	-6.14826600	0.67151900	1.21354500
H	-3.79393100	0.32800300	0.63139400
H	-3.81781100	4.01619500	-1.60212200
H	-6.19375100	4.35044100	-1.00696000
H	-7.36691100	2.67824800	0.40451300
C	-2.23291100	2.00651500	-0.91084400
H	-1.86450000	2.74113600	-1.62431900
C	-1.40792400	1.00015900	-0.47964800
C	-0.06469000	0.86677800	-0.87429400
O	0.59381900	1.82373500	-1.56121500
H	-1.79504300	0.25943800	0.20606000
H	2.79984400	2.84044800	3.11753200
H	0.20422000	2.69411900	-1.39261400

M3_{HAT}

C	-0.68955500	0.18198600	-0.56899400
C	-2.34126200	1.64862200	-0.59297300
C	-3.07737100	-0.66399000	-1.04565700
H	-2.61455300	-1.47282800	-1.60770800
N	-1.30400900	2.35511300	-0.27086900
N	-0.27306800	1.44276100	-0.24067000
N	-2.03478100	0.33385600	-0.79515600
C	-3.74779600	2.07328600	-0.85363300
H	-3.79165100	3.14278000	-1.05693500
H	-4.38849600	1.84598700	0.00990000
C	-4.28486200	-0.02268400	-1.82988500

O	-4.16839300	1.38071700	-2.01359500
C	-5.06360600	-0.99033700	0.26176000
C	-3.68109900	-1.15243900	0.25223600
C	-3.00274000	-1.68815400	1.34396100
C	-3.74156500	-2.05556900	2.46595700
C	-5.13024700	-1.89299200	2.48459100
C	-5.80060900	-1.36394600	1.38380700
C	-5.55843100	-0.40821900	-1.03718100
H	-1.92601600	-1.82483800	1.30010600
H	-5.69193300	-2.18274100	3.36693200
H	-6.87924700	-1.23999100	1.40249700
H	-6.19421100	0.47225900	-0.89847100
H	-6.14717700	-1.14131600	-1.59673200
C	0.99238800	1.84265400	0.29068300
C	1.34362400	1.42766800	1.58048500
C	1.83860500	2.60877600	-0.51541000
C	2.60843500	1.78140200	2.04641400
C	3.09141200	2.94404400	-0.00208700
C	3.49623900	2.52922100	1.26850800
H	2.90794800	1.46597500	3.04296600
H	3.76969700	3.53352000	-0.61355700
C	1.41265500	3.01742300	-1.89976200
H	0.52344400	3.65292700	-1.86525700
H	1.15737400	2.13826300	-2.50060800
H	2.21253400	3.56106700	-2.40417900
C	0.40779200	0.59635200	2.41675100
H	0.44680000	-0.45454100	2.10772300
H	-0.62830700	0.93158400	2.31293900
H	0.68754400	0.64972300	3.47006100
H	-4.31015700	-0.42309600	-2.84307900
C	4.87344200	2.85319100	1.78645300
H	5.52272800	1.97405900	1.71893600
H	5.33537700	3.65695000	1.21008700
H	4.83860200	3.15310300	2.83666400
C	5.87231600	-1.11852100	-0.33099000
C	4.48560100	-1.03725500	-0.33923100
C	3.69929000	-2.18245500	-0.56240700
C	4.35707500	-3.40792600	-0.75127600
C	5.74593600	-3.48853600	-0.74075700
C	6.51133500	-2.34290500	-0.53432500
H	6.46063700	-0.22268600	-0.15720000
H	4.00823300	-0.07827700	-0.15168300
H	3.76362700	-4.30363600	-0.91436800
H	6.23106000	-4.44745400	-0.89363700

H	7.59469900	-2.40229200	-0.52386600
C	2.23618100	-2.14236800	-0.59134900
H	1.71544100	-3.09746600	-0.56739900
C	1.49098600	-1.01880000	-0.65136200
C	0.03347600	-1.05862400	-0.66363600
O	-0.62273300	-2.14253700	-0.74552500
H	1.98011500	-0.05390200	-0.71968700
H	-3.23796100	-2.47410900	3.33124100

M04

C	-0.65774700	-1.49345400	0.06579000
C	-2.40716600	-2.02956000	1.23980600
C	-2.93433900	-0.65261900	-0.74692000
H	-2.37636300	0.15573000	-1.22945600
N	-1.40896200	-2.60755100	1.84824000
N	-0.32310800	-2.26974900	1.10003300
N	-1.98641800	-1.34512100	0.13680000
C	-3.85269800	-1.93200300	1.59663300
H	-4.00153800	-2.19316000	2.64384200
H	-4.44829200	-2.60675000	0.96654800
C	-4.14951100	-0.09350100	0.08909500
O	-4.20972500	-0.57791100	1.42234200
C	-4.95289700	-1.52818700	-1.69393800
C	-3.56389300	-1.63068700	-1.71907600
C	-2.92057100	-2.54988800	-2.54369700
C	-3.69945100	-3.37423400	-3.35214600
C	-5.09307000	-3.27308400	-3.33493100
C	-5.72864800	-2.34937800	-2.50852100
C	-5.40691400	-0.46795600	-0.72629000
H	-1.83744600	-2.61307000	-2.55937700
H	-5.68604400	-3.92396200	-3.96927100
H	-6.81170700	-2.27626800	-2.49212100
H	-6.20181900	-0.80502400	-0.05450300
H	-5.78524700	0.40989300	-1.26096900
C	0.95255400	-2.89215900	1.36243700
C	1.36499700	-3.90888300	0.49527400
C	1.70620500	-2.45776900	2.45654300
C	2.60378000	-4.49490300	0.74828400
C	2.93459600	-3.08212700	2.66389400
C	3.39925000	-4.09553000	1.82329300
H	2.95225100	-5.28559000	0.08939100
H	3.54628000	-2.76211100	3.50331300
C	1.25650200	-1.32697600	3.34336500
H	1.50046100	-0.35869900	2.88828200

H	1.76801600	-1.37914200	4.30574400
H	0.17928600	-1.35735700	3.52400200
C	0.52689900	-4.34486400	-0.67857700
H	-0.53315300	-4.41871100	-0.41806600
H	0.85759800	-5.32138200	-1.03411100
H	0.62154800	-3.64234700	-1.51490400
H	-4.04189600	0.98220300	0.21251300
C	4.72065600	-4.76549200	2.09248300
H	4.59571800	-5.57840100	2.81476700
H	5.13998000	-5.19261600	1.17951300
H	5.44085500	-4.05951800	2.51150400
C	5.79383100	0.48697000	-0.02470300
C	4.42899600	0.28966800	-0.19745100
C	3.94028600	-0.18763700	-1.42358200
C	4.83643000	-0.41958100	-2.47725800
C	6.20153100	-0.22800600	-2.29777300
C	6.68233600	0.21905200	-1.06751900
H	6.16826400	0.86059500	0.92272900
H	3.73007400	0.54217300	0.59551400
H	4.45429700	-0.76596000	-3.43350000
H	6.88860900	-0.42212300	-3.11461600
H	7.74724600	0.37235600	-0.92489900
C	2.52321900	-0.47246300	-1.62887000
H	2.18458500	-0.56110100	-2.66040100
C	1.61859100	-0.71299300	-0.65707000
C	0.24430600	-0.97777500	-1.02957600
O	-0.23908400	-0.89767700	-2.15062800
H	1.87440800	-0.65601200	0.39542900
H	-3.22009500	-4.09986700	-4.00068100
C	-2.46416900	2.80357600	0.98229500
C	-1.37450700	1.89221400	0.88735400
C	-1.10012800	1.04416600	1.97242400
C	-1.86068500	1.05323100	3.13581100
C	-2.93163100	1.93039900	3.23124700
C	-3.21139500	2.78674600	2.16687700
H	-0.25009500	0.37694400	1.87716600
H	-1.61733000	0.37857700	3.95213200
H	-3.55021400	1.95724200	4.12240800
H	-4.04738600	3.46695800	2.27748500
C	-2.80318200	3.80349600	-0.14034100
C	-1.62643000	4.77461600	-0.35287200
C	-3.11189500	3.08639700	-1.46796100
C	-4.03459500	4.65261400	0.20776200
H	-1.35215500	5.25981800	0.58915300

H	-0.74361600	4.26829000	-0.74494400
H	-1.92143600	5.55246900	-1.06637900
H	-4.01138100	2.46555400	-1.38064400
H	-3.30814800	3.83283900	-2.24572300
H	-2.27280600	2.46460500	-1.78153300
H	-4.24511300	5.32889000	-0.62597800
H	-4.92392300	4.03426000	0.36833100
H	-3.87193800	5.26524600	1.10004400
N	-0.63085900	1.77769900	-0.30225300
C	0.61658300	2.20485100	-0.35400000
C	1.34639200	2.32008500	-1.53254400
H	0.88727400	2.01374000	-2.46469200
C	2.69963400	2.77113000	-1.52874900
O	3.33627400	3.21664300	-0.57327600
O	3.28097800	2.66589700	-2.76044400
C	4.64884000	3.04847000	-2.80776300
H	4.98930200	2.82948800	-3.81989500
H	4.76563800	4.11513100	-2.59677800
H	5.23469200	2.47747100	-2.08290700
C	1.32204100	2.52477500	0.95352700
O	1.10071100	3.77213400	1.36175400
O	1.92181000	1.69824800	1.61030600
C	1.68186700	4.10909300	2.62456100
H	2.76712200	4.00139000	2.57616300
H	1.40744300	5.14465400	2.81331100
H	1.28710700	3.45797000	3.40713600

TS4(RR)

C	-2.00852500	-0.09032000	0.30563000
C	-2.95807600	-2.05463300	0.38176800
C	-0.54648600	-2.13145700	0.84696500
H	0.29718600	-1.53131000	0.49984700
N	-3.92781000	-1.22415500	0.12572400
N	-3.32207700	-0.00562400	0.08736700
N	-1.76586600	-1.39689200	0.50292700
C	-2.91632100	-3.54761500	0.41854000
H	-3.81299100	-3.96180200	-0.04055300
H	-2.83510600	-3.91157300	1.45090600
C	-0.53212800	-3.53873700	0.14715600
O	-1.80144800	-3.92180200	-0.36973200
C	-0.17872300	-3.78665700	2.53219200
C	-0.49953000	-2.44533600	2.32925100
C	-0.75442100	-1.59237800	3.40003300

C	-0.65268500	-2.09997200	4.69364100
C	-0.30843000	-3.43703100	4.90315400
C	-0.07437100	-4.28958300	3.82580000
C	-0.00702700	-4.51251400	1.22323000
H	-1.04448300	-0.55671900	3.24256400
H	-0.23667200	-3.81917300	5.91610700
H	0.17152900	-5.33375100	3.99212700
H	-0.55686100	-5.45708300	1.17882400
H	1.04770000	-4.73485000	1.02989100
C	-4.13679100	1.17579000	-0.06395000
C	-4.58524700	1.80623000	1.09466100
C	-4.46167400	1.59657700	-1.35396600
C	-5.41568600	2.91596700	0.92958100
C	-5.29478900	2.70543100	-1.46453300
C	-5.78354000	3.37203300	-0.33614700
H	-5.78259800	3.43180200	1.81281800
H	-5.56489900	3.06240700	-2.45507900
C	-3.88305900	0.89967900	-2.55239200
H	-4.08272900	-0.17609500	-2.52622400
H	-2.79630700	1.03505700	-2.56051700
H	-4.29527300	1.30770800	-3.47609100
C	-4.16691300	1.32306500	2.45823100
H	-3.10253300	1.51873000	2.63133300
H	-4.32845100	0.24659800	2.56919000
H	-4.73177600	1.83725000	3.23653500
H	0.11912700	-3.51056800	-0.72492700
C	-6.70485600	4.55341800	-0.49454300
H	-7.70727100	4.22233500	-0.78322000
H	-6.79159800	5.11603100	0.43678900
H	-6.34585600	5.22765300	-1.27598900
C	3.90094700	1.25289000	3.24324300
C	2.73909300	1.12540800	2.49280800
C	2.14279600	2.25237400	1.90795200
C	2.74510400	3.50510400	2.09120600
C	3.91257600	3.63204500	2.83600200
C	4.49317900	2.50522000	3.41509600
H	4.35295500	0.37312200	3.69005300
H	2.30544200	0.14023400	2.34553800
H	2.28434100	4.37944300	1.63940300
H	4.36659200	4.60892700	2.96731000
H	5.40381400	2.60013400	3.99766900
C	0.92148400	2.16440200	1.10276500
H	0.54249000	3.10108800	0.70428100
C	0.06780500	1.08040100	1.11509700

C	-1.07288000	1.10059200	0.26847900
O	-1.40553000	2.00304800	-0.50450400
H	0.29472500	0.19684900	1.69505100
H	-0.84946400	-1.45327200	5.54178100
C	1.25154700	-2.31210000	-2.67828600
C	1.73245500	-1.50899500	-1.60872300
C	2.56219500	-2.08623000	-0.63141600
C	2.97274100	-3.41267100	-0.71235000
C	2.55379700	-4.18960000	-1.78575700
C	1.70590100	-3.63411700	-2.74468000
H	2.86870500	-1.47019700	0.20993500
H	3.61039400	-3.83079000	0.06066500
H	2.86614800	-5.22479300	-1.87533400
H	1.37929000	-4.26931400	-3.55918700
C	0.24472500	-1.76988400	-3.70377800
C	-1.05522900	-1.36008100	-2.98122500
C	0.83088000	-0.56428600	-4.46089400
C	-0.12943500	-2.82948400	-4.74938700
H	-1.47590200	-2.21254200	-2.43156400
H	-0.86693700	-0.54125700	-2.28233500
H	-1.79727100	-1.03242400	-3.71815600
H	1.76111500	-0.84611800	-4.96543500
H	0.11951800	-0.22895500	-5.22366300
H	1.03809700	0.26967400	-3.78974300
H	-0.85068100	-2.39762000	-5.44925500
H	0.74056000	-3.15746900	-5.32716700
H	-0.59431400	-3.70824700	-4.29122500
N	1.29353100	-0.17976800	-1.47996000
C	2.15885100	0.78609800	-1.31268900
C	1.73763400	2.12385200	-1.16936400
H	0.69855400	2.34336100	-1.38480000
C	2.66426800	3.22192000	-1.10591900
O	3.88829400	3.18208200	-1.14531200
O	2.01005100	4.41073800	-0.95732100
C	2.85323500	5.55709000	-0.90507100
H	2.19199000	6.41145300	-0.76789500
H	3.55694500	5.48411000	-0.07195500
H	3.42042700	5.66339400	-1.83274500
C	3.65703200	0.52326200	-1.32700900
O	4.18324200	0.57900400	-0.10454500
O	4.28069900	0.26662200	-2.33038100
C	5.60647500	0.49038100	-0.04405100
H	6.04664000	1.30593900	-0.62134800
H	5.86256400	0.58483100	1.00991300

H	5.94886000	-0.46796800	-0.44028500
TS4(RR)'			
C	0.92975100	1.42733400	0.36579500
C	1.37255400	2.83438900	-1.25082400
C	-0.96458900	2.09887400	-1.27490000
H	-1.44933900	1.14389000	-1.06425100
N	2.49010500	2.71396600	-0.59666200
N	2.19924300	1.84306900	0.40588500
N	0.38939400	2.06367300	-0.69918500
C	1.06341200	3.57183800	-2.51154400
H	1.98601700	3.84343100	-3.02295000
H	0.48455400	4.48055000	-2.30015500
C	-0.92233800	2.28754900	-2.83701700
O	0.34970900	2.66943600	-3.33605800
C	-2.33744000	3.97769900	-1.81820000
C	-1.74011800	3.29237100	-0.76288300
C	-1.87358400	3.72373900	0.55395200
C	-2.64134100	4.85869900	0.80382200
C	-3.25613700	5.54192200	-0.24825800
C	-3.10702100	5.10945300	-1.56448200
C	-2.01948900	3.33272000	-3.14230700
H	-1.38357500	3.19784500	1.36988400
H	-3.84828300	6.42636500	-0.03697300
H	-3.57528300	5.65182100	-2.38001400
H	-1.65791000	4.04329100	-3.89149400
H	-2.90268200	2.84025500	-3.56065100
C	3.25245400	1.51000200	1.33503200
C	3.20668400	2.04692100	2.62277700
C	4.29206500	0.71117300	0.86398500
C	4.26595900	1.73838400	3.47118000
C	5.32728700	0.42865700	1.75681300
C	5.33004700	0.93110500	3.05736200
H	4.26123600	2.13772200	4.48248600
H	6.14875500	-0.20013000	1.42302400
C	4.28285000	0.17459800	-0.54127500
H	4.42454300	0.97696300	-1.27160400
H	3.32777800	-0.31035600	-0.76913300
H	5.07821100	-0.56057700	-0.67806000
C	2.05105300	2.89501000	3.08014300
H	1.17014900	2.27123200	3.26600400
H	1.77976200	3.64649300	2.33214700
H	2.30054200	3.41109600	4.00830000

H	-1.12898400	1.33009600	-3.31986100
C	6.45957500	0.62541200	4.00647100
H	7.01487500	1.53530800	4.25333100
H	6.07868100	0.21245000	4.94456700
H	7.15865300	-0.09230800	3.57334000
C	-5.41437200	-0.09795700	1.46505400
C	-4.03894000	-0.13132300	1.27484900
C	-3.19410400	-0.61801900	2.28574300
C	-3.76618300	-1.11527500	3.46312900
C	-5.14427200	-1.07792800	3.65380700
C	-5.97111800	-0.56125400	2.65908100
H	-6.05852400	0.27978900	0.67736800
H	-3.61418700	0.18650200	0.32665300
H	-3.11969900	-1.52312000	4.23476500
H	-5.57130800	-1.45397400	4.57784600
H	-7.04609300	-0.53096400	2.80581300
C	-1.73235000	-0.60646300	2.14157400
H	-1.16022300	-1.10113800	2.92051400
C	-1.08575600	0.33768000	1.36649700
C	0.32991000	0.43616100	1.35829900
O	1.12920400	-0.15269100	2.08852800
H	-1.67991900	0.99430300	0.75258200
H	-2.75810500	5.21669700	1.82099600
C	2.37142800	-2.60271300	-1.75075600
C	1.20709500	-1.84843000	-1.43142500
C	0.87880300	-0.73115100	-2.21483900
C	1.64788300	-0.34312600	-3.30759200
C	2.76484200	-1.09526700	-3.64538800
C	3.10310900	-2.20779200	-2.87399000
H	0.00258300	-0.15898700	-1.93804600
H	1.37472300	0.54493300	-3.86953900
H	3.38056300	-0.82001400	-4.49549900
H	3.98481900	-2.76956700	-3.15864800
C	2.83645700	-3.78308400	-0.88318100
C	3.23097700	-3.26911500	0.51562200
C	1.73428400	-4.85245200	-0.76285000
C	4.07043500	-4.47425100	-1.47985300
H	4.09726000	-2.60171700	0.44557100
H	2.40854800	-2.72634100	0.98325900
H	3.51021400	-4.11602000	1.15293300
H	1.39416700	-5.16756200	-1.75533600
H	2.13506500	-5.73240000	-0.24754600
H	0.87488400	-4.48806200	-0.20007600
H	4.36351200	-5.30178600	-0.82693400

H	3.86813000	-4.88692600	-2.47386300
H	4.92455800	-3.79374000	-1.55323000
N	0.49089300	-2.17779000	-0.27548000
C	-0.79759400	-2.30979000	-0.19745600
C	-1.38775000	-2.71848100	1.02845000
H	-0.68054800	-3.04459800	1.78243600
C	-2.71284100	-3.25823400	1.17864300
O	-3.12368100	-3.84856300	2.16899500
O	-3.52559100	-3.01198300	0.11710100
C	-4.88442800	-3.39875300	0.29165600
H	-5.40833900	-3.06333400	-0.60301200
H	-4.96924500	-4.48324000	0.39488600
H	-5.30410600	-2.91729400	1.17851700
C	-1.68208200	-1.95775200	-1.38052700
O	-1.68589900	-2.91741300	-2.29821000
O	-2.24871000	-0.89256900	-1.51284300
C	-2.42722800	-2.62068600	-3.48841600
H	-1.99406900	-1.75094200	-3.98751600
H	-2.34742300	-3.50440900	-4.11703500
H	-3.46970300	-2.41605900	-3.23844200

TS4(RR)"

C	-1.59893400	1.39905900	-0.15637700
C	-2.96904900	1.66615600	-1.83199900
C	-2.17894000	-0.64333200	-1.60165500
H	-1.28924700	-1.10302500	-1.16026700
N	-2.84410700	2.85325700	-1.31100000
N	-1.99168000	2.66615800	-0.26438100
N	-2.22755500	0.74489300	-1.14530500
C	-3.59832300	1.20206400	-3.10435800
H	-3.88576300	2.05553100	-3.71688300
H	-4.48098300	0.58226900	-2.90501900
C	-2.08586400	-0.68339500	-3.16376700
O	-2.58337400	0.49294900	-3.79487500
C	-3.80766400	-2.19080400	-2.38714900
C	-3.43987300	-1.41913700	-1.28454700
C	-4.17349900	-1.45122700	-0.10233400
C	-5.27185400	-2.30693600	-0.02487400
C	-5.62460100	-3.10529800	-1.11453400
C	-4.90049500	-3.04739900	-2.30461600
C	-2.89543500	-1.93400500	-3.56209500
H	-3.92229700	-0.80983100	0.73885500
H	-6.48205400	-3.76597200	-1.03970400

H	-5.19246500	-3.65145700	-3.15808000
H	-3.43690800	-1.74680300	-4.49335600
H	-2.22443000	-2.78108500	-3.74390400
C	-1.62639700	3.78062100	0.57211700
C	-2.36808800	4.01298100	1.73022000
C	-0.55749000	4.57394800	0.15993300
C	-2.00591500	5.11840900	2.49776100
C	-0.23602400	5.66766100	0.96116100
C	-0.95060100	5.95539100	2.12584900
H	-2.56108500	5.33076700	3.40785500
H	0.59516300	6.30468300	0.67110300
C	0.21688800	4.22762700	-1.08116400
H	-0.42783200	4.22785300	-1.96527000
H	0.64802900	3.22432400	-0.98369000
H	1.02359800	4.94412500	-1.24287100
C	-3.49247100	3.09429400	2.12998000
H	-3.11444800	2.09786100	2.38580200
H	-4.21528700	2.97343200	1.31740100
H	-4.01670500	3.48812500	3.00144300
H	-1.03936800	-0.73761900	-3.46507400
C	-0.60539000	7.15709500	2.96633300
H	-1.34518500	7.95073600	2.82257400
H	-0.60084700	6.90308400	4.02921200
H	0.37449800	7.55795800	2.70066300
C	-1.96728200	-3.98799500	3.68363000
C	-1.62622500	-2.90775800	2.87988900
C	-0.48162100	-2.14604400	3.15594600
C	0.31672800	-2.50364700	4.25097800
C	-0.02420700	-3.58431900	5.05571900
C	-1.16850600	-4.32967900	4.77383300
H	-2.85677700	-4.56690900	3.45748500
H	-2.25950300	-2.66026900	2.03231900
H	1.20993100	-1.92340600	4.46767700
H	0.60058100	-3.84595200	5.90337800
H	-1.43601000	-5.17445000	5.40027900
C	-0.10856300	-0.98571000	2.34120100
H	0.73677400	-0.39520400	2.68595100
C	-0.94601800	-0.39627500	1.42063600
C	-0.62249600	0.87478900	0.87565300
O	0.31458100	1.61786500	1.16688400
H	-1.84477600	-0.89220200	1.07896000
H	-5.85948000	-2.34524100	0.88601900
C	5.24255500	0.33890100	-0.66812600
C	3.89691200	0.46509100	-0.23017300

C	3.15695500	1.60930500	-0.56360300
C	3.70340800	2.62125400	-1.34611900
C	5.00687800	2.49744000	-1.80722400
C	5.75245300	1.36973900	-1.46291400
H	2.14898600	1.69195400	-0.16640700
H	3.11243100	3.49946400	-1.58892500
H	5.45263700	3.27111600	-2.42439700
H	6.76855800	1.30307500	-1.83331500
C	6.10998200	-0.87495600	-0.29841100
C	6.28957700	-0.94309200	1.22911400
C	5.46870100	-2.17858700	-0.80873100
C	7.50980200	-0.78708500	-0.92181200
H	6.80223200	-0.04565400	1.59169100
H	5.32531700	-1.02535100	1.73172200
H	6.90236900	-1.81289400	1.49134700
H	5.29888800	-2.12578100	-1.88928700
H	6.14293500	-3.01912100	-0.60891300
H	4.51315200	-2.38029900	-0.32404200
H	8.08773600	-1.66637700	-0.62187100
H	7.46854600	-0.77187300	-2.01580500
H	8.05432800	0.09984800	-0.58292000
N	3.31972400	-0.50569800	0.60860300
C	2.24143000	-1.13656500	0.25362100
C	1.67320000	-2.14786700	1.08216300
H	2.25525900	-2.40059500	1.96163500
C	0.77923600	-3.18032000	0.65229700
O	0.60272500	-4.25347700	1.21484500
O	0.03729200	-2.85482000	-0.45682600
C	-0.87213500	-3.86486800	-0.88122400
H	-1.30129700	-3.51330000	-1.81965700
H	-0.35657700	-4.81388700	-1.03954300
H	-1.66454200	-4.00951000	-0.14156900
C	1.64271600	-0.89934900	-1.12773300
O	2.31627900	-1.61511600	-2.02652100
O	0.72713800	-0.15569100	-1.40830100
C	1.85310600	-1.52177400	-3.37619300
H	1.78156200	-0.47761400	-3.68498300
H	2.58487000	-2.05321800	-3.98074600
H	0.87427900	-2.00168100	-3.46175200

TS4(RR)'''

C	3.04590200	-0.01952800	-0.19466300
C	4.43249500	1.39288000	-1.11272600

C	2.18347600	2.32162100	-0.81683200
H	1.18452100	1.88292900	-0.77323400
N	5.14171200	0.32129000	-0.89882000
N	4.26306700	-0.54508600	-0.32113000
N	3.14393200	1.22564300	-0.68714700
C	4.73704500	2.65594500	-1.85179900
H	5.65098500	2.54057000	-2.43320400
H	4.85285400	3.49678400	-1.15697000
C	2.37534400	3.04597600	-2.18927500
O	3.66601100	2.84914600	-2.75957000
C	2.35608900	4.66013400	-0.39266100
C	2.42691400	3.40534600	0.21204800
C	2.70304400	3.26842300	1.56839100
C	2.88088000	4.42329000	2.32964300
C	2.78890700	5.68259500	1.73444800
C	2.53105100	5.81028100	0.36961300
C	2.09541600	4.52983100	-1.87359900
H	2.80398400	2.28870800	2.02900100
H	2.93463800	6.57200800	2.33857500
H	2.48227000	6.79131200	-0.09260900
H	2.73061200	5.17416800	-2.48676100
H	1.05314400	4.77128900	-2.10782700
C	4.71617400	-1.82835100	0.14872700
C	4.97092800	-1.97344500	1.51130200
C	4.88522800	-2.84938800	-0.78721700
C	5.43055200	-3.21978200	1.93864100
C	5.34782100	-4.07243300	-0.31063700
C	5.62858400	-4.27260100	1.04467600
H	5.63861100	-3.36783700	2.99490100
H	5.48533200	-4.89159300	-1.01174600
C	4.54771600	-2.62315800	-2.23474500
H	5.19637100	-1.86223500	-2.67855500
H	3.51484800	-2.27205400	-2.32888400
H	4.65568600	-3.54648400	-2.80490100
C	4.74057000	-0.83884800	2.47519200
H	3.66942600	-0.64992400	2.61268800
H	5.19660000	0.08877600	2.11535600
H	5.16562200	-1.07476800	3.45140900
H	1.68164000	2.63492400	-2.92320200
C	6.15474400	-5.60084800	1.52265400
H	7.22742000	-5.68312900	1.32098200
H	6.00610700	-5.72200000	2.59730800
H	5.66003100	-6.42727200	1.00705500
C	-2.29021100	2.05873900	3.31287900

C	-1.33410700	1.50379900	2.47196300
C	-1.33824100	0.12678600	2.20584900
C	-2.32558000	-0.67168800	2.79235800
C	-3.28033100	-0.11688900	3.64024900
C	-3.26466400	1.25008900	3.90231100
H	-2.28144100	3.12624700	3.50777900
H	-0.59259300	2.14638200	2.00398600
H	-2.33416600	-1.73598400	2.57040300
H	-4.04189100	-0.75072800	4.08345600
H	-4.01103100	1.68880500	4.55646500
C	-0.35694500	-0.50755300	1.31576500
H	-0.51800900	-1.56255200	1.10589200
C	0.89886400	0.00495800	1.06088800
C	1.82553700	-0.76271600	0.30731700
O	1.76300600	-1.95801900	0.00537500
H	1.15567200	1.02144600	1.33483000
H	3.10076800	4.34100200	3.38852500
C	-6.28541000	0.04193700	-0.27415900
C	-5.10336700	-0.55555500	0.24226000
C	-5.20554100	-1.67148700	1.08803900
C	-6.43637500	-2.23204900	1.41108000
C	-7.59538100	-1.67237900	0.89193100
C	-7.50425300	-0.55305600	0.06469000
H	-4.29719900	-2.08716000	1.50818600
H	-6.48113100	-3.09390400	2.06972100
H	-8.56807300	-2.09111400	1.12881700
H	-8.42567800	-0.13592500	-0.32321900
C	-6.24074300	1.28345900	-1.18080600
C	-5.64543600	2.47674300	-0.41015000
C	-5.40640200	1.00277400	-2.44490300
C	-7.64281000	1.69728200	-1.65047900
H	-6.27363700	2.72147000	0.45285700
H	-4.63725200	2.25415200	-0.05996800
H	-5.60985400	3.35605300	-1.06312000
H	-5.79425500	0.12507100	-2.97293400
H	-5.46826900	1.86131600	-3.12271800
H	-4.35694000	0.82803400	-2.20706400
H	-7.55563100	2.58326600	-2.28628200
H	-8.12567700	0.90992200	-2.23825400
H	-8.29636200	1.95434300	-0.81116400
N	-3.85724600	0.03092400	-0.03586000
C	-2.83993100	-0.65082700	-0.45628400
C	-1.57505700	-0.01938400	-0.67398300
H	-1.53985000	1.04251900	-0.45950000

C	-0.57297000	-0.48279000	-1.58111500
O	0.44871800	0.14566500	-1.87304300
O	-0.79667200	-1.72343200	-2.08681900
C	0.27215600	-2.28270900	-2.84276800
H	-0.08997900	-3.24411800	-3.20519300
H	0.53328100	-1.63654700	-3.68360100
H	1.14577200	-2.41949000	-2.20003400
C	-2.92039500	-2.15758200	-0.64103700
O	-3.70043800	-2.49527000	-1.66434600
O	-2.38121900	-2.95179100	0.09774100
C	-3.88606000	-3.90335100	-1.84507700
H	-4.36606100	-4.33144400	-0.96251900
H	-4.52466200	-4.01052900	-2.71874400
H	-2.92341700	-4.39142500	-2.00798100

M4(RR)

C	-2.09952200	-0.28857900	0.26625000
C	-2.80447000	-2.36023000	0.14451000
C	-0.39467500	-2.17515700	0.58183100
H	0.34967000	-1.41322900	0.33212200
N	-3.87093800	-1.63788700	-0.03730700
N	-3.41338800	-0.35236300	0.04915500
N	-1.70235300	-1.57385200	0.34028600
C	-2.56040200	-3.82840500	0.00976500
H	-3.40379600	-4.31048200	-0.48299500
H	-2.39857700	-4.29319700	0.99069000
C	-0.20305100	-3.45683700	-0.30506500
O	-1.42691100	-3.95875400	-0.83340500
C	0.27608600	-3.97052300	2.01134600
C	-0.26136300	-2.68421300	2.00416800
C	-0.61744400	-2.04617200	3.18927900
C	-0.39033500	-2.70545000	4.39611500
C	0.17527000	-3.98167300	4.40912100
C	0.50504600	-4.62530900	3.21778500
C	0.51242800	-4.47177600	0.61047700
H	-1.08523500	-1.06523900	3.18384300
H	0.34361500	-4.48350900	5.35644200
H	0.92002900	-5.62858300	3.22969800
H	0.11746300	-5.47773800	0.44076300
H	1.58117900	-4.49140600	0.37148500
C	-4.34099600	0.74591900	0.01166300
C	-4.79442100	1.25442300	1.22720600
C	-4.75122400	1.22953000	-1.23171900

C	-5.72472900	2.29391000	1.17412800
C	-5.68211400	2.26375600	-1.23230500
C	-6.18164000	2.80246600	-0.04155200
H	-6.09865700	2.71223500	2.10494100
H	-6.02120600	2.66649400	-2.18367900
C	-4.14959200	0.67673600	-2.49247900
H	-4.29690700	-0.40541200	-2.56536500
H	-3.07143100	0.86988700	-2.47218000
H	-4.58764000	1.14835100	-3.37346200
C	-4.27776200	0.71394200	2.53498000
H	-3.21142100	0.93916700	2.65152300
H	-4.39275400	-0.37332300	2.58975000
H	-4.81345200	1.16016100	3.37387300
H	0.39675200	-3.21706900	-1.18335500
C	-7.20214000	3.91025700	-0.08296000
H	-8.16650900	3.53343900	-0.43735800
H	-7.35294300	4.34800200	0.90562700
H	-6.89043200	4.70284900	-0.76835600
C	3.54483700	0.30457900	3.07613900
C	2.40127400	0.53168200	2.31364400
C	1.95828900	1.83140000	2.05194400
C	2.67655400	2.89972500	2.59721100
C	3.82140700	2.67806800	3.35726700
C	4.26466700	1.37782800	3.59398100
H	3.87238100	-0.71380200	3.26353400
H	1.85714800	-0.31831200	1.90879300
H	2.33628100	3.91559800	2.41310800
H	4.36599300	3.52186600	3.77030500
H	5.15728300	1.20269400	4.18635700
C	0.79059400	2.10341300	1.12072100
H	0.34471200	3.06501400	1.40349300
C	-0.24827900	1.02017200	1.14325900
C	-1.26711400	0.96836100	0.23396300
O	-1.58836100	1.78210700	-0.69121700
H	-0.15749300	0.23688300	1.88292200
H	-0.66273900	-2.22541800	5.32995600
C	1.67295900	-1.73045700	-2.84009200
C	2.07382400	-1.04842500	-1.66675300
C	2.98232700	-1.63076800	-0.77321900
C	3.54004100	-2.87730100	-1.03092400
C	3.19042800	-3.54617000	-2.19755400
C	2.27789600	-2.96899400	-3.08129800
H	3.23335800	-1.09232800	0.13815800
H	4.23718100	-3.31617100	-0.32439300

H	3.61528900	-4.51889200	-2.42257800
H	2.01996100	-3.52225500	-3.97590300
C	0.61653600	-1.15509000	-3.79507400
C	-0.73300700	-0.98832700	-3.06379800
C	1.08201400	0.20275500	-4.35038500
C	0.37800000	-2.08473900	-4.99256500
H	-1.06796600	-1.94427500	-2.64003700
H	-0.67567700	-0.24078800	-2.26826600
H	-1.49127800	-0.66198400	-3.78498900
H	2.03610900	0.09567600	-4.87664900
H	0.34052600	0.58249200	-5.06125800
H	1.20597800	0.94582100	-3.56094900
H	-0.37037100	-1.63234700	-5.64938500
H	1.28964700	-2.23568000	-5.57931400
H	-0.00088700	-3.06262100	-4.67850100
N	1.44119500	0.15613000	-1.29297000
C	2.08908200	1.18435000	-0.91457600
C	1.30642700	2.34616800	-0.35274200
H	0.37780600	2.41135900	-0.94245100
C	2.02448700	3.66037800	-0.55423000
O	2.95779700	3.82723800	-1.31070800
O	1.46633600	4.66051400	0.13427900
C	2.06435900	5.94809300	-0.05716100
H	1.48911500	6.63502600	0.55935100
H	3.10844000	5.92735100	0.26064000
H	2.01207200	6.23641200	-1.10814200
C	3.60210100	1.28999900	-1.07609100
O	4.19024900	1.68788600	0.04564700
O	4.17682800	1.03341000	-2.10642100
C	5.59414200	1.94476500	-0.05045600
H	5.77236300	2.73712700	-0.78061300
H	5.90166300	2.25708900	0.94527900
H	6.12548700	1.04120000	-0.35455600

TS4(RS)

C	-2.82771000	0.82538600	-0.24373200
C	-4.73101600	0.21961400	-1.12262000
C	-3.11149300	-1.61580400	-1.00183700
H	-2.02008000	-1.66421600	-1.01922700
N	-4.89058900	1.47478300	-0.81407500
N	-3.69728200	1.83472100	-0.26384900
N	-3.48140100	-0.21794800	-0.77981700
C	-5.59200900	-0.73591800	-1.88408400

H	-6.38590200	-0.19866500	-2.40139200
H	-6.03622700	-1.47973500	-1.21099900
C	-3.67276200	-2.11327000	-2.37446200
O	-4.75534200	-1.32781500	-2.86286300
C	-4.28216900	-3.65569800	-0.61544700
C	-3.74915700	-2.53398500	0.01847900
C	-3.84741700	-2.36255900	1.39510300
C	-4.47610700	-3.35586000	2.14451000
C	-4.99485300	-4.49050800	1.51830600
C	-4.90534500	-4.64704300	0.13533700
C	-4.08117400	-3.57760100	-2.10896600
H	-3.46376800	-1.46891100	1.88114800
H	-5.48581600	-5.25356700	2.11349000
H	-5.32865200	-5.52199500	-0.34831600
H	-4.97591600	-3.83123300	-2.68351300
H	-3.27999100	-4.25234000	-2.42963300
C	-3.54323900	3.14417800	0.31918800
C	-3.78251300	3.27471600	1.68632800
C	-3.19526300	4.20664900	-0.51510100
C	-3.67564100	4.55631200	2.22706700
C	-3.10450000	5.46541300	0.07282900
C	-3.34135700	5.65709500	1.43743800
H	-3.86101000	4.69514600	3.28889300
H	-2.83774300	6.31723500	-0.54749300
C	-2.90434800	3.97019400	-1.97059100
H	-3.76235500	3.52169500	-2.48011600
H	-2.05972800	3.28002100	-2.06565200
H	-2.65280500	4.90550900	-2.47198300
C	-4.12115200	2.07965500	2.53853600
H	-3.25237700	1.42002900	2.64721000
H	-4.93289600	1.49071700	2.10038700
H	-4.42650200	2.39615000	3.53653500
H	-2.89985100	-2.02811600	-3.13961400
C	-3.20826900	7.02873400	2.04634700
H	-3.75571000	7.09825100	2.98836700
H	-2.15743100	7.25546000	2.25256700
H	-3.58298400	7.79810000	1.36727300
C	1.38822300	-3.60551200	2.45334700
C	0.73190900	-2.57683500	1.79118400
C	1.16626700	-1.25131400	1.93343400
C	2.27392100	-0.98334500	2.74546200
C	2.92629200	-2.01405600	3.41577200
C	2.48583200	-3.32682800	3.27008300
H	1.04869300	-4.62931600	2.33137600

H	-0.10794900	-2.80390100	1.13954600
H	2.62350800	0.04124500	2.84427600
H	3.78167200	-1.79114100	4.04639700
H	2.99600500	-4.13340900	3.78745100
C	0.49840500	-0.14371900	1.24275500
H	0.99465700	0.82222800	1.28827000
C	-0.84080200	-0.16604200	0.90468000
C	-1.38977600	0.94538600	0.21731000
O	-0.82816900	2.00767400	-0.06269800
H	-1.44012200	-1.05629700	1.05294900
H	-4.56855600	-3.24171800	3.21926300
C	5.99492400	1.50144300	-0.40436900
C	5.04626900	0.64388200	0.21425200
C	5.46673900	-0.25908200	1.20228700
C	6.80117200	-0.35445200	1.58145900
C	7.74075600	0.46538100	0.97220000
C	7.32806600	1.37305700	-0.00283900
H	4.71618000	-0.88110900	1.67850200
H	7.09576500	-1.06095800	2.35181000
H	8.78848000	0.41132300	1.25025700
H	8.08386400	2.00017000	-0.46031100
C	5.59286700	2.51915000	-1.48474700
C	4.94880400	1.80234300	-2.68589800
C	4.61200800	3.55152300	-0.89961100
C	6.80599500	3.29316500	-2.01840500
H	5.63252500	1.05054800	-3.09414000
H	4.01678300	1.30681900	-2.41235100
H	4.73416900	2.53158000	-3.47504800
H	5.08682300	4.10361300	-0.08157800
H	4.32887400	4.27197500	-1.67527400
H	3.71199100	3.06622700	-0.52152800
H	6.46636100	4.00614100	-2.77568400
H	7.30771300	3.86049000	-1.22823600
H	7.53934500	2.62975700	-2.48823200
N	3.67786600	0.75363400	-0.10113000
C	2.99791500	-0.27173200	-0.51116400
C	1.61953700	-0.12476500	-0.85825100
H	1.26018000	0.89327700	-0.96043900
C	0.78557100	-1.10300600	-1.47219900
O	-0.33980100	-0.86869000	-1.92237200
O	1.27934700	-2.37190100	-1.46237800
C	0.43843900	-3.37006400	-2.02677600
H	1.02277700	-4.28923200	-2.02722600
H	-0.46361200	-3.51054000	-1.42249200

H	0.14458200	-3.10672000	-3.04523200
C	3.68834100	-1.60705000	-0.75334100
O	3.51741200	-2.47069300	0.24238800
O	4.35203200	-1.82518100	-1.74128800
C	4.12259500	-3.74995600	0.04733600
H	5.20509900	-3.64587000	-0.05631700
H	3.87427300	-4.33056900	0.93327600
H	3.71702600	-4.22125000	-0.85094900

TS4(RS)'

C	-1.23268300	1.13033000	-0.51616500
C	-2.29228500	2.59430600	0.71622100
C	0.12357600	2.58269900	1.13129300
H	0.87551300	1.79022800	1.12980400
N	-3.21305300	2.05488300	-0.02825400
N	-2.53874000	1.15282900	-0.79286600
N	-1.06513600	2.05523600	0.45227000
C	-2.38623100	3.59342500	1.82270400
H	-3.41417600	3.66748900	2.17591900
H	-2.04928300	4.58110200	1.48088900
C	-0.20280600	2.99665000	2.61401700
O	-1.59255700	3.09617700	2.88282100
C	0.83615200	4.84447200	1.44158800
C	0.59253700	3.86871000	0.47673400
C	0.74725600	4.14223500	-0.88047900
C	1.18991700	5.40832600	-1.25809800
C	1.46024100	6.38039700	-0.29293400
C	1.27904500	6.10776300	1.06133100
C	0.54228700	4.33177800	2.82635300
H	0.51686200	3.39902800	-1.63960200
H	1.79995600	7.36307700	-0.60319300
H	1.46611500	6.87252400	1.80874100
H	-0.07472200	5.01451300	3.41740000
H	1.46774700	4.15966900	3.38508100
C	-3.26788600	0.41193600	-1.79226000
C	-3.07715000	0.73652600	-3.13639800
C	-4.15813800	-0.56578100	-1.35013800
C	-3.82492600	0.02262800	-4.07011500
C	-4.87937800	-1.25236800	-2.32656400
C	-4.72800800	-0.97098800	-3.68478600
H	-3.69784300	0.24879000	-5.12586400
H	-5.57289700	-2.02898500	-2.01413000
C	-4.31184500	-0.87332200	0.11376500

H	-4.80028500	-0.04726600	0.63979200
H	-3.33492000	-1.03968100	0.58146800
H	-4.90646900	-1.77686200	0.25372800
C	-2.09219400	1.79147000	-3.56422400
H	-1.06400200	1.42156300	-3.48028200
H	-2.17407300	2.69461100	-2.95131400
H	-2.26231900	2.06957500	-4.60527600
H	0.15008600	2.22437300	3.29672300
C	-5.54017100	-1.70477000	-4.72002100
H	-6.40038100	-1.10319400	-5.03071000
H	-4.94563300	-1.91241500	-5.61291800
H	-5.91916300	-2.65047200	-4.32736200
C	5.35023300	1.60556700	-1.99687600
C	4.03753900	1.33247900	-1.62953200
C	3.52127400	0.03605700	-1.75469000
C	4.35486700	-0.97883400	-2.24531200
C	5.66647900	-0.70415600	-2.61592100
C	6.16779000	0.59093600	-2.49393300
H	5.73772200	2.61446200	-1.89823500
H	3.41171700	2.13671500	-1.25242500
H	3.96159700	-1.99017700	-2.31951800
H	6.29748600	-1.49925300	-3.00088200
H	7.19079700	0.80939800	-2.78281100
C	2.13325400	-0.30579000	-1.41215600
H	1.81529600	-1.30152400	-1.71260700
C	1.12827100	0.60999500	-1.15680800
C	-0.23107800	0.19813500	-1.17895500
O	-0.71019600	-0.80198800	-1.72058600
H	1.37542400	1.61930100	-0.85963200
H	1.31674200	5.64062500	-2.30993400
C	-1.73385900	-2.31646300	2.42673800
C	-0.88667300	-2.26164400	1.28546400
C	-1.22305700	-3.00671200	0.14269500
C	-2.33831200	-3.83775500	0.11583500
C	-3.13875700	-3.94023000	1.24429400
C	-2.83219500	-3.17970100	2.37254700
H	-0.60491500	-2.89830800	-0.74007700
H	-2.57318400	-4.39795900	-0.78430500
H	-4.00869800	-4.58954300	1.25123100
H	-3.48360600	-3.26622400	3.23389200
C	-1.47727300	-1.45836400	3.67304400
C	-0.09028500	-1.75223300	4.27342300
C	-1.57889900	0.02452300	3.28144400
C	-2.51362700	-1.71603600	4.77530400

H	0.01295600	-2.82013000	4.49409600
H	0.71045500	-1.45997500	3.59394600
H	0.02923000	-1.19861800	5.21142000
H	-2.57671300	0.25498100	2.88796400
H	-1.40849200	0.66305000	4.15588600
H	-0.83541100	0.25992300	2.51706300
H	-2.28850000	-1.07117600	5.63002300
H	-3.53042700	-1.48461800	4.44277800
H	-2.48941500	-2.75367500	5.12365700
N	0.25219500	-1.43055000	1.28747200
C	1.40147100	-1.89602700	0.87969800
C	2.53669400	-1.04992500	0.77712400
H	2.40785100	-0.04619500	1.16517400
C	3.92398800	-1.46441100	0.77475400
O	4.85963900	-0.72574000	1.04170100
O	4.13095900	-2.75200800	0.39643800
C	5.49634800	-3.15751400	0.35171300
H	5.48874500	-4.20410200	0.05057200
H	6.04775000	-2.55543000	-0.37474700
H	5.96458900	-3.04872800	1.33231000
C	1.57891400	-3.36190900	0.51282600
O	1.75182500	-3.52942700	-0.80319400
O	1.55414000	-4.26612600	1.31223200
C	2.00026600	-4.87742800	-1.21111800
H	1.15605700	-5.51517100	-0.94084900
H	2.12648300	-4.84500800	-2.29110200
H	2.90691000	-5.24809000	-0.72799400

TS4(RS)"

C	2.33124000	0.57996900	0.02351200
C	2.83504700	2.36917000	-1.12875800
C	0.49611000	2.34273400	-0.38065900
H	-0.21397200	1.53400700	-0.20509500
N	3.93680900	1.67763400	-1.08351600
N	3.60927100	0.57314300	-0.35924000
N	1.82485200	1.72885400	-0.46451400
C	2.47176900	3.59121600	-1.90747900
H	3.22909200	3.79534700	-2.66295300
H	2.36417200	4.46402200	-1.25136000
C	0.14061400	3.08397300	-1.72191000
O	1.26138600	3.26707600	-2.57230400
C	-0.11591300	4.58620700	0.16483900
C	0.45683100	3.42412400	0.67682200

C	0.92559700	3.36024900	1.98611400
C	0.78642300	4.48585600	2.79453100
C	0.19630000	5.64800100	2.29279000
C	-0.25506400	5.70848000	0.97585000
C	-0.50727100	4.41468500	-1.27994300
H	1.40383500	2.46391300	2.37293000
H	0.10042100	6.51839200	2.93362800
H	-0.69617600	6.61988900	0.58465500
H	-0.16478700	5.23038400	-1.92309000
H	-1.59573000	4.35519500	-1.38131700
C	4.61296400	-0.43990700	-0.14128700
C	5.42451500	-0.34169300	0.98470900
C	4.72976300	-1.44479200	-1.10260300
C	6.40908000	-1.31982500	1.13778400
C	5.72440600	-2.39652000	-0.90351500
C	6.57366300	-2.34584400	0.20703700
H	7.05914700	-1.27649400	2.00756300
H	5.83961700	-3.19710600	-1.62968200
C	3.78627200	-1.48926300	-2.27178200
H	3.85391200	-0.57697100	-2.87390000
H	2.75651000	-1.58209700	-1.90758100
H	4.00392300	-2.34370800	-2.91454800
C	5.23023200	0.76124700	1.99106900
H	4.25752700	0.67399700	2.48724300
H	5.26951300	1.74456000	1.51285000
H	6.00472200	0.71998700	2.75781400
H	-0.54698500	2.47345800	-2.31155800
C	7.66254200	-3.37287500	0.37707500
H	8.53463300	-3.11020400	-0.23017100
H	7.98754700	-3.43717900	1.41733900
H	7.32405600	-4.36053500	0.05556500
C	-3.42281300	0.41080500	3.28848200
C	-2.25838800	0.15921900	2.57179800
C	-1.46117900	-0.95481700	2.87436000
C	-1.87892000	-1.82847700	3.88924700
C	-3.04167500	-1.57495500	4.60700500
C	-3.81503300	-0.45169300	4.30981900
H	-4.03212200	1.27345400	3.03886300
H	-1.98326000	0.81997300	1.75502400
H	-1.27862400	-2.70613100	4.11444400
H	-3.34787400	-2.25243400	5.39737200
H	-4.72568400	-0.25591900	4.86686000
C	-0.23059700	-1.23224400	2.12833100
H	0.24771300	-2.19740300	2.28043300

C	0.50064600	-0.22172300	1.53485800
C	1.65388900	-0.54815800	0.77781500
O	2.16018500	-1.66244800	0.63891200
H	0.16015800	0.80110800	1.60201700
H	1.14537500	4.46069100	3.81763100
C	-5.13071300	-0.35908600	-1.10671000
C	-3.73703100	-0.21447600	-0.86016900
C	-3.08033900	0.94619100	-1.30110100
C	-3.74297900	1.94192800	-2.00913400
C	-5.09726100	1.79653300	-2.27618100
C	-5.76599200	0.65937700	-1.82186600
H	-2.02715700	1.05564800	-1.06143300
H	-3.20617500	2.82531800	-2.34322600
H	-5.63865000	2.56072300	-2.82400800
H	-6.82416600	0.57574600	-2.03941000
C	-5.91024300	-1.59306300	-0.62445600
C	-5.30988700	-2.87534500	-1.23106000
C	-5.87964800	-1.67303500	0.91383600
C	-7.38365000	-1.53750900	-1.05150000
H	-5.31303800	-2.81841400	-2.32492800
H	-4.28571300	-3.03900500	-0.89402000
H	-5.91439000	-3.73992400	-0.93496700
H	-6.34427000	-0.78179100	1.35005100
H	-6.44908900	-2.54848500	1.24646800
H	-4.85621800	-1.75065100	1.28329500
H	-7.89289100	-2.43488200	-0.68749900
H	-7.89891200	-0.66892700	-0.62914200
H	-7.49274700	-1.51001300	-2.14054300
N	-3.07109200	-1.18434600	-0.10865100
C	-1.90358900	-1.66472700	-0.42786600
C	-1.27050100	-2.60409800	0.42287400
H	-1.87155800	-2.95269300	1.25306400
C	-0.14644900	-3.44894900	0.11185300
O	0.31961900	-4.27791700	0.88609200
O	0.37202900	-3.27539400	-1.13444800
C	1.55850600	-4.01714700	-1.39555700
H	1.79065900	-3.85201900	-2.44785900
H	2.37298600	-3.64986600	-0.76351600
H	1.39910400	-5.08038300	-1.20606900
C	-1.25964400	-1.30860600	-1.75945700
O	-0.18959100	-0.49484000	-1.65805200
O	-1.69945000	-1.68879500	-2.81614500
C	0.41427500	-0.18490000	-2.92238500
H	-0.32420200	0.25114400	-3.59859500

H	1.20932200	0.53388300	-2.72129200
H	0.82269900	-1.09347200	-3.37052200
TS4(RS)'''			
C	2.94130800	-0.01015700	-0.10683700
C	3.98815400	1.55656600	-1.21959300
C	1.60241100	2.05618800	-0.89383100
H	0.71425900	1.41533400	-0.88952400
N	4.89710100	0.66143900	-0.96403500
N	4.23416400	-0.30132000	-0.26936400
N	2.77081100	1.17975400	-0.72443300
C	4.04523200	2.79035800	-2.05806200
H	4.94720400	2.79026800	-2.66821700
H	4.02930700	3.69263300	-1.43269000
C	1.67613900	2.84000300	-2.26143800
O	2.92408700	2.71697300	-2.91948100
C	1.38373200	4.39060700	-0.41391800
C	1.57285700	3.13784900	0.16621000
C	1.71457600	2.99588600	1.54564700
C	1.62218100	4.13288200	2.34472900
C	1.40235900	5.38658900	1.76922100
C	1.28910900	5.52481300	0.38810100
C	1.31689100	4.30339200	-1.91522800
H	1.90522300	2.02637000	1.99854500
H	1.33470400	6.26346400	2.40462300
H	1.14076200	6.50277800	-0.05901900
H	2.01522100	4.98495400	-2.41100300
H	0.31599500	4.54822600	-2.28488900
C	4.97036800	-1.47874800	0.12651200
C	5.73908000	-1.41226800	1.28466900
C	4.91137700	-2.59463100	-0.70964300
C	6.48767100	-2.54420700	1.61102300
C	5.67848500	-3.69580400	-0.34071600
C	6.47206300	-3.68677800	0.81095700
H	7.09533200	-2.52891400	2.51191700
H	5.65469000	-4.58528000	-0.96517800
C	4.02812500	-2.59970900	-1.92732800
H	4.24336900	-1.74228900	-2.57429500
H	2.97096500	-2.54935500	-1.63736100
H	4.18416200	-3.51010900	-2.50827500
C	5.73751900	-0.18009700	2.14967200
H	4.73565000	0.01736800	2.54567100
H	6.04693400	0.70287500	1.58276400

H	6.41811700	-0.30363200	2.99289500
H	0.95970800	2.41352200	-2.96292900
C	7.31201100	-4.88678300	1.16414800
H	8.23693500	-4.89391200	0.57869300
H	7.58592000	-4.88124200	2.22106900
H	6.78003900	-5.81619400	0.94742100
C	-2.46974500	1.09803700	3.62275400
C	-1.46036400	0.68021500	2.76374900
C	-1.42027600	-0.64315700	2.29621200
C	-2.42881200	-1.52765800	2.70325000
C	-3.44158800	-1.10877600	3.55890000
C	-3.46339400	0.20446000	4.02386600
H	-2.47840500	2.12084800	3.98561800
H	-0.68179600	1.38136000	2.47675200
H	-2.41273400	-2.54999900	2.33635900
H	-4.21506600	-1.80703400	3.86196200
H	-4.25139900	0.53217100	4.69446500
C	-0.30611100	-1.13450500	1.47314900
H	-0.08570700	-2.19634300	1.55012200
C	0.72380100	-0.32714100	1.01836600
C	1.95923900	-0.90800200	0.63196300
O	2.35556500	-2.05315400	0.85585200
H	0.55763300	0.73365300	0.91864300
H	1.72834300	4.04273100	3.42040900
C	-6.20465300	-0.91284100	-0.35980200
C	-4.91368700	-0.56813000	0.12025200
C	-4.74053000	0.60732600	0.86721400
C	-5.80068200	1.46564900	1.13262300
C	-7.06446600	1.15056600	0.65186700
C	-7.24656800	-0.02318400	-0.07998700
H	-3.75342400	0.81524500	1.26996000
H	-5.63422200	2.36318800	1.72146300
H	-7.91079100	1.80143500	0.84716300
H	-8.24427400	-0.24327400	-0.44108000
C	-6.45446600	-2.19324300	-1.17173800
C	-5.59120100	-2.19188300	-2.44625600
C	-6.12877300	-3.43212600	-0.31735400
C	-7.91895700	-2.31452000	-1.61418800
H	-5.81648000	-1.31247900	-3.05887900
H	-4.52646200	-2.18474800	-2.21083400
H	-5.81003000	-3.08626300	-3.04010000
H	-6.77115900	-3.46095600	0.56918500
H	-6.31453300	-4.34164300	-0.89977500
H	-5.08690200	-3.42468600	0.00368500

H	-8.04094700	-3.23868700	-2.18723100
H	-8.60120400	-2.36111600	-0.75949600
H	-8.22231800	-1.48058400	-2.25525600
N	-3.82154000	-1.43427600	-0.05245100
C	-2.68295600	-1.00423600	-0.50371600
C	-1.52465900	-1.83280400	-0.47166400
H	-1.68695300	-2.84061200	-0.10556700
C	-0.39719800	-1.71357900	-1.35546000
O	0.47908300	-2.55374200	-1.50001200
O	-0.32996900	-0.52654200	-2.02945500
C	0.66424700	-0.46709800	-3.04910500
H	0.40079800	0.38074500	-3.68039300
H	1.66324500	-0.32367900	-2.62270900
H	0.67060200	-1.38562600	-3.63728100
C	-2.57554000	0.40851200	-1.05896800
O	-1.79395700	1.19152200	-0.30130200
O	-3.17448600	0.79960900	-2.03088900
C	-1.78638100	2.56999200	-0.67945800
H	-2.80489000	2.96453900	-0.68558900
H	-1.18177600	3.08438900	0.06768100
H	-1.35752000	2.68712900	-1.67978500

M4(RS)

C	-2.82148000	0.86009700	-0.28792500
C	-4.80005500	0.24196400	-0.99667200
C	-3.10687000	-1.52425400	-1.17051800
H	-2.01698500	-1.52464400	-1.26574800
N	-4.95598300	1.47710200	-0.61934000
N	-3.71426000	1.84282300	-0.17662200
N	-3.51017500	-0.17256100	-0.80519900
C	-5.69996500	-0.70755500	-1.71931200
H	-6.56712400	-0.18118800	-2.11667200
H	-6.03774300	-1.51026900	-1.05199500
C	-3.77360900	-1.94219400	-2.52247200
O	-4.95512000	-1.20303800	-2.82084400
C	-4.12125400	-3.66036500	-0.86326000
C	-3.60492900	-2.55860000	-0.18204400
C	-3.60888500	-2.49883600	1.20760000
C	-4.11493400	-3.58719500	1.91714700
C	-4.61056600	-4.70334700	1.24097700
C	-4.62279900	-4.74585800	-0.15288600
C	-4.05196400	-3.44986100	-2.35610000
H	-3.25315100	-1.61729000	1.73518100

H	-5.00535800	-5.54090000	1.80699600
H	-5.03199000	-5.60564300	-0.67459800
H	-4.97071500	-3.72634600	-2.87972100
H	-3.23270000	-4.03037000	-2.79445600
C	-3.50532600	3.13253800	0.42303500
C	-3.57621900	3.22312700	1.81163300
C	-3.25384400	4.22181700	-0.41289500
C	-3.40063800	4.48821800	2.37540800
C	-3.08799200	5.46180200	0.19661700
C	-3.16347300	5.61270800	1.58532000
H	-3.45046400	4.59338100	3.45600800
H	-2.88444200	6.33075400	-0.42453900
C	-3.12119400	4.02110700	-1.89629500
H	-4.03550500	3.59865200	-2.32387100
H	-2.30239900	3.31802200	-2.08206900
H	-2.90662400	4.96542500	-2.39855800
C	-3.80955600	1.99857300	2.65698300
H	-2.95708300	1.31294600	2.58603100
H	-4.69975500	1.45274000	2.32837600
H	-3.94092300	2.27338000	3.70437400
H	-3.09979800	-1.73655600	-3.35553900
C	-2.99527300	6.97484700	2.20740400
H	-3.85396500	7.61278900	1.97661700
H	-2.90604500	6.90667300	3.29325200
H	-2.10426600	7.47425300	1.81769700
C	1.16849600	-3.27531500	2.95608300
C	0.65498600	-2.37505000	2.02682100
C	1.16180600	-1.07501400	1.93878900
C	2.16944600	-0.69075200	2.82719500
C	2.68709600	-1.58788400	3.75854900
C	2.19239900	-2.88790600	3.81937100
H	0.76691200	-4.28276200	3.00840700
H	-0.13741100	-2.69402600	1.35470100
H	2.56063200	0.32306200	2.77591300
H	3.47330400	-1.26894800	4.43640400
H	2.59170800	-3.59213400	4.54255900
C	0.68918100	-0.09243200	0.89086100
H	1.01965600	0.91006900	1.19329500
C	-0.79055100	-0.07104600	0.67003300
C	-1.34049500	0.97354100	-0.02391100
O	-0.78922400	2.01502000	-0.49192900
H	-1.39941000	-0.90337200	0.99986100
H	-4.13187100	-3.56128600	3.00142900
C	5.83873900	1.50238900	-0.70876700

C	4.96502000	0.74948600	0.11127300
C	5.44686100	0.05405700	1.22603700
C	6.80041100	0.06658400	1.54529800
C	7.67891400	0.77773500	0.74023800
C	7.19398200	1.47696600	-0.36441200
H	4.73766300	-0.48613800	1.84625500
H	7.15585500	-0.47459900	2.41627000
H	8.74006000	0.79936300	0.96611700
H	7.90644800	2.02289100	-0.97050700
C	5.34389900	2.29412100	-1.92999600
C	4.68267800	1.34956000	-2.95028000
C	4.34335200	3.37758100	-1.48762300
C	6.49855700	3.00318200	-2.65083800
H	5.37497800	0.55472300	-3.24564200
H	3.77871200	0.88448700	-2.55514500
H	4.40827300	1.91569800	-3.84674500
H	4.82324700	4.07885800	-0.79720100
H	4.00448700	3.94190100	-2.36321800
H	3.47309500	2.94287700	-0.99476900
H	6.09441400	3.55995300	-3.50128600
H	7.00970000	3.71705100	-1.99763100
H	7.23632200	2.29269000	-3.03670200
N	3.56598600	0.75336300	-0.12850500
C	2.93967400	-0.33744800	-0.31732500
C	1.44119100	-0.26749400	-0.50363600
H	1.21026800	0.65377800	-1.04514400
C	0.83098400	-1.38668300	-1.31156500
O	0.03209200	-1.21911100	-2.20750900
O	1.21509400	-2.59917800	-0.90053100
C	0.61773800	-3.70835800	-1.58161700
H	1.06983500	-4.59918400	-1.15110200
H	-0.46236500	-3.71348900	-1.41450400
H	0.81977100	-3.64864200	-2.65193000
C	3.66143200	-1.66965100	-0.47231400
O	3.63441100	-2.40735200	0.62647700
O	4.19492900	-1.98219400	-1.51115200
C	4.24402500	-3.69843700	0.51902300
H	5.30672000	-3.59523300	0.29107500
H	4.09998200	-4.16919700	1.48886200
H	3.75564200	-4.27526100	-0.26901000

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C	0.94070100	1.55339200	0.02504500
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C	2.74569500	2.55745800	0.72839800
C	3.18531700	0.32785600	-0.22768900
H	2.60789000	-0.59717700	-0.26505300
N	1.78706100	3.41176600	0.94473400
N	0.67085300	2.77712700	0.49310700
N	2.26830600	1.40854100	0.16403600
C	4.19100500	2.58879300	1.10057800
H	4.37363100	3.36181300	1.84588600
H	4.81727000	2.77800900	0.21902500
C	4.36680400	0.21969700	0.80535500
O	4.46214000	1.33079200	1.68816600
C	5.24097400	0.47347000	-1.44027800
C	3.86179600	0.64098100	-1.54460200
C	3.26504900	1.04672200	-2.73460700
C	4.08460700	1.28740900	-3.83514000
C	5.46845700	1.11711900	-3.74012200
C	6.05596000	0.70744000	-2.54479900
C	5.63369800	0.02925300	-0.05485100
H	2.18725700	1.16164400	-2.79596900
H	6.09282600	1.31025200	-4.60649300
H	7.13194900	0.58190000	-2.47300400
H	6.46754700	0.59758800	0.36722800
H	5.92084400	-1.02807300	-0.05406600
C	-0.59366900	3.46624800	0.50392000
C	-1.12813900	3.89180100	-0.71556400
C	-1.23660700	3.62823100	1.73224400
C	-2.38584200	4.48826600	-0.67726600
C	-2.49301500	4.23542300	1.71327200
C	-3.08390200	4.65915800	0.52156100
H	-2.83545100	4.82292800	-1.60862500
H	-3.02536700	4.36638000	2.65137500
C	-0.61253200	3.13682600	3.01120000
H	0.30390800	3.68840000	3.23814600
H	-0.34489200	2.07673300	2.93977100
H	-1.30603200	3.25853300	3.84373200
C	-0.40196500	3.67969100	-2.01766800
H	-0.54073800	2.65373500	-2.37740500
H	0.67239700	3.85835600	-1.91770300
H	-0.79219800	4.35372600	-2.78129600
H	4.19513900	-0.62905200	1.46403100
C	-4.45594200	5.27965800	0.51180600
H	-4.42157800	6.29359300	0.10338900
H	-5.13333300	4.69642600	-0.11898600
H	-4.87751900	5.32770300	1.51724200

C	-5.67254200	1.39065900	-0.11104500
C	-4.30600900	1.13939600	-0.07829400
C	-3.74522800	0.15602700	-0.90628900
C	-4.58533800	-0.55292100	-1.77637700
C	-5.95027100	-0.29170100	-1.81694800
C	-6.49979600	0.67747800	-0.97937200
H	-6.09465600	2.14924800	0.54084400
H	-3.67592800	1.71819600	0.59158600
H	-4.15590800	-1.32427500	-2.41051800
H	-6.58666300	-0.84777100	-2.49813100
H	-7.56540200	0.88071800	-1.00614500
C	-2.30758300	-0.13981100	-0.91937600
H	-1.96647600	-0.80730200	-1.70854300
C	-1.35268300	0.61929800	-0.28317400
C	0.01423800	0.56337700	-0.66795100
O	0.54491900	-0.10205500	-1.56302300
H	-1.62997000	1.28701800	0.52131100
H	3.64530300	1.60837800	-4.77377900
C	2.13943200	-2.54146800	1.56326200
C	1.13158900	-2.49158500	0.55567900
C	1.48485700	-2.77286700	-0.77907400
C	2.77440500	-3.15559000	-1.12935200
C	3.74469900	-3.27371400	-0.14162800
C	3.41360500	-2.97222500	1.18096400
H	0.74388300	-2.62200000	-1.55434800
H	3.01593400	-3.35140700	-2.16949800
H	4.75382200	-3.58838100	-0.38823800
H	4.19463300	-3.05698000	1.92845100
C	1.85720200	-2.10164600	3.01009100
C	1.46356600	-0.60884900	3.02694900
C	0.73600100	-2.95164700	3.63579300
C	3.09227200	-2.25432100	3.90968300
H	2.30496000	0.01919700	2.70649900
H	0.60649100	-0.42612400	2.37489500
H	1.20172600	-0.30825400	4.04800500
H	1.00475300	-4.01299800	3.61016600
H	0.59780500	-2.66287800	4.68362700
H	-0.20730900	-2.81692300	3.10691400
H	2.83647500	-1.92153600	4.91995300
H	3.42428000	-3.29541800	3.97442400
H	3.93413300	-1.64275600	3.56725100
N	-0.14886000	-2.06791500	0.91111600
C	-1.23159400	-2.53714800	0.35000500
C	-2.49461900	-1.99463200	0.66138900

H	-2.53478000	-1.24927300	1.44551900
C	-3.73032300	-2.66236700	0.33141700
O	-3.88566300	-3.62378900	-0.41441200
O	-4.78583500	-2.08029200	0.95445400
C	-6.05214600	-2.66595300	0.67628900
H	-6.78833400	-2.04187300	1.18150400
H	-6.24533900	-2.67685800	-0.39821200
H	-6.09763600	-3.68938900	1.05782200
C	-1.22271400	-3.68956200	-0.64334200
O	-1.51977700	-3.27824300	-1.88251100
O	-0.96156100	-4.83268600	-0.35508200
C	-1.67260400	-4.32720600	-2.84156900
H	-2.48713000	-4.98481300	-2.53174500
H	-1.91024400	-3.83899900	-3.78428100
H	-0.74850100	-4.90192600	-2.92938800

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C	-1.99237400	0.91922600	-0.27330400
C	-3.29581500	0.41735900	-1.94318700
C	-3.07879200	-1.38379200	-0.25688100
H	-2.23431800	-1.66591900	0.37488800
N	-2.88004200	1.62546500	-2.20035700
N	-2.07345400	1.92613400	-1.14151800
N	-2.77867400	-0.04420700	-0.76742600
C	-4.07700500	-0.55855200	-2.75944100
H	-4.14496600	-0.22469400	-3.79399200
H	-5.08785500	-0.68964300	-2.35154100
C	-3.25156800	-2.38799000	-1.45484200
O	-3.32772100	-1.75991700	-2.72807900
C	-5.21381100	-2.43840600	-0.02566200
C	-4.40606200	-1.41608300	0.46574500
C	-4.83501100	-0.57538600	1.48912800
C	-6.10715400	-0.77674100	2.01889800
C	-6.92298200	-1.80260000	1.53394800
C	-6.48296300	-2.64102900	0.51179800
C	-4.52180800	-3.20512200	-1.12367300
H	-4.18016400	0.20651100	1.86131900
H	-7.91212500	-1.94562500	1.95717300
H	-7.12214500	-3.43382500	0.13515800
H	-5.13556000	-3.32300000	-2.02209000
H	-4.24655800	-4.20926700	-0.78543000
C	-1.45982200	3.22128500	-1.03442800
C	-1.95611200	4.11281200	-0.07887700

C	-0.39328700	3.51264600	-1.88599500
C	-1.33723500	5.35732200	0.00313000
C	0.19370100	4.77121300	-1.75817700
C	-0.26386500	5.70112000	-0.82311400
H	-1.70324400	6.07719500	0.73068800
H	1.03097900	5.02711800	-2.40205000
C	0.10278300	2.50734400	-2.89181500
H	-0.52445700	2.50913900	-3.78844700
H	0.08142200	1.48939300	-2.48722700
H	1.12693200	2.74165800	-3.18820700
C	-3.09556400	3.73797800	0.83211200
H	-2.75489700	3.07080000	1.63227300
H	-3.89425000	3.22484500	0.28855100
H	-3.51554600	4.62934900	1.29982700
H	-2.36455700	-3.01540900	-1.52285500
C	0.40075100	7.04545200	-0.68295600
H	-0.33952500	7.83316200	-0.52418100
H	1.07513500	7.04999900	0.17909700
H	0.98768100	7.29227000	-1.56955800
C	4.30494800	2.45966600	1.38932400
C	3.01206500	1.97992700	1.20261500
C	2.22877900	1.60528200	2.30282100
C	2.77791700	1.70733300	3.58974900
C	4.06708100	2.18882300	3.77618500
C	4.83466700	2.56705300	2.67339900
H	4.90302300	2.74167200	0.52877300
H	2.62031400	1.88029000	0.19501300
H	2.18012600	1.39973200	4.44414600
H	4.47625700	2.26905100	4.77798100
H	5.84347400	2.94098600	2.81596500
C	0.86683900	1.08282000	2.14808800
H	0.35161800	0.78868000	3.06018300
C	0.07909300	1.34139900	1.03511300
C	-1.22223800	0.80212300	1.01547100
O	-1.79282300	0.16933900	1.91784000
H	0.47715300	1.81017400	0.14297900
H	-6.46733500	-0.13345000	2.81494400
C	4.52800500	-1.61197500	-1.46522700
C	3.35745800	-0.97165900	-0.97866400
C	2.56814900	-0.21180900	-1.85777800
C	2.87586100	-0.10051500	-3.20883200
C	4.00075400	-0.74812000	-3.70067300
C	4.80493000	-1.48390500	-2.82920000
H	1.70534000	0.30162900	-1.44256100

H	2.24299100	0.49191300	-3.86327200
H	4.26550000	-0.67920800	-4.75081000
H	5.68072700	-1.97080100	-3.24141200
C	5.45371500	-2.41633700	-0.53967400
C	6.04992300	-1.48509900	0.53248200
C	4.68060800	-3.56477900	0.13321300
C	6.62393500	-3.04555900	-1.30742900
H	6.64601900	-0.69642100	0.06074200
H	5.26368800	-1.02137600	1.12957100
H	6.70868000	-2.05786800	1.19498200
H	4.23675100	-4.22326200	-0.62099800
H	5.36812800	-4.16063100	0.74386500
H	3.88200900	-3.19185700	0.77452700
H	7.25264100	-3.59965500	-0.60388400
H	6.27770200	-3.74897100	-2.07177100
H	7.25139300	-2.28957600	-1.78982200
N	3.02767500	-1.00078800	0.38436500
C	1.83635700	-1.34020500	0.77742000
C	1.44695200	-1.18853300	2.13660100
H	2.24247600	-0.92640300	2.82212400
C	0.29124500	-1.77736600	2.77203200
O	0.00760500	-1.62743500	3.95328800
O	-0.47846200	-2.54855500	1.95250400
C	-1.70702300	-2.99018100	2.52194500
H	-2.16013300	-3.65526500	1.78452400
H	-1.53138600	-3.52818300	3.45518800
H	-2.35924800	-2.13159100	2.71081400
C	0.83628000	-1.90707500	-0.22440500
O	1.21760000	-3.13589300	-0.56977900
O	-0.13164000	-1.34372200	-0.68789500
C	0.38372500	-3.81649100	-1.50985100
H	0.15535200	-3.16955700	-2.35856100
H	0.94510100	-4.69147000	-1.83051800
H	-0.54153300	-4.12667500	-1.01736700

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C	-2.77082900	0.44771100	0.02429800
C	-4.19979600	-0.12107300	-1.51999200
C	-3.88214700	-1.84156700	0.23040900
H	-3.02544100	-2.09293200	0.85426900
N	-3.79262100	1.06688100	-1.86843500
N	-2.90436400	1.41060800	-0.88871100
N	-3.60383400	-0.52845900	-0.35958500

C	-5.00021100	-1.14692400	-2.25351700
H	-5.12263800	-0.85952400	-3.29703000
H	-5.98726200	-1.28593900	-1.79435200
C	-4.08599800	-2.90338800	-0.91041300
O	-4.21545100	-2.32683900	-2.20555300
C	-6.01198600	-2.87224200	0.56772400
C	-5.18974200	-1.82949200	0.98534500
C	-5.58402300	-0.93798700	1.97767600
C	-6.84279600	-1.10495000	2.55054200
C	-7.67646000	-2.14787300	2.13619900
C	-7.26774400	-3.03944900	1.14646600
C	-5.34378400	-3.70351500	-0.49881700
H	-4.91441200	-0.14280900	2.29411500
H	-8.65513100	-2.26371200	2.59090500
H	-7.91960800	-3.84733300	0.82822900
H	-5.97829300	-3.88144400	-1.37241700
H	-5.05499000	-4.68263600	-0.10397500
C	-2.29701000	2.71486700	-0.86454100
C	-2.76032600	3.63238400	0.07888300
C	-1.24986000	2.97691500	-1.75462300
C	-2.12972400	4.87682300	0.11469700
C	-0.65491800	4.23243700	-1.67421100
C	-1.07985300	5.19080200	-0.74748700
H	-2.47018200	5.61506900	0.83571800
H	0.16618100	4.46756300	-2.34690000
C	-0.74827800	1.92087700	-2.70277400
H	-1.56907700	1.44804200	-3.24867200
H	-0.20467700	1.14321300	-2.15046000
H	-0.05588600	2.35852200	-3.42404300
C	-3.87373100	3.28869800	1.03409100
H	-3.52042200	2.61670700	1.82467600
H	-4.70441100	2.79278400	0.52337700
H	-4.25450400	4.19207100	1.51216900
H	-3.19546200	-3.52839000	-0.98054600
C	-0.40381400	6.53550700	-0.69212700
H	-0.83788600	7.16674800	0.08501100
H	0.66442700	6.42135600	-0.48640100
H	-0.49736300	7.05499100	-1.65004800
C	3.03406000	3.16433300	2.01439200
C	1.90560700	2.43981600	1.64745900
C	1.70638100	1.13764000	2.12975200
C	2.67664100	0.57606900	2.97153500
C	3.80727600	1.29917100	3.33604700
C	3.98625600	2.59764800	2.86247700

H	3.16742500	4.17603900	1.64454100
H	1.15843300	2.89376300	1.00371000
H	2.53439000	-0.43678900	3.33842300
H	4.54795000	0.85081700	3.99029400
H	4.86495500	3.16616300	3.15033300
C	0.46032000	0.40589300	1.86178500
H	0.16924600	-0.31332900	2.62498500
C	-0.56843100	0.87727300	1.05706800
C	-1.86566800	0.34385100	1.22653100
O	-2.34260300	-0.25678800	2.20150200
H	-0.34236600	1.50112600	0.20044500
H	-7.17916200	-0.42294000	3.32450000
C	6.02937000	-1.52311300	-0.01832000
C	4.89716200	-0.71296500	0.26080100
C	5.00277600	0.68379600	0.18720700
C	6.19233200	1.30446300	-0.17726000
C	7.30185200	0.52428900	-0.47269200
C	7.20529300	-0.86531400	-0.39070500
H	4.13278100	1.27733800	0.44930200
H	6.24535800	2.38856000	-0.21744900
H	8.24268600	0.98327900	-0.75953700
H	8.08768700	-1.44689100	-0.62927400
C	5.97345900	-3.05708900	0.06002700
C	5.65707600	-3.50028200	1.49984700
C	4.90743400	-3.60664300	-0.90573500
C	7.31169300	-3.69861300	-0.33182200
H	6.44206000	-3.15931200	2.18323500
H	4.70110600	-3.09677100	1.83403200
H	5.61695900	-4.59425100	1.54888200
H	5.12017200	-3.28816100	-1.93182300
H	4.91953800	-4.70201800	-0.88004600
H	3.90568600	-3.26683600	-0.64073900
H	7.21924500	-4.78635500	-0.25651700
H	7.59397200	-3.45789100	-1.36187800
H	8.12405800	-3.38741300	0.33242900
N	3.69009300	-1.29066300	0.69196500
C	2.56514400	-0.99306000	0.12325900
C	1.31963500	-1.44928000	0.65756600
H	1.38400900	-2.07687500	1.53943900
C	0.15656300	-1.68584200	-0.15504600
O	-0.88609200	-2.20783700	0.22568900
O	0.26311100	-1.22970700	-1.43217800
C	-0.81961500	-1.54333100	-2.30166500
H	-0.50314700	-1.23166200	-3.29656400

H	-1.03350300	-2.61412000	-2.28525000
H	-1.72736800	-1.00281600	-2.02076600
C	2.51398600	-0.06699100	-1.08662300
O	3.12421800	-0.60879800	-2.14118000
O	2.01314300	1.03396300	-1.08591200
C	3.16684100	0.22253800	-3.30429600
H	3.71799400	1.14046700	-3.08805900
H	3.67594400	-0.35876400	-4.06990700
H	2.15294300	0.47588300	-3.62243500

TS4(SR)'''

C	-2.83791500	0.11970800	-0.24968000
C	-4.33618200	1.07971300	1.00676800
C	-2.41049100	2.53219000	0.46452300
H	-1.36171200	2.29119600	0.29209200
N	-4.78888000	-0.12674100	0.81804300
N	-3.84469000	-0.70950500	0.02177700
N	-3.14719100	1.26983000	0.36429700
C	-4.79244500	2.17252800	1.91617000
H	-5.53949200	1.79874900	2.61517900
H	-5.21281900	3.01230100	1.34745300
C	-2.61637800	3.16814100	1.88852200
O	-3.64269800	2.54859500	2.65350600
C	-3.23705900	4.75533200	0.15848200
C	-2.95342200	3.56144300	-0.49919500
C	-3.16929000	3.41054100	-1.86535900
C	-3.68611600	4.49193600	-2.57453800
C	-3.97209500	5.69507100	-1.92281300
C	-3.74807700	5.83666100	-0.55486500
C	-2.90822400	4.66404700	1.62677600
H	-2.92902400	2.47118000	-2.35484800
H	-4.37618300	6.52823100	-2.48911800
H	-3.97460300	6.77209100	-0.05227600
H	-3.72281300	5.00343100	2.27403700
H	-2.02917800	5.26943400	1.86886300
C	-3.97934700	-2.08707400	-0.36529700
C	-4.41524000	-2.38617200	-1.65529500
C	-3.65580700	-3.05343700	0.59099300
C	-4.53374800	-3.73659600	-1.98248100
C	-3.78629800	-4.38672900	0.21216400
C	-4.22331600	-4.74368500	-1.06677400
H	-4.87698400	-4.00683600	-2.97767500
H	-3.53948300	-5.16475500	0.92997900

C	-3.16462300	-2.64721800	1.95590800
H	-3.97427400	-2.21220700	2.54995600
H	-2.37571300	-1.88724900	1.88104600
H	-2.76785000	-3.51076500	2.49252000
C	-4.72820500	-1.29639600	-2.64578300
H	-3.81210300	-0.80094400	-2.98596900
H	-5.37400100	-0.53122900	-2.20529500
H	-5.22905300	-1.70988300	-3.52196700
H	-1.71394700	3.01978400	2.48139800
C	-4.32945300	-6.19405100	-1.45910700
H	-5.08424400	-6.33871500	-2.23472600
H	-3.37391300	-6.55388600	-1.85373300
H	-4.58767500	-6.81643800	-0.59969100
C	1.61042400	-4.60126100	0.58443700
C	0.87617000	-3.45483700	0.31399800
C	1.23219500	-2.61691600	-0.75173600
C	2.35538600	-2.94048100	-1.52078700
C	3.08910000	-4.09268800	-1.25164200
C	2.71653200	-4.92661700	-0.20100600
H	1.32530000	-5.24126700	1.41338200
H	0.02974700	-3.19542700	0.94488700
H	2.64475200	-2.28630800	-2.33950100
H	3.95279400	-4.33775300	-1.86238000
H	3.28818400	-5.82454000	0.01114100
C	0.45187700	-1.41201100	-1.06974000
H	0.87662000	-0.75015600	-1.81988200
C	-0.91038100	-1.33150200	-0.81499000
C	-1.55704600	-0.09346000	-1.01478100
O	-1.12453800	0.89961200	-1.62035700
H	-1.40628300	-2.09886400	-0.23525600
H	-3.86738500	4.40123700	-3.64048200
C	5.62723600	1.49861800	-0.95013700
C	4.80007100	0.34684800	-0.86369800
C	5.36659700	-0.93079000	-0.98295900
C	6.73400500	-1.10254200	-1.16974900
C	7.55649300	0.01311800	-1.24049600
C	6.99749200	1.28610500	-1.12962100
H	4.70591300	-1.79022500	-0.93506500
H	7.14570200	-2.10286200	-1.26360300
H	8.62663900	-0.09551200	-1.38550900
H	7.66517200	2.13733000	-1.18672400
C	5.05920300	2.92414900	-0.84371100
C	4.09212400	3.19486900	-2.01043200
C	4.32830400	3.12203200	0.49764600

C	6.16640700	3.98521400	-0.91259700
H	4.61848200	3.11539600	-2.96748100
H	3.26276500	2.48715000	-2.00489400
H	3.69057100	4.21106900	-1.92766300
H	4.99573300	2.89750200	1.33619000
H	4.00823500	4.16627900	0.58682800
H	3.44671500	2.48578400	0.58101900
H	5.71184000	4.97701200	-0.83131500
H	6.88602600	3.87931000	-0.09424000
H	6.71172900	3.94709600	-1.86078000
N	3.40228600	0.48634900	-0.74988700
C	2.74981200	-0.02719800	0.24314700
C	1.33461600	0.17178000	0.34533600
H	0.92574000	0.92856500	-0.31653000
C	0.52471400	-0.10016700	1.49153100
O	-0.65104800	0.25784800	1.60807300
O	1.11570800	-0.87153100	2.43960500
C	0.32413100	-1.17148700	3.58358700
H	0.99138400	-1.66783500	4.28702700
H	-0.08355700	-0.25923400	4.02391300
H	-0.50188800	-1.83854800	3.32257800
C	3.48131800	-0.80520700	1.32774500
O	3.99042500	0.04300100	2.22825000
O	3.63719900	-2.00005000	1.35704500
C	4.72968000	-0.57350500	3.28629700
H	5.58155700	-1.12331700	2.88090000
H	5.06756400	0.23779900	3.92745600
H	4.08755200	-1.26058700	3.84160100

M4(SR)

C	0.63724600	1.68139000	0.06934900
C	2.29165400	2.88097100	0.85065000
C	2.99882500	0.72588800	-0.13605800
H	2.51275800	-0.24902300	-0.18872000
N	1.23601000	3.61185100	1.05549800
N	0.21284000	2.85607400	0.54981700
N	1.96961100	1.69798000	0.24610300
C	3.71154300	3.05507300	1.27775500
H	3.78855500	3.81933700	2.05020500
H	4.34542400	3.33559300	0.42617000
C	4.17352500	0.73814100	0.91238200
O	4.09876600	1.81367900	1.84031000
C	5.04160900	1.13036600	-1.31903500

C	3.65505000	1.10419800	-1.44535400
C	3.02495100	1.39610400	-2.65196400
C	3.82153200	1.73022800	-3.74496100
C	5.21416000	1.76169200	-3.62707100
C	5.83402500	1.45854100	-2.41668500
C	5.47240900	0.76095800	0.07661900
H	1.94183100	1.33588400	-2.71687400
H	5.81913600	2.02595300	-4.48867800
H	6.91601100	1.48460400	-2.32846900
H	6.18964700	1.46392300	0.51145800
H	5.93799300	-0.23077900	0.09035000
C	-1.12428200	3.38545700	0.51874700
C	-1.67275200	3.72673800	-0.72131400
C	-1.81134800	3.51718900	1.72567400
C	-2.97653900	4.21464300	-0.72435800
C	-3.11349600	4.01817000	1.66780500
C	-3.70985700	4.36726800	0.45581000
H	-3.43294700	4.48383300	-1.67384800
H	-3.67463200	4.12575900	2.59258600
C	-1.17738900	3.11262900	3.03017500
H	-0.37166800	3.79900700	3.30581400
H	-0.73909000	2.11077900	2.96264500
H	-1.91883500	3.11034500	3.83022100
C	-0.89376700	3.55616400	-1.99851900
H	-0.79693400	2.49708200	-2.26212300
H	0.11698900	3.96577300	-1.90480600
H	-1.39693700	4.06741700	-2.82040600
H	4.11572300	-0.15586700	1.53260100
C	-5.11404700	4.91113800	0.40844000
H	-5.10571000	5.98601400	0.20231200
H	-5.69039900	4.43006000	-0.38653000
H	-5.63217400	4.75395000	1.35682000
C	-5.59911600	1.11893400	-0.07733100
C	-4.25431700	0.77543500	0.05428500
C	-3.72309800	-0.30670800	-0.65046000
C	-4.56728500	-1.02190400	-1.50883500
C	-5.91112600	-0.68421000	-1.63959200
C	-6.43435800	0.38823600	-0.91808900
H	-5.99100400	1.96402500	0.48217400
H	-3.61839200	1.37595000	0.69739400
H	-4.16104000	-1.85805400	-2.07476400
H	-6.54745600	-1.25397400	-2.30997300
H	-7.48115200	0.65646800	-1.01912200
C	-2.26813700	-0.73248300	-0.52018500

H	-1.91592200	-1.03578600	-1.51143000
C	-1.35909500	0.33503800	-0.01485300
C	-0.14952200	0.58352500	-0.59720800
O	0.41873000	0.04672200	-1.60332600
H	-1.62516900	0.85471400	0.89863500
H	3.35827500	1.96429800	-4.69815700
C	2.55607800	-2.53580300	1.42316200
C	1.57952100	-2.48044700	0.39841300
C	1.95818600	-2.52044100	-0.95214700
C	3.29006600	-2.66997300	-1.31575200
C	4.25611900	-2.78876400	-0.32256100
C	3.88317300	-2.72532400	1.01991800
H	1.20377200	-2.32704300	-1.70658000
H	3.56895500	-2.67551600	-2.36443600
H	5.30248800	-2.91378000	-0.58330600
H	4.66393200	-2.80031200	1.76774200
C	2.19331400	-2.34165400	2.90418600
C	1.63520900	-0.91804000	3.12093500
C	1.15851700	-3.38886400	3.35389600
C	3.42021600	-2.49572200	3.81335600
H	2.40105000	-0.16014100	2.91691100
H	0.77255500	-0.72514300	2.48083500
H	1.33104300	-0.80360900	4.16742300
H	1.53819000	-4.40112600	3.18044100
H	0.96718600	-3.27707000	4.42651000
H	0.21146700	-3.27655000	2.82437300
H	3.10971200	-2.35589000	4.85289500
H	3.86890700	-3.49052000	3.72721400
H	4.19004200	-1.74742300	3.59708900
N	0.24426300	-2.19930600	0.74839900
C	-0.76344300	-2.62916300	0.10504800
C	-2.10544700	-2.01741600	0.41642300
H	-2.08572300	-1.65637100	1.44736400
C	-3.25111000	-2.99422300	0.28575100
O	-3.30534300	-3.92470000	-0.49034100
O	-4.23592600	-2.69129500	1.13365100
C	-5.43108900	-3.46460300	0.98435100
H	-6.12261400	-3.08973800	1.73562400
H	-5.84064500	-3.32051600	-0.01826500
H	-5.22188700	-4.52315900	1.14609800
C	-0.69410000	-3.69361100	-0.97965300
O	-1.12921500	-3.23886900	-2.15433300
O	-0.28850000	-4.81263400	-0.78190100
C	-1.22593600	-4.22741900	-3.18733700

H	-1.93785900	-4.99817100	-2.88564000
H	-1.57876300	-3.70026800	-4.07065800
H	-0.24948600	-4.67839500	-3.37118800

TS4(SS)

C	-0.79146500	1.63872300	0.02941100
C	-2.56180100	2.23112300	-1.09418200
C	-2.99967500	0.48414200	0.59649000
H	-2.37616300	-0.33038300	0.97808600
N	-1.60078900	2.96308400	-1.58229000
N	-0.50180700	2.58391300	-0.86743500
N	-2.10433600	1.40887400	-0.10519800
C	-3.98897100	2.07508800	-1.50117500
H	-4.15483300	2.51929000	-2.48204300
H	-4.65337400	2.55355300	-0.76906700
C	-4.10521900	-0.05212400	-0.38837500
O	-4.21369100	0.68334100	-1.60181400
C	-5.13624200	0.92064500	1.57885900
C	-3.77516700	1.19712700	1.68370900
C	-3.27536800	2.03379700	2.67683600
C	-4.17586800	2.60052900	3.57608200
C	-5.54267900	2.32589800	3.48001800
C	-6.03238000	1.48374200	2.48393600
C	-5.41636200	-0.01049200	0.42759400
H	-2.20853900	2.22359700	2.74519600
H	-6.23134000	2.77618500	4.18781600
H	-7.09558300	1.27665500	2.40897200
H	-6.24225500	0.31978200	-0.20913500
H	-5.66813300	-1.01288400	0.79125000
C	0.75060200	3.27232600	-1.05517800
C	1.11308900	4.23314400	-0.10896800
C	1.53510200	2.94477800	-2.16432600
C	2.32899700	4.88707400	-0.30265800
C	2.73918600	3.63012600	-2.31072200
C	3.15287700	4.59628400	-1.39115700
H	2.63784000	5.64270200	0.41480300
H	3.37151800	3.39815400	-3.16403200
C	1.14078500	1.85735100	-3.12881500
H	1.43739400	0.87292100	-2.74277900
H	1.64579500	1.99984100	-4.08563500
H	0.06292900	1.84268800	-3.30776700
C	0.23992700	4.53051400	1.08184000
H	-0.80890500	4.64967000	0.79376800

H	0.56738400	5.44751500	1.57305700
H	0.29320900	3.71997300	1.81797800
H	-3.84965100	-1.06047400	-0.71405300
C	4.47755300	5.29219800	-1.56206200
H	4.51076800	6.22487500	-0.99565600
H	5.29160000	4.65340200	-1.20475500
H	4.67226200	5.51473100	-2.61366900
C	5.72712600	0.09584700	-0.10424100
C	4.34516800	0.12494700	0.03930900
C	3.76703100	0.07310100	1.31621900
C	4.60348100	-0.03147800	2.43580000
C	5.98656200	-0.05198100	2.29054200
C	6.55199200	0.01255300	1.01839100
H	6.16556200	0.13447100	-1.09638400
H	3.70594200	0.15364600	-0.83744800
H	4.15903500	-0.09352500	3.42520400
H	6.62148900	-0.12228100	3.16806500
H	7.63075300	-0.00616700	0.90034900
C	2.31645600	0.15309200	1.52747200
H	1.98448600	0.07490100	2.55957000
C	1.44222200	0.76751200	0.65118900
C	0.10700900	0.99101900	1.05768800
O	-0.41810000	0.75326100	2.15505100
H	1.73333400	0.98312000	-0.36951200
H	-3.81352000	3.26001600	4.35777300
C	-2.13004900	-2.94714000	-1.12694300
C	-1.13148400	-1.95225600	-0.95393800
C	-0.95785000	-0.96438000	-1.93447900
C	-1.73340400	-0.93244400	-3.08773600
C	-2.69535700	-1.91454400	-3.28122000
C	-2.87345800	-2.90164100	-2.31252200
H	-0.18544800	-0.22030300	-1.76467400
H	-1.58412300	-0.14725100	-3.82312700
H	-3.31254000	-1.91664700	-4.17354000
H	-3.63396300	-3.65207300	-2.49132600
C	-2.41268100	-4.02184800	-0.06332500
C	-1.17239300	-4.90150500	0.17755900
C	-2.84226100	-3.35344600	1.25585200
C	-3.55228400	-4.95668000	-0.49254200
H	-0.82993000	-5.34975200	-0.76052400
H	-0.34537600	-4.33637100	0.60770400
H	-1.42994600	-5.71107600	0.86950200
H	-3.74788400	-2.75305700	1.10425400
H	-3.07498600	-4.12245200	2.00080100

H	-2.05297700	-2.71163700	1.65008800
H	-3.72446400	-5.69174600	0.29902900
H	-4.48925600	-4.41339200	-0.65202900
H	-3.30793500	-5.50469600	-1.40814500
N	-0.37441400	-1.89036700	0.23465300
C	0.90160500	-2.13778500	0.21903500
C	1.68586500	-2.14643200	1.39755600
H	1.15566700	-2.09740000	2.34074600
C	2.99965000	-2.73459800	1.38034800
O	3.64767400	-3.04974000	0.38854400
O	3.50402000	-2.88533200	2.63152200
C	4.82764700	-3.40898700	2.68566400
H	5.11769800	-3.38465500	3.73558300
H	4.85227600	-4.43605700	2.31262200
H	5.50767500	-2.79493200	2.09096700
C	1.60282900	-2.32197000	-1.11595200
O	1.44674400	-3.55535700	-1.58995200
O	2.14084800	-1.42210500	-1.72253400
C	2.02749000	-3.78772500	-2.87725300
H	3.10641400	-3.62669200	-2.83241600
H	1.80386600	-4.82343100	-3.12311600
H	1.58868100	-3.11275100	-3.61477700

TS4(SS)'

C	-1.78903700	-0.43881500	0.68477500
C	-3.59460500	0.63945600	1.26817200
C	-3.61834200	-0.07854500	-1.09230600
H	-2.83297000	-0.17403200	-1.84002400
N	-2.89276700	0.55071900	2.36178800
N	-1.77825400	-0.13124500	1.98619000
N	-2.95762500	0.04188900	0.21961200
C	-4.86846900	1.36432800	0.98357500
H	-5.05784500	2.10942400	1.75543700
H	-5.71461500	0.66556200	0.93989800
C	-4.53451900	1.17371200	-1.36467200
O	-4.66635400	2.03586000	-0.24462900
C	-5.84400600	-0.86689300	-1.49594500
C	-4.56930700	-1.25619500	-1.09327300
C	-4.28884900	-2.57251200	-0.73665800
C	-5.32074600	-3.50561900	-0.78908900
C	-6.60244000	-3.12315800	-1.19502200
C	-6.87258000	-1.80448600	-1.55256400
C	-5.89323900	0.60073400	-1.83059300

H	-3.28575000	-2.85920500	-0.43579000
H	-7.39660600	-3.86211600	-1.23005600
H	-7.87041700	-1.50991200	-1.86299200
H	-6.71256100	1.12917500	-1.33330000
H	-6.01873400	0.75343300	-2.90679700
C	-0.74847500	-0.42166300	2.94815700
C	-0.53668100	-1.75138900	3.32376100
C	0.02307900	0.64840500	3.40609200
C	0.55142900	-2.00326500	4.15555100
C	1.10729400	0.33699100	4.22751800
C	1.39464700	-0.97862000	4.59557300
H	0.75223600	-3.02761500	4.45968900
H	1.74195000	1.14516600	4.58179400
C	-0.30374800	2.06709500	3.03052100
H	-0.35369800	2.18944600	1.94286000
H	0.46271300	2.74615700	3.40335100
H	-1.27226400	2.36093300	3.44478600
C	-1.41009700	-2.87080800	2.82275700
H	-2.45554900	-2.56263300	2.73597900
H	-1.35793400	-3.72219000	3.50308100
H	-1.07299400	-3.20932900	1.83671900
H	-4.07616300	1.79683800	-2.13178400
C	2.59330000	-1.30366500	5.44761400
H	2.30205900	-1.88505500	6.32657100
H	3.31038500	-1.90636500	4.88141300
H	3.09956000	-0.39732400	5.78421400
C	4.62189900	-2.26154800	1.54582400
C	3.32374700	-1.93231200	1.17360100
C	2.79199200	-2.39370200	-0.03979000
C	3.59191900	-3.20465500	-0.85735500
C	4.89180100	-3.52921800	-0.48790400
C	5.41251100	-3.05531300	0.71529100
H	5.01879600	-1.89888300	2.48884000
H	2.71834300	-1.32893000	1.84518900
H	3.17716200	-3.58177100	-1.78861600
H	5.49719300	-4.15608900	-1.13485800
H	6.42591200	-3.31027700	1.00828200
C	1.41522400	-2.09570800	-0.45854000
H	0.99950400	-2.74277000	-1.22628700
C	0.52788600	-1.36509900	0.31043900
C	-0.80086500	-1.22493300	-0.15157600
O	-1.26939400	-1.69081000	-1.20259200
H	0.85780300	-0.78275300	1.15907500
H	-5.12827000	-4.53760700	-0.51500800

C	0.81495500	3.51811900	-0.16131600
C	1.44962400	2.24829600	-0.09316600
C	2.38965500	2.00147400	0.92336700
C	2.76938400	2.99150800	1.82232500
C	2.19275300	4.25136000	1.72972100
C	1.22361800	4.49119900	0.75530700
H	2.81527400	1.00512600	0.99558300
H	3.50169900	2.77107900	2.59361400
H	2.47396800	5.04242700	2.41763500
H	0.77567500	5.47710300	0.71867300
C	-0.28761900	3.81530900	-1.18802900
C	0.24955400	3.65639000	-2.62150200
C	-1.47489800	2.85942500	-0.96054700
C	-0.82335500	5.24731500	-1.05650100
H	1.08771400	4.34051100	-2.79179600
H	0.59071200	2.63854700	-2.81191500
H	-0.54018300	3.90130900	-3.34065100
H	-1.87833100	2.98028000	0.05272100
H	-2.27849200	3.09724000	-1.66690600
H	-1.16537700	1.82084100	-1.10323900
H	-1.60780800	5.40280400	-1.80305000
H	-1.26022400	5.43012700	-0.06956800
H	-0.04172500	5.99288800	-1.23364500
N	1.07413700	1.21315900	-0.96589600
C	1.98216000	0.52308700	-1.60004300
C	1.63417600	-0.64511200	-2.31381500
H	0.57880600	-0.85422200	-2.44808500
C	2.56239300	-1.32049500	-3.18219100
O	3.72400200	-1.01740600	-3.42240800
O	2.00060200	-2.43533700	-3.73338800
C	2.84813000	-3.16293600	-4.61699700
H	2.27334600	-4.02969600	-4.93969400
H	3.12715100	-2.55241500	-5.47906900
H	3.76002700	-3.48228500	-4.10542700
C	3.45210300	0.92074200	-1.55690800
O	3.66081500	1.97037400	-2.36129400
O	4.31023100	0.41818400	-0.87358700
C	5.00568900	2.45564900	-2.37736700
H	5.68342800	1.67177300	-2.72147900
H	5.01273300	3.29824900	-3.06562100
H	5.30244000	2.77487900	-1.37606300

TS4(SS)"

C	-0.78680400	1.80863500	-0.13351200
C	-0.39451900	3.69268800	0.89432400
C	1.65477400	2.57705100	0.10401000
H	1.92932300	1.53404000	-0.03349700
N	-1.69212000	3.59699600	0.86734700
N	-1.92245800	2.42058900	0.21742600
N	0.19630000	2.62309400	0.28379400
C	0.50603500	4.66774300	1.57979500
H	-0.04672900	5.22395700	2.33624900
H	0.94434900	5.37274800	0.86126800
C	2.37067000	3.18953700	1.35837000
O	1.49029400	3.88779400	2.23309900
C	3.10324300	4.31584700	-0.66346800
C	2.08078800	3.45338200	-1.05005500
C	1.58051600	3.44728400	-2.34792000
C	2.12243300	4.34199100	-3.26826600
C	3.14809000	5.21227300	-2.88872400
C	3.64821800	5.20355500	-1.58793900
C	3.47258000	4.11024500	0.78452700
H	0.79337900	2.75272600	-2.62908600
H	3.55902500	5.90473600	-3.61641600
H	4.44493200	5.88234700	-1.29877700
H	3.51836900	5.04187100	1.35671600
H	4.45137200	3.62816700	0.87167200
C	-3.26966500	1.99786100	-0.05447500
C	-3.70411500	1.97299400	-1.38077200
C	-4.06070700	1.59191700	1.02704300
C	-4.98835500	1.48118300	-1.61899500
C	-5.33386000	1.11083200	0.73132900
C	-5.80783000	1.03519700	-0.58281100
H	-5.35294200	1.44691100	-2.64219900
H	-5.97096200	0.78179700	1.54891700
C	-3.54067400	1.64065800	2.43888900
H	-2.64360800	1.01805800	2.53418800
H	-4.29671100	1.26418400	3.13058900
H	-3.28328700	2.66292300	2.72736200
C	-2.82646800	2.42469800	-2.51843100
H	-2.22618800	3.29699500	-2.24561400
H	-3.43666300	2.68571700	-3.38424200
H	-2.14152900	1.62541200	-2.82325000
H	2.77372300	2.38044600	1.96798800
C	-7.17244800	0.46458700	-0.86557900
H	-7.50581300	0.71541600	-1.87422500
H	-7.15353600	-0.62660900	-0.77838100

H	-7.91018200	0.83758300	-0.15105000
C	-4.54691900	-3.61184200	-1.12517500
C	-3.59691800	-2.61860400	-0.90971200
C	-2.23506400	-2.88067400	-1.10871300
C	-1.85496200	-4.15735600	-1.54312400
C	-2.80336900	-5.14915000	-1.76397100
C	-4.15496400	-4.87975200	-1.55107100
H	-5.59811600	-3.39327600	-0.96529400
H	-3.92435600	-1.62937400	-0.60023300
H	-0.79908400	-4.36687900	-1.70014100
H	-2.48925700	-6.13127100	-2.10217600
H	-4.89860300	-5.65180400	-1.71990600
C	-1.19677300	-1.84722500	-0.90552300
H	-0.23872700	-2.04804600	-1.38212000
C	-1.51538900	-0.50995700	-0.67210500
C	-0.53581600	0.48772900	-0.83127700
O	0.54223600	0.41803900	-1.44207700
H	-2.43651900	-0.25671500	-0.16575300
H	1.74865300	4.36241100	-4.28664200
C	4.15649000	-2.87808600	-0.51939500
C	3.28757900	-2.86370800	0.60511600
C	3.82977400	-2.78671400	1.89820400
C	5.19939500	-2.67798700	2.10982700
C	6.05519000	-2.65852300	1.01758000
C	5.52629200	-2.76141100	-0.26896100
H	3.15435200	-2.84235600	2.74609800
H	5.58760400	-2.62160200	3.12204400
H	7.12849600	-2.57660700	1.15562600
H	6.21805900	-2.75427800	-1.10272100
C	3.62536100	-2.98196800	-1.95652400
C	2.83786900	-4.29208500	-2.14633900
C	2.72554300	-1.77244200	-2.25370200
C	4.75688200	-2.98061400	-2.99239900
H	3.48675300	-5.15552200	-1.96377800
H	1.98665200	-4.34501700	-1.46733300
H	2.47481200	-4.35380900	-3.17836600
H	3.30537000	-0.84351700	-2.21519200
H	2.29539200	-1.86077400	-3.25833800
H	1.90870700	-1.67858600	-1.53862600
H	4.31933800	-3.05793700	-3.99234400
H	5.34357100	-2.05730200	-2.95725500
H	5.43557100	-3.82925100	-2.85849400
N	1.90232700	-3.05004600	0.44698600
C	1.03424500	-2.33158500	1.07948300

C	-0.36715300	-2.65892400	1.03447900
H	-0.60126000	-3.69254300	0.81325100
C	-1.31767800	-1.91196100	1.81155700
O	-1.19745100	-0.73980900	2.15922500
O	-2.46526700	-2.60360200	2.01664400
C	-3.54161000	-1.85921700	2.57617200
H	-4.35308600	-2.57062600	2.72361100
H	-3.25274300	-1.40748900	3.52820400
H	-3.86238800	-1.06707400	1.89160600
C	1.44141100	-1.09077100	1.86738500
O	1.31862400	-1.27196200	3.18176900
O	1.85826600	-0.07261500	1.36568000
C	1.55806100	-0.10235600	3.97086400
H	0.89819400	0.70326200	3.64055100
H	1.33914200	-0.38456200	4.99824200
H	2.59890800	0.21407900	3.87356700

TS4(SS)'''

C	-2.94271400	0.38178600	-0.22926400
C	-4.80240400	0.33765900	-1.37557000
C	-4.29730700	-1.81969200	-0.29717100
H	-3.36909700	-2.34189700	-0.08152400
N	-4.38959500	1.56997100	-1.45820700
N	-3.23910900	1.58449300	-0.73468500
N	-3.94633600	-0.42461200	-0.63285600
C	-5.94988100	-0.34721300	-2.04124200
H	-6.28899500	0.23567100	-2.89683300
H	-6.78551600	-0.48121900	-1.34138000
C	-5.09135500	-2.48952700	-1.48053600
O	-5.44171600	-1.57985800	-2.51191000
C	-6.39003500	-2.58831500	0.57230300
C	-5.24919100	-1.85121900	0.87569200
C	-5.07297700	-1.25441000	2.12016200
C	-6.08053100	-1.39867600	3.07020600
C	-7.23232700	-2.13311200	2.77270200
C	-7.39382400	-2.73561900	1.52699100
C	-6.32788600	-3.14945200	-0.82481800
H	-4.16860900	-0.69624100	2.34679200
H	-8.00937900	-2.23639800	3.52309600
H	-8.28964000	-3.30599400	1.30160300
H	-7.22374200	-2.93593700	-1.41624500
H	-6.20820400	-4.23670100	-0.80387800
C	-2.55460100	2.83776600	-0.54339500

C	-2.82363400	3.55092900	0.62542200
C	-1.64384200	3.25036100	-1.51785900
C	-2.12012200	4.73911000	0.81481200
C	-0.96712200	4.44517100	-1.27883700
C	-1.18561800	5.19317400	-0.11801200
H	-2.30266700	5.31819500	1.71606100
H	-0.24619600	4.79628200	-2.01255000
C	-1.36967400	2.39993700	-2.72771900
H	-0.90226000	1.45299600	-2.42992700
H	-0.69555700	2.91602500	-3.41244100
H	-2.29326900	2.16195300	-3.26375100
C	-3.78465200	3.02803800	1.65925700
H	-4.70933800	2.66116600	1.20516700
H	-4.03747100	3.81116800	2.37495500
H	-3.33314300	2.19939400	2.21681900
H	-4.45594800	-3.22445900	-1.97484200
C	-0.39846600	6.45136600	0.13684700
H	-0.94655300	7.13552400	0.78760800
H	0.54940500	6.21014100	0.62943400
H	-0.16409000	6.96692700	-0.79684100
C	2.90624500	3.24795700	1.55825800
C	1.81051200	2.48755400	1.17211300
C	1.65668200	1.17536800	1.64698800
C	2.62918200	0.64837000	2.50341900
C	3.72125200	1.41445000	2.89981200
C	3.86270100	2.71579700	2.42701900
H	3.02062800	4.25824600	1.17834300
H	1.08399000	2.90938800	0.48164100
H	2.51613200	-0.37666400	2.84820900
H	4.46818400	0.98773700	3.56177700
H	4.71785800	3.31420700	2.72422100
C	0.52463100	0.32520900	1.27128500
H	0.54774300	-0.69790000	1.63848300
C	-0.66444400	0.80948800	0.77390200
C	-1.73970400	-0.09464400	0.56526400
O	-1.79186200	-1.27461900	0.93188000
H	-0.74859600	1.83817100	0.46062900
H	-5.96986300	-0.94143400	4.04772000
C	6.39578300	-0.60841600	-0.37939100
C	5.19053800	-0.81374600	0.34855400
C	5.25197000	-1.39955900	1.62427900
C	6.45562300	-1.81407600	2.18293000
C	7.63352600	-1.63835400	1.47016800
C	7.58652900	-1.04138100	0.21079100

H	4.33335800	-1.51236500	2.18836900
H	6.46575800	-2.26192600	3.17215600
H	8.58593100	-1.95305000	1.88462000
H	8.52147300	-0.91378100	-0.32138900
C	6.40281500	0.04463100	-1.77167300
C	5.53497100	-0.76743800	-2.75135800
C	5.88389500	1.49173000	-1.68092200
C	7.81652100	0.10486700	-2.36757200
H	5.87513600	-1.80794900	-2.79130800
H	4.48368300	-0.75786200	-2.46288700
H	5.62231000	-0.34312900	-3.75790600
H	6.53607800	2.08841200	-1.03410600
H	5.88764800	1.94760500	-2.67774900
H	4.87049000	1.51832200	-1.28037300
H	7.76462000	0.57845000	-3.35264600
H	8.49583100	0.69963800	-1.74890600
H	8.24870300	-0.89246000	-2.49813100
N	3.98127900	-0.35241500	-0.19043300
C	2.89481200	-1.06248200	-0.21210700
C	1.67451000	-0.55489100	-0.73381200
H	1.67924000	0.45627400	-1.12195100
C	0.66153000	-1.45344800	-1.20126700
O	0.63138600	-2.67667600	-1.09672100
O	-0.35309600	-0.78488700	-1.83599800
C	-1.36700400	-1.62147200	-2.37598400
H	-2.12219500	-0.95507100	-2.79832600
H	-0.96397400	-2.26945100	-3.15812700
H	-1.79665800	-2.25175200	-1.59200300
C	2.84058700	-2.45411800	0.39757800
O	3.55158800	-3.33855900	-0.29823200
O	2.27562400	-2.70326900	1.44034900
C	3.61725500	-4.64652700	0.27836600
H	2.61326700	-5.05998100	0.38890200
H	4.20793600	-5.24791400	-0.40907900
H	4.09995500	-4.59706600	1.25714900

M4(SS)

C	-0.57879000	1.78044600	0.08641400
C	-2.27809300	2.56588200	-1.04667500
C	-2.88495600	0.76223800	0.53341300
H	-2.33170500	-0.11419500	0.87831300
N	-1.25839200	3.25139800	-1.47311000
N	-0.20585900	2.75460000	-0.75124500

N	-1.90583400	1.65596700	-0.09768100
C	-3.69683700	2.52663600	-1.50661200
H	-3.80031700	3.02883200	-2.46798200
H	-4.35914000	3.00786200	-0.77399000
C	-4.01976700	0.38342900	-0.49306700
O	-4.00506500	1.15809800	-1.68631100
C	-4.98956500	1.35833000	1.50870100
C	-3.60972800	1.46489700	1.65946400
C	-3.04215200	2.14770800	2.73117400
C	-3.89437000	2.74352700	3.65789300
C	-5.28134400	2.64621700	3.51187800
C	-5.83854500	1.95043700	2.44101000
C	-5.34547700	0.55299800	0.28552800
H	-1.96085500	2.18294900	2.83079300
H	-5.93207300	3.11732200	4.24191300
H	-6.91647800	1.87636400	2.33182300
H	-6.09280700	1.03697700	-0.35079500
H	-5.74727900	-0.42574700	0.56823100
C	1.10695200	3.31592800	-0.91827100
C	1.56665100	4.21247200	0.04767900
C	1.86259000	2.92402100	-2.02643300
C	2.85149600	4.72705500	-0.12014200
C	3.13903300	3.46957100	-2.14964800
C	3.65058300	4.36283600	-1.20527600
H	3.23680500	5.42758500	0.61612200
H	3.75163400	3.18240600	-3.00068200
C	1.35280000	1.89783400	-3.00418700
H	1.48750800	0.88672400	-2.59738100
H	1.91108500	1.95375700	-3.94032700
H	0.29150700	2.03774600	-3.22495800
C	0.71734300	4.57565300	1.23624900
H	-0.29688800	4.85304400	0.93420100
H	1.15821400	5.41202700	1.78022000
H	0.63769300	3.72659200	1.92472700
H	-3.87305600	-0.64042900	-0.84107500
C	5.05227100	4.89705600	-1.34407900
H	5.18102400	5.82409600	-0.78184100
H	5.77566900	4.17004500	-0.96088400
H	5.29975400	5.08676200	-2.39107100
C	5.70818100	-0.12075500	-0.18860200
C	4.32413200	-0.09148500	-0.02664200
C	3.74226600	-0.40399800	1.20577300
C	4.59040000	-0.73266300	2.27122400
C	5.97303300	-0.77194000	2.11028600

C	6.53844600	-0.46586400	0.87475800
H	6.13854100	0.12728400	-1.15423700
H	3.69575600	0.16175000	-0.87228200
H	4.15731600	-0.95685900	3.24264300
H	6.60600100	-1.02946000	2.95396700
H	7.61562500	-0.48884800	0.74382900
C	2.24222700	-0.38221700	1.45166700
H	2.10141300	-0.14526200	2.51260600
C	1.48367800	0.63025500	0.65015500
C	0.21382900	0.94205300	1.04619500
O	-0.42764800	0.53314700	2.06829300
H	1.89677300	1.01289200	-0.27117900
H	-3.47975500	3.28453800	4.50247700
C	-2.40760600	-2.93259900	-1.16215500
C	-1.35738100	-1.99640900	-1.01724700
C	-1.17026900	-0.97589600	-1.95944700
C	-1.99818900	-0.86690100	-3.07110900
C	-3.01294600	-1.79737600	-3.24990900
C	-3.19945800	-2.81028800	-2.30850000
H	-0.37193200	-0.25707800	-1.78869100
H	-1.85075800	-0.05894500	-3.78054300
H	-3.66960800	-1.73790400	-4.11148100
H	-4.00227300	-3.51761100	-2.47701500
C	-2.67895700	-4.02342200	-0.11648700
C	-1.44536000	-4.92615300	0.06167400
C	-3.05776200	-3.36564300	1.22373800
C	-3.84722400	-4.92705000	-0.53305800
H	-1.15683400	-5.37471600	-0.89435300
H	-0.58722300	-4.37923500	0.45416900
H	-1.68214500	-5.73453300	0.76165200
H	-3.95524400	-2.74824700	1.10187500
H	-3.27927600	-4.14064600	1.96553500
H	-2.25105500	-2.73832600	1.60585200
H	-4.00243900	-5.68468900	0.24031700
H	-4.78029100	-4.36503100	-0.63975400
H	-3.64409200	-5.44693300	-1.47477100
N	-0.54839000	-1.98639100	0.14237900
C	0.72051900	-1.98172800	0.05976700
C	1.52516900	-1.81108500	1.32361200
H	0.79701200	-1.85162400	2.13486100
C	2.52840100	-2.92306700	1.47375500
O	3.05052100	-3.51004600	0.55046100
O	2.81403500	-3.15783900	2.75688000
C	3.88040200	-4.08646800	2.98758000

H	3.96732000	-4.17639000	4.06814700
H	3.64654200	-5.05265800	2.53812000
H	4.80681000	-3.69690400	2.55873300
C	1.44492200	-2.17034200	-1.26345800
O	1.13202200	-3.34331500	-1.80399700
O	2.17629000	-1.35457100	-1.77402500
C	1.71973800	-3.59986400	-3.08512500
H	2.80793500	-3.56634700	-3.01130300
H	1.38284100	-4.59322500	-3.37169300
H	1.37910000	-2.85411100	-3.80639600

TS5D(SS)

C	2.44497700	-0.58498800	-0.26600800
C	4.05579400	-1.04834700	-1.66072000
C	4.12221800	1.26806400	-0.81443100
H	3.35858600	1.96235200	-0.46087800
N	3.40393500	-2.16737400	-1.52390900
N	2.40756600	-1.86325400	-0.64235200
N	3.50543000	-0.05980900	-0.89512300
C	5.16091000	-0.64436500	-2.58132300
H	5.26381000	-1.36553700	-3.39122300
H	6.11375600	-0.56649400	-2.04193300
C	4.68094800	1.68069100	-2.22671000
O	4.75545900	0.59265600	-3.14028000
C	6.43385600	1.82373400	-0.56159700
C	5.34199600	1.24687500	0.08242200
C	5.44019900	0.73941800	1.37478200
C	6.67231200	0.81709000	2.01973100
C	7.77267900	1.39624000	1.38174000
C	7.66178100	1.90508900	0.08936500
C	6.06686400	2.30008700	-1.94306600
H	4.57021700	0.30725000	1.86019100
H	8.72578100	1.44735100	1.89842600
H	8.51977300	2.35086400	-0.40443400
H	6.77893000	1.99181800	-2.71413600
H	6.00440800	3.39252800	-1.97417900
C	1.52008900	-2.88991200	-0.16329100
C	1.64314400	-3.31137500	1.16181400
C	0.59140100	-3.42396200	-1.06272600
C	0.75075700	-4.29358100	1.59781600
C	-0.28484700	-4.38657800	-0.57042900
C	-0.22760500	-4.82321800	0.75687000
H	0.81960200	-4.64144600	2.62555800

H	-1.02973800	-4.80769800	-1.24088900
C	0.56162900	-2.98761700	-2.50201200
H	0.55308500	-1.89682300	-2.58939200
H	-0.32701000	-3.37875900	-2.99871200
H	1.44618500	-3.35145100	-3.03258700
C	2.67081900	-2.72615200	2.09547800
H	3.63359600	-2.58016600	1.59648500
H	2.82421800	-3.38999500	2.94732900
H	2.34735300	-1.75387600	2.48476200
H	4.00427300	2.38845500	-2.70471100
C	-1.21938800	-5.83602400	1.26510800
H	-0.89109400	-6.27364400	2.20994300
H	-2.19212200	-5.36206400	1.43188000
H	-1.36702600	-6.63975200	0.53975400
C	-2.11712500	-2.43463100	3.36567600
C	-1.29840900	-1.58991000	2.61822000
C	-1.60281100	-0.23589400	2.47679200
C	-2.75373500	0.26056200	3.09742300
C	-3.57503300	-0.58051900	3.84380000
C	-3.25993900	-1.93237200	3.98240200
H	-1.85825400	-3.48601100	3.46073900
H	-0.41327500	-1.99157300	2.13385300
H	-3.01994600	1.30842600	2.97020200
H	-4.46905700	-0.18024700	4.31284700
H	-3.90350400	-2.58644400	4.56202600
C	-0.67767600	0.68604000	1.71577200
H	0.00812000	1.16011000	2.42526400
C	0.19365000	0.04497900	0.63270500
C	1.59855900	0.14505400	0.75606100
O	2.25517100	0.84490200	1.54490400
H	-0.22949700	-0.76674300	0.04455100
H	6.77891800	0.42539500	3.02587300
C	-4.51870900	-0.23315600	-2.01500800
C	-4.21334900	0.13107600	-0.68018600
C	-5.22518300	0.15632600	0.29019800
C	-6.54342700	-0.15212700	-0.02758500
C	-6.86160000	-0.49518000	-1.33397800
C	-5.85543900	-0.53053400	-2.29891100
H	-4.94712800	0.40743700	1.30954900
H	-7.30711600	-0.12525100	0.74357800
H	-7.88236200	-0.73918600	-1.61010500
H	-6.13537700	-0.79876400	-3.31046400
C	-3.45085500	-0.27733200	-3.11695300
C	-2.80473100	1.10763000	-3.30122100

C	-2.36566700	-1.30764700	-2.76452800
C	-4.04479200	-0.68594400	-4.47202700
H	-3.56633900	1.86361500	-3.51617700
H	-2.25675700	1.42230700	-2.41214400
H	-2.10402700	1.07288300	-4.14299800
H	-2.79732000	-2.31086900	-2.67494400
H	-1.61761700	-1.32953400	-3.56414600
H	-1.86810900	-1.05811300	-1.82450700
H	-3.24310000	-0.71565900	-5.21596300
H	-4.50132700	-1.67994900	-4.43380600
H	-4.79680100	0.02905500	-4.82046500
N	-2.89328000	0.40425900	-0.25447800
C	-2.60549600	1.55490600	0.24329400
C	-1.33278200	1.82003900	0.90311700
H	-0.28602900	1.21533200	0.05437700
C	-1.04996900	3.21898400	1.18688600
O	-1.53043600	4.16366200	0.57157800
O	-0.13537500	3.40880800	2.16441200
C	0.24225600	4.76521400	2.38699400
H	0.98768100	4.74117500	3.18012800
H	0.66665400	5.20048100	1.47955300
H	-0.62021400	5.36036200	2.69367800
C	-3.65419400	2.66244000	0.27063400
O	-4.00441300	3.06360900	-0.94803700
O	-4.16448900	3.05649600	1.29432900
C	-5.09470800	3.98923400	-0.99180000
H	-4.84627500	4.89263900	-0.43210100
H	-5.24934800	4.21848500	-2.04391100
H	-5.98828400	3.52947800	-0.56352100

TS5B(SS)

C	-0.81185400	2.28234700	-0.23484700
C	-0.11279900	4.05107200	0.84170000
C	1.69655500	2.58648800	-0.00763100
H	1.72836800	1.50252800	-0.16170800
N	-1.41144800	4.12116700	0.91084000
N	-1.83189800	3.00804200	0.22650700
N	0.28925400	2.94482400	0.14882000
C	0.96860600	4.85587700	1.48258800
H	0.55830100	5.51681000	2.24528900
H	1.50142400	5.45445000	0.73151600
C	2.50544700	3.00675100	1.27514400
O	1.81933900	3.92285400	2.12281400

C	3.55174000	3.92111900	-0.71207700
C	2.35706300	3.34566700	-1.13720500
C	1.90083600	3.48696800	-2.44481400
C	2.67285600	4.23356800	-3.33257700
C	3.87227100	4.81738700	-2.91436500
C	4.32185700	4.66343800	-1.60433100
C	3.82511200	3.60270400	0.73597300
H	0.97609100	2.99861700	-2.74127700
H	4.45998300	5.39877000	-3.61790300
H	5.25332100	5.11993900	-1.28282100
H	4.11078000	4.47696300	1.32797000
H	4.63402700	2.86936900	0.82567700
C	-3.22184100	2.72611700	-0.00963700
C	-3.69516000	2.87426100	-1.31968600
C	-4.00235300	2.23613500	1.03582300
C	-5.01080200	2.49859800	-1.56744900
C	-5.32256000	1.89002200	0.73655000
C	-5.83571100	1.99877700	-0.55387400
H	-5.40470300	2.59512000	-2.57630700
H	-5.95402000	1.50456600	1.53322200
C	-3.44359000	1.99989900	2.41518800
H	-3.05556400	0.97592000	2.49645300
H	-4.22862200	2.11091700	3.16602700
H	-2.63566700	2.69356900	2.65705500
C	-2.79984400	3.38733700	-2.41788500
H	-2.29294400	4.30948300	-2.11598600
H	-3.38292800	3.59508500	-3.31629500
H	-2.02487200	2.65453900	-2.67266700
H	2.67413500	2.13396000	1.90831600
C	-7.24553400	1.57225500	-0.86897100
H	-7.77705200	2.35071700	-1.42289100
H	-7.23753400	0.67098800	-1.49012700
H	-7.80582600	1.35037200	0.04132600
C	-5.37503800	-2.13672100	-0.48330100
C	-4.00918000	-1.98436800	-0.25800200
C	-3.14673900	-1.64145600	-1.30521200
C	-3.69102600	-1.44300400	-2.57615800
C	-5.05782300	-1.59160600	-2.80501500
C	-5.90721100	-1.94334700	-1.75815200
H	-6.02853300	-2.40619400	0.34154500
H	-3.60166500	-2.12153900	0.74068200
H	-3.03366800	-1.16282100	-3.39614100
H	-5.45858700	-1.43711400	-3.80258900
H	-6.97172200	-2.06695000	-1.93310000

C	-1.66658100	-1.34999400	-1.07055700
H	-1.17906400	-1.36396400	-2.05446000
C	-1.60796400	0.05610100	-0.54831700
C	-0.80792300	1.03047900	-1.05311400
O	-0.01317300	1.05674200	-2.05919000
H	-2.20594500	0.25989000	0.33710400
H	2.34158300	4.36317600	-4.35791800
C	2.30639000	-0.43890900	2.91848400
C	1.05874000	-0.27984900	2.26636200
C	0.17161600	0.72601200	2.68055500
C	0.47762700	1.57741300	3.73590300
C	1.68613300	1.41951800	4.39998700
C	2.57116500	0.42287700	3.98900800
H	-0.76767600	0.82344500	2.14304400
H	-0.22194200	2.35507100	4.02778500
H	1.95203700	2.06735200	5.22867800
H	3.50533200	0.32448900	4.52840100
C	3.31468200	-1.52524000	2.51685700
C	2.70806200	-2.91826500	2.75972500
C	3.69483000	-1.37128500	1.03447500
C	4.60922000	-1.43364400	3.33593600
H	2.39800500	-3.02515200	3.80403200
H	1.83229000	-3.09281000	2.13021000
H	3.45561200	-3.69031200	2.54386600
H	4.06680800	-0.35797800	0.83805500
H	4.49312300	-2.07806700	0.77622200
H	2.83529000	-1.56064100	0.38865500
H	5.30124900	-2.20733700	2.99093200
H	5.10077300	-0.46346700	3.21032100
H	4.43270400	-1.59877500	4.40328400
N	0.68646700	-1.04145400	1.13597300
C	-0.38295400	-1.74920600	1.14654600
C	-0.93212800	-2.32850300	-0.09760500
H	0.26042800	-2.68159200	-0.83323000
C	-1.50492300	-3.64661100	0.11496300
O	-1.51438500	-4.27421200	1.17185000
O	-1.94871700	-4.20984900	-1.03480800
C	-2.54549900	-5.49456000	-0.89500100
H	-2.84222100	-5.79942000	-1.89754100
H	-1.83384200	-6.20979200	-0.47625000
H	-3.42122800	-5.44317400	-0.24269900
C	-1.16852200	-1.92322700	2.44148800
O	-0.44542400	-2.45628300	3.42180000
O	-2.31364000	-1.54621700	2.57313400

C	-1.08765000	-2.50615800	4.69899200
H	-1.99833700	-3.10507900	4.64303800
H	-0.36875700	-2.96252700	5.37609200
H	-1.33740000	-1.49522900	5.02932500
C	2.85834200	-0.19809800	-2.38696900
C	4.13556000	-0.18823000	-3.22219700
C	4.98427300	-1.45140900	-3.08637500
C	1.85633000	-1.31143900	-2.72780400
C	4.23055000	-2.72073700	-3.48911800
C	2.16772500	-2.66092800	-2.13931300
H	3.11211600	-0.26000100	-1.32209900
H	3.86656000	-0.06173400	-4.28018400
H	5.34044100	-1.56895800	-2.05465200
H	3.66008300	-2.54644000	-4.40863600
H	1.77339900	-1.41797200	-3.81812000
H	2.31872800	0.74405700	-2.52019200
H	4.73555300	0.68653100	-2.94728700
H	5.87005500	-1.36433600	-3.72450200
H	0.87866100	-0.99652800	-2.36097600
H	4.93816500	-3.52289900	-3.70950600
C	3.77091100	-4.49625800	-1.81062000
H	4.84300300	-4.40928100	-1.60752500
H	3.63044000	-5.32636600	-2.51409500
C	3.00503900	-4.73961400	-0.52243000
H	3.20369100	-5.75088800	-0.16073700
H	3.33727300	-4.03247200	0.24213600
C	1.52071200	-4.52918800	-0.77824800
H	0.94479600	-4.59205000	0.15112800
H	1.13346500	-5.29987200	-1.45778000
N	1.28466600	-3.21002800	-1.34912200
N	3.33981400	-3.24758600	-2.44935000

M5B(R)

C	-0.66437400	2.48254700	-0.32352500
C	0.07869200	4.51122200	0.02218800
C	1.83287300	2.76831200	-0.04848000
H	1.80622300	1.70316300	0.19642900
N	-1.21425400	4.64684600	-0.04671500
N	-1.66299100	3.37016000	-0.27793900
N	0.44840900	3.20902500	-0.14890200
C	1.17251600	5.45286900	0.40625600
H	0.76338000	6.37285400	0.82197900
H	1.80195900	5.69325200	-0.46035200

C	2.57238300	3.59142900	1.06194800
O	1.90256600	4.79714700	1.42986400
C	3.83020300	3.65853000	-1.00727100
C	2.62045200	3.03735000	-1.31014600
C	2.26721600	2.71467500	-2.61695200
C	3.15698200	3.04688800	-3.63697700
C	4.37100500	3.67574800	-3.34459300
C	4.71903700	3.98154300	-2.02969000
C	3.97706400	3.85841400	0.48125200
H	1.32783600	2.20075900	-2.80174000
H	5.05151600	3.92838700	-4.15159400
H	5.66406600	4.46828700	-1.80823400
H	4.32184800	4.85800300	0.76028100
H	4.68831400	3.13556000	0.89928500
C	-3.06152400	3.08830700	-0.44642300
C	-3.50982200	2.66217100	-1.69794400
C	-3.89455300	3.19879100	0.67122400
C	-4.86014500	2.32850300	-1.80992200
C	-5.23534700	2.86316400	0.50300600
C	-5.73233800	2.41912400	-0.72556400
H	-5.23461100	1.97763900	-2.76803400
H	-5.90434000	2.92920300	1.35762100
C	-3.34913700	3.63071600	2.00680200
H	-2.47206500	3.03538500	2.28370800
H	-4.10513800	3.51057800	2.78387600
H	-3.03395900	4.67753500	1.98590600
C	-2.57243400	2.53542100	-2.86987300
H	-1.95160700	3.43028000	-2.97895300
H	-3.13779300	2.39479400	-3.79247400
H	-1.89616400	1.68227600	-2.74534500
H	2.61484700	3.01201400	1.98414900
C	-7.18620700	2.05287700	-0.86777000
H	-7.81880500	2.94475500	-0.81829800
H	-7.37460000	1.55212000	-1.81951900
H	-7.49620500	1.38184800	-0.06191000
C	-5.58334100	-1.06460700	0.27246700
C	-4.23581500	-1.09741500	0.61310500
C	-3.25219200	-1.29194800	-0.36380500
C	-3.65739000	-1.44736800	-1.69019300
C	-5.00834400	-1.41639200	-2.03725100
C	-5.97810900	-1.22497200	-1.05728200
H	-6.33183000	-0.91234400	1.04535400
H	-3.92874300	-0.97657300	1.64957800
H	-2.90256300	-1.58712000	-2.46115100

H	-5.30112800	-1.54121800	-3.07581200
H	-7.03054200	-1.19855900	-1.32278300
C	-1.76974000	-1.17933300	-0.01969100
H	-1.20777300	-1.49886400	-0.91066400
C	-1.55507500	0.30676200	0.12739100
C	-0.66739800	1.01716800	-0.60869100
O	0.20235700	0.66209200	-1.48844400
H	-2.19601400	0.82542000	0.83606600
H	2.90852800	2.81364800	-4.66746300
C	3.01956400	0.02588200	2.18274700
C	1.59607100	-0.04492500	2.28608400
C	0.95594400	0.77445300	3.24025700
C	1.66185800	1.57427400	4.13215800
C	3.04879700	1.60137800	4.07101700
C	3.69648000	0.84348500	3.09303600
H	-0.13014300	0.76459900	3.26015400
H	1.12512900	2.17583000	4.85975100
H	3.62711200	2.21465100	4.75428000
H	4.77845900	0.89365800	3.05198000
C	3.80225000	-0.79550400	1.15048700
C	3.56716200	-2.29391800	1.40425100
C	3.37088500	-0.40231500	-0.27375800
C	5.31697300	-0.56118900	1.23404800
H	3.98799900	-2.58299600	2.37336700
H	2.50481900	-2.52854800	1.42083400
H	4.05926800	-2.88778200	0.62473600
H	3.73589200	0.60563600	-0.50923700
H	3.82621600	-1.08880700	-0.99588100
H	2.28504200	-0.40328800	-0.40818600
H	5.80956200	-1.16135400	0.46251700
H	5.57895400	0.48708600	1.05663400
H	5.72673100	-0.86291600	2.20301700
N	0.79398700	-0.81644500	1.44105500
C	-0.20347900	-1.51802200	1.95608000
C	-1.32972200	-1.94440700	1.22575600
H	0.88459800	-2.11746100	-0.21979600
C	-1.86191500	-3.22469500	1.60056500
O	-1.54481000	-3.89633400	2.58700800
O	-2.74004200	-3.74530800	0.69394700
C	-3.28686100	-5.01125300	1.03582700
H	-3.96286800	-5.27458500	0.22279800
H	-2.50164800	-5.76581000	1.13226000
H	-3.83638000	-4.96029700	1.97894000
C	-0.10906400	-1.94370700	3.41955400

O	0.98831200	-2.68587800	3.62944700
O	-0.86153800	-1.60376600	4.30257300
C	1.17823100	-3.11036300	4.97873400
H	0.32982700	-3.71556000	5.30552300
H	2.09280800	-3.70019400	4.98345100
H	1.27770800	-2.24533600	5.63793700
C	2.46575100	-1.78700700	-3.53951000
C	2.59827400	-2.60910400	-4.82079700
C	2.58738900	-4.12043600	-4.59464000
C	1.13704900	-1.98591200	-2.78722300
C	1.31430300	-4.61997600	-3.91247400
C	1.12313800	-3.20891300	-1.92120700
H	3.30042900	-2.01794500	-2.86822600
H	1.77404500	-2.34769800	-5.49738000
H	3.45258300	-4.42741400	-3.99434100
H	0.42978400	-4.14749500	-4.35128600
H	0.31079400	-2.07117200	-3.50578000
H	2.54691500	-0.72261700	-3.78111600
H	3.52468200	-2.32985200	-5.33227800
H	2.67143700	-4.62917000	-5.55999600
H	0.90305000	-1.11892000	-2.15879500
H	1.20255000	-5.69584500	-4.05742500
C	1.48850100	-5.62598400	-1.64002000
H	2.31962000	-6.18282800	-2.08166500
H	0.58619000	-6.24104500	-1.72379300
C	1.77785600	-5.27994500	-0.18877900
H	1.68315400	-6.17900800	0.42221200
H	2.79747400	-4.89782100	-0.08309200
C	0.79025000	-4.21528900	0.26084500
H	0.94946500	-3.88858400	1.28960200
H	-0.23813600	-4.58753400	0.18542200
N	0.93749900	-3.06175800	-0.62261600
N	1.29771600	-4.41367400	-2.45517000

TS6B(R)

C	0.54627200	0.99583000	1.03707300
C	1.82810900	2.18513200	2.34933500
C	2.47428700	2.31174100	-0.02033900
H	2.43808400	1.57889400	-0.82559300
N	0.93444400	1.66977600	3.14190900
N	0.13985900	0.93340800	2.31019000
N	1.62817800	1.79364900	1.05820600
C	3.01664200	3.04085500	2.63642000

H	3.26935200	2.99491000	3.69550600
H	2.80960500	4.08456200	2.36129800
C	3.94595000	2.53406800	0.48548500
O	4.09045400	2.49660700	1.90046500
C	3.07745800	4.57811800	-0.49320400
C	2.00992900	3.68449400	-0.45815100
C	0.71841500	4.08413100	-0.78670200
C	0.50648500	5.41022300	-1.15497000
C	1.57342900	6.31196900	-1.19558700
C	2.86450800	5.90270700	-0.86756900
C	4.36581200	3.90129000	-0.10057800
H	-0.09642900	3.36780600	-0.76232000
H	1.39322700	7.34336600	-1.48163000
H	3.69003400	6.60760700	-0.89473000
H	4.94544400	4.46397100	0.63722800
H	5.00801700	3.75379500	-0.97561800
C	-1.07041200	0.37630000	2.85815800
C	-2.21497100	1.17522100	2.81936400
C	-1.02613200	-0.88837400	3.44443600
C	-3.36571600	0.66006000	3.41072700
C	-2.21317100	-1.36913700	3.99657400
C	-3.38649300	-0.61210700	3.98727700
H	-4.27134300	1.26220500	3.40966900
H	-2.21758100	-2.35715900	4.44961600
C	0.23907000	-1.70143700	3.44121200
H	0.52461300	-2.00669200	2.42612700
H	0.11297000	-2.60891400	4.03379200
H	1.07362100	-1.13033000	3.86072300
C	-2.19114300	2.53505700	2.17487600
H	-1.53949500	3.22221100	2.72446400
H	-3.19571100	2.96111500	2.13845100
H	-1.81481600	2.47570800	1.14768900
H	4.57953400	1.72014800	0.13266400
C	-4.66755500	-1.16771600	4.55092300
H	-5.26221400	-0.38406500	5.02600900
H	-5.27488000	-1.60293100	3.74959300
H	-4.47272900	-1.95252900	5.28439800
C	-3.82614900	-3.96672300	0.00994200
C	-2.58506500	-3.34125400	-0.03610300
C	-2.22795700	-2.52217300	-1.11579500
C	-3.16023300	-2.32370300	-2.13235100
C	-4.40809300	-2.94774700	-2.09086600
C	-4.74654800	-3.77363000	-1.02195800
H	-4.07937600	-4.60357100	0.85251300

H	-1.86467300	-3.50085300	0.76345600
H	-2.90205500	-1.68539100	-2.97426400
H	-5.11704800	-2.78879800	-2.89860900
H	-5.71536900	-4.26231600	-0.99158700
C	-0.86856500	-1.83212800	-1.13319700
H	-0.72938200	-1.35933900	-2.11652900
C	-0.94244100	-0.70245200	-0.08095500
C	-0.05105000	0.39715600	-0.23503900
O	0.21453300	1.02491200	-1.26793200
H	-0.93538000	-1.13211200	0.91990300
H	-0.49356800	5.74422000	-1.41349500
C	4.40928000	-0.75987100	-0.94828800
C	3.34557700	-0.93834000	-0.01583700
C	3.60551900	-0.80809700	1.35708800
C	4.88340300	-0.55519600	1.84524600
C	5.93536300	-0.42807900	0.94969400
C	5.68472200	-0.52803200	-0.42077700
H	2.76772700	-0.92783300	2.04051900
H	5.04718300	-0.45647900	2.91401000
H	6.94470700	-0.23996400	1.30156500
H	6.52546700	-0.41399700	-1.09489900
C	4.19422300	-0.81439000	-2.47297200
C	3.67841500	-2.19252200	-2.92566800
C	3.18931700	0.26802900	-2.90563500
C	5.49872200	-0.55127100	-3.23962300
H	4.35576600	-2.98728600	-2.59992900
H	2.68647100	-2.40883700	-2.52770400
H	3.62321000	-2.21130300	-4.02040400
H	3.58962400	1.26804700	-2.69378100
H	3.02494000	0.20440700	-3.98767200
H	2.22934800	0.14816000	-2.39680000
H	5.28624300	-0.56357200	-4.31282700
H	5.92539900	0.42710200	-2.99572900
H	6.25358400	-1.31888100	-3.04095900
N	2.03135400	-1.18930800	-0.44417300
C	1.51841400	-2.39244200	-0.30676500
C	0.25427800	-2.80834900	-0.77644600
H	-2.22221600	-0.05118000	-0.20045300
C	0.16492400	-4.21671400	-1.06659100
O	0.83919600	-5.12836800	-0.57968500
O	-0.74316900	-4.51053200	-2.04319500
C	-1.03070200	-5.88950500	-2.21487100
H	-1.79438400	-5.94342500	-2.99113500
H	-0.14160400	-6.44487600	-2.52210800

H	-1.41312200	-6.32514400	-1.28694800
C	2.37072300	-3.41967700	0.42922600
O	3.38993300	-3.87259100	-0.30401900
O	2.22988300	-3.67150300	1.60606600
C	4.28938100	-4.74006300	0.38399500
H	3.76388900	-5.63584500	0.72263300
H	5.06407200	-5.00110700	-0.33498800
H	4.72427300	-4.22948100	1.24642500
C	-2.94544900	2.55252700	-2.98779300
C	-3.89320800	3.69424900	-3.35563600
C	-5.31191600	3.54747700	-2.80599200
C	-2.70416200	2.38225600	-1.47607800
C	-5.35157300	3.40750400	-1.28374500
C	-3.77639100	1.57223600	-0.79537900
H	-3.31346700	1.60372500	-3.39812700
H	-3.46790400	4.63361600	-2.97641300
H	-5.80891600	2.67573400	-3.25019500
H	-4.67667400	4.13094700	-0.81420500
H	-2.61904900	3.36703300	-0.99786700
H	-1.97346000	2.73904500	-3.45522000
H	-3.93546500	3.78865500	-4.44550400
H	-5.89794900	4.42823100	-3.08813700
H	-1.76068200	1.85911100	-1.32787200
H	-6.35305600	3.62970200	-0.90799400
C	-6.19014900	1.22383800	-0.45409300
H	-6.97278100	1.41115400	-1.19668200
H	-6.57515200	1.53720600	0.52411400
C	-5.79589300	-0.24094600	-0.44464600
H	-6.59376800	-0.84143400	-0.00143800
H	-5.63252900	-0.59260600	-1.46803300
C	-4.50190200	-0.38652800	0.34179800
H	-4.15921300	-1.42128700	0.36551300
H	-4.66170000	-0.06188100	1.37741100
N	-3.45289400	0.42407500	-0.26662800
N	-5.03543300	2.05806600	-0.80841800

TS5(RR)

C	-0.27037500	2.22754600	0.18739600
C	-1.32223500	3.40424300	1.69392400
C	-1.64206800	0.98747400	1.97386100
H	-1.68987000	0.14819800	1.27846000
N	-0.67169200	4.27777300	0.97826100
N	-0.02078800	3.52859300	0.04896800

N	-1.09832400	2.13385300	1.24064400
C	-2.31896600	3.56723200	2.79677000
H	-2.70689000	4.58508300	2.80603300
H	-1.86253600	3.34445700	3.77002800
C	-3.07559300	1.30432200	2.53185000
O	-3.38884500	2.69021000	2.49308200
C	-1.62983000	0.52966000	4.31795100
C	-0.80981900	0.70710300	3.20630400
C	0.57690600	0.66419300	3.31016000
C	1.14086600	0.38463200	4.55283900
C	0.32353500	0.16908800	5.66491500
C	-1.06373400	0.24913800	5.55829100
C	-3.08161400	0.71610700	3.96010300
H	1.21262500	0.87257600	2.45175000
H	0.77644700	-0.04143900	6.62817300
H	-1.69241600	0.11209800	6.43264000
H	-3.61004600	1.38761000	4.64314100
H	-3.61608300	-0.23965700	3.95867500
C	0.88640900	4.15658500	-0.88016500
C	2.23486000	4.21587500	-0.53236600
C	0.35991800	4.67333700	-2.06492400
C	3.09180600	4.83360400	-1.44508000
C	1.25576400	5.28544200	-2.93579500
C	2.62055200	5.37363600	-2.64208700
H	4.15080200	4.89753400	-1.20856100
H	0.88224900	5.69534600	-3.87066100
C	-1.10121000	4.52195700	-2.38372000
H	-1.72967300	4.92946500	-1.58588400
H	-1.34385800	3.45912400	-2.49126700
H	-1.34828800	5.03343600	-3.31479500
C	2.74069600	3.63192500	0.76095500
H	2.72566400	2.53461200	0.74006300
H	2.13406400	3.95740500	1.61153400
H	3.77209300	3.94122000	0.93824000
H	-3.83290700	0.83647700	1.90267300
C	3.55834100	6.06214600	-3.59872300
H	3.46091700	7.14909800	-3.51416700
H	4.59781100	5.80128000	-3.39115800
H	3.33101100	5.79281900	-4.63302500
C	0.54675100	-4.11203900	1.39536900
C	0.40962800	-2.86376700	0.79103500
C	1.04310500	-2.57854600	-0.42335300
C	1.84722600	-3.56749500	-0.99976400
C	1.98428800	-4.81665500	-0.39968400

C	1.32821500	-5.09667600	0.79766100
H	0.04139200	-4.31089300	2.33544000
H	-0.21393100	-2.11963900	1.28044300
H	2.34403900	-3.35834700	-1.94144600
H	2.60914400	-5.57172900	-0.86681000
H	1.43451600	-6.07020600	1.26540200
C	0.79175800	-1.28106000	-1.17521600
H	1.64609700	-1.11211700	-1.84320200
C	0.67581900	-0.08664400	-0.22713500
C	0.23010300	1.15960600	-0.78211800
O	0.26906200	1.51460600	-1.95594800
H	0.23209500	-0.30245800	0.74085900
H	2.21992200	0.34705300	4.65951100
C	-4.65088800	-0.30487200	-0.25279700
C	-3.49711500	-1.09304000	-0.03791700
C	-3.42089500	-1.99007400	1.03297200
C	-4.49300200	-2.15207900	1.90229500
C	-5.65368500	-1.41875200	1.68712800
C	-5.72251400	-0.52219200	0.62101100
H	-2.50206300	-2.55429100	1.17664900
H	-4.41786000	-2.84547000	2.73346600
H	-6.50613500	-1.53250800	2.34837900
H	-6.64024100	0.03723000	0.48811700
C	-4.72860400	0.74625400	-1.37140700
C	-3.65047600	1.83008300	-1.15887000
C	-4.54664500	0.08296300	-2.74878700
C	-6.08972400	1.45483200	-1.37966700
H	-3.75391600	2.29525200	-0.17007400
H	-2.64373800	1.41681900	-1.25606100
H	-3.77213600	2.61441300	-1.91364300
H	-5.30373600	-0.69223000	-2.90256800
H	-4.66292300	0.83579500	-3.53523200
H	-3.56171600	-0.37313400	-2.86447100
H	-6.10006900	2.19331500	-2.18609800
H	-6.91157400	0.75459200	-1.55786300
H	-6.27756000	1.98317300	-0.43982700
N	-2.33363300	-0.86945100	-0.81132000
C	-1.72128700	-1.78665200	-1.44156300
C	-0.42938500	-1.41020200	-2.13545500
H	-0.60416500	-0.40960200	-2.55071700
C	-0.12811000	-2.25743300	-3.35592000
O	0.97223500	-2.55029200	-3.75732500
O	-1.25758700	-2.56627100	-4.00686100
C	-1.09319400	-3.35386200	-5.19302700

H	-2.09758400	-3.53927000	-5.56650700
H	-0.50292200	-2.80536600	-5.92856500
H	-0.59157100	-4.29254500	-4.95044500
C	-2.26752600	-3.20302300	-1.59424300
O	-1.27841300	-4.08977500	-1.60470100
O	-3.43741100	-3.46467800	-1.72074300
C	-1.66389000	-5.45667700	-1.79672500
H	-2.14332900	-5.57367200	-2.77076000
H	-0.73971000	-6.02762800	-1.74521200
H	-2.35457500	-5.76401200	-1.00989600
C	3.71015000	-2.66224200	2.11961900
C	5.07669500	-3.19789200	2.54448700
C	6.21971100	-2.84332800	1.59579900
C	3.59719900	-1.13049000	2.05606400
C	6.39153700	-1.33501400	1.41804500
C	4.14964500	-0.51640300	0.79319600
H	3.42343900	-3.07787500	1.14675500
H	5.31634300	-2.80610500	3.54257000
H	6.05851400	-3.29714700	0.60996800
H	6.31456600	-0.82696700	2.38585100
H	4.08751600	-0.67384100	2.92593500
H	2.95937200	-3.01465200	2.83380100
H	5.01248700	-4.28653400	2.64342600
H	7.15551900	-3.25330500	1.98936900
H	2.54257800	-0.84917800	2.09849200
H	7.38524400	-1.10842100	1.02453800
C	5.96980200	-0.42280400	-0.85578200
H	6.57382800	-1.27678800	-1.17948900
H	6.63339400	0.44733000	-0.78319400
C	4.84113300	-0.15894900	-1.83828500
H	5.24599200	0.26444900	-2.75959700
H	4.33420100	-1.09811900	-2.08671500
C	3.84487500	0.78514800	-1.17725800
H	2.98792600	0.99418900	-1.82689500
H	4.32801300	1.74811800	-0.95746600
N	3.33864400	0.19025500	0.05420900
N	5.44045300	-0.73651200	0.47718800
H	1.93980400	0.12198100	0.06321300

M5(RR)

C	-0.10562400	2.20750500	0.21018300
C	-0.93813100	3.41495100	1.82064600
C	-1.59850500	1.05236600	1.96819000

S150

H	-1.78843300	0.29434200	1.20989000
N	-0.23368200	4.24494800	1.10182600
N	0.27780200	3.48098100	0.10597000
N	-0.87906300	2.15045800	1.30789500
C	-1.89074700	3.64932900	2.94815400
H	-2.11498100	4.71138100	3.03640700
H	-1.47775500	3.28254500	3.89638100
C	-2.97443200	1.55662800	2.54738000
O	-3.07923200	2.97183500	2.58022900
C	-1.69495100	0.42210800	4.26785700
C	-0.84314300	0.52549200	3.16968000
C	0.50165000	0.17192600	3.25899000
C	0.97581800	-0.31951800	4.47327800
C	0.12073900	-0.44916900	5.57007400
C	-1.21689500	-0.07481700	5.47715900
C	-3.08237400	0.90806200	3.94365300
H	1.18221600	0.29486100	2.41851600
H	0.50849600	-0.83238800	6.50811400
H	-1.87499200	-0.15579600	6.33653000
H	-3.46119900	1.63576100	4.66745700
H	-3.79478500	0.07749900	3.90960300
C	1.17509200	4.07686500	-0.85770100
C	2.51303600	4.21818200	-0.48658700
C	0.64509300	4.52460400	-2.06971600
C	3.36313700	4.80379600	-1.42506100
C	1.53795900	5.10781100	-2.96466300
C	2.89546700	5.24805000	-2.66274000
H	4.41446200	4.92150600	-1.17590600
H	1.16296800	5.46407100	-3.92053100
C	-0.81662700	4.37545800	-2.38919000
H	-1.44358300	4.70452400	-1.55447100
H	-1.05536900	3.32752500	-2.59536500
H	-1.07753900	4.96700800	-3.26762900
C	3.00367100	3.77519700	0.86564600
H	2.85429500	2.70055000	1.02459500
H	2.48139200	4.31384400	1.66237000
H	4.07201800	3.97652400	0.96156600
H	-3.78514500	1.23627300	1.89208700
C	3.82749600	5.90565300	-3.64610000
H	3.73769300	6.99494900	-3.58603400
H	4.86736200	5.64394100	-3.44150400
H	3.58807200	5.61266300	-4.67091400
C	0.60486400	-4.24863600	1.24932500
C	0.29659400	-3.06456900	0.58711900

C	1.00350100	-2.67031700	-0.55408800
C	2.03824400	-3.48965500	-1.01279300
C	2.35401900	-4.67442900	-0.34914800
C	1.63758400	-5.05828000	0.78226300
H	0.04228900	-4.53312900	2.13255200
H	-0.50347200	-2.44310700	0.98114100
H	2.58634700	-3.20318000	-1.90538900
H	3.16298200	-5.29775600	-0.71768300
H	1.88535300	-5.98000200	1.29892800
C	0.67144200	-1.36985700	-1.26829700
H	1.48919200	-1.14337900	-1.96024400
C	0.59804600	-0.23703000	-0.23597500
C	0.27226800	1.11406800	-0.78034900
O	0.36407400	1.44250800	-1.94014500
H	-0.07997500	-0.47741000	0.58358600
H	2.02020100	-0.59692400	4.57397100
C	-4.65951300	0.05807000	-0.25150000
C	-3.59540900	-0.84706700	-0.03420000
C	-3.62113500	-1.75259200	1.03156400
C	-4.70907400	-1.80433100	1.89503300
C	-5.78378000	-0.95073200	1.67897700
C	-5.75215200	-0.04862000	0.61647500
H	-2.77031300	-2.41251100	1.18227700
H	-4.71113300	-2.50473700	2.72352700
H	-6.64703100	-0.97603300	2.33529900
H	-6.60447900	0.60491400	0.48075800
C	-4.63098700	1.11020100	-1.37072600
C	-3.45350800	2.08417700	-1.16040400
C	-4.51353800	0.42902400	-2.74613200
C	-5.91493000	1.95122100	-1.38314100
H	-3.50792100	2.56104600	-0.17277600
H	-2.49123600	1.57600600	-1.26142900
H	-3.49959100	2.87534500	-1.91604900
H	-5.33951500	-0.27259000	-2.89745700
H	-4.55815900	1.18702000	-3.53488600
H	-3.57619000	-0.11817700	-2.86090700
H	-5.84886600	2.68506200	-2.19097700
H	-6.80194000	1.33609100	-1.56245000
H	-6.05136400	2.49790600	-0.44494100
N	-2.40677700	-0.73911800	-0.80128400
C	-1.89774900	-1.70835100	-1.44568300
C	-0.58748800	-1.45144100	-2.16939700
H	-0.71577500	-0.46223200	-2.62594100
C	-0.36033200	-2.37235800	-3.35486800

O	0.70784100	-2.80741600	-3.70756700
O	-1.50464800	-2.57398900	-4.01874700
C	-1.41290100	-3.43271100	-5.16420800
H	-2.42476700	-3.51529800	-5.55347700
H	-0.74632500	-2.99431900	-5.90803000
H	-1.03183700	-4.41108400	-4.86520500
C	-2.58980300	-3.05592600	-1.61351700
O	-1.69833400	-4.04098400	-1.60131500
O	-3.77690000	-3.18883500	-1.76712400
C	-2.22183500	-5.35601900	-1.84145600
H	-2.70202800	-5.38757400	-2.82158300
H	-1.36426800	-6.02321600	-1.80699700
H	-2.94798800	-5.61495000	-1.06970400
C	3.51492400	-2.39566800	2.34565300
C	4.60205700	-3.47092000	2.28789400
C	5.54960100	-3.37067200	1.09196500
C	4.05467900	-0.95597300	2.40532400
C	6.27409300	-2.02415700	1.00136100
C	4.38779200	-0.42084500	1.03323800
H	2.85070200	-2.48689900	1.47689800
H	5.19927100	-3.41615500	3.20872300
H	4.99754400	-3.52979000	0.15593400
H	6.62045000	-1.70950100	1.99169700
H	4.92349300	-0.90189600	3.07178600
H	2.89431800	-2.57558000	3.23094200
H	4.12133900	-4.45559000	2.28133600
H	6.29640600	-4.16874900	1.16514000
H	3.30123500	-0.27681600	2.80674700
H	7.16818500	-2.11612300	0.37965200
C	5.68846200	-0.73461100	-1.03189900
H	5.95699400	-1.68999100	-1.49593400
H	6.53811900	-0.05231600	-1.16424000
C	4.43810100	-0.16911000	-1.68127600
H	4.66106000	0.17585500	-2.69346900
H	3.68301800	-0.96148900	-1.74876600
C	3.89694700	0.95411500	-0.80455700
H	2.98075700	1.37643600	-1.23752800
H	4.62397700	1.78033800	-0.76784300
N	3.60291700	0.48670600	0.54515200
N	5.46215600	-0.97007300	0.39611600
H	1.59897900	-0.12023500	0.22920800

TS5(RS)

C	-2.67323800	0.38094000	-1.34486500
C	-4.71385700	-0.10866400	-1.93774900
C	-3.42474700	-2.07752400	-1.24415200
H	-2.36985500	-2.35450100	-1.28115300
N	-4.63794500	1.18820400	-2.03454200
N	-3.36245900	1.47667100	-1.65935600
N	-3.52691300	-0.64027300	-1.51463000
C	-5.79315300	-1.07238000	-2.31502300
H	-6.51462600	-0.59072500	-2.97393200
H	-6.30989300	-1.44585800	-1.42159800
C	-4.22774400	-2.89755000	-2.31326400
O	-5.15786900	-2.10810500	-3.04251900
C	-4.92430200	-3.52594900	-0.08044600
C	-4.09691800	-2.41560200	0.06886800
C	-3.99091400	-1.74248400	1.28125300
C	-4.71201500	-2.22405500	2.37160100
C	-5.52271900	-3.35338200	2.23701600
C	-5.63957800	-4.00825600	1.01173500
C	-4.90756700	-4.02443800	-1.50411400
H	-3.38122600	-0.84573100	1.37423900
H	-6.08262000	-3.71403600	3.09366600
H	-6.29150400	-4.87008900	0.90814800
H	-5.90451600	-4.22574300	-1.90558800
H	-4.32610400	-4.94828200	-1.58828000
C	-2.94529100	2.85389700	-1.55594600
C	-3.09304000	3.48708100	-0.32044200
C	-2.46140100	3.48377600	-2.70162300
C	-2.73880200	4.83398100	-0.25993900
C	-2.11029500	4.82718000	-2.58234500
C	-2.24621900	5.51549500	-1.37507700
H	-2.84763600	5.36227700	0.68429100
H	-1.72076900	5.34652700	-3.45387200
C	-2.30237100	2.72279000	-3.98812900
H	-3.25020600	2.27856800	-4.30656700
H	-1.58009700	1.91199500	-3.85028400
H	-1.94459000	3.37916800	-4.78218400
C	-3.58683600	2.74580100	0.89401900
H	-2.80866200	2.08465500	1.29905700
H	-4.46297700	2.13187900	0.66486000
H	-3.86099800	3.45018700	1.68137400
H	-3.54831300	-3.28876300	-3.07072600
C	-1.88412200	6.97381200	-1.27007400
H	-2.78586500	7.59393600	-1.26412100
H	-1.34190700	7.17515000	-0.34242700

H	-1.26412900	7.28959100	-2.11109000
C	0.90618400	-3.43767400	2.83890600
C	0.54644400	-2.71472300	1.70487600
C	1.08517500	-1.44670500	1.47033700
C	1.98013700	-0.91054100	2.39796400
C	2.33706800	-1.62692300	3.53870600
C	1.80254800	-2.89520400	3.75914300
H	0.48145000	-4.42207600	3.00796600
H	-0.16501500	-3.14565900	1.00220400
H	2.40281100	0.07749900	2.22322900
H	3.03314100	-1.19595200	4.25204100
H	2.07841600	-3.45682300	4.64577000
C	0.72577600	-0.66784600	0.22508700
H	1.19039100	0.32298200	0.29484800
C	-0.77873300	-0.46496100	0.10641100
C	-1.19654100	0.37669500	-0.97574500
O	-0.50440900	1.18711200	-1.58587400
H	-1.38489600	-1.35785100	0.25838000
H	-4.65281900	-1.71334400	3.32735000
C	5.72037200	0.61868800	-1.70149400
C	4.86123300	0.03132400	-0.74417900
C	5.33062200	-0.32037600	0.52655300
C	6.66213800	-0.12407100	0.87489000
C	7.52960700	0.42631500	-0.05834600
C	7.05539700	0.78463200	-1.31969000
H	4.62834000	-0.73322100	1.24585600
H	7.00939400	-0.39805500	1.86564200
H	8.57417100	0.58731100	0.18727400
H	7.75971800	1.21286500	-2.02224400
C	5.23322200	1.03530500	-3.09791500
C	4.69838900	-0.18811900	-3.86353700
C	4.13517800	2.10885300	-2.98151100
C	6.37042200	1.63323600	-3.93754200
H	5.47056500	-0.95992600	-3.94271500
H	3.82515400	-0.62833200	-3.38014000
H	4.40961700	0.11242800	-4.87630000
H	4.52178900	2.99308900	-2.46442400
H	3.81704000	2.41443700	-3.98388600
H	3.26390400	1.74043300	-2.43876100
H	5.97436200	1.92057300	-4.91584900
H	6.79322500	2.52965300	-3.47330700
H	7.17720900	0.91240500	-4.10295500
N	3.47737200	-0.12602700	-1.00995400
C	2.91070600	-1.25735900	-0.88742700

C	1.40100800	-1.27381000	-1.06028000
H	1.17472600	-0.56437900	-1.86304100
C	0.74782400	-2.57378800	-1.46866400
O	-0.37562800	-2.62154500	-1.92576200
O	1.49260200	-3.65642300	-1.26755800
C	0.88727500	-4.90888100	-1.62040300
H	1.65021100	-5.66399500	-1.44858100
H	0.01571000	-5.08960600	-0.98833300
H	0.58292400	-4.89512000	-2.66732400
C	3.71840200	-2.52365200	-0.62729200
O	3.51908100	-3.00745500	0.59062000
O	4.47238900	-2.98657200	-1.44822700
C	4.21680600	-4.22092700	0.89395800
H	5.29488800	-4.05585300	0.84573000
H	3.91013300	-4.48762500	1.90281600
H	3.93484500	-5.00002500	0.18284800
C	-0.19622900	4.06544400	1.92994900
C	0.78257100	4.86175700	2.79337200
C	1.03089500	4.28597400	4.18672000
C	0.23781200	2.61751500	1.63241200
C	1.55446000	2.84996200	4.15500300
C	-0.09337700	1.66202900	2.75480400
H	-1.19104900	4.04978100	2.39572100
H	1.74302100	4.92051100	2.26409900
H	0.11179200	4.30831100	4.78531200
H	2.32738000	2.73926400	3.38639700
H	1.31384700	2.58881100	1.41848500
H	-0.31124400	4.57882700	0.97069800
H	0.41538000	5.88891400	2.88690500
H	1.76644600	4.91040700	4.70399300
H	-0.27313200	2.26079100	0.73415600
H	2.02520100	2.59590100	5.10699600
C	0.10174700	1.08009100	5.13048700
H	0.10167200	1.76273500	5.98555400
H	0.84942200	0.29908400	5.31845500
C	-1.27424000	0.46980200	4.92840100
H	-1.48558500	-0.23604600	5.73438900
H	-2.03728200	1.25470700	4.95194200
C	-1.29724300	-0.22473200	3.57505200
H	-2.28167200	-0.65284200	3.36635900
H	-0.57126900	-1.04992600	3.56821800
N	-0.97406300	0.72515400	2.51501300
N	0.50277600	1.84960900	3.94657000
H	-1.02610300	0.22446800	1.22537800

M5(RS)

C	-2.79799700	0.49482100	-1.36938000
C	-4.93031500	0.17283000	-1.65067100
C	-3.69769800	-1.91459200	-1.23894900
H	-2.67900800	-2.25148900	-1.44485800
N	-4.76805500	1.46435500	-1.73576800
N	-3.43527100	1.64818300	-1.55534500
N	-3.73928200	-0.45766400	-1.41902600
C	-6.11974100	-0.69808000	-1.89554100
H	-6.89837300	-0.13668400	-2.41008000
H	-6.51684500	-1.08942800	-0.95076700
C	-4.69812400	-2.61174600	-2.23059200
O	-5.67316000	-1.72464200	-2.76220400
C	-5.10424500	-3.36035800	0.03406700
C	-4.19658200	-2.30739100	0.13795400
C	-3.87184100	-1.74874900	1.37168800
C	-4.45773800	-2.28666900	2.51583100
C	-5.35043700	-3.35603800	2.41971800
C	-5.68370200	-3.89677400	1.17967600
C	-5.32307600	-3.75440500	-1.40424800
H	-3.19768000	-0.89931800	1.45760900
H	-5.79980500	-3.76018100	3.32083700
H	-6.39438100	-4.71394700	1.10604600
H	-6.37805800	-3.87300000	-1.66584800
H	-4.81914100	-4.69944800	-1.63120600
C	-2.89052700	2.98266200	-1.46634700
C	-2.91865400	3.60559600	-0.21541300
C	-2.41070200	3.58139100	-2.63028200
C	-2.42098500	4.90556500	-0.15670700
C	-1.91552900	4.87953100	-2.50986000
C	-1.91123900	5.55121300	-1.28665200
H	-2.43288900	5.42723900	0.79720000
H	-1.52823000	5.37598400	-3.39533600
C	-2.42427700	2.84907400	-3.94366900
H	-3.42901000	2.48937600	-4.18479200
H	-1.75793200	1.98189900	-3.90276800
H	-2.09072900	3.50369900	-4.74948400
C	-3.44594500	2.90551900	1.00928200
H	-2.72613300	2.17048400	1.39656400
H	-4.38713100	2.38817400	0.80067500
H	-3.62546000	3.63184000	1.80412100
H	-4.16102700	-2.98081400	-3.10415700

C	-1.37260200	6.95301000	-1.17143500
H	-2.15043200	7.63924400	-0.82464400
H	-0.55553900	6.99403700	-0.44459800
H	-0.99713800	7.31494800	-2.12994800
C	0.71551300	-3.33965600	2.85705000
C	0.35494500	-2.64700000	1.70442500
C	0.96616800	-1.43077700	1.38800400
C	1.93398200	-0.91479400	2.25036500
C	2.29740400	-1.60470700	3.40486300
C	1.68977000	-2.82127700	3.70892100
H	0.23400300	-4.28381700	3.09073100
H	-0.40969300	-3.06584200	1.05251100
H	2.40906200	0.03492600	2.01107000
H	3.05474600	-1.19152400	4.06465500
H	1.96973500	-3.36157200	4.60748400
C	0.63141900	-0.70075900	0.10488800
H	1.10557100	0.28649900	0.13374800
C	-0.87576800	-0.48510900	-0.00421400
C	-1.30025800	0.37132900	-1.14291900
O	-0.57941000	1.06433400	-1.82227800
H	-1.43716500	-1.42067900	0.00406200
H	-4.22527800	-1.86564100	3.48827500
C	5.64215600	0.38256000	-1.80755700
C	4.77704000	-0.18981600	-0.84655300
C	5.24540400	-0.55078300	0.42205300
C	6.58094800	-0.37516300	0.76556100
C	7.45345700	0.16244500	-0.17045500
C	6.98089400	0.52737900	-1.43049000
H	4.54080400	-0.95407800	1.14473900
H	6.92744000	-0.65524200	1.75482700
H	8.50108800	0.30762000	0.07183700
H	7.68942600	0.94430200	-2.13554500
C	5.15782500	0.80230200	-3.20409400
C	4.60195800	-0.41593100	-3.96286000
C	4.07800000	1.89457500	-3.09086500
C	6.30269500	1.37790800	-4.04912300
H	5.36347300	-1.19810700	-4.04429700
H	3.72570500	-0.84310600	-3.47304100
H	4.31130400	-0.11497500	-4.97491300
H	4.47918300	2.77328700	-2.57556100
H	3.76621800	2.20306600	-4.09434100
H	3.19982100	1.54286400	-2.54823700
H	5.90915000	1.66571600	-5.02828700
H	6.73986600	2.27041700	-3.59068300

H	7.09819000	0.64408900	-4.21195100
N	3.38957500	-0.31716000	-1.10823800
C	2.78864100	-1.42722700	-0.96459300
C	1.27667600	-1.39329000	-1.14064400
H	1.08878300	-0.72710000	-1.98981100
C	0.56795100	-2.68626000	-1.48685100
O	-0.59790000	-2.71036200	-1.82764800
O	1.31733200	-3.77492000	-1.39050700
C	0.67191400	-5.01790200	-1.71162200
H	1.44862400	-5.77562300	-1.64687400
H	-0.12312200	-5.21568500	-0.99088700
H	0.25475100	-4.97155300	-2.71776700
C	3.55284500	-2.71421900	-0.67669200
O	3.29839900	-3.18550400	0.53577000
O	4.32178200	-3.19991900	-1.46955500
C	3.96166000	-4.40964800	0.87367300
H	5.04388000	-4.27148300	0.83848700
H	3.63388300	-4.64844900	1.88278300
H	3.67067700	-5.19603100	0.17424500
C	0.25287500	4.15043800	1.93968000
C	1.51812400	4.73187800	2.57151900
C	1.93705500	4.08865200	3.89353800
C	0.34414700	2.65519100	1.58796400
C	2.15885100	2.57783500	3.78335900
C	0.05653500	1.74484100	2.76167200
H	-0.61163500	4.30715200	2.59918600
H	2.34305100	4.62083000	1.85449900
H	1.18138700	4.27173300	4.66803100
H	2.73109800	2.34627400	2.87636400
H	1.33509100	2.43884500	1.16624200
H	0.04421300	4.70102500	1.01669100
H	1.37916700	5.80784300	2.72105800
H	2.86709100	4.55502300	4.23603300
H	-0.39281900	2.41176600	0.81627900
H	2.76324800	2.22508300	4.62333900
C	0.60914800	1.15336200	5.08916500
H	0.86740200	1.84946100	5.89547100
H	1.23346400	0.25743800	5.20873700
C	-0.86299700	0.78475500	5.15320100
H	-1.04209000	0.12279700	6.00401300
H	-1.46695000	1.68800000	5.29312600
C	-1.25324300	0.12404300	3.83554600
H	-2.31450600	-0.14544500	3.83887300
H	-0.68111100	-0.80898800	3.70741300

N	-1.00437400	1.00621800	2.70301500
N	0.92470000	1.79758800	3.81383700
H	-1.17934800	0.07421400	0.90856300

TS5(SR)

C	0.06322900	-2.10838700	-0.65003800
C	1.17149800	-3.90433500	-1.19181300
C	2.60057000	-2.06724300	-0.39201800
H	2.50974800	-0.97972500	-0.40798300
N	-0.07985600	-4.20994000	-1.38827200
N	-0.76111800	-3.07665800	-1.04304100
N	1.29376000	-2.62529800	-0.73300400
C	2.44858600	-4.63452600	-1.46383300
H	2.27046800	-5.47380300	-2.13511600
H	2.88150600	-5.00428800	-0.52590000
C	3.67420800	-2.53896700	-1.42498400
O	3.30275300	-3.72143100	-2.12954900
C	4.44341000	-2.94647000	0.82685900
C	3.10385400	-2.58426800	0.93594200
C	2.41345800	-2.67620300	2.13899600
C	3.10122600	-3.14714500	3.25534400
C	4.44908600	-3.50448600	3.15852700
C	5.13025100	-3.40552600	1.94641700
C	4.94860400	-2.72142900	-0.57691000
H	1.37198300	-2.37342800	2.20416600
H	4.97037800	-3.86793600	4.03842200
H	6.17627900	-3.68800700	1.87652300
H	5.55870900	-3.53863200	-0.97004800
H	5.54787600	-1.80255400	-0.61399300
C	-2.20280900	-3.09489300	-1.02451200
C	-2.84552900	-3.11254600	0.21471000
C	-2.87484800	-3.19209600	-2.24802800
C	-4.23730600	-3.21601900	0.20528100
C	-4.26059800	-3.31327400	-2.19854600
C	-4.95569900	-3.32561400	-0.98502000
H	-4.76768200	-3.22319700	1.15465900
H	-4.81292300	-3.39188800	-3.13138800
C	-2.12984100	-3.19002200	-3.55591700
H	-1.56781200	-4.11925500	-3.68560400
H	-1.41253800	-2.36524400	-3.60671600
H	-2.82747800	-3.09000400	-4.38802700
C	-2.07646700	-3.05831600	1.50832100
H	-1.55895600	-2.10268500	1.63976500

H	-1.32048700	-3.84959100	1.55113000
H	-2.75320300	-3.18670500	2.35476700
H	3.80532900	-1.78702800	-2.20427200
C	-6.45944900	-3.40591900	-0.97617400
H	-6.83917900	-3.64584300	0.01902800
H	-6.89349100	-2.44691800	-1.28230600
H	-6.81768300	-4.16229400	-1.67875900
C	-3.16215200	2.77132900	-3.64454100
C	-2.13155000	2.17352500	-2.92240900
C	-2.04216100	2.33920000	-1.53702200
C	-2.98864900	3.13840600	-0.89314400
C	-4.02087700	3.73739400	-1.61126800
C	-4.11431000	3.54897100	-2.98898000
H	-3.22101600	2.62832200	-4.71872800
H	-1.39510500	1.56859500	-3.44658300
H	-2.91807700	3.28145000	0.18170300
H	-4.75416300	4.34807700	-1.09359500
H	-4.92050300	4.01182200	-3.54883800
C	-0.94140700	1.65519800	-0.74256700
H	-1.07814200	1.90784600	0.31444300
C	-1.07510800	0.13764300	-0.90910500
C	-0.18959200	-0.69492300	-0.14475600
O	0.38666000	-0.41946800	0.90330500
H	-1.18177500	-0.19478900	-1.94462400
H	2.58869300	-3.23475300	4.20765700
C	5.02125100	1.28869700	-0.06062000
C	3.68603500	1.10201300	0.36925100
C	3.40156900	0.55490900	1.62551400
C	4.42562800	0.18260100	2.48905600
C	5.74233000	0.36781400	2.09364700
C	6.02286300	0.92049300	0.84334500
H	2.36420400	0.36685100	1.88971800
H	4.18783900	-0.27417300	3.44441300
H	6.55947600	0.07890300	2.74674900
H	7.06227000	1.05808900	0.57155100
C	5.36579400	1.88110000	-1.43595000
C	4.90316500	0.92524000	-2.55094200
C	4.70194900	3.25966700	-1.61553500
C	6.87857600	2.08004600	-1.60071400
H	5.43495700	-0.03013500	-2.47562200
H	3.82855100	0.74091100	-2.49901500
H	5.13367900	1.36047800	-3.52936800
H	4.96652200	3.92575600	-0.78810300
H	5.05538000	3.71437400	-2.54685600

H	3.61432600	3.19079700	-1.66911900
H	7.07441800	2.50418900	-2.58964200
H	7.28149100	2.77034900	-0.85292700
H	7.42349600	1.13366000	-1.53213900
N	2.61221600	1.34344900	-0.52746700
C	1.57174000	1.98045700	-0.17330500
C	0.45691700	2.19051400	-1.18072100
H	0.77495700	1.70840800	-2.10859200
C	0.38578700	3.68473600	-1.47168900
O	0.68781400	4.19932300	-2.52031700
O	-0.04688200	4.35941300	-0.40206300
C	-0.18817500	5.77531700	-0.57581200
H	-0.53173200	6.15816700	0.38229500
H	0.77097800	6.21807800	-0.84871700
H	-0.92295400	5.97810700	-1.35722700
C	1.41851600	2.68295700	1.17148300
O	2.35427000	3.61925400	1.30150500
O	0.55657700	2.44852400	1.98297000
C	2.29390300	4.37612300	2.51848700
H	2.45826100	3.71830500	3.37398900
H	3.08581700	5.11731800	2.44468100
H	1.31830900	4.85736400	2.60788000
C	-2.76964600	1.63770300	3.15635200
C	-3.68408400	1.64115100	4.38221900
C	-5.15556500	1.35055900	4.08590900
C	-2.70606000	0.28521200	2.42072500
C	-5.37883000	0.01196000	3.37834100
C	-3.84526000	0.12297700	1.44169700
H	-3.08812100	2.41353000	2.44762000
H	-3.31524100	0.88841100	5.09194800
H	-5.58763800	2.14639900	3.46581400
H	-4.77859200	-0.77451100	3.84975100
H	-2.69803900	-0.53443700	3.14855800
H	-1.75389800	1.89893400	3.46603100
H	-3.60298000	2.61000900	4.88569600
H	-5.71264400	1.34020500	5.02856800
H	-1.77323400	0.22701200	1.85532900
H	-6.42181300	-0.29681500	3.47628300
C	-6.25284500	0.09144400	1.03641300
H	-7.06424900	0.61593900	1.54843600
H	-6.59298200	-0.93317900	0.83031700
C	-5.88252000	0.80489600	-0.25447800
H	-6.70888400	0.74359700	-0.96677800
H	-5.68901500	1.86257800	-0.04292700

C	-4.62281000	0.16978800	-0.82379600
H	-4.25319200	0.74049700	-1.68366800
H	-4.83365000	-0.84741500	-1.17210200
N	-3.56362300	0.13670800	0.17415800
N	-5.10103400	0.05463600	1.94087500
H	-2.21792800	-0.02388700	-0.36831600

M5(SR)

C	-0.44638400	2.28047600	-0.54399600
C	-1.80150400	3.95727800	-0.81437900
C	-2.90940000	1.91059100	0.00190200
H	-2.69308200	0.85173300	-0.14074000
N	-0.62705600	4.40955400	-1.16603800
N	0.20556400	3.34908100	-0.99199400
N	-1.72399300	2.65418600	-0.42158400
C	-3.17490300	4.54671700	-0.87396800
H	-3.17790500	5.44716600	-1.48621200
H	-3.52684300	4.79030600	0.13634200
C	-4.14701700	2.32620300	-0.86022000
O	-3.99255400	3.58280300	-1.51289100
C	-4.68224200	2.43448800	1.49666800
C	-3.30793100	2.22247900	1.42428200
C	-2.49913600	2.24840400	2.55499200
C	-3.10179200	2.49590800	3.78684800
C	-4.48134500	2.70445800	3.87098500
C	-5.28126600	2.67458100	2.72945200
C	-5.32263600	2.30242300	0.13764600
H	-1.42963900	2.07353700	2.47927900
H	-4.93461300	2.89559000	4.83823500
H	-6.35199300	2.83819600	2.80115600
H	-6.03948000	3.09350700	-0.09653100
H	-5.84467900	1.34018700	0.06320900
C	1.62273400	3.45683000	-1.22322200
C	2.47897000	3.38926000	-0.12238300
C	2.05937200	3.60075800	-2.54544100
C	3.84633600	3.46241300	-0.38603100
C	3.43435000	3.66036700	-2.74781700
C	4.33970300	3.58622100	-1.68406700
H	4.53864200	3.41536800	0.45051500
H	3.81008400	3.76297600	-3.76229300
C	1.08721500	3.68140300	-3.69234300
H	0.53205900	4.62310700	-3.66864400
H	0.35289000	2.87032500	-3.65604800

H	1.61874600	3.61821300	-4.64218800
C	1.97549700	3.21193500	1.28532900
H	1.79816200	2.15194500	1.50089500
H	1.05014000	3.76456700	1.46976400
H	2.72790100	3.55665200	1.99645400
H	-4.28847600	1.61304200	-1.67330000
C	5.82183000	3.61028700	-1.94657800
H	6.38252900	3.82660400	-1.03514600
H	6.15448700	2.63757100	-2.32403800
H	6.07617600	4.35910300	-2.70036300
C	3.77187000	-1.81024800	-3.70644200
C	2.65540600	-1.34646000	-3.01337600
C	2.43301000	-1.72393400	-1.68600500
C	3.33854600	-2.59423800	-1.07420200
C	4.45060300	-3.06612100	-1.76665900
C	4.67436400	-2.66906100	-3.08381100
H	3.93247300	-1.50283200	-4.73465600
H	1.95527300	-0.68855200	-3.52184800
H	3.16835300	-2.89552400	-0.04399500
H	5.14647900	-3.73846000	-1.27438100
H	5.54375200	-3.03095200	-3.62283800
C	1.21252400	-1.23952400	-0.91920300
H	1.34354100	-1.50911300	0.13315500
C	1.13323800	0.29076400	-1.01640600
C	0.07042600	0.90501100	-0.17389700
O	-0.43416900	0.40267500	0.80606100
H	1.03446400	0.64479800	-2.04778900
H	-2.49658000	2.52633400	4.68651700
C	-4.75202900	-1.84259900	-0.38919200
C	-3.46855700	-1.50428800	0.10166600
C	-3.29723600	-1.04939600	1.41491300
C	-4.38402500	-0.90750500	2.27064000
C	-5.64948600	-1.24875800	1.81480900
C	-5.81525200	-1.71866200	0.51102500
H	-2.30490200	-0.74890800	1.74088800
H	-4.23537800	-0.50955900	3.26982600
H	-6.51446000	-1.14624400	2.46185700
H	-6.81550100	-1.98360900	0.19155500
C	-4.97956600	-2.32724900	-1.82940100
C	-4.67100800	-1.18404500	-2.81402100
C	-4.09631900	-3.54996100	-2.14281700
C	-6.43692400	-2.75213400	-2.05843000
H	-5.35966500	-0.34832200	-2.64729400
H	-3.64513000	-0.82752400	-2.70449600

H	-4.80984900	-1.53414500	-3.84248000
H	-4.24580700	-4.33637900	-1.39630400
H	-4.36960700	-3.95336000	-3.12320000
H	-3.03538800	-3.29790700	-2.17100200
H	-6.54659500	-3.09639700	-3.09058500
H	-6.72874600	-3.57373700	-1.39667800
H	-7.13358200	-1.92151500	-1.91155400
N	-2.35365600	-1.48384200	-0.77851400
C	-1.23923100	-2.00852300	-0.46674800
C	-0.08408300	-1.93457500	-1.45139100
H	-0.45623200	-1.41294700	-2.33750800
C	0.23960900	-3.35529400	-1.89977600
O	0.14768800	-3.75895500	-3.03233700
O	0.64752500	-4.09860000	-0.86718700
C	1.06757700	-5.43138000	-1.18738000
H	1.33253900	-5.89347500	-0.23940800
H	0.25616900	-5.97609800	-1.67130500
H	1.93366800	-5.38998600	-1.85116000
C	-1.01149200	-2.81011900	0.80915400
O	-1.81365900	-3.86833700	0.83987600
O	-0.20745200	-2.52189100	1.66217300
C	-1.68504600	-4.69579800	2.00479900
H	-1.93800000	-4.12098400	2.89746800
H	-2.38453600	-5.51566400	1.86313600
H	-0.66206100	-5.06727300	2.08537500
C	2.52850100	-1.58492500	3.34287300
C	3.26563800	-1.73910400	4.67425000
C	4.77722900	-1.52648700	4.60162900
C	2.62288500	-0.18349300	2.71075500
C	5.15714700	-0.15907600	4.02885200
C	3.88612000	0.00771000	1.90006600
H	2.90030200	-2.32205000	2.61798900
H	2.84671900	-1.01627500	5.38795000
H	5.24509600	-2.30437700	3.98442300
H	4.53452700	0.62265000	4.47859400
H	2.52875400	0.58631600	3.48763900
H	1.47089200	-1.81631500	3.49488800
H	3.05973200	-2.73391600	5.08355700
H	5.20049300	-1.61802500	5.60781100
H	1.79162800	-0.05029300	2.01392500
H	6.19072600	0.08448500	4.28983900
C	6.33374100	-0.26453200	1.85097200
H	6.91862800	-1.03104600	2.37253200
H	6.91555300	0.66690000	1.87779500

C	6.06164900	-0.68583100	0.41701200
H	6.98409000	-0.64374200	-0.16786900
H	5.69459800	-1.71773400	0.40013900
C	4.98760100	0.22905300	-0.16102400
H	4.74307500	-0.05680000	-1.19156700
H	5.37229300	1.25887800	-0.19599200
N	3.76187000	0.17646300	0.62550100
N	5.07457100	-0.08434100	2.57362000
H	2.09571000	0.66452800	-0.61114400

TS5(SS)

C	-0.88745000	-1.47736700	0.58614900
C	-2.67509500	-2.36781400	1.45066700
C	-2.94988000	-1.71801700	-0.92528200
H	-2.56876600	-0.85867700	-1.48096000
N	-1.78454000	-2.41397800	2.40099500
N	-0.67325600	-1.85423300	1.84758700
N	-2.16070200	-1.80632900	0.31695200
C	-4.12388100	-2.72753500	1.45136300
H	-4.49715200	-2.77950300	2.47361400
H	-4.27968400	-3.69693000	0.95823100
C	-4.48366200	-1.55478900	-0.59068600
O	-4.78970300	-1.67525000	0.78755200
C	-4.13075000	-3.51914500	-1.97507900
C	-2.86160400	-3.01972800	-1.69405800
C	-1.71094400	-3.69753200	-2.08959300
C	-1.85357800	-4.90029900	-2.77607200
C	-3.12456400	-5.40652300	-3.06291100
C	-4.26976300	-4.71971400	-2.66803800
C	-5.21154600	-2.60993600	-1.45486600
H	-0.72854800	-3.28890400	-1.87450900
H	-3.21907800	-6.34611500	-3.59749800
H	-5.25571900	-5.11641500	-2.88948300
H	-5.96180700	-3.13305100	-0.85379800
H	-5.74283400	-2.12242100	-2.27831900
C	0.57529700	-1.91758400	2.56907500
C	1.50668800	-2.87735200	2.15989300
C	0.75576500	-1.08802800	3.67914100
C	2.66542900	-2.99879400	2.92300000
C	1.94206700	-1.24164100	4.39467100
C	2.90302500	-2.18790400	4.03388000
H	3.40383100	-3.74332700	2.63610800
H	2.11385500	-0.60937100	5.26159000

C	-0.26238100	-0.05431500	4.08108300
H	-0.21358200	0.82044600	3.42086200
H	-0.06640900	0.29090700	5.09719700
H	-1.27860100	-0.45569400	4.04700600
C	1.28286600	-3.73795600	0.94499700
H	0.26904500	-4.14845600	0.91213500
H	1.98758400	-4.57025400	0.93744500
H	1.45031200	-3.16108300	0.02709100
H	-4.79728400	-0.54182000	-0.83579000
C	4.19338600	-2.30074100	4.80011800
H	4.58964300	-3.31744200	4.76111400
H	4.94744500	-1.63359700	4.36708200
H	4.06073100	-2.01446200	5.84538100
C	3.91421000	3.10004000	1.54601300
C	2.83716400	2.31568100	1.13483200
C	2.60819900	2.07400100	-0.22262600
C	3.50079900	2.62380800	-1.15324000
C	4.57058800	3.41755300	-0.74606100
C	4.77882000	3.66153300	0.60978500
H	4.07416700	3.27353300	2.60547300
H	2.16875200	1.90293200	1.88142300
H	3.34622200	2.43667700	-2.21282900
H	5.24461600	3.83400800	-1.48792400
H	5.61295400	4.27509500	0.93400600
C	1.43474800	1.25389300	-0.73910100
H	1.76417400	0.80775800	-1.68406200
C	1.03582300	0.10947500	0.18495200
C	0.03028000	-0.75243200	-0.37689100
O	-0.17332000	-0.96526500	-1.57068500
H	0.81191400	0.41748300	1.20875400
H	-0.97185700	-5.44757300	-3.09208100
C	-4.41227200	1.92452300	0.06348100
C	-3.12355200	1.49888900	0.46047000
C	-2.90190400	0.95822500	1.73140400
C	-3.93845200	0.82074500	2.64661400
C	-5.21235400	1.22812800	2.27819900
C	-5.43005800	1.77068700	1.01198100
H	-1.89335400	0.64654500	1.99108100
H	-3.74711000	0.39618500	3.62729000
H	-6.04352700	1.12836600	2.96799800
H	-6.43551800	2.08832500	0.76513200
C	-4.68117700	2.59616300	-1.29512500
C	-3.88932700	3.91502400	-1.37982800
C	-4.29087900	1.68382700	-2.47345700

C	-6.16643900	2.94309900	-1.46708900
H	-4.13799500	4.56781500	-0.53757900
H	-2.81011200	3.75234200	-1.37225300
H	-4.14750100	4.43514900	-2.30818400
H	-4.93358600	0.79772600	-2.51180800
H	-4.43509300	2.23007800	-3.41139700
H	-3.24862800	1.36573700	-2.42160100
H	-6.31196400	3.39268900	-2.45331700
H	-6.80022900	2.05262100	-1.40843000
H	-6.50714300	3.66489800	-0.71876300
N	-2.03224600	1.52453400	-0.44695800
C	-0.97031300	2.17524100	-0.18400200
C	0.17023900	2.11532800	-1.17241600
H	-0.24544800	1.62460100	-2.05515700
C	0.59366400	3.51862200	-1.54240900
O	0.50689300	4.47350300	-0.80289000
O	1.10944600	3.56741300	-2.76930800
C	1.66875300	4.83322100	-3.14863600
H	2.04523900	4.69841000	-4.15972000
H	0.90076800	5.60703100	-3.12153200
H	2.47968700	5.09572000	-2.46554400
C	-0.82417800	2.99831300	1.08430300
O	-1.71233600	3.97547100	1.14229100
O	-0.02558300	2.72948100	1.95316500
C	-1.70951400	4.73753200	2.35846000
H	-0.73520200	5.20632600	2.50230600
H	-2.48590400	5.48829800	2.23570400
H	-1.93288200	4.08335200	3.20331100
C	3.34590700	-0.82190100	-3.32073200
C	4.50010700	-1.21784700	-4.24211200
C	5.87473400	-1.18531000	-3.57581000
C	3.12682400	-1.76467100	-2.12245100
C	5.96089600	-2.08439300	-2.34184200
C	4.02271800	-1.44332800	-0.95211200
H	3.51128100	0.19664400	-2.94571800
H	4.31474800	-2.23159300	-4.62135900
H	6.13362200	-0.16033100	-3.28114200
H	5.50142000	-3.05722800	-2.54579100
H	3.27366000	-2.80737100	-2.42973300
H	2.41843600	-0.79697900	-3.90116000
H	4.50482000	-0.55418200	-5.11249800
H	6.63114400	-1.51254400	-4.29637800
H	2.09546200	-1.68121100	-1.77495000
H	7.00521100	-2.28106200	-2.08805800

C	6.29529900	-0.88235100	-0.19449200
H	7.02656500	-0.31313400	-0.77820800
H	6.83703700	-1.67185500	0.34038100
C	5.55604000	0.02442700	0.77432500
H	6.22010500	0.31151100	1.59295800
H	5.22531400	0.93365300	0.26289000
C	4.33716400	-0.73186400	1.28550800
H	3.75167900	-0.14115500	1.99767400
H	4.65973600	-1.64386400	1.80460300
N	3.46770600	-1.08876700	0.17280400
N	5.35800600	-1.49981800	-1.14141200
H	2.15152300	-0.60493900	0.22682200

M5(SS)

C	-1.02854500	-1.45013900	0.73843100
C	-2.81164300	-2.33947300	1.60017400
C	-3.08004800	-1.71364800	-0.78211600
H	-2.68530500	-0.86607300	-1.34926200
N	-1.92986700	-2.34592700	2.56368200
N	-0.82358400	-1.78551700	2.01250200
N	-2.29202400	-1.79981100	0.45986700
C	-4.25324200	-2.72595300	1.58363400
H	-4.63722000	-2.79489300	2.60078000
H	-4.38382900	-3.69292300	1.07889600
C	-4.60897900	-1.51013800	-0.44680000
O	-4.92891600	-1.67653800	0.92469200
C	-4.30718700	-3.46884500	-1.84776900
C	-3.02456300	-3.02290600	-1.53993200
C	-1.89465600	-3.74807000	-1.90900500
C	-2.07282700	-4.94465200	-2.59794200
C	-3.35703400	-5.39693000	-2.91272200
C	-4.48126100	-4.66271900	-2.54303200
C	-5.35861600	-2.51234900	-1.35240100
H	-0.89857800	-3.38804000	-1.67133400
H	-3.47909300	-6.33332400	-3.44739500
H	-5.47785500	-5.01847100	-2.78543900
H	-6.15683100	-3.00186400	-0.78653700
H	-5.83100900	-1.98611400	-2.18814600
C	0.41942300	-1.75663000	2.74868000
C	1.40665100	-2.67976500	2.39043200
C	0.56337600	-0.83148500	3.78745300
C	2.59112300	-2.65169600	3.12227400
C	1.77621100	-0.83997500	4.47350900

C	2.79842600	-1.73575800	4.15416900
H	3.37493200	-3.36116500	2.87003200
H	1.92091700	-0.12839900	5.28198800
C	-0.50803600	0.16643000	4.13886600
H	-0.44706700	1.04725300	3.48732000
H	-0.37368400	0.51343800	5.16455100
H	-1.50946900	-0.26211900	4.05396700
C	1.24003900	-3.63744900	1.24179200
H	0.21470700	-4.00353800	1.14179300
H	1.89635000	-4.49866100	1.37531700
H	1.53962800	-3.14974000	0.30572400
H	-4.89086300	-0.47803300	-0.65341700
C	4.11481300	-1.69461900	4.88222500
H	4.54033300	-2.69511400	4.98590900
H	4.83423400	-1.08650500	4.32229600
H	4.00637300	-1.25398100	5.87511000
C	4.03012000	2.88150100	1.60507800
C	2.92447100	2.13454000	1.19926500
C	2.67570600	1.91304600	-0.15712800
C	3.57667500	2.43770000	-1.09421500
C	4.66916900	3.20125800	-0.69205400
C	4.89737300	3.42906300	0.66367800
H	4.20776600	3.03940000	2.66417700
H	2.25485600	1.73231800	1.95209200
H	3.41368600	2.25132500	-2.15256300
H	5.34914000	3.60233500	-1.43707200
H	5.75159200	4.01719900	0.98292400
C	1.47453000	1.13022700	-0.66454200
H	1.81162100	0.57666700	-1.54689700
C	0.98257900	0.09672100	0.34744700
C	-0.06524400	-0.79713000	-0.22705000
O	-0.21459300	-1.04196800	-1.40413200
H	0.61251500	0.56298600	1.26749900
H	-1.20797000	-5.52949600	-2.89230600
C	-4.34962000	2.05053600	-0.16612300
C	-3.10509300	1.59625700	0.32617500
C	-2.97703500	1.10986500	1.63064100
C	-4.06978800	1.05407100	2.48745400
C	-5.30182300	1.49663300	2.02767800
C	-5.42391500	1.98936000	0.72861700
H	-1.99887400	0.77268200	1.96407500
H	-3.95380600	0.66464100	3.49405600
H	-6.17414100	1.46316600	2.67139000
H	-6.39877000	2.33518300	0.40802000

C	-4.51933400	2.62403500	-1.58296700
C	-3.66101100	3.89293800	-1.74108600
C	-4.12237000	1.58857600	-2.65195400
C	-5.97634200	3.02217700	-1.85562000
H	-3.91410200	4.62817200	-0.97106000
H	-2.59226800	3.68409700	-1.66855900
H	-3.85031100	4.34091900	-2.72214200
H	-4.76972500	0.70579400	-2.59773400
H	-4.25186600	2.02947700	-3.64576100
H	-3.08239100	1.27244500	-2.55349800
H	-6.05194600	3.40729300	-2.87627500
H	-6.65457900	2.16735000	-1.76940900
H	-6.31788500	3.80929600	-1.17661300
N	-1.96845800	1.52954000	-0.52130700
C	-0.90117000	2.16969800	-0.25604300
C	0.27438200	2.01667600	-1.19545700
H	-0.12803800	1.51057700	-2.07579700
C	0.75967400	3.39042900	-1.60868200
O	0.70066900	4.37093500	-0.90172800
O	1.28025000	3.37812900	-2.83280100
C	1.88961800	4.60881100	-3.25131900
H	2.27639800	4.42154400	-4.25012200
H	1.14839100	5.40884200	-3.26648000
H	2.69873000	4.86847100	-2.56483900
C	-0.76613100	3.06568800	0.96314500
O	-1.62371300	4.06857300	0.93871500
O	0.00895000	2.82416000	1.86167000
C	-1.60081900	4.92609200	2.09097100
H	-0.61002500	5.36805900	2.20398500
H	-2.34762700	5.69250300	1.90058600
H	-1.85409100	4.35130500	2.98347400
C	3.27909600	-1.07955000	-3.23590500
C	4.35965800	-1.40457200	-4.26806900
C	5.78806600	-1.32470500	-3.73022700
C	3.21588600	-2.04901800	-2.04124200
C	6.02386500	-2.23649200	-2.52388000
C	4.18937700	-1.69577900	-0.94019500
H	3.43671900	-0.06097200	-2.85581300
H	4.18398100	-2.41893900	-4.65165600
H	6.03007700	-0.29391400	-3.44015200
H	5.58583800	-3.22405700	-2.70911300
H	3.37137900	-3.07873200	-2.38697500
H	2.30261900	-1.08328400	-3.73194000
H	4.25571600	-0.72581000	-5.12107900

H	6.48615400	-1.60653200	-4.52600400
H	2.22222300	-2.00785600	-1.58926100
H	7.09571300	-2.39757100	-2.37906700
C	6.50664900	-1.05719700	-0.39735100
H	7.17445000	-0.45736800	-1.02729900
H	7.11996500	-1.82524000	0.09353100
C	5.81542700	-0.18095800	0.63378700
H	6.53133500	0.13292100	1.39824800
H	5.41475000	0.71712500	0.15233400
C	4.65553200	-0.96436400	1.23532000
H	4.12171600	-0.36069200	1.97863100
H	5.04151000	-1.85152300	1.76218000
N	3.70214800	-1.36886300	0.21085100
N	5.51787800	-1.69851500	-1.26464100
H	1.84957800	-0.55272400	0.59971000

TS6(RR)

C	-0.16129200	-1.99741200	-0.69170400
C	-1.21500800	-3.85517100	-0.26963500
C	-2.68994700	-1.89265700	-0.20261400
H	-2.53247600	-0.84256500	0.03990600
N	0.02063200	-4.20853800	-0.48821000
N	0.66610900	-3.04548800	-0.75263700
N	-1.36917100	-2.50307400	-0.40234400
C	-2.38024800	-4.62080500	0.26839700
H	-2.04755200	-5.57980300	0.66308900
H	-3.14078000	-4.78618700	-0.50424500
C	-3.44232000	-2.59353400	0.98804300
O	-2.86828700	-3.84269500	1.34842700
C	-4.84219300	-2.56043900	-0.98872700
C	-3.59049200	-2.10598600	-1.39942700
C	-3.29521900	-1.90766800	-2.74412000
C	-4.28986400	-2.15920600	-3.68596600
C	-5.55134900	-2.60076600	-3.28027200
C	-5.83576200	-2.80649100	-1.93178400
C	-4.90310600	-2.71978600	0.50822000
H	-2.31117900	-1.58033200	-3.06672400
H	-6.31544700	-2.79392400	-4.02603000
H	-6.81261300	-3.16345100	-1.62106900
H	-5.32294200	-3.67806900	0.82677100
H	-5.50675300	-1.92721300	0.96360800
C	2.08064800	-3.06611100	-1.04582800
C	2.52826700	-2.61534000	-2.29212000

C	2.93661900	-3.54559300	-0.04958500
C	3.90466500	-2.61714700	-2.50843700
C	4.30325300	-3.53278900	-0.32596500
C	4.80567700	-3.06335500	-1.53971700
H	4.28082100	-2.26299600	-3.46504300
H	4.99205700	-3.88966200	0.43580300
C	2.42831200	-4.03465500	1.27945300
H	1.64643700	-3.37900700	1.67067000
H	3.24347500	-4.06789900	2.00440200
H	2.00243500	-5.03790000	1.19357900
C	1.59968200	-2.11832200	-3.36927100
H	1.47281000	-1.03157100	-3.30259100
H	0.61388900	-2.58942800	-3.32465400
H	2.02501800	-2.32851500	-4.35192700
H	-3.36055000	-1.98267500	1.88813200
C	6.28662800	-3.04830800	-1.81252100
H	6.54474000	-3.78543700	-2.57894200
H	6.60467400	-2.06920700	-2.18128800
H	6.85729800	-3.28087300	-0.91129600
C	-3.20990400	3.71762400	-2.92874400
C	-2.30122800	3.10133300	-2.07119000
C	-1.09734700	2.59112600	-2.55874500
C	-0.82450900	2.70171600	-3.92363300
C	-1.73074000	3.31556300	-4.78458900
C	-2.92856100	3.82631000	-4.28875200
H	-4.13860500	4.11568900	-2.53166400
H	-2.51982300	3.04777500	-1.00886500
H	0.11159000	2.30774500	-4.31361100
H	-1.49925000	3.39867800	-5.84193400
H	-3.63544600	4.30740400	-4.95703500
C	-0.12694900	1.83559900	-1.65893100
H	0.84304700	1.82214300	-2.17115000
C	-0.61596600	0.37879100	-1.64613200
C	0.28785500	-0.55886900	-0.90356300
O	1.41409700	-0.30183600	-0.56131700
H	-1.64282200	0.30984000	-1.28113700
H	-4.08121200	-2.01461500	-4.74036800
C	-2.05338000	-0.11162700	3.23843200
C	-2.15787700	0.62316300	2.03298800
C	-3.41565800	1.05520500	1.58414300
C	-4.57770900	0.79961000	2.30321700
C	-4.48628000	0.10821300	3.50341000
C	-3.23957400	-0.32674700	3.95073600
H	-3.47096300	1.58118200	0.63418000

H	-5.53549500	1.14070700	1.92426600
H	-5.37336800	-0.10335300	4.09078300
H	-3.20200600	-0.87001000	4.88644000
C	-0.72211100	-0.66671800	3.75744200
C	-0.10089300	-1.59675100	2.70038200
C	0.24478900	0.48162100	4.08563800
C	-0.90529900	-1.50043300	5.03309000
H	-0.82421200	-2.35920800	2.38018600
H	0.25221600	-1.03809700	1.82808000
H	0.75311000	-2.11647100	3.14642700
H	-0.13378800	1.06922900	4.92769400
H	1.22457500	0.07484400	4.36345200
H	0.37096400	1.16127400	3.24254200
H	0.07173100	-1.87191200	5.35519700
H	-1.32005800	-0.90733700	5.85329100
H	-1.55452500	-2.36564900	4.86316200
N	-1.06663600	0.86423300	1.14738100
C	-0.75780100	2.08362900	0.86374200
C	0.12336800	2.46287100	-0.26448000
H	1.42804200	2.17425400	-0.04230400
C	0.43701000	3.90970500	-0.36562500
O	0.63653400	4.53066700	-1.39072300
O	0.65083700	4.45909600	0.84988400
C	0.99406600	5.84523500	0.84746200
H	1.07456800	6.13334300	1.89408500
H	1.94558500	5.99770600	0.33416300
H	0.21837700	6.42967200	0.34788200
C	-1.33648300	3.18914200	1.75828700
O	-2.09150900	4.03923300	1.06070400
O	-1.16454900	3.24821500	2.94952500
C	-2.65034600	5.12050500	1.81859100
H	-1.85031400	5.69226000	2.29303000
H	-3.19221400	5.73430500	1.10298500
H	-3.32424800	4.73137200	2.58380400
C	3.35486500	-0.66050800	1.89193200
C	4.74256600	-1.07846500	2.37644500
C	5.88680500	-0.63624200	1.46945700
C	3.08575600	0.85289900	1.83072000
C	5.92405300	0.88048200	1.29270000
C	3.64025100	1.52914200	0.60202500
H	3.15831500	-1.08988600	0.90347200
H	4.90974500	-0.66815200	3.38181300
H	5.79403500	-1.10700600	0.48134100
H	5.76472500	1.37647100	2.25648300

H	3.47010200	1.34708300	2.73297400
H	2.61449600	-1.09010100	2.57396100
H	4.76369500	-2.16964700	2.47961200
H	6.84003200	-0.96524500	1.89652600
H	2.00626900	1.02723400	1.80707400
H	6.90589700	1.20140700	0.93523700
C	5.49212300	1.64101200	-1.02217500
H	6.07935600	0.76355300	-1.31791000
H	6.17430500	2.49880200	-0.97883800
C	4.36771100	1.90171500	-2.00812200
H	4.77355500	2.32711300	-2.92836300
H	3.85452000	0.96548200	-2.25670200
C	3.37398300	2.84435800	-1.33989000
H	2.55381600	3.11572200	-2.00485600
H	3.88005900	3.77819200	-1.05533000
N	2.82043500	2.20230200	-0.15037500
N	4.95623300	1.38839800	0.32011300
H	-0.64314800	0.02464400	-2.68785000

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C	1.93291700	0.17448300	0.01054400
C	2.85500000	2.13666200	0.20320000
C	0.51554900	2.11157600	0.94856500
H	-0.35772000	1.52362400	0.66503500
N	3.80414000	1.36103300	-0.24176600
N	3.21782800	0.13984000	-0.34934300
N	1.69414400	1.43892200	0.38693500
C	2.79236700	3.61835500	0.38998600
H	3.62454300	4.09742300	-0.12414400
H	2.82323400	3.88007100	1.45523400
C	0.38936700	3.56821800	0.37454400
O	1.59011800	4.03338400	-0.23247200
C	0.33847300	3.61626900	2.79512000
C	0.66242900	2.30705200	2.44310600
C	1.06538100	1.37889800	3.39713900
C	1.12815200	1.77938600	4.72985300
C	0.79198800	3.08587900	5.09096300
C	0.39694300	4.01257700	4.12784100
C	-0.03974600	4.42690600	1.58214200
H	1.34198200	0.36611500	3.11895200
H	0.84864800	3.38490200	6.13253000
H	0.15008900	5.03128500	4.41043500
H	0.44487000	5.40650300	1.54253000

H	-1.12240800	4.59011400	1.54349000
C	4.03767400	-1.01481200	-0.64846500
C	4.66128400	-1.65249500	0.42625300
C	4.21414700	-1.39163900	-1.98021000
C	5.48828000	-2.73447400	0.12615200
C	5.05091100	-2.47779100	-2.22361000
C	5.68973400	-3.16187400	-1.18661500
H	5.99053200	-3.24962700	0.94062900
H	5.20990900	-2.79513100	-3.25089300
C	3.51498700	-0.66508400	-3.09270400
H	3.66476200	0.41622600	-3.01656900
H	2.43865600	-0.85702000	-3.04255500
H	3.88502200	-0.99919600	-4.06281600
C	4.44622900	-1.20658200	1.84870400
H	3.47145800	-1.53814000	2.22170300
H	4.49162500	-0.11833700	1.94581700
H	5.20795200	-1.63832900	2.49898100
H	-0.35035700	3.59150200	-0.42591400
C	6.56480900	-4.35130900	-1.48224500
H	7.05703400	-4.24616500	-2.45144700
H	7.32930600	-4.48107100	-0.71352600
H	5.96526300	-5.26665900	-1.51311900
C	-3.39259500	-2.08482800	3.76238900
C	-2.80447400	-1.90193800	2.51228500
C	-1.65832300	-2.61547600	2.15517200
C	-1.11264000	-3.51276400	3.07638200
C	-1.70044700	-3.70204400	4.32494700
C	-2.84393800	-2.98550200	4.67326200
H	-4.28570300	-1.52529900	4.02422200
H	-3.24963600	-1.22337000	1.78861100
H	-0.22175400	-4.07614000	2.80626100
H	-1.26901000	-4.41210400	5.02400200
H	-3.30599300	-3.13183400	5.64449300
C	-0.95446000	-2.36524200	0.81949200
H	-0.40599700	-3.28344600	0.57515800
C	0.08734400	-1.27712700	1.08677300
C	1.00772700	-1.03370000	-0.06771000
O	1.18679100	-1.78051000	-0.99750300
H	-0.38424100	-0.34670800	1.41168900
H	1.44502200	1.07300400	5.48955900
C	-1.55376000	2.28404700	-2.32629200
C	-1.90745700	1.48356600	-1.20478300
C	-2.76636200	2.02229400	-0.22847200
C	-3.28279300	3.31028300	-0.31937100

C	-2.94587700	4.09492600	-1.41457800
C	-2.10175800	3.57100600	-2.39336300
H	-3.00523300	1.39801100	0.62988100
H	-3.93619800	3.69085900	0.46000200
H	-3.33211600	5.10375300	-1.51646500
H	-1.86288300	4.20403100	-3.23926700
C	-0.60348400	1.79516100	-3.42875800
C	0.77811600	1.49883800	-2.82609400
C	-1.14439200	0.52170700	-4.09871900
C	-0.40479500	2.84683000	-4.52929100
H	1.15985800	2.36284800	-2.26604500
H	0.71535400	0.63193400	-2.16510500
H	1.48729100	1.27382500	-3.62912400
H	-2.11994700	0.71119000	-4.55510000
H	-0.44881400	0.20040300	-4.88275200
H	-1.26167300	-0.28824100	-3.37835600
H	0.27341300	2.44137100	-5.28582000
H	-1.34614500	3.10011500	-5.02685900
H	0.04245400	3.76747200	-4.14077400
N	-1.36871300	0.20310200	-0.95200900
C	-2.20437200	-0.81993700	-0.86828900
C	-1.94213900	-2.07710300	-0.29469400
C	-2.72077000	-3.23603200	-0.62829100
O	-2.65176600	-4.32785100	-0.06687200
O	-3.55485200	-3.07433600	-1.70295900
C	-4.43809400	-4.15776100	-1.95568500
H	-5.03347800	-3.86468400	-2.82005000
H	-3.88120000	-5.07154400	-2.17430700
H	-5.08943900	-4.34160000	-1.09679300
C	-3.60901200	-0.59571700	-1.43966600
O	-4.53940900	-0.72970200	-0.48151500
O	-3.86578400	-0.25217600	-2.56811100
C	-5.88286100	-0.52438400	-0.92057300
H	-6.14128700	-1.25730900	-1.68870000
H	-6.51024500	-0.65611600	-0.04123100
H	-6.00013300	0.48141300	-1.32965900
H	0.72921800	-1.60652400	1.91888600

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C	-2.76446900	-0.19466900	-0.67893400
C	-4.19623500	1.39023900	-1.09050400
C	-1.88610100	2.22117300	-0.91064200
H	-1.01515700	1.88895200	-0.34009700

N	-4.90750400	0.29942000	-1.02411800
N	-4.00401600	-0.67840500	-0.76876300
N	-2.86891000	1.12615400	-0.89275400
C	-4.60772900	2.82479300	-1.13953600
H	-5.67646700	2.91526900	-0.95036500
H	-4.36838000	3.27606000	-2.11071300
C	-2.50523000	3.51491900	-0.24950700
O	-3.91006400	3.43568100	-0.06978700
C	-1.63976900	4.02241400	-2.46125800
C	-1.54213900	2.63965800	-2.32361100
C	-1.16593200	1.83016100	-3.39173700
C	-0.86668000	2.43367500	-4.61029600
C	-0.94550500	3.82148800	-4.74907500
C	-1.33465700	4.62379700	-3.67913800
C	-2.10015000	4.67576700	-1.18519100
H	-1.12141200	0.74952000	-3.29501700
H	-0.71209400	4.27807600	-5.70535500
H	-1.41069900	5.70040700	-3.79543400
H	-2.95236000	5.34609500	-1.33299500
H	-1.29869900	5.26984300	-0.73634100
C	-4.45289900	-2.04929400	-0.67740400
C	-4.61348300	-2.75263900	-1.87504900
C	-4.76011200	-2.57069800	0.57880000
C	-5.08802800	-4.05748800	-1.77910400
C	-5.23528900	-3.88169300	0.61491600
C	-5.40331300	-4.63566900	-0.54621900
H	-5.22061100	-4.63482800	-2.69035000
H	-5.48227300	-4.31989400	1.57838700
C	-4.57408300	-1.77878000	1.84418700
H	-4.73073700	-0.70905100	1.67942400
H	-3.55981100	-1.92158000	2.23238500
H	-5.27960800	-2.11135400	2.60729100
C	-4.29068300	-2.12417500	-3.20512100
H	-3.22151300	-1.90698000	-3.29860200
H	-4.83214200	-1.18343000	-3.34027900
H	-4.56601800	-2.79705600	-4.01772800
H	-2.10853100	3.63294300	0.75987300
C	-5.94814600	-6.03809500	-0.48209100
H	-7.01975500	-6.04092300	-0.70523900
H	-5.45852500	-6.68314000	-1.21525300
H	-5.81166300	-6.47116100	0.51055400
C	3.33336300	-1.15657100	-3.39857600
C	2.41994000	-0.91160400	-2.37535000
C	1.89415600	-1.95785000	-1.61369600

C	2.28260900	-3.26411200	-1.92255600
C	3.18827900	-3.51698900	-2.95115300
C	3.72399000	-2.46325700	-3.68792000
H	3.72922400	-0.32936900	-3.98115000
H	2.09946500	0.10846000	-2.17804800
H	1.87972400	-4.08295000	-1.33566800
H	3.47719000	-4.53934200	-3.17443800
H	4.43296200	-2.65656500	-4.48669500
C	0.85906700	-1.70363200	-0.52607700
H	0.41335800	-2.67912000	-0.30137900
C	-0.27476000	-0.84466100	-1.09357700
C	-1.55712300	-1.05487700	-0.34418400
O	-1.73937000	-1.92752200	0.46940600
H	-0.02716700	0.22071500	-1.13415400
H	-0.57565700	1.82167900	-5.45700300
C	-0.47126800	2.81333400	2.70337500
C	-0.73191200	1.52448800	2.17817300
C	-1.98553800	0.92883400	2.37868400
C	-3.00436000	1.57950300	3.06553700
C	-2.76550300	2.84445900	3.58189500
C	-1.51190100	3.42931100	3.40911200
H	-2.14901400	-0.07681000	2.00163500
H	-3.96505900	1.09304300	3.20257400
H	-3.53914100	3.37652700	4.12493400
H	-1.34826500	4.40810900	3.84269800
C	0.86555400	3.53911100	2.49941600
C	2.05515400	2.65572700	2.91768000
C	0.96127800	3.94982700	1.01962200
C	0.95623600	4.82412300	3.33542500
H	1.94314100	2.34027900	3.95913500
H	2.15752200	1.76161700	2.30324800
H	2.98207800	3.23414700	2.83154000
H	0.18504300	4.68894700	0.79445300
H	1.93211800	4.41235800	0.80860900
H	0.83563200	3.09402700	0.35157600
H	1.93699500	5.28071000	3.17415700
H	0.20093200	5.56066800	3.04634900
H	0.85227300	4.61788900	4.40538100
N	0.19686100	0.82975000	1.34824400
C	0.63083900	-0.32987200	1.69754700
C	1.46438500	-1.18538200	0.81167900
H	2.58085100	-0.37182800	0.56543200
C	2.09023500	-2.31653100	1.52814300
O	2.26474700	-3.44243700	1.10462400

O	2.56126100	-1.93959200	2.74548500
C	3.11279700	-2.98818000	3.54235400
H	3.34389800	-2.53899800	4.50667500
H	2.38848600	-3.79741500	3.65867800
H	4.01995700	-3.38408100	3.07883500
C	0.31509900	-0.82406500	3.11455600
O	-0.25821700	-2.02871000	3.07959400
O	0.51849000	-0.19267600	4.12070000
C	-0.61327100	-2.56569500	4.36085000
H	-1.33994400	-1.91371500	4.84957400
H	-1.04429400	-3.54449500	4.16433500
H	0.27505800	-2.65220200	4.98975300
C	5.38464100	-2.35039000	-0.34984900
C	6.77658100	-2.33036600	-0.98057900
C	7.16513000	-1.00099200	-1.63025800
C	5.18237000	-1.28824700	0.74240200
C	7.13729100	0.18876100	-0.66468700
C	4.82442600	0.05393100	0.16221000
H	4.61915700	-2.20608800	-1.11852600
H	7.51979700	-2.56976700	-0.20783500
H	6.49658100	-0.77850100	-2.47253600
H	7.57191400	-0.08788300	0.30159400
H	6.08032200	-1.19709900	1.36351500
H	5.20275900	-3.33556400	0.09123500
H	6.83836100	-3.12540500	-1.73159600
H	8.17757100	-1.08903400	-2.03768900
H	4.37149000	-1.56863500	1.41053200
H	7.74759500	1.00544500	-1.05391400
C	5.50049600	2.01426900	-1.14381400
H	6.12889300	2.07159900	-2.03592900
H	5.77676200	2.84508900	-0.48368300
C	4.03325500	2.08668600	-1.52851400
H	3.79007900	3.09083300	-1.88307800
H	3.84864100	1.38182500	-2.34327300
C	3.18383400	1.72661700	-0.31875300
H	2.12200300	1.64091800	-0.57866600
H	3.25849700	2.51992400	0.43371900
N	3.58828100	0.46177200	0.28005200
N	5.79178300	0.74311200	-0.47246200
H	-0.48000300	-1.16183600	-2.12624900

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C	-1.33401500	-1.18054500	0.13953300
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C	-1.18985700	-3.08722500	-0.90999200
C	0.99831300	-2.23973900	-0.19870800
H	1.40351900	-1.23085100	-0.09512600
N	-2.46355400	-2.81495700	-0.88295500
N	-2.54076200	-1.63205900	-0.22416600
N	-0.46167000	-2.10907100	-0.29415500
C	-0.44409500	-4.18502500	-1.59273100
H	-1.09251400	-4.68837600	-2.30912700
H	-0.07153900	-4.91655200	-0.86364600
C	1.58183100	-2.92092000	-1.49554200
O	0.59984400	-3.55261200	-2.30380800
C	2.33896100	-4.09420100	0.48989900
C	1.39520800	-3.16844000	0.92955400
C	0.93035200	-3.17623200	2.24120400
C	1.44561700	-4.12251300	3.12418300
C	2.40765500	-5.03941300	2.69447200
C	2.85800000	-5.03414100	1.37610000
C	2.64254100	-3.91601700	-0.97457500
H	0.17122600	-2.47430600	2.57530700
H	2.79925200	-5.77130300	3.39332400
H	3.59196900	-5.76008800	1.03999000
H	2.58615700	-4.85092000	-1.54009800
H	3.64835800	-3.50900900	-1.12404600
C	-3.85366400	-1.10591100	0.07573800
C	-4.50367500	-1.62077200	1.19835700
C	-4.41756300	-0.16827100	-0.78790300
C	-5.78975600	-1.14946100	1.45464100
C	-5.70803800	0.26462100	-0.48933300
C	-6.40631800	-0.21400100	0.62096900
H	-6.32195200	-1.52376500	2.32539400
H	-6.17644600	0.99838800	-1.14012100
C	-3.64924500	0.38180800	-1.95683200
H	-3.15068900	-0.41305500	-2.52089000
H	-2.88258200	1.08304100	-1.60445200
H	-4.31527400	0.91601500	-2.63668100
C	-3.83497900	-2.63235400	2.09122000
H	-2.90362500	-2.23865900	2.51327600
H	-3.58490700	-3.54249900	1.53775700
H	-4.49054200	-2.90321300	2.91939000
H	2.01409800	-2.16071500	-2.14470800
C	-7.81121800	0.25052800	0.90271700
H	-8.53804800	-0.45270800	0.48388000
H	-7.99661200	0.31478700	1.97725300
H	-7.99982000	1.22934100	0.45712600

C	4.03775300	2.15953600	2.87954600
C	2.82237800	2.14301000	2.19863200
C	1.63474400	1.83569300	2.86435000
C	1.68965600	1.55135700	4.23223900
C	2.90136700	1.57164100	4.91874600
C	4.08222000	1.87443600	4.24260600
H	4.95115700	2.39930100	2.34261500
H	2.78380200	2.37182400	1.13859500
H	0.77024400	1.32009400	4.76640600
H	2.92294700	1.35660000	5.98276500
H	5.02748100	1.89243800	4.77581100
C	0.30317000	1.76803600	2.12630800
H	-0.45471800	2.15574100	2.81417600
C	-0.03333000	0.26600000	1.90602400
C	-1.16886200	0.09546900	0.94413100
O	-2.06406600	0.90192900	0.83325200
H	0.84413400	-0.30008800	1.59644000
H	1.09453000	-4.14869200	4.15011000
C	2.56240600	0.29505000	-2.45310400
C	1.26749600	0.51905400	-1.90700000
C	0.13787500	0.14468500	-2.65417200
C	0.24050300	-0.42972300	-3.91624800
C	1.50009200	-0.63395900	-4.46379600
C	2.63083800	-0.26524200	-3.73436600
H	-0.83888600	0.31930900	-2.21037200
H	-0.65657900	-0.71409600	-4.45832800
H	1.61319200	-1.07890100	-5.44698600
H	3.60023800	-0.43762100	-4.18685000
C	3.84651900	0.64709000	-1.68429800
C	3.91607000	2.16674000	-1.45282400
C	3.89093600	-0.10294100	-0.33942000
C	5.10996700	0.24554300	-2.45789100
H	4.03270700	2.68781800	-2.40872400
H	3.01208200	2.55074100	-0.97969500
H	4.77995200	2.40956800	-0.82283900
H	3.87405500	-1.18787900	-0.50647600
H	4.82234900	0.13509100	0.18700200
H	3.05398100	0.17498900	0.30265500
H	5.98892500	0.51498100	-1.86455300
H	5.14744700	-0.83355400	-2.64194600
H	5.18591800	0.76486000	-3.41810300
N	1.08609500	0.99450100	-0.59393100
C	0.50896300	2.16666400	-0.37931700
C	0.19993600	2.64125000	0.89669500

C	-0.30900600	3.96378400	1.14822700
O	-0.72511500	4.37926700	2.22680000
O	-0.26994100	4.79697700	0.06740500
C	-0.83860100	6.08485100	0.26479200
H	-0.72311500	6.61039300	-0.68252600
H	-1.89707300	6.00932500	0.52640700
H	-0.31789400	6.62137000	1.06080800
C	0.13650800	2.97871900	-1.60903400
O	-1.18226400	2.91619800	-1.84053500
O	0.92260700	3.51027700	-2.35620300
C	-1.61445800	3.56908400	-3.03612100
H	-1.12554600	3.12397000	-3.90567200
H	-2.69169500	3.42123700	-3.08548000
H	-1.37492000	4.63369000	-2.99059400
H	-0.37119500	-0.14885700	2.86665300

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C	-0.02182600	2.53407000	0.26381800
C	1.10073900	3.37136600	1.92576600
C	2.39843100	1.79816100	0.52769400
H	2.10069300	0.94079300	-0.07536200
N	-0.09152700	3.89747600	2.02287300
N	-0.78075600	3.35986800	0.97893000
N	1.17915300	2.53979000	0.84626300
C	2.28712300	3.37124300	2.83693300
H	2.02196600	3.77730700	3.81180600
H	3.10928300	3.95584600	2.40605800
C	3.09945400	1.32491100	1.84744200
O	2.63045800	2.00497200	3.00740000
C	4.67386800	2.48189100	0.41362700
C	3.42505600	2.64734200	-0.17843400
C	3.24357700	3.44107400	-1.30558200
C	4.35646100	4.08723100	-1.83813000
C	5.61567100	3.92660300	-1.25231700
C	5.78484000	3.12332300	-0.12637800
C	4.60533200	1.53244200	1.58317300
H	2.26361100	3.54787000	-1.76271000
H	6.47277500	4.43553400	-1.68136400
H	6.76571300	3.00135600	0.32256600
H	5.10106100	1.90334300	2.48464600
H	5.06550600	0.57337600	1.31724700
C	-2.12548900	3.77216800	0.65765600
C	-2.28779100	4.62125900	-0.44223700

C	-3.18636800	3.28757500	1.42827100
C	-3.59279900	4.97315600	-0.78073700
C	-4.46784300	3.67745400	1.04621200
C	-4.69033200	4.50683900	-0.05504000
H	-3.75357600	5.63400000	-1.62793400
H	-5.31572400	3.31920000	1.62424500
C	-2.98688100	2.35070500	2.59071600
H	-3.79243100	2.47625600	3.31600000
H	-2.03792900	2.51906600	3.10457600
H	-3.01758500	1.30677200	2.25406800
C	-1.11084600	5.12895000	-1.23550700
H	-0.71293800	4.35861200	-1.90593600
H	-0.29671500	5.46011100	-0.58437500
H	-1.41393000	5.97292200	-1.85585800
H	2.86073200	0.27539500	2.03592500
C	-6.09333900	4.87630900	-0.45621100
H	-6.71205900	5.07451600	0.42202800
H	-6.10252600	5.75930000	-1.09752500
H	-6.55861300	4.05357300	-1.00810800
C	-5.54459900	-0.79353500	-0.76523800
C	-4.16428500	-0.64801300	-0.69281800
C	-3.40445200	-0.45474600	-1.85171300
C	-4.05800900	-0.39249400	-3.07997600
C	-5.44293400	-0.53869200	-3.15784400
C	-6.19001300	-0.74101600	-2.00162000
H	-6.11909000	-0.95186000	0.14231000
H	-3.66561100	-0.71627500	0.27313400
H	-3.47686900	-0.23966200	-3.98570800
H	-5.93607600	-0.49218400	-4.12396300
H	-7.26781100	-0.85464800	-2.05982400
C	-1.89797400	-0.25509900	-1.77408800
H	-1.55290400	0.01766800	-2.77916100
C	-1.72000600	0.99282300	-0.88109200
C	-0.38850400	1.67118200	-0.93192800
O	0.42154000	1.60490500	-1.82467900
H	-1.97421200	0.77697300	0.16223600
H	4.24714000	4.71687400	-2.71477800
C	3.62723300	-1.94927600	-0.47149500
C	2.66679000	-1.14201400	-1.12948200
C	3.07123600	-0.14007400	-2.02003700
C	4.41721200	0.13114900	-2.23995400
C	5.37447800	-0.62495700	-1.57894500
C	4.97119400	-1.65544500	-0.72980600
H	2.30571000	0.46284200	-2.50099000

H	4.70333500	0.94300600	-2.90173100
H	6.43176200	-0.42667500	-1.72160400
H	5.74329900	-2.24578300	-0.25172500
C	3.24103700	-3.14274800	0.41722300
C	2.38823100	-2.68871500	1.61124200
C	2.45288400	-4.17320200	-0.41105900
C	4.47720600	-3.85260400	0.98604200
H	2.94881700	-1.97925300	2.23210300
H	1.45626900	-2.22342300	1.28240800
H	2.13950400	-3.55378300	2.23805400
H	3.04446200	-4.50462100	-1.27080100
H	2.23516500	-5.04834700	0.21269400
H	1.50674700	-3.77706900	-0.78556800
H	4.14867200	-4.68613100	1.61364400
H	5.11227700	-4.26293500	0.19509700
H	5.08267000	-3.18498300	1.60770000
N	1.28719900	-1.20876400	-0.79360000
C	0.36950100	-1.48458900	-1.63456700
C	-1.09791300	-1.49288400	-1.27886500
H	-1.12441800	-1.44751800	0.28306900
C	-1.54002600	-2.84086700	-1.63752900
O	-0.76111400	-3.78853700	-1.75554500
O	-2.86945800	-3.04728100	-1.75076800
C	-3.27033500	-4.38974000	-2.01016600
H	-4.35316400	-4.35457700	-2.12209900
H	-2.80397300	-4.76577500	-2.92261300
H	-2.99842900	-5.04483400	-1.17845700
C	0.67713900	-1.88309800	-3.08116400
O	1.72309900	-2.69141800	-3.20359600
O	0.00600500	-1.49799900	-4.01321000
C	2.04934500	-3.07742900	-4.54286900
H	2.32607500	-2.19945000	-5.12975400
H	2.89079500	-3.76131600	-4.45679100
H	1.19629800	-3.57221400	-5.01023700
C	-1.31425100	-4.63608800	1.59555500
C	-1.36312600	-5.41425800	2.91161400
C	-1.00534000	-4.60798600	4.16300300
C	-2.25145800	-3.41381500	1.58549700
C	-1.90006800	-3.38750700	4.40173000
C	-1.59659500	-2.23893700	2.25919800
H	-0.29237600	-4.29938200	1.37564000
H	-2.37753400	-5.81516000	3.03785300
H	0.03706300	-4.26747500	4.11886000
H	-2.95097000	-3.63044800	4.21403000

H	-3.19629300	-3.65241700	2.08348900
H	-1.60105000	-5.29986000	0.77515800
H	-0.69339400	-6.27729600	2.84309300
H	-1.08922400	-5.26413600	5.03517700
H	-2.49948900	-3.11641700	0.56680400
H	-1.83501600	-3.06796200	5.44217100
C	-0.85151800	-1.09459100	4.26662100
H	-0.47019500	-1.44992500	5.22468500
H	-1.59617400	-0.31414700	4.46407800
C	0.28368400	-0.56574900	3.40442400
H	0.72715000	0.32752100	3.85171200
H	1.05818700	-1.33406100	3.33672800
C	-0.25526700	-0.23622900	2.02003000
H	0.55824900	-0.10310700	1.29611800
H	-0.83311200	0.69582700	2.07536000
N	-1.09415700	-1.30372300	1.48654400
N	-1.50416300	-2.22431100	3.59255400
H	-2.43930100	1.76277300	-1.20332400

M6(R')

C	-0.67461000	-1.63760500	-0.01983600
C	-2.40984600	-2.36608900	1.06709800
C	-2.92449000	-0.54413000	-0.52035300
H	-2.34371500	0.30142800	-0.89151100
N	-1.42734500	-3.12941200	1.45794000
N	-0.35017900	-2.66527600	0.76617300
N	-1.98520000	-1.44961100	0.14625100
C	-3.82359900	-2.24029200	1.53366200
H	-3.94718800	-2.72199500	2.50274500
H	-4.51458400	-2.69290200	0.81071100
C	-4.02952900	-0.08217600	0.49754300
O	-4.04752300	-0.85266100	1.69594600
C	-5.05510600	-1.06321900	-1.46917800
C	-3.68440000	-1.26516700	-1.61053700
C	-3.16013200	-2.03360600	-2.64447600
C	-4.04600100	-2.61830600	-3.54615400
C	-5.42324200	-2.42341200	-3.41103200
C	-5.93730000	-1.64345900	-2.37713400
C	-5.35673300	-0.18070400	-0.28436800
H	-2.08670200	-2.16575900	-2.74817100
H	-6.10128400	-2.88626800	-4.12080100
H	-7.00829100	-1.49654200	-2.27663700
H	-6.14874100	-0.57109800	0.36136600

H	-5.66409900	0.81820100	-0.61243900
C	0.89595400	-3.39288000	0.75679200
C	1.18102800	-4.15430600	-0.38209700
C	1.76048700	-3.28054200	1.84768900
C	2.41678900	-4.79725700	-0.42071300
C	2.97966300	-3.94813400	1.75712800
C	3.33072800	-4.69375200	0.62955300
H	2.66929500	-5.39398700	-1.29295700
H	3.67683200	-3.87564900	2.58763900
C	1.42312800	-2.43723500	3.04596300
H	2.03335600	-2.73294300	3.90053700
H	0.36968000	-2.52499500	3.32156600
H	1.62694100	-1.38065300	2.84020700
C	0.21198600	-4.26439200	-1.53179600
H	0.24477100	-3.37421100	-2.17036000
H	-0.81738400	-4.39251100	-1.18379700
H	0.46798900	-5.12118000	-2.15594800
H	-3.82184800	0.93214000	0.83369500
C	4.68112400	-5.35300800	0.54125200
H	5.02765700	-5.67611600	1.52506400
H	4.65780700	-6.21806500	-0.12420600
H	5.41826300	-4.64660500	0.14584300
C	5.45292000	0.94850600	1.13170100
C	4.20510800	1.11620700	0.53355800
C	3.83610500	0.34564400	-0.57036200
C	4.73899900	-0.60176300	-1.05908100
C	5.98700000	-0.77242700	-0.46512900
C	6.34864300	0.00410900	0.63471900
H	5.72557000	1.55678200	1.98880500
H	3.50812600	1.85841000	0.91514100
H	4.45890000	-1.20863400	-1.91774100
H	6.67956100	-1.50762800	-0.86383700
H	7.32142200	-0.12485800	1.09846900
C	2.43496400	0.44634400	-1.17521300
H	2.50845700	0.07938900	-2.20818200
C	1.60727700	-0.57910700	-0.39998600
C	0.24145700	-0.85041900	-0.94585700
O	-0.16741800	-0.60907200	-2.05696300
H	1.51465700	-0.30096800	0.65507600
H	-3.66512300	-3.22692800	-4.35938900
C	-1.74658200	2.35670200	1.87887100
C	-1.36897900	2.24325800	0.51121200
C	-2.25564000	2.72747200	-0.47160300
C	-3.45761800	3.34922800	-0.15292800

C	-3.80948500	3.49756200	1.18309200
C	-2.95851500	2.99713400	2.16785000
H	-1.97051800	2.60462300	-1.51190700
H	-4.10883700	3.70816100	-0.94435200
H	-4.73794800	3.98365000	1.46462900
H	-3.26194100	3.11694800	3.20080300
C	-0.88018600	1.79698800	3.01570300
C	-0.79624500	0.26791400	2.87764200
C	0.53566800	2.39930300	2.98903700
C	-1.47648500	2.09546900	4.39861400
H	-1.80067500	-0.17289500	2.85201000
H	-0.26608600	0.00495200	1.95839500
H	-0.25484900	-0.15393800	3.73108000
H	0.48979300	3.49012300	3.06826400
H	1.11075000	2.01717700	3.84042000
H	1.06056500	2.14482500	2.06770500
H	-0.81449700	1.68276100	5.16564000
H	-1.56726400	3.17132400	4.57899000
H	-2.46191300	1.63716600	4.52928600
N	-0.17322600	1.61250300	0.11106800
C	0.69548400	2.31160700	-0.61233000
C	1.89195300	1.86227600	-1.18589000
C	2.74239800	2.83990200	-1.82785400
O	2.70594400	4.06359200	-1.72116100
O	3.68881400	2.25766300	-2.61988300
C	4.65242400	3.14542900	-3.16938200
H	5.35145100	2.52284900	-3.72697100
H	4.18233700	3.87235700	-3.83584500
H	5.17819400	3.68581800	-2.37806300
C	0.35844400	3.78411200	-0.85341600
O	0.53435700	4.49766000	0.26383700
O	-0.12323200	4.23235000	-1.86767800
C	0.11676900	5.85978600	0.17486000
H	-0.94936400	5.91085700	-0.05956400
H	0.31416700	6.30027000	1.15036800
H	0.68136000	6.37889700	-0.60249700
H	2.14841800	-1.53486300	-0.43310500

TS6(SS)

C	0.45601000	-2.18966000	-0.33939000
C	-0.44679500	-3.89559300	0.65103900
C	-2.09873700	-2.23157700	-0.16578800
H	-2.04655800	-1.13936900	-0.21717400

N	0.83591200	-4.14347500	0.65523200
N	1.38613100	-3.06995200	0.03134200
N	-0.71952900	-2.70962900	0.03178000
C	-1.59349100	-4.61612200	1.28000300
H	-1.23300200	-5.30229400	2.04539400
H	-2.15613900	-5.17849100	0.52252400
C	-3.01512100	-2.71286400	1.02700000
O	-2.37784500	-3.62323900	1.90623600
C	-3.93364400	-3.46322600	-1.09030600
C	-2.71598200	-2.86130400	-1.39857200
C	-2.20482300	-2.88714100	-2.69468400
C	-2.94180100	-3.52774200	-3.68698700
C	-4.16702100	-4.12803000	-3.38422000
C	-4.67084000	-4.09908300	-2.08670100
C	-4.27739800	-3.30888300	0.36614500
H	-1.25779000	-2.41279200	-2.92814800
H	-4.72888000	-4.62495100	-4.16826100
H	-5.61987400	-4.57065900	-1.85163700
H	-4.54027300	-4.25543500	0.84831900
H	-5.12765600	-2.63260600	0.49913500
C	2.77350200	-3.06519900	-0.37224800
C	3.03602100	-3.30149400	-1.72674000
C	3.76969300	-2.80985000	0.57460400
C	4.36578100	-3.23150100	-2.13733200
C	5.08093500	-2.75585900	0.10729900
C	5.39590600	-2.94544300	-1.23989400
H	4.60001100	-3.41024000	-3.18294700
H	5.87789400	-2.55516500	0.81843200
C	3.46645000	-2.56007200	2.02777900
H	3.25570600	-1.49801900	2.20599300
H	4.33083100	-2.82548700	2.63845100
H	2.61310500	-3.14834800	2.37278100
C	1.93718500	-3.60514000	-2.71375900
H	1.17582600	-4.26434200	-2.28669100
H	2.35255300	-4.09419000	-3.59544400
H	1.43923900	-2.69080200	-3.05778900
H	-3.25213300	-1.86295600	1.66481700
C	6.82059000	-2.82923200	-1.71146300
H	6.95759700	-3.30945300	-2.68182900
H	7.09822400	-1.77540600	-1.81435000
H	7.50943600	-3.28233600	-0.99509100
C	5.51662700	2.24121700	-0.48765800
C	4.20191000	1.84326600	-0.25812700
C	3.26506000	1.86548400	-1.29685000

C	3.66951000	2.28314600	-2.56432400
C	4.98492300	2.68243600	-2.79455800
C	5.91264800	2.66350300	-1.75622900
H	6.23415300	2.22214000	0.32679200
H	3.89437000	1.52294600	0.73562900
H	2.94619100	2.30628800	-3.37534900
H	5.28260400	3.01192500	-3.78508800
H	6.93653400	2.97669900	-1.93267100
C	1.83572800	1.38539700	-1.06484900
H	1.28259000	1.55474900	-1.99703200
C	1.93322900	-0.13669400	-0.85623300
C	0.65220200	-0.88574100	-1.07960200
O	-0.21023300	-0.57811200	-1.86924700
H	2.34895900	-0.36540200	0.13258500
H	-2.56105400	-3.56068600	-4.70209600
C	-1.92088400	-0.10408400	2.99618800
C	-0.68833600	-0.30526600	2.33037100
C	0.17910300	-1.32369200	2.73993200
C	-0.12892800	-2.16609800	3.80092800
C	-1.33120700	-1.98275200	4.46864000
C	-2.19621900	-0.96745100	4.06537800
H	1.12016300	-1.43079800	2.21050700
H	0.56450100	-2.94768000	4.09632000
H	-1.60566300	-2.62327600	5.29986400
H	-3.12205700	-0.84922100	4.61464200
C	-2.88621700	1.04486400	2.65117000
C	-2.22828600	2.38473200	3.02849700
C	-3.24855400	1.06348600	1.15586600
C	-4.20162600	0.93508500	3.43557800
H	-1.88875500	2.37085300	4.06826400
H	-1.36370700	2.60115400	2.39605800
H	-2.95475500	3.19659800	2.91450200
H	-3.77408500	0.14605900	0.86315000
H	-3.93081600	1.89827500	0.95486600
H	-2.36414700	1.18832200	0.52801500
H	-4.87103900	1.73835400	3.11525900
H	-4.70776600	-0.01825800	3.24980800
H	-4.04824200	1.04367300	4.51310000
N	-0.30716800	0.47300900	1.20173300
C	0.68580300	1.28557200	1.28275400
C	1.12408100	2.09461900	0.12598400
H	-0.06652600	2.62891600	-0.40466800
C	1.73423300	3.36439700	0.55037800
O	1.91831200	3.73491400	1.70138700

O	1.97350900	4.17347100	-0.49957700
C	2.65469700	5.38926800	-0.19541900
H	2.79027600	5.90157100	-1.14610000
H	2.06336700	6.00189100	0.48820500
H	3.62397100	5.17352200	0.26090800
C	1.49957200	1.34902300	2.57028700
O	0.83396300	1.79736100	3.61997500
O	2.62792000	0.90253000	2.60335300
C	1.53809100	1.73075600	4.86682300
H	2.45034600	2.32687500	4.81279200
H	0.85688900	2.13422800	5.61211900
H	1.78973500	0.69298300	5.09437500
C	-2.95418300	0.97720800	-2.52831500
C	-4.15795500	1.34678100	-3.39398200
C	-4.82366600	2.66887600	-3.01521900
C	-1.78899600	1.97977800	-2.58537900
C	-3.87243800	3.86406700	-3.09928100
C	-1.95523500	3.18866300	-1.70401300
H	-3.27244000	0.85218100	-1.48629200
H	-3.83329700	1.40687200	-4.44146400
H	-5.23301500	2.61865500	-1.99829300
H	-3.26592900	3.80484800	-4.00969900
H	-1.63086500	2.31069600	-3.61962700
H	-2.56577900	0.00616000	-2.85280000
H	-4.89610100	0.53987300	-3.34133500
H	-5.66480300	2.85272700	-3.69139400
H	-0.87468300	1.48511800	-2.26364300
H	-4.44088100	4.79389800	-3.16467400
C	-3.31486100	5.12136200	-1.02643700
H	-4.40216300	5.14947000	-0.90675100
H	-3.00457900	6.06451100	-1.49202800
C	-2.63596100	4.92989000	0.31867300
H	-2.72642700	5.84190900	0.91219600
H	-3.12416000	4.11713700	0.86409000
C	-1.17730600	4.56514500	0.08693400
H	-0.66504600	4.35202400	1.03096900
H	-0.64421400	5.39793700	-0.39092600
N	-1.08068900	3.37870700	-0.75397600
N	-2.99675700	4.01102400	-1.93148900
H	2.64202200	-0.54393000	-1.59109400

M6(R)

C	0.73358300	-1.41463800	0.03699000
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C	2.25763600	-1.83085400	-1.46183700
C	3.12087200	-0.54326400	0.44893600
H	2.67197200	0.21926000	1.08662800
N	1.18067400	-2.41872000	-1.90585600
N	0.24339200	-2.16138300	-0.95478800
N	2.02509900	-1.20401100	-0.27569100
C	3.62255400	-1.70065200	-2.05429500
H	3.59310800	-1.92188200	-3.12066100
H	4.31451700	-2.39652000	-1.56044500
C	4.14040400	0.10677000	-0.55501500
O	4.00839800	-0.35266800	-1.89427100
C	5.30225800	-1.36937000	0.97357100
C	3.94349200	-1.55786000	1.21912400
C	3.49479700	-2.57739100	2.05384100
C	4.43811900	-3.41012400	2.65147200
C	5.80205800	-3.21951800	2.41702300
C	6.24320300	-2.19876300	1.57771700
C	5.53132900	-0.21651900	0.03159200
H	2.43556800	-2.72360400	2.23765200
H	6.52426100	-3.87827800	2.88819800
H	7.30293100	-2.05867000	1.38825100
H	6.23425200	-0.44619000	-0.77395400
H	5.92263800	0.65277600	0.57025000
C	-1.07170500	-2.73479200	-1.09634200
C	-1.42481600	-3.80274100	-0.26232100
C	-1.90846300	-2.21178300	-2.08081000
C	-2.71090400	-4.31471300	-0.40446100
C	-3.18241500	-2.77219500	-2.18692500
C	-3.60553500	-3.80379600	-1.35163400
H	-3.02191000	-5.13545800	0.23673700
H	-3.85596800	-2.38486300	-2.94702600
C	-1.46709600	-1.11529700	-3.00624200
H	-0.71528400	-0.47092600	-2.54927600
H	-2.31339100	-0.47951800	-3.26897100
H	-1.03685000	-1.53820100	-3.92005100
C	-0.47685900	-4.34837900	0.77344600
H	0.54630200	-4.41824100	0.39328700
H	-0.79400100	-5.34396100	1.08612100
H	-0.45962000	-3.71822400	1.67130800
H	3.95796600	1.17981400	-0.61795800
C	-5.00184400	-4.35842200	-1.45298400
H	-4.98983000	-5.45113400	-1.47551500
H	-5.59644500	-4.05573600	-0.58537400
H	-5.50663800	-3.99714500	-2.35090700

C	-4.99414500	0.11270100	3.66825500
C	-3.89817000	-0.23197200	2.87833100
C	-3.11428800	0.75220600	2.27505500
C	-3.45833700	2.09222300	2.48012400
C	-4.55022100	2.44231200	3.26819000
C	-5.32408300	1.45028900	3.86892200
H	-5.59321300	-0.66948400	4.12439600
H	-3.67384800	-1.28200300	2.71642900
H	-2.85792000	2.86535100	2.00567800
H	-4.79512400	3.48955100	3.41652000
H	-6.17617700	1.71789300	4.48544900
C	-1.89061400	0.46203900	1.41310200
H	-1.09891800	1.11683300	1.80136800
C	-1.36512600	-0.98764500	1.59994800
C	0.11549300	-1.02227400	1.36198900
O	0.90962300	-0.77309300	2.24619300
H	-1.93291500	-1.66302600	0.96036300
H	4.11008700	-4.21323300	3.30274600
C	1.97878800	3.20665600	-0.09088800
C	1.28517000	2.16293800	-0.76938900
C	1.72954200	1.76149000	-2.03969600
C	2.79881800	2.38092700	-2.67656500
C	3.46938000	3.40963400	-2.03040400
C	3.05787600	3.80006900	-0.75461800
H	1.20764300	0.94332700	-2.52667900
H	3.11365100	2.04071300	-3.65787700
H	4.31168200	3.90611100	-2.50139100
H	3.60166600	4.60414700	-0.27345600
C	1.55920800	3.68962900	1.30736500
C	0.09743400	4.17529100	1.29822100
C	1.72791700	2.55041400	2.32786500
C	2.41966000	4.86567400	1.79137900
H	-0.03324600	4.98148100	0.56870100
H	-0.59638800	3.37270200	1.04607400
H	-0.16528700	4.56508100	2.28820300
H	2.77997600	2.24548600	2.38580200
H	1.42391600	2.89193800	3.32389300
H	1.12257800	1.68490000	2.05485900
H	2.07845900	5.16801900	2.78592500
H	3.47671900	4.59363100	1.87194500
H	2.33381300	5.73368200	1.12998000
N	0.22319100	1.47819700	-0.15391600
C	-0.98169200	1.46817100	-0.68556200
C	-2.06902900	0.86421400	-0.03119200

C	-3.27611300	0.60486600	-0.75873800
O	-3.60465700	1.06587200	-1.85369300
O	-4.08762600	-0.28239000	-0.11613700
C	-5.35977800	-0.49790400	-0.70703100
H	-5.89576000	-1.16309200	-0.02961300
H	-5.90428600	0.44317400	-0.81814400
H	-5.26290100	-0.96554800	-1.69006500
C	-1.26785400	2.24655800	-1.96697200
O	-1.78261600	3.44070900	-1.64557800
O	-1.00888700	1.92039200	-3.10125200
C	-2.11707000	4.26969800	-2.76046100
H	-2.87461300	3.77678200	-3.37338800
H	-2.50739600	5.19428900	-2.34018700
H	-1.23320400	4.46830600	-3.36943900
H	-1.47356100	-1.29286600	2.64482400

TS7(S')

C	-1.51165100	-0.10367300	-0.33645200
C	-3.20213000	1.19663700	0.16322300
C	-1.08359100	2.39531300	0.15516100
H	-0.03170400	2.15245800	0.28923900
N	-3.74115300	0.05593600	-0.14361300
N	-2.68496200	-0.74373200	-0.47022700
N	-1.83975600	1.14602000	0.03838500
C	-3.78927000	2.44073500	0.74930200
H	-4.75938600	2.21985200	1.19410300
H	-3.90979300	3.22065700	-0.01246500
C	-1.60363700	3.22084900	1.38005400
O	-2.90980300	2.82998200	1.78910400
C	-1.56968200	4.60456000	-0.60155000
C	-1.32041600	3.30304300	-1.03377300
C	-1.31220000	2.97536200	-2.38439400
C	-1.54941200	3.98548900	-3.31459000
C	-1.78801900	5.29390000	-2.88942400
C	-1.80136800	5.61278700	-1.53209000
C	-1.54501900	4.68658500	0.90459300
H	-1.13610300	1.95563300	-2.71514300
H	-1.97376900	6.06960500	-3.62510600
H	-2.00150300	6.62888800	-1.20635100
H	-2.37673800	5.25737800	1.32629100
H	-0.61509200	5.14950800	1.25282200
C	-3.00287800	-2.05280800	-1.00466300
C	-2.72872300	-2.32089900	-2.35210800

C	-3.69472000	-2.94901400	-0.18661400
C	-3.11549000	-3.56135300	-2.85118700
C	-4.05004500	-4.18155800	-0.73709800
C	-3.76191900	-4.51131000	-2.05859300
H	-2.90840000	-3.78816400	-3.89425400
H	-4.57836800	-4.89503800	-0.10967700
C	-4.11167300	-2.61867300	1.22031800
H	-5.11440300	-2.17963900	1.22598900
H	-3.43906400	-1.90311300	1.68666300
H	-4.13374300	-3.52366600	1.83134300
C	-2.03274400	-1.34476900	-3.26013000
H	-0.95278500	-1.51557400	-3.22844200
H	-2.22604800	-0.30472200	-2.97999300
H	-2.37007600	-1.48167500	-4.28893600
H	-0.97591900	3.03860700	2.25148400
C	-4.12987800	-5.85796500	-2.62335700
H	-4.90589900	-6.33985400	-2.02529500
H	-4.48820800	-5.76840400	-3.65176800
H	-3.25766000	-6.51925800	-2.63627800
C	4.72139200	1.90243700	-2.61175300
C	3.91143400	1.02360300	-1.89661700
C	3.01532500	0.18168300	-2.55979300
C	2.94598500	0.24087700	-3.95334000
C	3.75361200	1.11944400	-4.67207100
C	4.64507000	1.95472000	-4.00233900
H	5.41731900	2.54564200	-2.08150400
H	3.98435600	0.96942700	-0.81287200
H	2.25238100	-0.41229300	-4.47882700
H	3.68918100	1.14857700	-5.75551600
H	5.27795500	2.63749300	-4.56029700
C	2.05783100	-0.72106000	-1.79263700
H	1.81956700	-1.57875200	-2.43355900
C	0.75479400	0.06138300	-1.56921300
C	-0.14763400	-0.75364100	-0.64448800
O	-0.21513400	-1.98398600	-0.78787100
H	0.96706300	1.05588600	-1.16588200
H	-1.55208800	3.75229900	-4.37387400
C	-0.10021400	0.34293400	3.14982700
C	0.75364500	0.50713200	2.03828800
C	1.60588000	1.63491200	1.99084200
C	1.61761800	2.60769600	2.97599400
C	0.74573200	2.47451900	4.05517600
C	-0.08613700	1.36588400	4.11777000
H	2.27107300	1.72029800	1.13377200

H	2.29179400	3.45479000	2.90108700
H	0.71549600	3.22058400	4.84249400
H	-0.74232300	1.27508900	4.97744700
C	-0.98748500	-0.87208800	3.46973900
C	-2.45117500	-0.40286300	3.52827300
C	-0.86122200	-2.05311300	2.49974800
C	-0.57771300	-1.42130500	4.85256800
H	-2.59788100	0.37367600	4.28407500
H	-2.76896700	0.01890500	2.56685300
H	-3.10993700	-1.24175100	3.77675800
H	0.16889500	-2.41329600	2.46331300
H	-1.50580600	-2.86180600	2.86369700
H	-1.15977800	-1.82570300	1.47586300
H	-1.18124500	-2.30339600	5.09012700
H	0.47568200	-1.71606800	4.83741800
H	-0.72219800	-0.69452600	5.65514000
N	0.87160100	-0.39610200	0.94663400
C	2.10211100	-0.90708200	0.73550400
C	2.63663000	-1.22841400	-0.49227300
C	3.78410500	-2.11033500	-0.64453000
O	4.36263900	-2.32005100	-1.69964400
O	4.15381000	-2.75165300	0.49340900
C	5.32213800	-3.55990500	0.38619200
H	5.17966600	-4.34211700	-0.36178800
H	6.18721500	-2.95474200	0.10508700
H	5.47223800	-3.99974100	1.37091500
C	2.91855800	-1.12523000	2.00052100
O	4.04780000	-0.41181900	1.98124600
O	2.55826400	-1.79301300	2.94147200
C	4.88374600	-0.58138300	3.12863100
H	5.18652700	-1.62736100	3.21692000
H	5.75042500	0.05533000	2.96449800
H	4.35050000	-0.28146300	4.03293200
H	0.25945200	0.19674900	-2.53837300

M7(S')

C	-1.43140600	-0.23541700	-0.26167600
C	-3.35431400	0.81016900	-0.03002800
C	-1.47315600	2.28462700	0.36237600
H	-0.42467000	2.20323300	0.64203300
N	-3.67151800	-0.37721300	-0.44312300
N	-2.47484500	-1.01513000	-0.60681300
N	-1.99582100	0.94691400	0.07301000

C	-4.20468800	1.93020900	0.47696700
H	-5.19423700	1.55306100	0.73468300
H	-4.30480300	2.72657200	-0.27010400
C	-2.28556400	2.93754600	1.53137700
O	-3.58824800	2.38032000	1.67091900
C	-2.14093400	4.46877200	-0.32434100
C	-1.67635400	3.24134500	-0.79641400
C	-1.46401600	3.02218400	-2.15205100
C	-1.71175500	4.06615300	-3.04197900
C	-2.16217000	5.30179300	-2.57394600
C	-2.38209300	5.51121200	-1.21284500
C	-2.32095300	4.43516900	1.17289200
H	-1.12540900	2.05809500	-2.51826700
H	-2.35361400	6.10386300	-3.27932300
H	-2.74900400	6.46762300	-0.85341100
H	-3.25597500	4.88711300	1.51389400
H	-1.49681100	4.95358300	1.67594400
C	-2.56530500	-2.32743800	-1.22694900
C	-2.17824700	-2.46846800	-2.56666900
C	-3.21187000	-3.34602300	-0.52727800
C	-2.37719600	-3.70617700	-3.16782400
C	-3.37369300	-4.57526600	-1.17503800
C	-2.95492900	-4.77977600	-2.48424000
H	-2.07574300	-3.83477800	-4.20480100
H	-3.86029900	-5.38381400	-0.63493700
C	-3.79744700	-3.15792200	0.84538800
H	-4.85530200	-2.88641400	0.76832800
H	-3.29674700	-2.36935900	1.40008300
H	-3.72774600	-4.08447700	1.41993900
C	-1.54964400	-1.35232300	-3.35071700
H	-0.47344700	-1.35206700	-3.16024900
H	-1.94999400	-0.37374200	-3.06552600
H	-1.72541400	-1.49050300	-4.41896200
H	-1.79826300	2.74943100	2.48712300
C	-3.12364600	-6.11441500	-3.16222900
H	-3.76202400	-6.77848400	-2.57619700
H	-3.56574100	-5.99622600	-4.15519000
H	-2.15466100	-6.60595600	-3.29355600
C	4.55686400	2.62212900	-2.29393200
C	3.85724400	1.60533900	-1.64899700
C	3.01949300	0.74981600	-2.36909900
C	2.89371300	0.93850600	-3.74697500
C	3.58967300	1.95622900	-4.39516200
C	4.42517000	2.80275600	-3.66972100

H	5.20946900	3.27307700	-1.72008000
H	3.97603900	1.45603000	-0.57809000
H	2.24376100	0.27760800	-4.31664600
H	3.48157400	2.08554700	-5.46779000
H	4.97103700	3.59460100	-4.17255300
C	2.17323000	-0.31120000	-1.68281800
H	2.00391500	-1.12932000	-2.39279000
C	0.80431200	0.30480200	-1.35654600
C	0.06562400	-0.70221200	-0.43601400
O	0.09154300	-1.92103500	-0.82818000
H	0.92714600	1.28532500	-0.87780500
H	-1.55734700	3.91439000	-4.10488300
C	-0.30454000	0.12004700	3.08075600
C	0.59176000	0.37390200	2.02350200
C	1.35712200	1.55853200	2.02538200
C	1.22011500	2.52738200	3.00604700
C	0.29562900	2.31492100	4.02596300
C	-0.43696800	1.13629000	4.04649300
H	2.07130700	1.70232300	1.21789400
H	1.82368600	3.42812800	2.97504000
H	0.15334300	3.05415200	4.80733400
H	-1.13276200	0.98727800	4.86563000
C	-1.10286800	-1.16857100	3.34161900
C	-2.60234700	-0.82496500	3.29518700
C	-0.79811900	-2.33930100	2.39731500
C	-0.74761100	-1.67503100	4.75626100
H	-2.86273500	-0.05458100	4.02684800
H	-2.89757600	-0.44491000	2.30939300
H	-3.20154400	-1.71447300	3.51659500
H	0.25877300	-2.60806100	2.45131200
H	-1.39754400	-3.19762100	2.72183900
H	-1.02433200	-2.15231400	1.34695500
H	-1.28155500	-2.61021900	4.95242100
H	0.32685100	-1.87094600	4.82306100
H	-1.02012200	-0.96699000	5.54198800
N	0.85784200	-0.53645400	0.94904800
C	2.18757400	-0.82895000	0.77244800
C	2.81265600	-0.87905000	-0.43717000
C	4.10188100	-1.55685100	-0.62814500
O	4.77094200	-1.49175500	-1.64220600
O	4.46913200	-2.33291500	0.41475200
C	5.74999000	-2.95160600	0.29668500
H	5.77316700	-3.61635200	-0.56874000
H	6.53143600	-2.19642100	0.18815000

H	5.89240800	-3.51760200	1.21544700
C	2.93092600	-1.08723400	2.06663500
O	3.98816600	-0.28167700	2.18660700
O	2.57716000	-1.87375200	2.91294400
C	4.79150900	-0.50952000	3.34785300
H	5.17286900	-1.53313100	3.33999900
H	5.60960800	0.20485700	3.28902800
H	4.20400300	-0.34798900	4.25359700
H	0.25994700	0.45787700	-2.29227100

TS7(S)

C	-0.95856500	-1.15068000	-0.28176100
C	-2.48566900	-2.44950600	0.61306900
C	-3.04757200	-0.10946100	0.88831200
H	-2.52601100	0.83584700	1.00184100
N	-1.67656900	-3.25794200	0.00295800
N	-0.74400800	-2.44508100	-0.56464400
N	-2.09373700	-1.14777500	0.45969800
C	-3.66204600	-2.74437700	1.48613100
H	-3.59356300	-3.76454900	1.86287700
H	-4.60337500	-2.62599300	0.93410200
C	-3.72214400	-0.49011000	2.25546400
O	-3.57092900	-1.86067900	2.58654600
C	-5.41577000	0.01010300	0.59759500
C	-4.20310700	-0.01838500	-0.08775000
C	-4.15447500	0.00564900	-1.47781700
C	-5.35335400	0.08419300	-2.18317100
C	-6.57126300	0.13259800	-1.50176900
C	-6.61187200	0.09235900	-0.10910400
C	-5.20030100	-0.07568700	2.08692600
H	-3.20980000	-0.05417100	-2.01265700
H	-7.49738300	0.18847900	-2.06442500
H	-7.56187000	0.11019200	0.41597000
H	-5.85242600	-0.80288400	2.57890600
H	-5.37239400	0.89492100	2.56297300
C	0.24698400	-3.10964000	-1.38312500
C	0.14038400	-3.02923500	-2.77556400
C	1.14325200	-3.95910100	-0.73183000
C	1.08364300	-3.73278100	-3.52117700
C	2.06711500	-4.63746800	-1.52702700
C	2.06899200	-4.51650500	-2.91617800
H	1.03294500	-3.68250700	-4.60595900
H	2.79112400	-5.28926500	-1.04426600

C	1.07463400	-4.19534800	0.75194100
H	0.21347100	-4.82688800	0.98979700
H	0.96826300	-3.25773700	1.30600600
H	1.98070600	-4.69305700	1.09803500
C	-0.96935900	-2.27304400	-3.45500000
H	-0.75189600	-1.20323800	-3.47713900
H	-1.92054300	-2.41518400	-2.93119000
H	-1.09280600	-2.63020500	-4.47879600
H	-3.23928400	0.04421900	3.07273600
C	3.10009600	-5.22942900	-3.75123600
H	2.67898800	-5.55559200	-4.70516700
H	3.94041300	-4.56367300	-3.97309700
H	3.49731900	-6.10251400	-3.22911800
C	-2.17762100	5.54306200	-1.75091500
C	-1.48405800	4.35688200	-1.98258000
C	-0.61634300	3.83707200	-1.02008400
C	-0.46350400	4.52477600	0.18629200
C	-1.15404400	5.71083900	0.42225600
C	-2.01342400	6.22498300	-0.54711600
H	-2.84282600	5.93752400	-2.51293000
H	-1.61048700	3.82975400	-2.92559200
H	0.21595900	4.12792800	0.93723100
H	-1.01917800	6.23509100	1.36343400
H	-2.54874600	7.15166700	-0.36635400
C	0.08796500	2.50770100	-1.25401500
H	0.15847500	2.35189600	-2.33867200
C	-0.79611300	1.40486500	-0.67265900
C	-0.15895400	0.03815700	-0.86440300
O	0.50373500	-0.22851600	-1.86632500
H	-0.94854500	1.60970300	0.38769000
H	-5.33935300	0.10055500	-3.26750400
C	1.92798300	-1.00751300	2.54434400
C	1.95464000	-0.65146800	1.17026800
C	2.80046100	-1.33976100	0.28692000
C	3.67938200	-2.32150700	0.73181500
C	3.69905300	-2.64255300	2.08212600
C	2.82059700	-2.00420200	2.95696000
H	2.76794600	-1.05640300	-0.76144500
H	4.33352100	-2.82712900	0.02749400
H	4.38158200	-3.39656900	2.46193800
H	2.85401500	-2.29072200	4.00114800
C	1.02565400	-0.30084100	3.56830100
C	1.43220600	1.17616200	3.71706400
C	-0.44447800	-0.36993500	3.12876000

C	1.11712000	-0.94988500	4.95651700
H	2.48542500	1.26208700	3.99784700
H	1.28829600	1.72131700	2.78300700
H	0.82117400	1.64392300	4.49766000
H	-0.77979500	-1.40709000	3.00328800
H	-1.07466000	0.09961700	3.89298200
H	-0.57800500	0.16706300	2.18758500
H	0.41856900	-0.44521700	5.63054800
H	0.85022100	-2.01131400	4.92815400
H	2.11826600	-0.85453700	5.38762200
N	1.20293900	0.43513600	0.65058800
C	1.93880400	1.45611300	0.15348500
C	1.47970600	2.46504700	-0.66806100
C	2.34216300	3.53392600	-1.15624500
O	2.14231800	4.16384700	-2.18316600
O	3.38900000	3.83142700	-0.34641200
C	4.34441800	4.73672200	-0.89218900
H	5.10772000	4.86461300	-0.12614100
H	4.78702900	4.32462000	-1.80280300
H	3.87584100	5.69439700	-1.12626200
C	3.41896400	1.46065100	0.52517100
O	4.18969500	1.20676600	-0.53968100
O	3.84856800	1.60853200	1.64346300
C	5.58987500	1.15112500	-0.26061000
H	5.79698900	0.35396400	0.45738900
H	6.07759100	0.94744900	-1.21167400
H	5.93050600	2.10465000	0.14958100
H	-1.76922500	1.42619700	-1.18224500

M7(S)

C	-0.55764200	-1.33163400	-0.16204400
C	-1.84405200	-2.99500500	0.50902400
C	-2.85750600	-0.86405200	0.99389300
H	-2.55880000	0.16513400	1.17239100
N	-0.86365500	-3.56651500	-0.11351100
N	-0.08666700	-2.53122100	-0.54731900
N	-1.71137800	-1.63302400	0.49083700
C	-2.95990000	-3.59316900	1.30328500
H	-2.70642500	-4.61780900	1.57429600
H	-3.89863100	-3.59295000	0.73624400
C	-3.40586000	-1.47273500	2.32858700
O	-3.05313200	-2.83764600	2.49791100
C	-5.21384800	-1.15378900	0.76154900

C	-4.03603600	-0.95717800	0.04215900
C	-4.03617500	-0.91375500	-1.34790600
C	-5.25478500	-1.02627800	-2.01563700
C	-6.44144900	-1.18839900	-1.29885600
C	-6.42893200	-1.26151600	0.09361700
C	-4.93080800	-1.25630200	2.23923000
H	-3.11074200	-0.82213500	-1.91095100
H	-7.38183200	-1.27924000	-1.83265100
H	-7.35022900	-1.41989000	0.64566300
H	-5.45879600	-2.07927200	2.72799800
H	-5.20591000	-0.33146200	2.75761200
C	1.02928100	-2.93055500	-1.37839600
C	0.88865900	-2.85472400	-2.76905800
C	2.09230300	-3.58307600	-0.75633100
C	1.94841700	-3.32768400	-3.53742300
C	3.12960500	-4.03923300	-1.57291200
C	3.08690600	-3.89691100	-2.95776700
H	1.87433600	-3.26963300	-4.62067700
H	3.98169700	-4.52892700	-1.10786500
C	2.09485900	-3.85705300	0.72239400
H	1.39932200	-4.67031400	0.95333600
H	1.78567600	-2.98061200	1.29805200
H	3.09199100	-4.14930600	1.05399600
C	-0.37162100	-2.33869600	-3.40597100
H	-0.47173300	-1.27222400	-3.19113100
H	-1.24807400	-2.85805200	-3.00130900
H	-0.34880000	-2.50231400	-4.48486000
H	-2.97114800	-0.96445100	3.18903200
C	4.23183600	-4.36024100	-3.82038700
H	3.86977800	-4.79271100	-4.75646000
H	4.88348600	-3.51916900	-4.07882400
H	4.83996900	-5.10648800	-3.30454200
C	-3.51615900	4.70345200	-1.97458200
C	-2.51698300	3.74238600	-2.11484500
C	-1.59523300	3.51638200	-1.09095800
C	-1.69687400	4.27017900	0.08173800
C	-2.69138700	5.23397700	0.22482200
C	-3.60568700	5.45355500	-0.80401300
H	-4.22269200	4.86939500	-2.78196900
H	-2.44751800	3.16147300	-3.03154200
H	-0.98076900	4.10273100	0.88367600
H	-2.75142400	5.81520200	1.13986500
H	-4.38004100	6.20602000	-0.69450900
C	-0.55337200	2.42106800	-1.22511800

H	-0.38500000	2.21727200	-2.28978900
C	-1.07959100	1.14210800	-0.57743700
C	0.04110800	0.07163500	-0.62452600
O	0.61604600	-0.07115800	-1.76675400
H	-1.35307000	1.38408400	0.45463100
H	-5.27796100	-0.99766000	-3.09964200
C	2.21936600	-0.54786500	2.37720600
C	2.06946400	-0.26004500	0.99821800
C	3.02607800	-0.67751000	0.06694700
C	4.17537500	-1.35104600	0.46576700
C	4.36259200	-1.60692900	1.81668100
C	3.39253800	-1.22342400	2.74057100
H	2.83551400	-0.43618800	-0.97382700
H	4.90830300	-1.66516700	-0.27091700
H	5.25744600	-2.11542500	2.16259900
H	3.57411800	-1.45649300	3.78182700
C	1.20340100	-0.14507800	3.46319500
C	1.14381200	1.38099400	3.64880900
C	-0.20200100	-0.63869100	3.09716400
C	1.55829600	-0.75961100	4.82587600
H	2.12306000	1.78248200	3.91724400
H	0.81225700	1.88478900	2.73837100
H	0.43465700	1.61240500	4.45174900
H	-0.22013400	-1.71724300	2.89749900
H	-0.88292900	-0.43517100	3.93074900
H	-0.56570900	-0.10157200	2.22037000
H	0.77534800	-0.49939500	5.54391500
H	1.62065600	-1.85140600	4.77568000
H	2.50381200	-0.37380700	5.21789800
N	1.02218600	0.60450600	0.50675900
C	1.46367600	1.87819300	0.16736300
C	0.77034500	2.76778500	-0.59232900
C	1.33736900	4.06572300	-0.99346400
O	1.03713300	4.64644100	-2.01822500
O	2.20399400	4.58843700	-0.10270400
C	2.88063000	5.77109400	-0.53068100
H	3.53491000	6.05351400	0.29191800
H	3.46445300	5.56844400	-1.43152300
H	2.16183700	6.56524700	-0.73922000
C	2.87984500	2.22554600	0.60105500
O	3.68874800	2.24266300	-0.46302900
O	3.25103100	2.41700500	1.73134800
C	5.06130400	2.51430500	-0.16493300
H	5.45354400	1.75047900	0.51036500

H	5.58345500	2.48914300	-1.11879300
H	5.15747800	3.49694300	0.30206700
H	-1.96967600	0.80236900	-1.11523400

TS(R')

C	-0.90948900	-1.13178700	0.17774700
C	-2.70869900	-1.78960100	1.22234300
C	-3.19672900	-0.36801400	-0.72209300
H	-2.67985000	0.45033200	-1.21853000
N	-1.73534000	-2.40873300	1.82379600
N	-0.61676400	-2.00370500	1.15533800
N	-2.24541800	-1.00429600	0.20455100
C	-4.17101300	-1.73544900	1.52292400
H	-4.35387500	-2.03576900	2.55453000
H	-4.72982200	-2.39863900	0.84905000
C	-4.45766800	0.14365300	0.06269200
O	-4.55699100	-0.38262300	1.38243600
C	-5.13432500	-1.32877800	-1.74011700
C	-3.74338900	-1.38324700	-1.70075800
C	-3.02520800	-2.26990200	-2.49642000
C	-3.73307100	-3.12856100	-3.33395900
C	-5.12932900	-3.08551700	-3.37405700
C	-5.83904200	-2.18392000	-2.58333300
C	-5.66293800	-0.26322100	-0.81366600
H	-1.93936200	-2.27731700	-2.47076600
H	-5.66753500	-3.76233500	-4.02991300
H	-6.92368200	-2.15295700	-2.61982200
H	-6.49058600	-0.60086000	-0.18308500
H	-6.01826300	0.60138900	-1.38403000
C	0.61813900	-2.72103700	1.39725900
C	0.84977900	-3.85206800	0.61332700
C	1.52669400	-2.24529400	2.34680300
C	2.07257400	-4.50487900	0.77791900
C	2.73392700	-2.92633600	2.46442300
C	3.03052000	-4.04564100	1.68076800
H	2.28477700	-5.38046400	0.17042300
H	3.47122600	-2.56174500	3.17530200
C	1.24697400	-1.00954800	3.15416900
H	2.06122600	-0.81960500	3.85492200
H	0.31610900	-1.10914900	3.71878300
H	1.14008200	-0.13110300	2.50473200
C	-0.14537300	-4.30586400	-0.42239100
H	-0.11410900	-3.65344500	-1.30381500

H	-1.16887500	-4.29512500	-0.03691300
H	0.08625000	-5.31779600	-0.75656500
H	-4.38868700	1.22209700	0.20442700
C	4.37386700	-4.71407200	1.80032700
H	4.61193400	-4.93241100	2.84461200
H	4.40686300	-5.64614600	1.23348100
H	5.15545800	-4.05039100	1.41552100
C	5.55531600	-0.94968200	0.60707800
C	4.36908600	-0.32137200	0.23613800
C	3.83410400	-0.50494400	-1.04186600
C	4.51195400	-1.32720100	-1.94207800
C	5.70147600	-1.95445400	-1.57778800
C	6.22613000	-1.76942200	-0.30003600
H	5.95712100	-0.80089000	1.60491500
H	3.84517800	0.31932500	0.94342600
H	4.10142600	-1.47521500	-2.93797500
H	6.21859600	-2.58801100	-2.29188200
H	7.15185300	-2.25856000	-0.01311500
C	2.47151600	0.07871300	-1.39675700
H	2.32016400	-0.05680300	-2.47659000
C	1.46880000	-0.78578600	-0.64266700
C	0.01032900	-0.48549100	-0.86080600
O	-0.50319800	-0.25354800	-1.95208300
H	1.69416000	-0.71304400	0.41990400
H	-3.19708600	-3.83310400	-3.96118100
C	-1.78984000	2.61217100	1.26999000
C	-1.05055000	2.19182700	0.12575500
C	-1.52569900	2.53810700	-1.15467500
C	-2.69502400	3.26156900	-1.35295000
C	-3.41304700	3.68427900	-0.24256800
C	-2.95244000	3.35936200	1.03225500
H	-0.93039900	2.21792300	-2.00436100
H	-3.02404800	3.50283500	-2.35888300
H	-4.32209900	4.26689600	-0.35451800
H	-3.53195900	3.71540900	1.87463900
C	-1.40876600	2.27544100	2.72300400
C	-1.65934700	0.77769900	2.93343300
C	0.05542100	2.61011100	3.05173700
C	-2.27146300	3.02946600	3.74673400
H	-2.70393900	0.53039400	2.71717200
H	-1.01056100	0.20111500	2.27480100
H	-1.43761600	0.49203200	3.96823100
H	0.21990100	3.69112000	3.02049300
H	0.28007800	2.25918200	4.06580200

H	0.74859500	2.14558800	2.35195500
H	-1.91458100	2.78265000	4.75122400
H	-2.19613500	4.11434400	3.62122000
H	-3.32628700	2.74354400	3.69530900
N	0.16941900	1.45801900	0.15855200
C	1.20598800	2.09257000	-0.44410800
C	2.31838000	1.54070100	-1.04858100
C	3.37898400	2.44327800	-1.48400000
O	3.62893500	3.55346000	-1.03579700
O	4.12194500	1.91012100	-2.48289600
C	5.22985200	2.69785600	-2.90670200
H	5.74399300	2.10922500	-3.66495500
H	4.89035600	3.64623800	-3.32900600
H	5.89903000	2.90504500	-2.06847000
C	1.09064600	3.61736600	-0.53921900
O	1.12173000	4.18784100	0.66549700
O	0.90123300	4.22583200	-1.56571300
C	0.86348500	5.59285700	0.67668600
H	-0.11911100	5.79491000	0.24378800
H	0.88964900	5.89394900	1.72237000
H	1.62759500	6.12378200	0.10539800
H	1.62539500	-1.83175800	-0.94076500

M7(R')

C	-1.00821300	-0.89735800	0.37672700
C	-2.84716700	-1.66998700	1.28527600
C	-3.28385400	-0.19258500	-0.61943900
H	-2.77066600	0.64904400	-1.08046600
N	-1.89304400	-2.27226600	1.92691900
N	-0.74907500	-1.79736900	1.34283400
N	-2.35252600	-0.82951400	0.32752700
C	-4.32388100	-1.68378100	1.50580000
H	-4.54942900	-2.04107700	2.51036200
H	-4.82302900	-2.33026400	0.77184900
C	-4.59624800	0.25160100	0.12197500
O	-4.75385600	-0.33946100	1.40871800
C	-5.14750100	-1.17368700	-1.75462500
C	-3.75885000	-1.19487900	-1.65050300
C	-2.98113600	-2.04645500	-2.42967900
C	-3.63089100	-2.90531200	-3.31364200
C	-5.02480500	-2.89715600	-3.41792000
C	-5.79248500	-2.02737000	-2.64532500
C	-5.74417500	-0.14069900	-0.83320600

H	-1.89824800	-1.99674400	-2.35355300
H	-5.51418900	-3.57425200	-4.11096200
H	-6.87487000	-2.02069300	-2.73193000
H	-6.60345900	-0.50255400	-0.26112800
H	-6.07391700	0.73649100	-1.40027000
C	0.47944600	-2.49377400	1.65944400
C	0.68641100	-3.71426500	1.01011600
C	1.39990400	-1.93838700	2.54871700
C	1.89135000	-4.37240600	1.25055700
C	2.58979500	-2.63409500	2.75350400
C	2.85907600	-3.84040900	2.10416800
H	2.08336000	-5.31538000	0.74546000
H	3.33132300	-2.21272300	3.42743300
C	1.15470000	-0.60590500	3.19775300
H	1.99616000	-0.32732700	3.83365200
H	0.24649400	-0.61973900	3.80703400
H	1.02637500	0.17165900	2.43500200
C	-0.33705100	-4.27322000	0.05748700
H	-0.58429800	-3.54921600	-0.72813800
H	-1.26773500	-4.51768800	0.57761600
H	0.04042900	-5.17703600	-0.42184300
H	-4.56765000	1.32295300	0.31925000
C	4.18649700	-4.52714200	2.28682900
H	4.57561500	-4.37632600	3.29617400
H	4.10776300	-5.59971400	2.09787600
H	4.91905500	-4.11565300	1.58377000
C	5.55027000	-1.26850800	0.09530200
C	4.37169000	-0.57212400	-0.15478800
C	3.63945600	-0.80139800	-1.32374000
C	4.10922100	-1.74641200	-2.23556800
C	5.28855700	-2.44786600	-1.98807300
C	6.01309600	-2.21172000	-0.82215100
H	6.10696800	-1.07693500	1.00771900
H	4.00988000	0.16072400	0.56452800
H	3.54609600	-1.93495700	-3.14621900
H	5.64226900	-3.17892200	-2.70860700
H	6.93207300	-2.75603800	-0.62902000
C	2.29653200	-0.11621000	-1.52751600
H	1.97038700	-0.25062500	-2.56528000
C	1.31455500	-0.80573500	-0.58821400
C	-0.06933200	-0.14937900	-0.63390800
O	-0.63364400	-0.13286600	-1.79681000
H	1.74404900	-0.77040100	0.41472300
H	-3.05010800	-3.58270700	-3.93141200

C	-1.83631500	2.67895500	0.86737600
C	-0.98983100	2.18296400	-0.15404600
C	-1.22748900	2.53005600	-1.49387300
C	-2.33537200	3.26821600	-1.88072700
C	-3.22202500	3.69528700	-0.90010800
C	-2.95200800	3.41975800	0.43529200
H	-0.52621700	2.16114400	-2.23123300
H	-2.49994600	3.50367800	-2.92706000
H	-4.10623200	4.26828000	-1.16120700
H	-3.64199800	3.81187300	1.17067800
C	-1.60833500	2.53313200	2.38762900
C	-1.90632100	1.10304400	2.85204700
C	-0.16630300	2.90926300	2.75200200
C	-2.52533100	3.46320100	3.19982100
H	-2.93026100	0.81179700	2.59494200
H	-1.20894700	0.39834700	2.40322800
H	-1.79150400	1.03383400	3.93989200
H	0.05128800	3.93496000	2.43472900
H	-0.03217600	2.85012700	3.83756500
H	0.55558000	2.24291000	2.28444000
H	-2.25255400	3.38097700	4.25584700
H	-2.41261000	4.51027200	2.90259500
H	-3.57995700	3.18535400	3.11419200
N	0.15582100	1.29854500	0.04000200
C	1.34225400	1.90380300	-0.38774200
C	2.31602400	1.34570700	-1.15571200
C	3.37671400	2.21942600	-1.69996300
O	3.60639500	3.37489100	-1.38989700
O	4.05956100	1.60126000	-2.67713000
C	5.08283500	2.38006000	-3.29758000
H	5.54088400	1.72910700	-4.03956400
H	4.65320100	3.26305400	-3.77493000
H	5.82117300	2.69736900	-2.55860600
C	1.56515700	3.31986300	0.12738200
O	2.46999600	3.28775500	1.11050800
O	0.99100700	4.31602100	-0.23483000
C	2.87650700	4.57117100	1.59082900
H	2.02430100	5.12053600	1.99588300
H	3.61172800	4.37962400	2.36953200
H	3.32130600	5.13809300	0.77002000
H	1.20755300	-1.85549800	-0.87792200

TS7(R)

C	1.11814800	-0.96272500	-0.28847600
C	2.68337800	-1.54143900	-1.70558500
C	3.56624400	-0.29132700	0.22474000
H	3.16930300	0.53811000	0.80611800
N	1.59979400	-2.08605500	-2.17397900
N	0.63641500	-1.73504800	-1.27490400
N	2.43893400	-0.85523000	-0.55080800
C	4.05270600	-1.47232500	-2.29516700
H	4.00772600	-1.66909500	-3.36597500
H	4.72180300	-2.20494700	-1.82359700
C	4.72568600	0.17593900	-0.73649500
O	4.49631100	-0.14456700	-2.10024700
C	5.56105800	-1.47610900	0.83635800
C	4.19397000	-1.37130100	1.08103500
C	3.55838900	-2.20314900	1.99956200
C	4.32025200	-3.15402600	2.67292100
C	5.69282200	-3.26327000	2.43243500
C	6.32228200	-2.42459800	1.51661700
C	6.01855700	-0.47217500	-0.18785700
H	2.49593700	-2.09385600	2.19005700
H	6.27262200	-4.01082700	2.96438300
H	7.38823300	-2.51260300	1.32918200
H	6.59061600	-0.92331000	-1.00532300
H	6.65953300	0.28922700	0.26678700
C	-0.67645500	-2.31036700	-1.43549300
C	-0.97317900	-3.46694500	-0.70366600
C	-1.57317800	-1.70768000	-2.31348000
C	-2.27641700	-3.94930900	-0.78193100
C	-2.86898600	-2.22674300	-2.35132200
C	-3.24615900	-3.31552400	-1.56777700
H	-2.54770900	-4.82737600	-0.20113200
H	-3.59622000	-1.75065800	-3.00441100
C	-1.15954500	-0.58076000	-3.21160500
H	-0.40522400	0.05639700	-2.74887900
H	-2.01649800	0.04904100	-3.45157200
H	-0.73576200	-0.98226100	-4.13858400
C	0.05413700	-4.11001900	0.18951200
H	1.02816500	-4.17886400	-0.30308400
H	-0.26314600	-5.11503400	0.47076300
H	0.18918700	-3.53505100	1.11400000
H	4.78259900	1.26295200	-0.71986500
C	-4.67631000	-3.78325000	-1.53402200
H	-4.73964000	-4.86650500	-1.40790900
H	-5.19488500	-3.31970000	-0.68656100

H	-5.21002200	-3.50349000	-2.44497300
C	-4.78394800	-2.11066500	2.76813900
C	-3.66554300	-1.67389100	2.06417800
C	-3.25949900	-0.33779000	2.12663900
C	-3.99139600	0.54464600	2.92251000
C	-5.11199900	0.11316300	3.62896700
C	-5.51349300	-1.21796000	3.55239600
H	-5.08762100	-3.15139500	2.70415500
H	-3.12104100	-2.37971500	1.44102500
H	-3.67829100	1.58472900	2.98288200
H	-5.66836900	0.81559300	4.24203900
H	-6.38465100	-1.55871700	4.10306700
C	-2.05142400	0.18474600	1.37192000
H	-1.65774200	1.02821500	1.96025300
C	-0.91758700	-0.85608200	1.36302300
C	0.46434400	-0.33671200	0.96412300
O	1.29813900	-0.07998800	1.84992700
H	-1.22526600	-1.68724000	0.73589700
H	3.84618200	-3.81409300	3.39195500
C	1.43294300	3.32924300	0.58040100
C	1.05128300	2.23527900	-0.24294000
C	1.78197600	1.95506700	-1.40864100
C	2.89444600	2.69646800	-1.78119400
C	3.30119200	3.74365700	-0.96427600
C	2.57269000	4.04533900	0.18266500
H	1.43619200	1.14708700	-2.04670100
H	3.43793100	2.44288900	-2.68569800
H	4.17334100	4.33730100	-1.21955500
H	2.90745300	4.88499100	0.77788000
C	0.64810000	3.78960300	1.82777000
C	-0.83155000	4.04880900	1.49085500
C	0.74078200	2.74928200	2.95266100
C	1.20307000	5.10998400	2.38753100
H	-0.92857700	4.73431800	0.64307300
H	-1.37585300	3.13529300	1.24978200
H	-1.31914700	4.50855000	2.35763800
H	1.78354300	2.60078400	3.25387700
H	0.18090600	3.10676900	3.82486100
H	0.34804100	1.78264500	2.64249900
H	0.59616400	5.40623100	3.24787300
H	2.23546600	5.00980900	2.73558700
H	1.15873500	5.91910800	1.65137300
N	-0.02852800	1.37511100	0.08556300
C	-1.21621200	1.45745000	-0.52214200

C	-2.29788500	0.75716600	-0.01214700
C	-3.48155500	0.63570700	-0.84201700
O	-3.59332900	1.07716900	-1.98366300
O	-4.50073100	-0.03656500	-0.26757500
C	-5.67484100	-0.17213700	-1.05829500
H	-6.37475800	-0.74340200	-0.44895800
H	-6.09535500	0.80587100	-1.30367400
H	-5.46019800	-0.70567100	-1.98768300
C	-1.40201000	2.44021500	-1.67025800
O	-2.23067700	3.42277300	-1.31021900
O	-0.82621700	2.40762600	-2.73226700
C	-2.53643700	4.35829300	-2.34565900
H	-3.03975300	3.84269900	-3.16659800
H	-3.19643500	5.09708000	-1.89586000
H	-1.62572700	4.83122700	-2.71741400
H	-0.77313100	-1.23680900	2.37918500

M7(R)

C	1.05970800	-0.88244400	-0.35617600
C	2.57164100	-1.71664800	-1.71315600
C	3.55850600	-0.36044500	0.08598800
H	3.21864100	0.52885500	0.61191400
N	1.44937300	-2.21299200	-2.13610400
N	0.51601600	-1.69862200	-1.27574000
N	2.38458800	-0.91011100	-0.62732600
C	3.93849000	-1.79997600	-2.30699000
H	3.87437200	-2.10056400	-3.35230500
H	4.56229300	-2.52178900	-1.76290200
C	4.73031300	-0.05452600	-0.92112900
O	4.46918800	-0.49062300	-2.24742900
C	5.47894500	-1.62183300	0.77713200
C	4.12515500	-1.40615800	1.02192200
C	3.44449900	-2.10967700	2.01260100
C	4.14820000	-3.05603800	2.75328800
C	5.50625800	-3.28275500	2.50911500
C	6.18166900	-2.56456300	1.52506800
C	5.98898200	-0.72553600	-0.32076300
H	2.39835100	-1.88611200	2.20003500
H	6.04016800	-4.02494400	3.09407500
H	7.23695100	-2.74078400	1.33948900
H	6.53701000	-1.26489300	-1.10014100
H	6.66766600	0.03422100	0.07865900
C	-0.81585300	-2.24700700	-1.40516700

C	-1.07764600	-3.43804100	-0.71306000
C	-1.72666300	-1.66104900	-2.28178300
C	-2.33118000	-4.01851500	-0.88463300
C	-2.97359400	-2.27944500	-2.41243600
C	-3.29172500	-3.45146500	-1.72827300
H	-2.56423600	-4.93335400	-0.34637400
H	-3.70804800	-1.82825800	-3.07567300
C	-1.39708900	-0.44712200	-3.09934000
H	-0.48600000	0.04718000	-2.76309800
H	-2.21136100	0.27708900	-3.03358900
H	-1.26246300	-0.72942700	-4.14840900
C	-0.04411500	-4.04507600	0.19793000
H	0.90035900	-4.20943000	-0.32992200
H	-0.39288500	-5.00135800	0.58909700
H	0.16761400	-3.38755600	1.04923600
H	4.85196500	1.02397800	-1.01068500
C	-4.64697400	-4.08760300	-1.89926500
H	-4.79007100	-4.91129300	-1.19710200
H	-5.44221200	-3.35373500	-1.73960800
H	-4.76580900	-4.48082300	-2.91332000
C	-4.78276000	-2.37674400	1.65783200
C	-3.77996000	-1.53585800	1.19049900
C	-3.19885200	-0.57949100	2.02928300
C	-3.63529900	-0.48759700	3.34876700
C	-4.64238000	-1.32970500	3.82293600
C	-5.21904600	-2.27535400	2.98026300
H	-5.22265900	-3.11394600	0.99196600
H	-3.44360600	-1.61037700	0.15773500
H	-3.18682800	0.24848900	4.01096300
H	-4.97464200	-1.24450900	4.85286000
H	-6.00174200	-2.93046400	3.34896900
C	-2.05460000	0.27254800	1.52030100
H	-1.81692600	1.04007900	2.27424400
C	-0.82630700	-0.64594600	1.38270600
C	0.46551100	0.01028200	0.83100800
O	1.40293000	0.18083300	1.70066300
H	-1.14300900	-1.49731600	0.78266500
H	3.64096000	-3.61951600	3.52976200
C	1.58223600	3.31581200	0.53387600
C	1.15662500	2.21956800	-0.25895800
C	1.81514300	1.91667400	-1.45760500
C	2.93102200	2.61937400	-1.88791600
C	3.40291800	3.65474600	-1.09192700
C	2.72835100	3.98994200	0.07755200

H	1.41331800	1.11853100	-2.07335800
H	3.42065800	2.35139200	-2.81852500
H	4.28225600	4.22026900	-1.38357600
H	3.11472000	4.82355500	0.64798800
C	0.86600600	3.84299600	1.80014900
C	-0.62764800	4.09094200	1.52878600
C	1.01009000	2.87479700	2.98289400
C	1.44934000	5.19413800	2.25165400
H	-0.77227800	4.71722300	0.64345800
H	-1.18840200	3.16661300	1.38902500
H	-1.06388500	4.61165600	2.38776700
H	2.06624300	2.74150400	3.24202200
H	0.49622700	3.29850700	3.85363000
H	0.60933300	1.88915600	2.75196400
H	0.87323800	5.54908700	3.11064200
H	2.49138900	5.10930400	2.57290100
H	1.38509700	5.95428500	1.46652300
N	0.06813800	1.35013000	0.10411400
C	-1.19441300	1.55203900	-0.37898400
C	-2.28644700	0.98031900	0.20300000
C	-3.60340100	1.19055600	-0.41271400
O	-3.81569300	1.27471400	-1.61194300
O	-4.58560000	1.30301100	0.49346500
C	-5.90797000	1.37004900	-0.03961000
H	-6.57359400	1.40436000	0.82064100
H	-6.02991500	2.26389000	-0.65404900
H	-6.11545700	0.48606600	-0.64715600
C	-1.37286800	2.54827100	-1.51281200
O	-2.20293500	3.52957400	-1.15857300
O	-0.82203200	2.49033800	-2.58584200
C	-2.55331400	4.43322400	-2.21087000
H	-3.07191500	3.88705400	-3.00176200
H	-3.21100000	5.17262400	-1.75988700
H	-1.65989700	4.90824100	-2.61861200
H	-0.54065900	-1.02234100	2.36858800

TS8(S')

C	1.63765600	0.38737200	-0.31345500
C	3.74512600	-0.36645100	-0.34147800
C	2.14165700	-2.00687100	0.45614200
H	1.16663600	-1.97757600	0.94149300
N	3.83438200	0.83613300	-0.81322800
N	2.52964200	1.28064900	-0.80162600

N	2.44634200	-0.67101000	-0.03249500
C	4.79645800	-1.35776600	0.03437900
H	5.77261800	-0.87603400	0.08357400
H	4.83902300	-2.18429800	-0.68612400
C	3.23046100	-2.49363700	1.47245900
O	4.47134900	-1.80824600	1.34005100
C	2.86594900	-4.18393500	-0.21523700
C	2.18098500	-3.04816000	-0.64341600
C	1.64508000	-2.96412200	-1.92269500
C	1.79281700	-4.05478600	-2.77861400
C	2.46791100	-5.20045500	-2.35197400
C	3.01048800	-5.27303300	-1.06903500
C	3.36224700	-4.00656200	1.19894300
H	1.13384300	-2.06436700	-2.25397400
H	2.57986900	-6.03989200	-3.03049500
H	3.54727600	-6.16026700	-0.74728400
H	4.39506000	-4.33279600	1.34688700
H	2.73343400	-4.56532500	1.90159700
C	2.33368200	2.61892600	-1.30593500
C	1.76472100	2.81102300	-2.56785400
C	2.83954000	3.68643100	-0.55257400
C	1.64717700	4.11919800	-3.03803200
C	2.68934800	4.97559300	-1.06162000
C	2.08616000	5.21409500	-2.29632800
H	1.20262000	4.28121300	-4.01737600
H	3.06853500	5.81294100	-0.48068200
C	3.58793500	3.47360600	0.73545700
H	4.64462400	3.27313300	0.53194700
H	3.19862200	2.62442500	1.29436200
H	3.52499300	4.36348100	1.36552100
C	1.26908500	1.67951800	-3.42423000
H	0.18177700	1.60767200	-3.33294200
H	1.70263600	0.71913100	-3.13566800
H	1.50993200	1.86491400	-4.47338200
H	2.91209100	-2.28840900	2.49500600
C	1.90786400	6.61897500	-2.81070500
H	0.95699700	7.03754000	-2.46536500
H	2.70524500	7.27481100	-2.45387300
H	1.90114200	6.64176800	-3.90274300
C	-4.24470000	-3.22364800	-2.01916500
C	-3.74074800	-2.05722800	-1.44888800
C	-3.08556100	-1.10711600	-2.23664300
C	-2.94736600	-1.34821200	-3.60543900
C	-3.44986500	-2.51401600	-4.17803900

C	-4.09947400	-3.45771800	-3.38510300
H	-4.75720000	-3.94882100	-1.39486800
H	-3.87914200	-1.87061800	-0.38654200
H	-2.44164700	-0.61279200	-4.22698800
H	-3.33638900	-2.68330700	-5.24419600
H	-4.49434400	-4.36576600	-3.82891300
C	-2.43129400	0.12705200	-1.63538700
H	-2.48655100	0.93896200	-2.37176000
C	-0.92907800	-0.18144800	-1.39834300
C	-0.46222700	0.90860600	-0.45730800
O	-0.44792500	2.08270100	-0.78847800
H	-0.80041400	-1.16804200	-0.94263800
H	1.38585700	-4.01116300	-3.78329600
C	0.37404500	-0.16309700	2.83364100
C	-0.56311600	-0.40188600	1.80938300
C	-1.15133400	-1.67273300	1.67142000
C	-0.79794000	-2.74098100	2.48164100
C	0.16138200	-2.53538200	3.46817500
C	0.71280900	-1.27047100	3.63218300
H	-1.89998000	-1.81187100	0.89684100
H	-1.26371600	-3.71055800	2.34378100
H	0.46739700	-3.34579800	4.12172600
H	1.42875900	-1.13205200	4.43587900
C	1.01217600	1.17998900	3.22876100
C	2.54468900	1.01930200	3.23138100
C	0.63655900	2.37989500	2.34952800
C	0.53899200	1.51805400	4.65779000
H	2.88246300	0.28241600	3.96502400
H	2.91480400	0.69955600	2.25003700
H	3.01671200	1.97440700	3.48409900
H	-0.43703200	2.57141800	2.38941600
H	1.16716500	3.25819400	2.73523000
H	0.91184400	2.25155100	1.30066600
H	0.98200800	2.46755000	4.97558300
H	-0.55026700	1.62041300	4.67647600
H	0.82828700	0.75205100	5.38216700
N	-1.03972500	0.61717900	0.91275800
C	-2.42313900	0.67074400	0.82026400
C	-3.09979300	0.59292500	-0.35444400
C	-4.50903400	1.01694400	-0.47284200
O	-5.22679200	0.75735300	-1.41699400
O	-4.91767100	1.78949400	0.55150700
C	-6.29660600	2.16355800	0.52358500
H	-6.51639600	2.73169700	-0.38165100

H	-6.93194000	1.27604100	0.55456500
H	-6.45506800	2.77727300	1.40786600
C	-3.10384800	0.79271600	2.16481800
O	-4.04383600	-0.13942100	2.31937900
O	-2.78365200	1.59121000	3.01259000
C	-4.79360100	-0.04553900	3.53553300
H	-5.31152500	0.91510100	3.57682100
H	-5.50741700	-0.86530500	3.50892200
H	-4.13040200	-0.13857000	4.39692400
H	-0.39476500	-0.16502100	-2.34816500

M8(S')

C	-5.30659500	-0.08834900	1.32374900
C	-3.94187100	-0.10520400	1.05334500
C	-3.41693500	-0.98477200	0.10226200
C	-4.27912400	-1.85406500	-0.56395300
C	-5.64601300	-1.84264600	-0.29187900
C	-6.16334400	-0.95854500	0.65152700
H	-5.70193100	0.60531200	2.05896200
H	-3.27724700	0.57690700	1.58010200
H	-3.87801200	-2.54263400	-1.30311300
H	-6.30611000	-2.52257300	-0.82118000
H	-7.22795900	-0.94567300	0.86120400
C	-1.92106500	-1.04975000	-0.14706600
H	-1.75526700	-1.56230900	-1.10519200
C	-1.27365800	-1.86663100	0.98221400
C	0.23549900	-1.84365100	0.98984400
O	0.92307000	-2.79005700	1.31504700
H	-1.59182900	-1.44593600	1.94573700
C	3.18515800	-0.71472100	-0.14654900
C	2.23139800	-0.45410900	0.84857900
C	2.59430000	0.00319100	2.12000600
C	3.92162000	0.22315600	2.44703800
C	4.89372800	-0.02626100	1.48096000
C	4.52285300	-0.48427800	0.22542400
H	1.80361000	0.18943400	2.83993300
H	4.19268000	0.57957100	3.43465600
H	5.94348600	0.13406000	1.70424900
H	5.30698800	-0.67462300	-0.49963600
C	2.95034900	-1.24588200	-1.57383500
C	3.64278600	-2.61743200	-1.68548700
C	1.48795200	-1.43920000	-1.99908400
C	3.57567700	-0.26010700	-2.57981700

H	4.71702700	-2.55122000	-1.49472800
H	3.20965000	-3.32100800	-0.96757800
H	3.50288200	-3.02131100	-2.69327200
H	0.92670300	-0.50171500	-1.98056600
H	1.48608400	-1.80175500	-3.03168700
H	0.97712700	-2.19137100	-1.39293700
H	3.42368200	-0.63382200	-3.59740700
H	3.09696100	0.71971800	-2.49378100
H	4.65066800	-0.13595000	-2.43014700
N	0.80836000	-0.62124000	0.65089000
C	0.03604000	0.43758500	0.17057500
C	-1.24813800	0.30276800	-0.21303600
C	-1.94926200	1.40669400	-0.90602800
O	-2.80300300	1.23657500	-1.74813700
O	-1.53511600	2.61940200	-0.51030500
C	-2.06380900	3.72353800	-1.25239900
H	-1.81365800	3.62173800	-2.30990700
H	-3.14797200	3.76737000	-1.13835700
H	-1.59809800	4.61188800	-0.83131900
C	0.83133800	1.70957600	-0.02610300
O	0.93835000	2.38775900	1.10697800
O	1.34528400	2.01117000	-1.07510600
C	1.78304200	3.54664300	1.04444300
H	1.39551500	4.25144600	0.30723100
H	1.76270800	3.97986200	2.04136500
H	2.79748100	3.24798300	0.77233800
H	-1.59393100	-2.90877600	0.95258900

TS8(S)

C	-0.95437400	-1.36959300	-0.11167600
C	-2.66257600	-2.68057600	0.49685700
C	-3.05388900	-0.34557900	0.98342900
H	-2.46340000	0.54907900	1.18157700
N	-1.83922700	-3.48618300	-0.09501900
N	-0.80713300	-2.65612700	-0.47474300
N	-2.17509700	-1.40065500	0.49869000
C	-3.92634900	-2.94534300	1.25042500
H	-3.98774700	-3.99858600	1.52370500
H	-4.80861400	-2.67681200	0.65628500
C	-3.79455200	-0.78101700	2.29294200
O	-3.84539900	-2.19305700	2.45161600
C	-5.39065700	0.06781000	0.69033000
C	-4.18237600	-0.06752100	0.00954600

C	-4.11971200	0.00865900	-1.37670000
C	-5.29247900	0.27370900	-2.08226200
C	-6.50041700	0.44557900	-1.40341900
C	-6.56036800	0.33471300	-0.01437900
C	-5.19706200	-0.14672700	2.17136600
H	-3.18504900	-0.16502100	-1.90341400
H	-7.40660600	0.64836800	-1.96501600
H	-7.50781800	0.43828000	0.50577700
H	-5.94913200	-0.80346200	2.61708800
H	-5.22551100	0.80472100	2.71349400
C	0.23283100	-3.25988100	-1.26273700
C	0.16640700	-3.13413200	-2.65348200
C	1.18468600	-4.04567000	-0.61551300
C	1.15938000	-3.76330300	-3.40028500
C	2.15795200	-4.65889600	-1.40588000
C	2.17014200	-4.51422700	-2.79299500
H	1.13715900	-3.67644500	-4.48402300
H	2.92078900	-5.26524500	-0.92292300
C	1.13682500	-4.23685800	0.87517500
H	0.23879500	-4.79329200	1.16166000
H	1.10914400	-3.27134500	1.39078700
H	2.01469800	-4.78420000	1.22221400
C	-0.94698200	-2.36317600	-3.30977600
H	-0.81367900	-1.29357200	-3.12418800
H	-1.92090200	-2.66272200	-2.90844000
H	-0.95030400	-2.53706600	-4.38739000
H	-3.26087000	-0.42422500	3.17475900
C	3.25300200	-5.15093100	-3.62562200
H	2.86185700	-5.49607000	-4.58581700
H	4.05031700	-4.43056000	-3.83599100
H	3.70278900	-6.00122900	-3.10830200
C	-2.29174900	5.43416900	-1.92011300
C	-1.45385400	4.34257900	-2.13756300
C	-0.74152200	3.77142700	-1.08295700
C	-0.88385200	4.31019400	0.19870800
C	-1.71846900	5.40216100	0.41978400
C	-2.42542400	5.96770300	-0.64021000
H	-2.83566200	5.87153900	-2.75162100
H	-1.34480100	3.93066700	-3.13771800
H	-0.32939800	3.87025300	1.02552100
H	-1.81671100	5.81363500	1.41954400
H	-3.07499900	6.82015600	-0.46897800
C	0.12443200	2.54718500	-1.31203400
H	0.31781200	2.46315000	-2.38932100

C	-0.63134800	1.28391300	-0.86250800
C	0.35853000	0.13580400	-0.82031700
O	0.84879800	-0.33568100	-1.84097400
H	-1.04729300	1.45425400	0.13323500
H	-5.26775600	0.33667100	-3.16497500
C	2.06537800	-0.90056100	2.33453100
C	2.06383900	-0.66432800	0.93672100
C	2.92346100	-1.36276100	0.08452300
C	3.82778600	-2.29548600	0.58123200
C	3.87706300	-2.51422600	1.95020600
C	3.00338000	-1.83474400	2.79631700
H	2.86710600	-1.14432100	-0.97561100
H	4.48567400	-2.83047600	-0.09618600
H	4.58543100	-3.22158000	2.37024800
H	3.06604400	-2.04809200	3.85542200
C	1.12457500	-0.20627700	3.34136000
C	1.42339000	1.29706200	3.47304400
C	-0.33606500	-0.37333600	2.90620900
C	1.24914600	-0.81645800	4.74584800
H	2.45714500	1.46757600	3.77908800
H	1.25890700	1.83253300	2.53550100
H	0.75577000	1.72336300	4.23015300
H	-0.61275900	-1.43077600	2.81592400
H	-0.99078000	0.09231700	3.65171700
H	-0.49696900	0.11494700	1.94531800
H	0.51759300	-0.33651300	5.40221800
H	1.04242400	-1.89128200	4.74138400
H	2.23900300	-0.65201300	5.18140000
N	1.28207900	0.40174300	0.35473300
C	1.97150300	1.58900600	0.10460400
C	1.46647400	2.62179800	-0.61823700
C	2.27243000	3.80436100	-0.96979900
O	2.03783100	4.51059400	-1.93011700
O	3.28647500	4.05357300	-0.12208800
C	4.16037300	5.11752700	-0.50481700
H	4.91538300	5.17644800	0.27668900
H	4.62403800	4.90037600	-1.46940400
H	3.60688400	6.05540800	-0.57455500
C	3.42229200	1.60410200	0.56328500
O	4.21125400	1.38073400	-0.49010200
O	3.81817400	1.73337300	1.69266300
C	5.60801800	1.29923000	-0.18432900
H	5.78689400	0.48355700	0.51966800
H	6.10813500	1.10857900	-1.13104300

H	5.95050200	2.24016000	0.25114700
H	-1.44027200	1.06862400	-1.56319800
M8(S)			
C	5.65959900	-1.74816000	0.80944300
C	4.37944700	-1.46810200	1.28268000
C	3.38856600	-1.00641000	0.41704300
C	3.69656500	-0.83144000	-0.93520000
C	4.97578800	-1.10557700	-1.40945600
C	5.96145500	-1.56622900	-0.53769000
H	6.42110700	-2.10554600	1.49525200
H	4.14713100	-1.60788100	2.33525100
H	2.93145100	-0.47021100	-1.62008300
H	5.20330900	-0.95869100	-2.46048600
H	6.95909100	-1.77970500	-0.90750800
C	1.97965200	-0.77559100	0.92984400
H	2.02577100	-0.66605800	2.02212700
C	1.11758200	-1.99934800	0.58303400
C	-0.35387400	-1.82648800	0.87284700
O	-1.07160500	-2.72272300	1.26994600
H	1.19873600	-2.19099900	-0.49671500
C	-3.28796100	-0.70986600	-0.06582800
C	-2.26652200	-0.31972800	0.81203200
C	-2.53221400	0.36707700	2.00059100
C	-3.83192200	0.67766700	2.36904000
C	-4.87142600	0.27574200	1.53543700
C	-4.59318100	-0.40079000	0.35531200
H	-1.69303000	0.64569000	2.63151000
H	-4.02851000	1.21110800	3.29243500
H	-5.90176400	0.49097200	1.79934000
H	-5.42885300	-0.69501300	-0.27091800
C	-3.14838900	-1.42503100	-1.42392800
C	-1.71845600	-1.67134500	-1.92692300
C	-3.84072700	-2.79586900	-1.31638500
C	-3.84547100	-0.56495800	-2.49650800
H	-1.14095800	-0.74655800	-1.99171100
H	-1.18812000	-2.40238400	-1.31293400
H	-1.78991000	-2.09468800	-2.93377600
H	-4.90029700	-2.70129900	-1.06384300
H	-3.76660600	-3.32411200	-2.27258300
H	-3.35526700	-3.40305000	-0.54601800
H	-3.77395400	-1.06455700	-3.46782000
H	-4.90472600	-0.40519200	-2.28321100

H	-3.35519000	0.41017100	-2.56965600
N	-0.86814600	-0.57462100	0.56033900
C	-0.02986400	0.49405500	0.22779600
C	1.30856200	0.45391000	0.35951800
C	2.13522400	1.65885200	0.10404200
O	3.09091000	1.96776900	0.77926500
O	1.72234300	2.35839600	-0.96234600
C	2.39539300	3.60546100	-1.17236600
H	1.96140900	4.02718900	-2.07621300
H	2.22916700	4.26771900	-0.31992000
H	3.46568200	3.43770100	-1.29998900
C	-0.76533200	1.70688200	-0.29251100
O	-0.62793000	2.74547900	0.52389700
O	-1.41649600	1.70206900	-1.30810700
C	-1.25672900	3.95488500	0.07507300
H	-2.32994700	3.79561400	-0.04048500
H	-1.05603500	4.69539400	0.84520000
H	-0.82679600	4.26254500	-0.88035900
H	1.46176700	-2.89132600	1.10786100

TS8(R')

C	1.11329400	-1.06999700	-0.40995700
C	2.96852100	-2.00899400	-1.21441700
C	3.38424700	-0.17412700	0.35163900
H	2.84920100	0.73031700	0.64641000
N	2.01245100	-2.72578600	-1.72126000
N	0.87893200	-2.13496000	-1.20110400
N	2.46861300	-1.01582500	-0.41383200
C	4.44138200	-2.01213600	-1.46172200
H	4.67562800	-2.54879900	-2.38089200
H	4.98189500	-2.47740700	-0.62673700
C	4.65858400	0.17488600	-0.49589200
O	4.81892800	-0.65586600	-1.64109100
C	5.31905300	-0.79220600	1.62327300
C	3.93283200	-0.90864400	1.55705400
C	3.21594600	-1.62590900	2.50867000
C	3.92095400	-2.24252800	3.54069400
C	5.31252700	-2.13407100	3.61196900
C	6.02103000	-1.40563000	2.65771500
C	5.84374700	0.04813100	0.48602800
H	2.13225900	-1.67532600	2.44710800
H	5.84718500	-2.62411400	4.41954200
H	7.10248000	-1.32524100	2.71629800

H	6.70953500	-0.38897600	-0.02000100
H	6.13981000	1.04043500	0.84398900
C	-0.38563000	-2.80329100	-1.35628500
C	-0.68884400	-3.81521100	-0.43851600
C	-1.28086400	-2.39525200	-2.34562100
C	-1.94790900	-4.40674800	-0.51516700
C	-2.52943100	-3.01722300	-2.38445100
C	-2.88156400	-4.01795100	-1.47889600
H	-2.20842100	-5.18501400	0.19831100
H	-3.24786500	-2.70266700	-3.13788700
C	-0.93629600	-1.28811800	-3.30289500
H	-1.64363500	-1.26434100	-4.13366600
H	0.07370600	-1.40793800	-3.70365800
H	-0.97276200	-0.31485900	-2.79981900
C	0.30800600	-4.21780400	0.61585000
H	0.59469600	-3.35886600	1.23357400
H	1.22564200	-4.60445500	0.16251200
H	-0.10888100	-4.98576000	1.26876500
H	4.57105700	1.18336700	-0.90268800
C	-4.22665200	-4.69093500	-1.55804000
H	-4.96814400	-4.03313300	-2.01694100
H	-4.16503800	-5.60439500	-2.15891400
H	-4.58540400	-4.96778400	-0.56370300
C	-5.39054100	-1.37051800	-0.49356400
C	-4.30916600	-0.58325400	-0.10809700
C	-3.71615800	-0.75701200	1.14518600
C	-4.21458000	-1.74113500	1.99841600
C	-5.29444100	-2.53387600	1.61388300
C	-5.88819600	-2.34766900	0.36771100
H	-5.84367000	-1.22459500	-1.46968800
H	-3.91783200	0.17563200	-0.78323900
H	-3.75178200	-1.88721900	2.97131200
H	-5.67315600	-3.29427200	2.28990100
H	-6.72946600	-2.96374500	0.06596200
C	-2.46419200	0.01640800	1.52752600
H	-2.33245700	-0.05134900	2.61462500
C	-1.29412900	-0.67289800	0.81609300
C	-0.04152600	0.15478200	0.94428200
O	0.66161600	0.15049400	1.94799400
H	-1.55247200	-0.78586800	-0.23912700
H	3.38698200	-2.80980700	4.29617400
C	1.71740900	2.63021200	-1.00266100
C	0.96383800	2.28931000	0.14595500
C	1.35494800	2.74522300	1.41345400

C	2.53844900	3.43670600	1.61364500
C	3.34450500	3.69950500	0.51231900
C	2.91691300	3.32453200	-0.75495600
H	0.71162000	2.51156800	2.25250000
H	2.82387400	3.75912100	2.60923800
H	4.28910500	4.22184400	0.62682600
H	3.54910200	3.59333900	-1.59121100
C	1.35850700	2.34539500	-2.47958000
C	1.77816400	0.92528600	-2.88036700
C	-0.13963600	2.52786700	-2.74860100
C	2.08443200	3.31810600	-3.42952700
H	2.83592100	0.73871100	-2.66247800
H	1.17892100	0.18494100	-2.35377100
H	1.61940300	0.78678000	-3.95609900
H	-0.44133200	3.56066900	-2.54631700
H	-0.34687100	2.32011300	-3.80375100
H	-0.75506000	1.85988800	-2.14732900
H	1.67307200	3.18903700	-4.43472200
H	1.93801000	4.36115700	-3.13279100
H	3.15744800	3.11914300	-3.49559800
N	-0.20935800	1.42549700	0.15553700
C	-1.43739500	2.03601200	0.43183700
C	-2.47690200	1.46788600	1.10425500
C	-3.58405200	2.33743700	1.55962200
O	-3.70402600	3.53183200	1.35481100
O	-4.44999700	1.66160300	2.32962000
C	-5.52084400	2.43497900	2.87311300
H	-6.13292600	1.73518000	3.43839800
H	-5.13117400	3.21776800	3.52691300
H	-6.10332000	2.89452400	2.07267300
C	-1.61412600	3.44883200	-0.10369200
O	-2.52297800	3.45110400	-1.07928500
O	-0.99833600	4.41851000	0.26138700
C	-2.88327100	4.75057400	-1.55474600
H	-2.00990800	5.26935700	-1.95597900
H	-3.62367500	4.58802900	-2.33473600
H	-3.30772100	5.32890100	-0.73120000
H	-1.11538400	-1.66140200	1.24380700

M8(R')

C	4.35029500	-1.57666800	1.65783600
C	3.21978600	-1.10462800	0.99702000
C	3.24249500	-0.89304300	-0.38408500

C	4.41135700	-1.16625000	-1.09311600
C	5.54299000	-1.64302100	-0.43460700
C	5.51562200	-1.84803300	0.94278900
H	4.32187600	-1.73185900	2.73168800
H	2.31166900	-0.89190500	1.55809000
H	4.43601500	-1.00023000	-2.16699200
H	6.44712500	-1.85127100	-0.99785500
H	6.39769600	-2.21539500	1.45725900
C	1.99182600	-0.42693400	-1.11188500
H	2.29656800	-0.04271000	-2.09394600
C	1.05783200	-1.63234500	-1.31201600
C	-0.39145800	-1.31561100	-1.59137000
O	-1.09150700	-1.97307900	-2.33125400
H	1.03780700	-2.21769600	-0.38105600
C	-3.20991300	-0.72162700	0.11247900
C	-2.35725400	-0.08476500	-0.81406400
C	-2.83692200	0.80137400	-1.77743000
C	-4.18933400	1.10651400	-1.85534600
C	-5.05434500	0.50680900	-0.95037100
C	-4.56722700	-0.38466800	0.00237300
H	-2.12365800	1.25507000	-2.45866900
H	-4.55393600	1.79865400	-2.60622400
H	-6.11678200	0.72610700	-0.97870300
H	-5.28260600	-0.82701900	0.68259300
C	-2.75899900	-1.76447800	1.15895000
C	-2.28812200	-3.05009600	0.45445000
C	-1.63779800	-1.24935100	2.07814500
C	-3.92490500	-2.16334100	2.07918800
H	-3.02115900	-3.38466200	-0.28556100
H	-1.33150700	-2.92277900	-0.05198400
H	-2.16251000	-3.84260600	1.19920800
H	-1.96488700	-0.37495500	2.64560300
H	-1.37842400	-2.04247500	2.78713200
H	-0.72964100	-0.97983700	1.53595700
H	-3.55084500	-2.86055200	2.83367400
H	-4.34579300	-1.29845100	2.60083400
H	-4.72673900	-2.66839400	1.53277600
N	-0.92456400	-0.28635600	-0.81035500
C	-0.08348400	0.71294300	-0.30416600
C	1.25944100	0.68213100	-0.39307900
C	2.01118000	1.84687600	0.13091800
O	1.60907100	2.61011000	0.98611300
O	3.20137500	1.97165300	-0.46263100
C	4.01703500	3.04608100	0.01523100

H	4.94536100	2.98585600	-0.54832600
H	3.52218100	4.00295300	-0.15882700
H	4.20711100	2.92646400	1.08341200
C	-0.81692500	1.93566800	0.21439600
O	-1.33051900	1.73142000	1.41721300
O	-0.96265200	2.93278800	-0.44725700
C	-2.15620900	2.79327000	1.91552100
H	-2.98190400	2.97266600	1.22401100
H	-2.52651900	2.45042500	2.87876200
H	-1.56553900	3.70373500	2.02806900
H	1.42306500	-2.28863100	-2.10249700

TS8(R)

C	1.06083100	-0.98258200	-0.41578100
C	2.57405200	-2.05847900	-1.63149900
C	3.55961500	-0.45265300	-0.06758700
H	3.23610100	0.49837300	0.35203700
N	1.44793000	-2.59952500	-1.97852900
N	0.52669100	-1.92927300	-1.20631800
N	2.38684000	-1.08223700	-0.69085100
C	3.94808900	-2.24525900	-2.18477800
H	3.89905600	-2.71542600	-3.16683400
H	4.56366900	-2.86609400	-1.52016200
C	4.71523000	-0.26363300	-1.11527500
O	4.48832200	-0.94506000	-2.34234400
C	5.51817500	-1.53969000	0.78686700
C	4.15187300	-1.36145200	0.98753000
C	3.48374700	-1.98296600	2.03815200
C	4.21460600	-2.80509900	2.89291600
C	5.58616400	-2.99126500	2.69639700
C	6.24789000	-2.35776800	1.64613700
C	5.99968200	-0.75349800	-0.40579400
H	2.42268000	-1.80016400	2.18386000
H	6.14221100	-3.63705300	3.36876000
H	7.31303000	-2.50687900	1.49543100
H	6.60856000	-1.34393000	-1.09760900
H	6.60655700	0.10113900	-0.09021600
C	-0.83146500	-2.40241400	-1.28658500
C	-1.16983200	-3.51294200	-0.50217400
C	-1.71207800	-1.82808900	-2.20430500
C	-2.45231900	-4.03916500	-0.64413800
C	-2.99208400	-2.38028500	-2.29646900
C	-3.37500000	-3.48574900	-1.53606500

H	-2.73848600	-4.89648100	-0.04020100
H	-3.70114800	-1.93572600	-2.99123800
C	-1.30267100	-0.69732400	-3.10347500
H	-0.42882100	-0.16487700	-2.72691400
H	-2.11755800	0.02320000	-3.19068900
H	-1.06129200	-1.08048900	-4.10074900
C	-0.17351200	-4.10623800	0.45811100
H	0.73114500	-4.42828500	-0.06675900
H	-0.60196300	-4.96612500	0.97460900
H	0.13443200	-3.37173500	1.21102200
H	4.78481600	0.78694300	-1.39807500
C	-4.76462500	-4.05378900	-1.67091900
H	-4.92784900	-4.87506500	-0.96976300
H	-5.51770900	-3.28293200	-1.47988700
H	-4.93543700	-4.43094600	-2.68351900
C	-4.63880400	-2.35136100	1.73242600
C	-3.66118500	-1.48671800	1.25525700
C	-3.15775100	-0.46258800	2.06089700
C	-3.64660400	-0.32061300	3.35755100
C	-4.63026700	-1.18496200	3.84051400
C	-5.12813100	-2.20190800	3.03112300
H	-5.01515100	-3.14493300	1.09261900
H	-3.28355400	-1.59520500	0.24052700
H	-3.25842000	0.47024200	3.99436600
H	-5.00619800	-1.06174300	4.85142600
H	-5.89114200	-2.87527600	3.40820200
C	-2.03558800	0.41072000	1.54295300
H	-1.88696000	1.24841100	2.24238200
C	-0.75040600	-0.43802500	1.52107000
C	0.48858300	0.26716800	0.93603400
O	1.49860500	0.40908400	1.66131900
H	-0.98075300	-1.35005500	0.97051200
H	3.71751000	-3.30387500	3.71865600
C	1.48113600	3.52951700	0.49076400
C	1.16999700	2.36201900	-0.24696300
C	1.90159800	2.02042100	-1.38858100
C	2.97593400	2.78531500	-1.82343800
C	3.32727200	3.91072400	-1.08997200
C	2.58496900	4.26639200	0.03147800
H	1.59417500	1.14590700	-1.95247700
H	3.52004400	2.50511100	-2.71991300
H	4.16780100	4.52682800	-1.39298300
H	2.88314200	5.16197700	0.55948800
C	0.68186600	4.05387600	1.70576500

C	-0.79351400	4.28025500	1.33229900
C	0.76356700	3.09820100	2.90590800
C	1.22042300	5.41271000	2.18580400
H	-0.88363500	4.89405400	0.43057100
H	-1.33161200	3.34723400	1.16305600
H	-1.29479500	4.80421600	2.15289700
H	1.80455100	2.93312800	3.20075100
H	0.23199500	3.54686800	3.75271500
H	0.32989800	2.12412200	2.68984900
H	0.60885400	5.74952900	3.02728200
H	2.25440700	5.34648800	2.53709300
H	1.16330700	6.17701900	1.40443600
N	0.10869300	1.46050300	0.12700100
C	-1.14672200	1.56448400	-0.42618500
C	-2.23382700	1.00302600	0.16283700
C	-3.53800100	1.10818200	-0.51572800
O	-3.70708400	1.06404400	-1.72154700
O	-4.54873000	1.27604000	0.34652700
C	-5.85613800	1.24047200	-0.22745600
H	-6.54877800	1.36041800	0.60313500
H	-5.98006300	2.04764400	-0.95144900
H	-6.02068500	0.28173900	-0.72539500
C	-1.30649200	2.43366800	-1.65808000
O	-2.18482600	3.41088500	-1.43645500
O	-0.70719100	2.28670000	-2.69557000
C	-2.52373100	4.19244800	-2.58675100
H	-2.99306400	3.55127400	-3.33615500
H	-3.22242400	4.94829400	-2.23580200
H	-1.63051200	4.65593100	-3.00817800
H	-0.47107700	-0.72113000	2.53996200

M8(R)

C	-5.19465100	-0.48831500	-1.36471000
C	-3.81990000	-0.41891800	-1.16187700
C	-3.23179200	-1.04833200	-0.06041300
C	-4.04092000	-1.75677800	0.82583200
C	-5.41764600	-1.83299500	0.62146900
C	-5.99813700	-1.19724800	-0.47260700
H	-5.63963600	0.01050400	-2.21975500
H	-3.19917600	0.13950400	-1.86038500
H	-3.59108100	-2.24749300	1.68485700
H	-6.03578700	-2.38743300	1.32045700
H	-7.07031600	-1.25228500	-0.63030300

C	-1.72773500	-1.00670200	0.13721400
H	-1.50215600	-1.36839600	1.15053900
C	-1.07057100	-1.94257200	-0.89000500
C	0.43778600	-1.87756900	-0.92867700
O	1.13771100	-2.82177000	-1.22926800
H	-1.42052100	-1.67015600	-1.89456500
C	3.31730600	-0.61880600	0.30771800
C	2.42437600	-0.47919800	-0.77331600
C	2.86621700	-0.21032600	-2.06846100
C	4.21602200	-0.04283000	-2.34050500
C	5.12148500	-0.15553200	-1.29284700
C	4.67378600	-0.43898100	-0.00640500
H	2.12297800	-0.11877200	-2.85357700
H	4.54977100	0.17196400	-3.34970000
H	6.18455900	-0.02833200	-1.47045100
H	5.41767900	-0.52913700	0.77379600
C	2.89645100	-0.95896900	1.75213800
C	2.03718700	0.16481300	2.35457700
C	2.11518600	-2.28482900	1.80758200
C	4.12324000	-1.12458900	2.66314600
H	2.55694300	1.12624100	2.30578500
H	1.07558000	0.27323400	1.84941300
H	1.83299900	-0.06305600	3.40609800
H	2.62942500	-3.07350900	1.25147000
H	2.02027800	-2.60202400	2.85090000
H	1.10568500	-2.18418000	1.40704600
H	3.77907100	-1.37104500	3.67111500
H	4.77680000	-1.93484100	2.32548200
H	4.71117100	-0.20455900	2.73085600
N	0.99236400	-0.63228700	-0.62794600
C	0.17092300	0.47991700	-0.41123000
C	-1.11661900	0.36847700	-0.03466400
C	-1.87942200	1.60833900	0.25326100
O	-1.72884000	2.67038300	-0.31592800
O	-2.75434400	1.42022800	1.24304800
C	-3.61269000	2.52999500	1.52571300
H	-4.25776800	2.20471500	2.33873200
H	-3.02465400	3.39925300	1.82368600
H	-4.20411800	2.77720700	0.64174600
C	0.79962800	1.83176300	-0.67124500
O	0.99838500	2.51154300	0.44970900
O	1.07725900	2.21594800	-1.77977100
C	1.43395100	3.86552200	0.26526100
H	0.65926100	4.42122500	-0.26667100

H	1.58092300	4.26794400	1.26449800
H	2.36411100	3.88939000	-0.30362400
H	-1.35071500	-2.98264900	-0.71582300

TS9

C	-5.08341900	-1.71118800	-0.68768300
C	-3.75903500	-1.28868300	-0.75030700
C	-2.89242300	-1.50291600	0.32776400
C	-3.37338100	-2.15866400	1.46027100
C	-4.69730600	-2.59035900	1.52178900
C	-5.55600800	-2.36506200	0.44965400
H	-5.74575400	-1.53214200	-1.52844000
H	-3.40360100	-0.77469300	-1.64092900
H	-2.70823100	-2.32914000	2.30221500
H	-5.05661100	-3.09932600	2.41029500
H	-6.58790700	-2.69679500	0.49786900
C	-1.45149400	-1.04367400	0.26475700
H	-0.96207800	-1.26704200	1.22176100
C	-0.67536800	-1.76618400	-0.84830400
C	0.71785700	-1.20738500	-1.09074000
O	1.42900400	-1.65785600	-1.95145100
H	-1.21946900	-1.71686900	-1.79687700
C	3.55776400	-0.40151300	0.42962400
C	2.29035400	0.25631300	0.42532300
C	2.13701700	1.39217500	1.24869500
C	3.18862800	2.00067200	1.91282100
C	4.45675900	1.45677500	1.79825500
C	4.59779600	0.27108300	1.09248600
H	1.15122600	1.81049300	1.40637200
H	2.99915200	2.88112900	2.51721700
H	5.31494600	1.91071500	2.28126100
H	5.58265200	-0.17460100	1.07215200
C	3.91210500	-1.77234100	-0.18350600
C	2.82521200	-2.82788600	0.16905500
C	4.21279200	-1.59196900	-1.68899900
C	5.21036200	-2.36370500	0.41277000
H	1.88824900	-2.39087700	0.51797800
H	2.60179400	-3.47225100	-0.68419100
H	3.17859600	-3.45762600	0.98989100
H	5.17850400	-1.08636300	-1.79179500
H	4.28699800	-2.56815800	-2.18026800
H	3.46053200	-1.00424900	-2.20465100
H	5.31669800	-3.38299700	0.02861800

S229

H	6.10900900	-1.81658200	0.11848400
H	5.16883400	-2.41715900	1.50482400
N	1.06352500	-0.11794700	-0.23779300
C	0.00330200	0.83113400	-0.25108200
C	-1.25366600	0.43539700	-0.01631900
C	-2.41836700	1.35267200	-0.21288200
O	-2.67108900	1.93449500	-1.24309600
O	-3.16770600	1.40541600	0.88557900
C	-4.40036500	2.12428700	0.75002200
H	-4.88409400	2.06769800	1.72207900
H	-4.20530000	3.16145900	0.47428200
H	-5.01820800	1.65112300	-0.01638800
C	0.33537400	2.19924400	-0.78200700
O	-0.31080400	3.15509900	-0.11858800
O	1.08677800	2.38244500	-1.70727100
C	-0.18366000	4.47407500	-0.66695300
H	-0.59602100	4.49368700	-1.67718300
H	-0.75268700	5.12384300	-0.00688000
H	0.86613000	4.76891700	-0.69121200
H	-0.54247700	-2.82714800	-0.61035700

TS10

C	-4.95291900	-2.30741900	-0.87006300
C	-3.69659700	-1.71125200	-0.81731700
C	-2.95684200	-1.71514600	0.37058600
C	-3.49242200	-2.33704400	1.49747600
C	-4.74734500	-2.94160200	1.44491100
C	-5.48164600	-2.92570100	0.26248900
H	-5.51824900	-2.29087800	-1.79619200
H	-3.29718300	-1.22562300	-1.70523700
H	-2.92595300	-2.34362800	2.42457400
H	-5.15131600	-3.42089600	2.33076300
H	-6.46042100	-3.39208400	0.22158600
C	-1.59005700	-1.06597600	0.42961200
H	-1.20831300	-1.13166600	1.45681200
C	-0.59735900	-1.77652800	-0.50234800
C	0.76644600	-1.11126000	-0.58268400
O	1.70373200	-1.66083600	-1.10613000
H	-1.00097400	-1.82125900	-1.52021200
C	3.32869000	0.45934100	0.49557600
C	1.96878000	0.84912300	0.55479400
C	1.65011400	2.01030700	1.28685400
C	2.61727400	2.85026700	1.81507800

C	3.96077100	2.53822700	1.65164300
C	4.28323800	1.34530900	1.02371100
H	0.61087400	2.26038400	1.46490200
H	2.30981200	3.73672600	2.35918800
H	4.74030200	3.18348400	2.04072400
H	5.32399000	1.04470000	0.95112800
N	0.83379200	0.18513900	-0.02298600
C	-0.35355500	0.94181800	-0.19534600
C	-1.55695400	0.39183900	0.00889800
C	-2.81294400	1.12652400	-0.33334700
O	-3.04801500	1.63035600	-1.40840000
O	-3.66071900	1.11521700	0.69294500
C	-4.96571500	1.63730700	0.41358100
H	-5.52574300	1.54509000	1.34098300
H	-4.89817400	2.68109200	0.10405900
H	-5.43360900	1.04933700	-0.37921700
C	-0.19297900	2.29956700	-0.82794300
O	-0.96458200	3.21133400	-0.24198700
O	0.54031400	2.50714700	-1.76231100
C	-1.00824300	4.48586500	-0.89751500
H	-1.41537600	4.36687100	-1.90313500
H	-1.66042700	5.10792700	-0.28974600
H	-0.00591900	4.91249300	-0.95278100
H	-0.41946100	-2.80663800	-0.18274700
C	3.91692700	-0.83957700	0.04824100
C	4.76931500	-0.88775700	-1.05581900
C	3.74270400	-1.98870500	0.82430800
C	5.40280800	-2.07772800	-1.40585800
H	4.92432200	0.00924100	-1.64839000
C	4.37904700	-3.17632700	0.47848000
H	3.09711100	-1.94841000	1.69753400
C	5.20677800	-3.22611400	-0.64227600
H	6.05344900	-2.10610900	-2.27429600
H	4.23216800	-4.06346300	1.08653800
H	5.70281700	-4.15255200	-0.91318800

TS11

C	-4.87928100	-3.32458400	-0.91543100
C	-3.82291300	-2.42308500	-0.82663800
C	-3.21118600	-2.16355800	0.40504200
C	-3.66702800	-2.83304700	1.53973300
C	-4.71976900	-3.74239100	1.45177900
C	-5.33023500	-3.98805500	0.22512700
H	-5.34868700	-3.51073000	-1.87595300

S231

H	-3.48383100	-1.90656400	-1.72219600
H	-3.19858400	-2.63765900	2.50032500
H	-5.06395800	-4.25504300	2.34415800
H	-6.15259400	-4.69243100	0.15606200
C	-2.06112700	-1.18355800	0.50427100
H	-1.76741600	-1.08396400	1.55737000
C	-0.84364400	-1.67414600	-0.29373900
C	0.31236700	-0.68926100	-0.33001000
O	1.40135500	-1.01112900	-0.73726100
H	-1.13062900	-1.88266000	-1.33062200
C	2.30095600	1.53409900	0.79354300
C	0.88673500	1.58029900	0.71457000
C	0.23295400	2.68247200	1.29960200
C	0.91669200	3.77671500	1.80513700
C	2.30458500	3.79480800	1.76868800
C	2.96094300	2.66995300	1.29404800
H	-0.84770800	2.68253100	1.37792200
H	0.35596100	4.60086100	2.23254300
H	2.86721800	4.64262000	2.14284000
H	4.04485600	2.62938800	1.33258000
N	0.00411800	0.61197500	0.12723100
C	-1.31288800	1.02918700	-0.19724800
C	-2.35480000	0.20458600	-0.03443900
C	-3.71662200	0.56997200	-0.53129600
O	-3.96774400	0.92286000	-1.66144700
O	-4.62657900	0.41352600	0.42735100
C	-5.98844300	0.56819000	0.00876100
H	-6.59171200	0.40185500	0.89788200
H	-6.15143200	1.57115600	-0.38786000
H	-6.22182500	-0.17241400	-0.75942100
C	-1.43638900	2.33380800	-0.94014200
O	-2.45857200	3.06043000	-0.49631700
O	-0.69543500	2.65162000	-1.83662500
C	-2.75345900	4.23290500	-1.26750900
H	-3.02283800	3.94411600	-2.28495100
H	-3.59262700	4.71080600	-0.76845400
H	-1.88643100	4.89440300	-1.28847300
H	-0.44395900	-2.60320100	0.12118600
C	3.22041800	0.38463700	0.54035300
C	4.22004000	0.47815900	-0.39637400
C	3.17304500	-0.75079000	1.39792400
C	5.17881500	-0.55766900	-0.55492100
H	4.27893500	1.35063800	-1.04243500
C	4.09132500	-1.75806300	1.27948000

H	2.39286400	-0.80569900	2.15223300
C	5.11659700	-1.69607200	0.29616100
H	4.05040300	-2.62039600	1.93927600
C	6.20461700	-0.48748000	-1.53550400
C	7.12109900	-1.50062400	-1.66391700
H	7.89977800	-1.43778400	-2.41716200
H	6.24858800	0.38367800	-2.18338700
C	7.05900300	-2.63393500	-0.81541200
H	7.79037300	-3.42776300	-0.92691100
C	6.08012300	-2.72756700	0.14187000
H	6.02705700	-3.59345900	0.79617400