

SUPPORTING INFORMATION FOR

Insights to N-heterocyclic carbene-catalyzed [3 + 4] annulation reactions of 2-bromoaldehydes with N-Ts hydrazones

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Part 1: Computational details

In the distortion/interaction theory, the activation energy ($\Delta E^\ddagger$) is divided into two main components: the distortion ($\Delta E^\ddagger_{\text{dist}}$) and interaction ($\Delta E^\ddagger_{\text{int}}$) energies. The distortion energy involves geometric and electronic changes to deform the reactants to their transition state geometry. The interaction energy is obtained by the relationship: $\Delta E^\ddagger_{\text{int}} = \Delta E^\ddagger - \Delta E^\ddagger_{\text{dist}}$.

For the global reactivity index (GRI) analysis, the relevant parameters of GIR, *i.e.*, electrophilicity index ω^1 , electronic chemical potential μ , chemical hardness η , one-electron energies of the frontier molecular orbital HOMO (E_L) and LUMO (E_H), were computed to determine what is the role (Lewis base or nucleophile) of the catalyst NHC. The HOMO energies obtained within the Kohn–Sham scheme,² nucleophilicity index N^3 was generally utilized to judge the nucleophilicity character.

In addition, 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:

$$\frac{[R]}{[S]} = \frac{\exp(-\Delta G^\ddagger_{[R]} / RT)}{\exp(-\Delta G^\ddagger_{[S]} / RT)} = \exp(\Delta\Delta G^\ddagger / RT)$$
$$ee = \frac{[R] - [S]}{[R] + [S]} \times 100\% = \frac{\frac{[R]}{[S]} - 1}{\frac{[R]}{[S]} + 1} \times 100\%$$

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.

Part 2: The relative Gibbs free energy (GFE) profiles of other possible pathways of steps 1-4

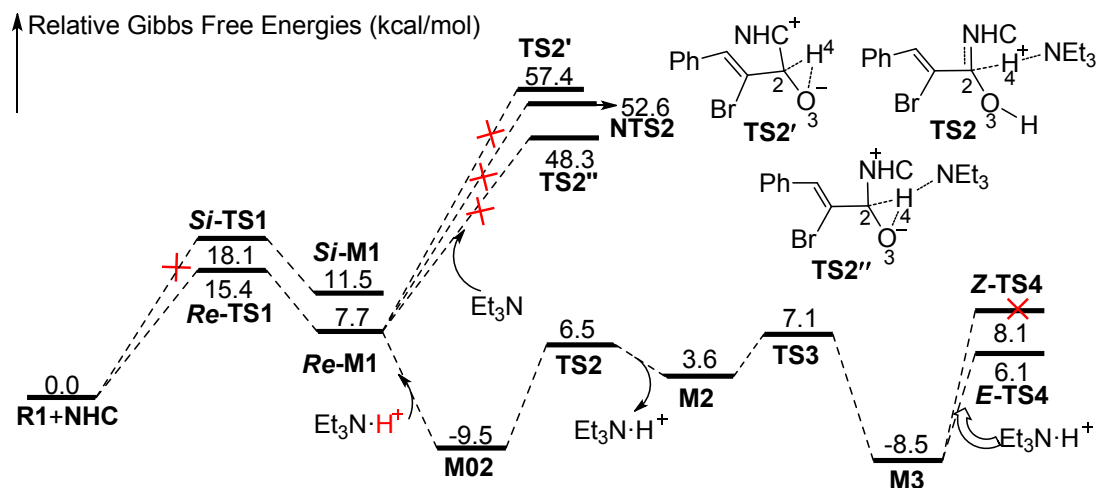


Fig. S1 The relative Gibbs free energy profiles of the NHC-catalyzed reaction pathways (unit: kcal/mol).

Part 3: The deprotonation of pre-R2 by base Et₃N generating R2

It should be noted that the **pre-R2** should be firstly deprotonated by base Et₃N to generate the reactive **R2** via transition state **TS0**. As shown in **Fig. S2**, the energy barrier via **TS0** is 15.6 kcal/mol, indicating that this step can happen under the experimental condition.

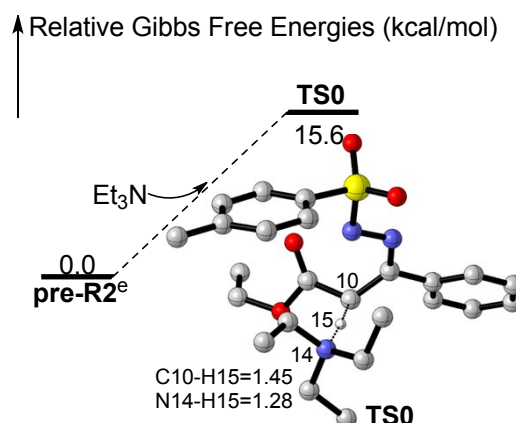


Fig. S2 The relative Gibbs free energy profiles of the deprotonation of **pre-R2** generating **R2**. (“^e” represents adding the energies of Et₃N, unit: kcal/mol)

Part 4: Test results of the different computational methods

We have compared the relative energies ($\Delta\Delta G$) of the *Re/Si-TS1* and *Re/Si-M1* calculated at the M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM_{toluene}//M06-2X/6-31G(d, p)/IEF-PCM_{toluene} (L1), M06-2X/6-311++G(2df, 2pd)/SMD_{toluene}//M06-2X/6-31G(d, p)/SMD_{toluene} (L2), ω b97X-D/6-311++G(2df, 2pd)/IEF-PCM_{toluene}// ω b97X-D/6-31G(d,p)/IEF-PCM_{toluene} (L3), B3PW91-D3/6-311++G(2df, 2pd)/IEF-PCM_{toluene}//B3PW91/6-31G(d, p)/IEF-PCM_{toluene} (L4) levels. As shown in **Table S1**, there are small differences for the $\Delta\Delta G$ of the stationary points (SPs), indicating the selected method is proper and reliable in this kind of reaction system.

Table S1 Comparison of relative Gibbs free energies ($\Delta\Delta G$) of the *Re/Si-TS1* and *Re/Si-M1* calculated by using the different levels.

	<i>Re-TS1</i>	<i>Si-TS1</i>	<i>Re-M1</i>	<i>Si-M1</i>
L1	10.4	7.6	4.8	0.0
L2	9.6	6.5	4.5	0.0
L3	8.2	5.2	4.1	0.0
L4	9.2	5.3	3.6	0.0

Part 5: The electrophilic and nucleophilic Parr functions (P_k^+ and P_k^-) of the key atoms of intermediates *E-M4*

Table S2 The electrophilic and nucleophilic Parr functions (P_k^+ and P_k^-) of the key atoms of intermediates *E-M4*.

<i>E-M4</i>	C9	C2
P_k^+	0.33	0.21
P_k^-	-0.01	-0.01

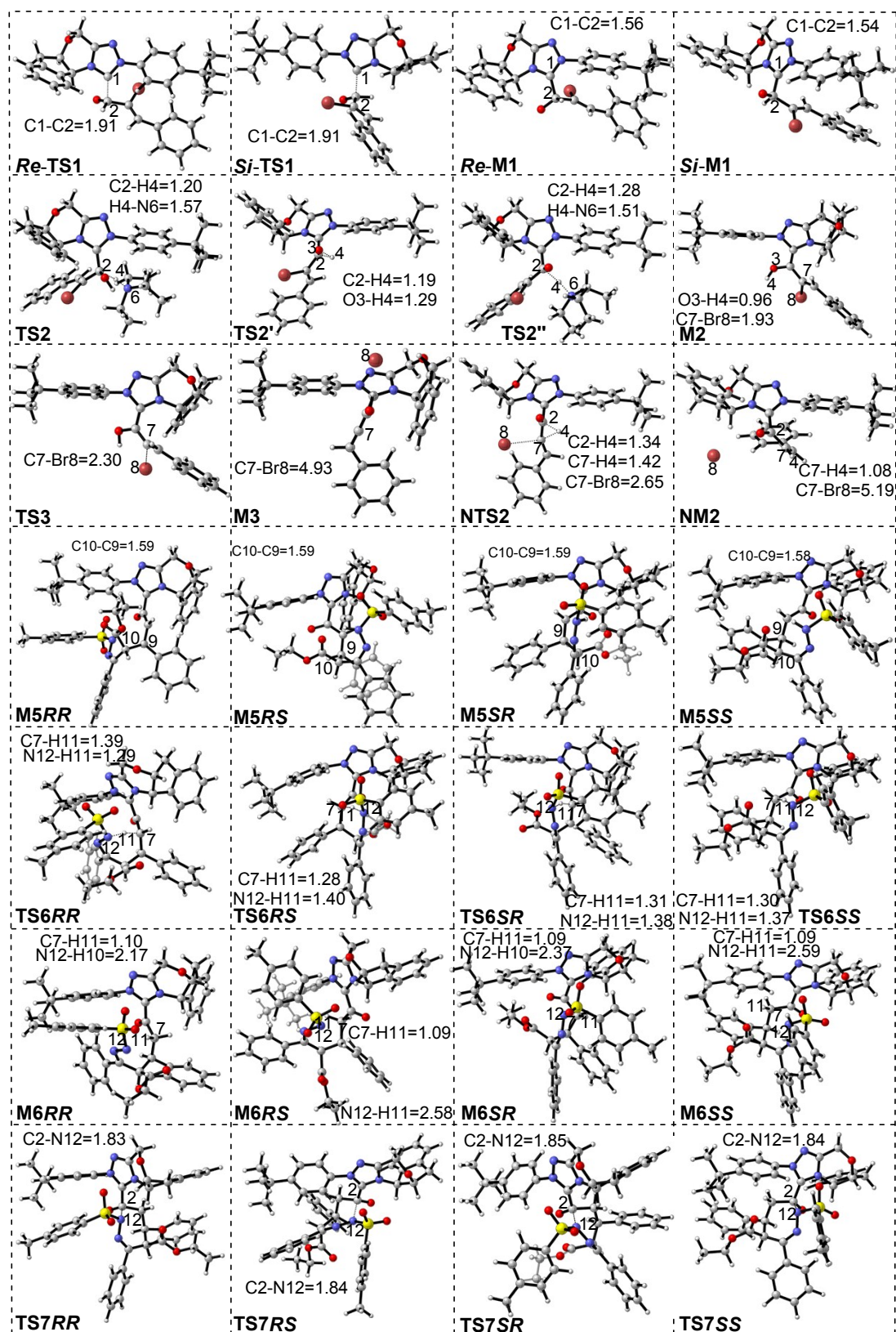
Part 6: Different conformations and configurations of TS5s

The enolate intermediate **E-M4** reacts with the reactant **R2** for the formation of intermediates **M5RR&RS&SR&SS** via the corresponding transition states **TS5RR&RS&SR&SS**. Different conformational possibilities of the transition states were explored for the nucleophilic addition of reactant **R2** to the enolate intermediate **E-M4**. We have considered and investigated the different conformations of **TS5RR&RS&SR&SS** in the C–C bond formation step. By rotating dihedral angle $\Phi_1(\text{C7–C9–C10–C13})$ from 0–360° at intervals of 90° in the four transition states **TS5RR&RS&SR&SS**, there should be sixteen (4×4) possible initial conformations obtained in theory. Actually, we have obtained sixteen conformations (*i.e.*, **TS5RR&RS&SR&SS**, **TS5'RR&RS&SR&SS**, **TS5''RR&RS&SR&SS** and **TS5'''RR&RS&SR&SS**) after optimizations. The energy barriers of the sixteen conformations have been provided in **Table S3**. As summarized in **Table S3**, the conformers **TS5RR** (1.4 kcal/mol), **TS5RS** (–0.1 kcal/mol), **TS5SR** (–4.0 kcal/mol), and **TS5SS** (4.2 kcal/mol) have the lowest energies compared to their conformers respectively, so they should be the most energetically favorable conformers, and we only discussed them in the main text of the manuscript.

Table S3 The relative Gibbs free energies ($\Delta\Delta G$) for different conformations of **TS5RR&RS&SR&SS**, **TS5'RR&RS&SR&SS**, **TS5''RR&RS&SR&SS** and **TS5'''RR&RS&SR&SS** with the energy of **R1+pre-R2+NHC** as 0.0 kcal/mol (unit: kcal/mol).

SP	Energy	SP	Energy	SP	Energy	SP	Energy
TS5RR	1.4	TS5RS	–0.1	TS5RS	–4.0	TS5SS	4.2
TS5'RR	6.5	TS5'RS	–0.1	TS5'RS	2.8	TS5'SS	6.4
TS5''RR	6.8	TS5''RS	6.4	TS5''RS	8.4	TS5''SS	6.8
TS5'''RR	10.6	TS5'''RS	7.2	TS5'''RS	8.6	TS5'''SS	9.7

Part 7: Optimized geometries of some stationary points



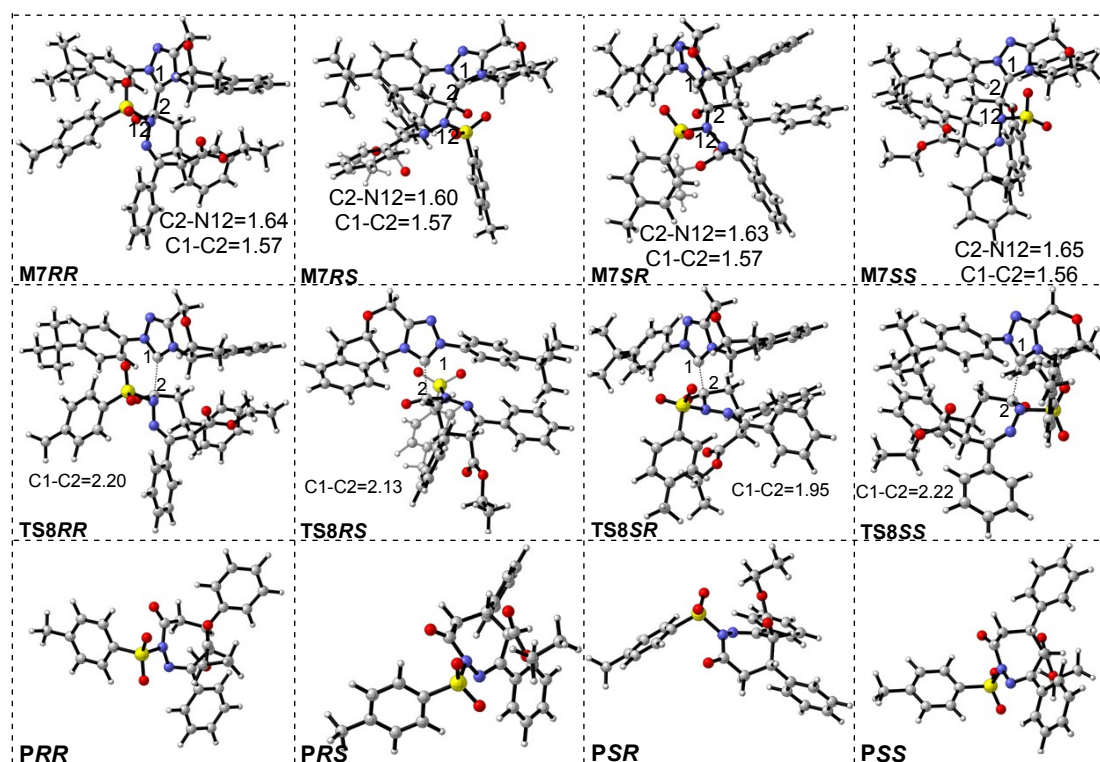


Fig. S3 Optimized geometries of some stationary points.

Part 8: Absolute single-point energies and GFE of the optimized structures by the M06-2X

Table S4 The single-point and GFE (=E+GFEC) energies of the stationary points involved in the [3 + 4] annulations reaction of 2-bromoenal with N-Ts hydrazone (unit: a.u.).

SP	E (M06-2X-D3/6-311++G(2df, 2pd)/IEF-PCM _{toluene})	GFEC (M06-2X/6-31G(d, p)/IEF-PCM _{toluene})	GFE
R1	-1506.432798	0.302317	-1506.130481
pre-R2	-2996.502221	0.097152	-2996.405069
NHC	-1091.534364	0.363119	-1091.171245
Et₃N	-292.361398	0.175101	-292.186297
Et₃NH⁺	-292.7819847	0.191431	-292.5905537
HBr	-2574.767771	-0.01312	-2574.780891
Re-TS1	-4088.039271	0.485914	-4087.5534
Si-TS1	-4088.043332	0.487568	-4087.5558
Re-M1	-4088.053045	0.489017	-4087.564
Si-M1	-4088.045219	0.488933	-4087.5563
M02	-4380.882085	0.700067	-4380.182018
TS2	-4380.85714	0.700663	-4380.156477
TS2'	-4087.967945	0.483059	-4087.484886
TS2''	-4380.369692	0.684063	-4379.685629
M2	-4088.056459	0.485885	-4087.570574
TS3	-4088.051418	0.486402	-4087.565016
NTS2	-4087.973161	0.480646	-4087.492515
M3	-4088.077215	0.487261	-4087.589954
E-TS4	-4380.849754	0.692623	-4380.157131
Z-TS4	-4380.850953	0.697057	-4380.153896
E-M4	-1513.729294	0.489637	-1513.239657
Z-M4	-1513.71883	0.490864	-1513.227966
TS5RR	-3019.736112	0.812581	-3018.923531
TS5RR'	-3019.727401	0.811932	-3018.915469
TS5RR''	-3019.721422	0.806508	-3018.914914
TS5RR'''	-3019.718215	0.809322	-3018.908893
TS5RS	-3019.737834	0.811691	-3018.926143
TS5RS'	-3019.738869	0.812749	-3018.92612
TS5RS''	-3019.727057	0.811305	-3018.915752
TS5RS'''	-3019.724279	0.809759	-3018.91452
TS5SR	-3019.743218	0.810906	-3018.932312

TS5SR'	-3019.738429	0.814175	-3018.924254
TS5SR''	-3019.724649	0.809246	-3018.915403
TS5SR'''	-3019.727045	0.811967	-3018.915078
TS5SS	-3019.733767	0.814577	-3018.91919
TS5SS'	-3019.727863	0.812169	-3018.915694
TS5SS''	-3019.72431	0.809289	-3018.915021
TS5SS'''	-3019.722477	0.812024	-3018.910453
NTS5	-3019.730605	0.818599	-3018.912006
M5RR	-3019.75839	0.81228	-3018.94611
M5RS	-3019.770987	0.817897	-3018.95309
M5SR	-3019.770928	0.817233	-3018.953695
M5SS	-3019.753209	0.813443	-3018.939766
TS6RR	-3019.739999	0.811516	-3018.928483
TS6RS	-3019.749645	0.81201	-3018.937635
TS6SR	-3019.749023	0.808798	-3018.940225
TS6SS	-3019.733791	0.812014	-3018.921777
M6RR	-3019.758033	0.816633	-3018.9414
M6RS	-3019.758951	0.81633	-3018.942621
M6SR	-3019.768523	0.817508	-3018.951015
M6SS	-3019.75433	0.817572	-3018.936758
TS7RR	-3019.753903	0.813068	-3018.940835
TS7RS	-3019.755174	0.815099	-3018.940075
TS7SR	-3019.758531	0.814085	-3018.944446
TS7SS	-3019.747717	0.81717	-3018.930547
TS7SR'	-3019.729231	0.817641	-3018.91159
M7RR	-3019.75688	0.814737	-3018.942143
M7RS	-3019.755933	0.815733	-3018.9402
M7SR	-3019.763828	0.817042	-3018.946786
M7SS	-3019.748333	0.816609	-3018.931724
TS8RR	-3019.743693	0.814534	-3018.929159
TS8RS	-3019.746189	0.815623	-3018.930566
TS8SR	-3019.749863	0.814095	-3018.935768
TS8SS	-3019.732826	0.816357	-3018.916469
PRR	-1928.208005	0.425622	-1927.782383
PRS	-1928.214421	0.422193	-1927.792228
PSR	-1928.214421	0.422193	-1927.792228
PSS	-1928.208005	0.425622	-1927.782383
TS0	-1798.791726	0.499903	-1798.291823
Re-TS1(L2)	-4088.067331	0.486723	-4087.580608
Si-TS1(L2)	-4088.062559	0.486994	-4087.575565
Re-M1(L2)	-4088.079533	0.488622	-4087.590911
Si-M1(L2)	-4088.072816	0.4890451	-4087.58377
Re-TS1(L3)	-4088.153337	0.488061	-4087.665276

<i>Si</i>-TS1(L3)	-4088.152752	0.492145	-4087.660607
<i>Re</i>-M1(L3)	-4088.16368	0.490064	-4088.16368
<i>Si</i>-M1(L3)	-4088.156846	0.489781	-4087.667065
<i>Re</i>-TS1(L4)	-4088.09718	0.477834	-4087.619346
<i>Si</i>-TS1(L4)	-4088.091205	0.478077	-4087.613128
<i>Re</i>-M1(L4)	-4088.107434	0.479635	-4087.627799
<i>Si</i>-M1(L4)	-4088.103708	0.481672	-4087.622036
NHC1	-1256.737767	0.330431	-1256.407336
NHC2	-1052.231563	0.332477	-1051.89909
<i>E</i>-M4_{NHC1}	-1678.932559	0.459665	-1678.472894
<i>E</i>-M4_{NHC2}	-1513.724998	0.492927	-1513.232071
TS5SR_{NHC1}	-3184.950487	0.782219	-3184.168268
TS5SR_{NHC2}	-2980.441318	0.785272	-2979.656046

Part 9: IRC results of Z-TS4 and E-TS4

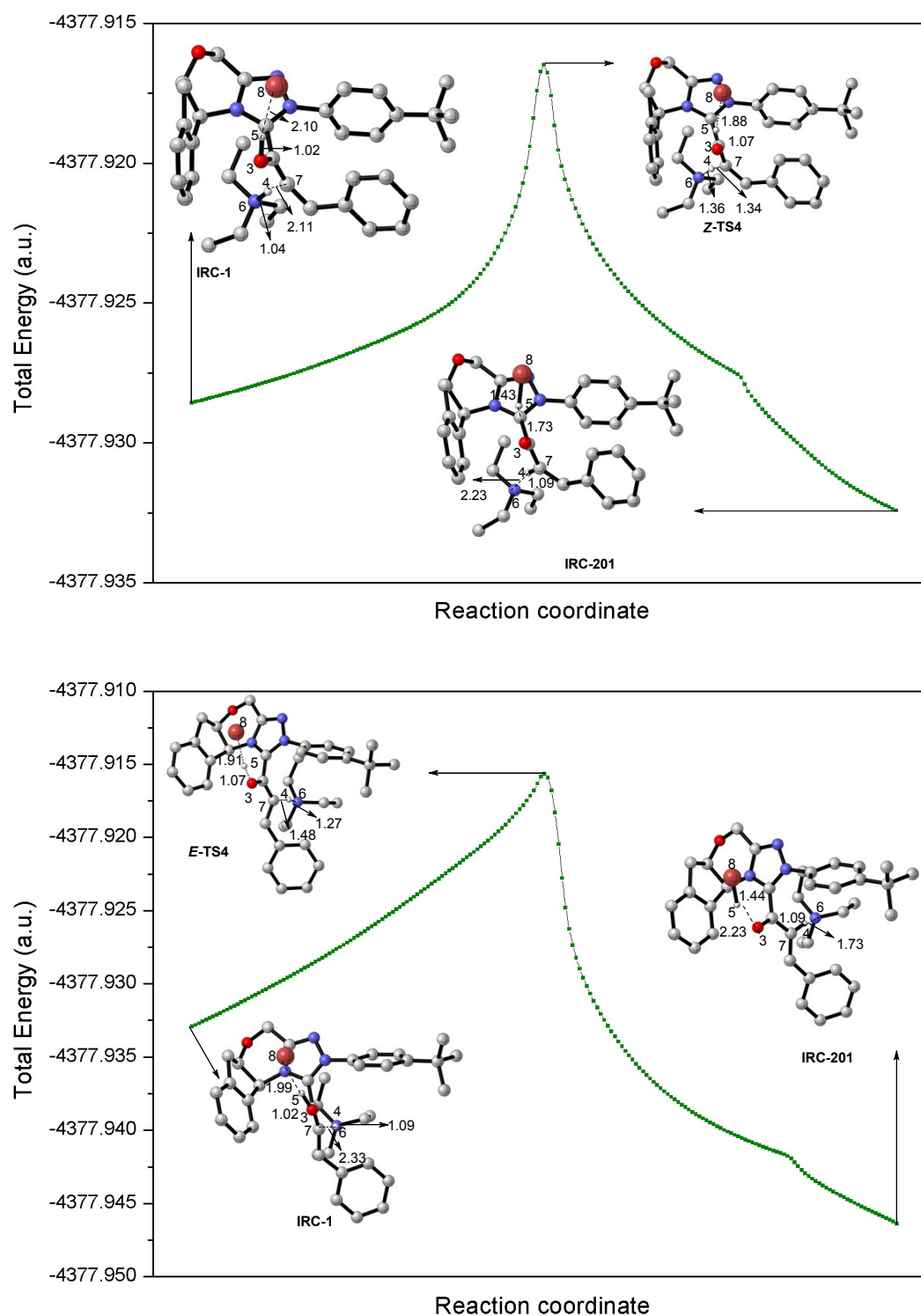
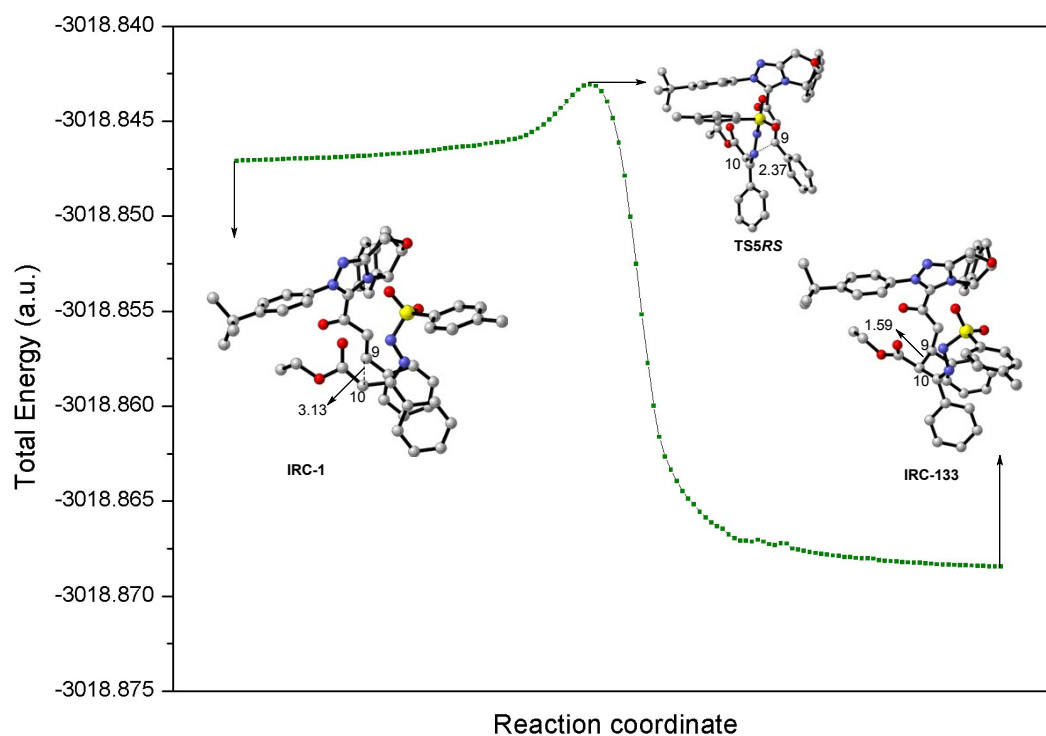
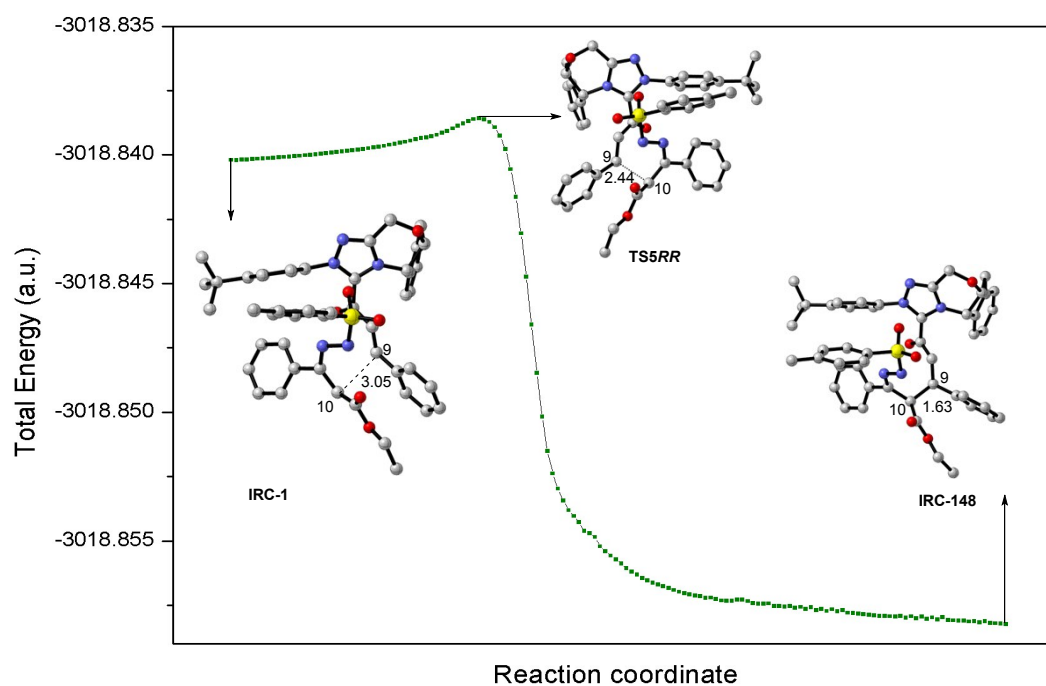


Fig. S4 IRC results of Z-TS4 and E-TS4 (distance unit: Å).

Part 10: IRC results of TS5RR, TS5RS, TS5SR, and TS5SS



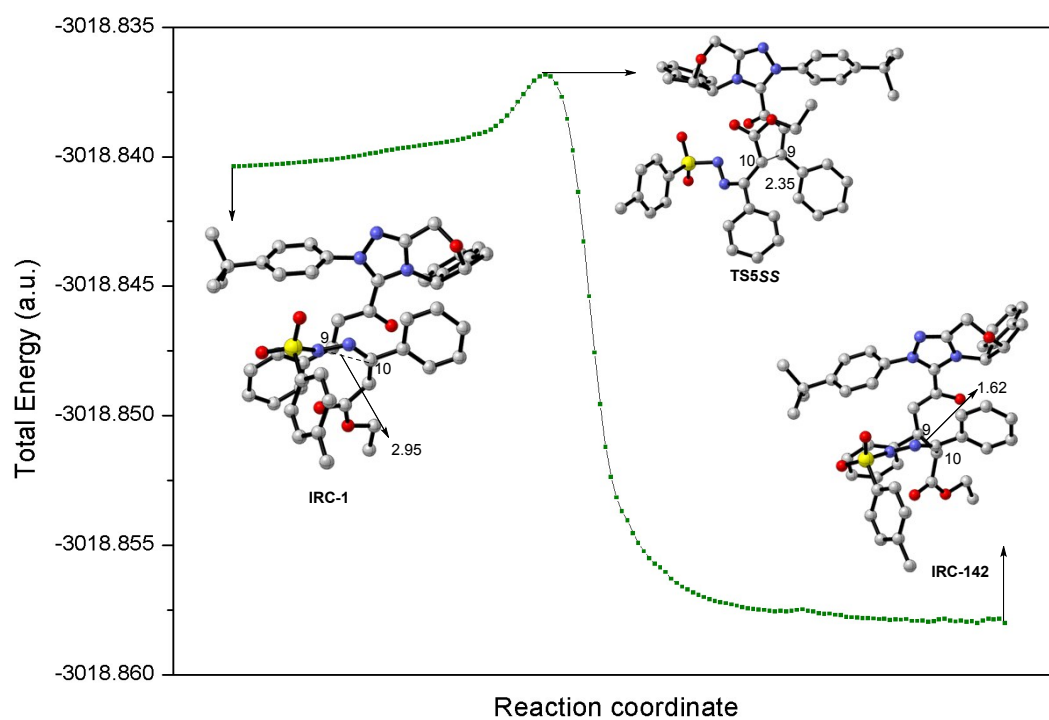
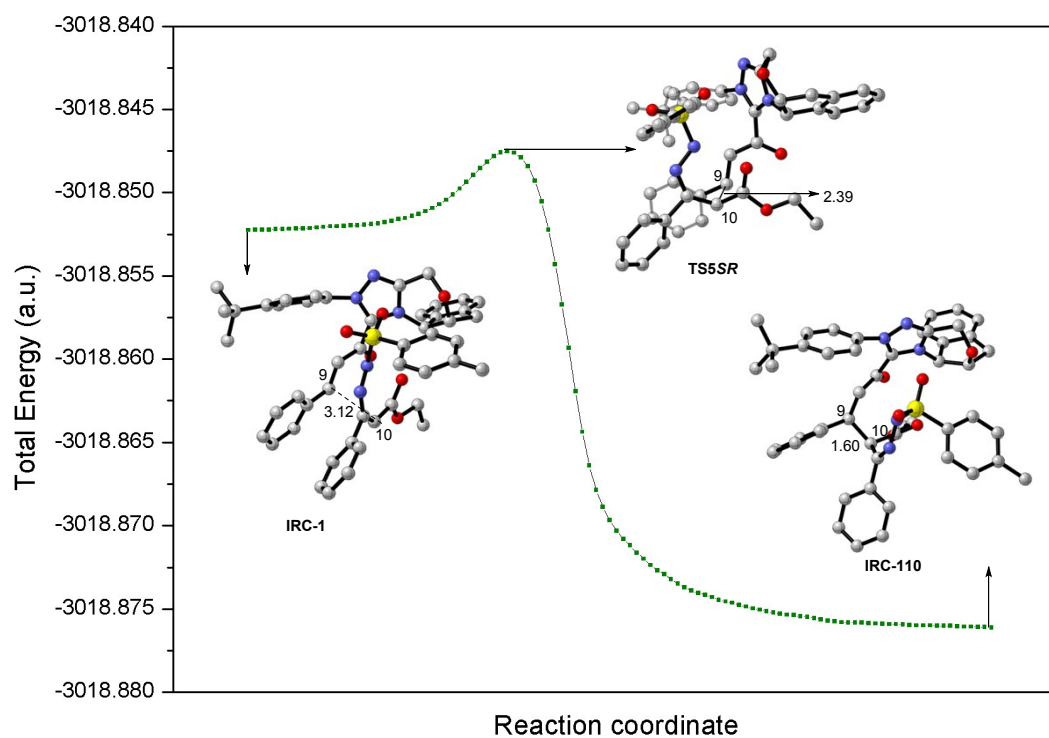


Fig. S5 IRC results of TS5RR, TS5SR, TS5RS, and TS5SS (distance unit: Å).

**Part 11: List of the cartesian coordinates of all the SPs involved in
the reaction**

R1

C	-0.04707500	1.16772900	-0.00002400
C	1.21537500	0.70443700	0.00004900
H	-0.09279300	2.25822200	-0.00025600
C	-1.36855100	0.54046000	-0.00006700
C	-2.47042600	1.41314500	0.00029100
C	-1.61288500	-0.84300900	-0.00044700
C	-3.77122000	0.92941400	0.00031200
H	-2.29573700	2.48551600	0.00056100
C	-2.91672700	-1.32343600	-0.00042800
H	-0.78985900	-1.54337600	-0.00076200
C	-3.99795800	-0.44494900	-0.00004600
H	-4.60606200	1.62207500	0.00060100
H	-3.08839000	-2.39472900	-0.00072000
H	-5.01249600	-0.82998700	-0.00002900
Br	1.76235600	-1.09604800	0.00020300
C	2.33281000	1.67709600	-0.00009700
O	3.50373900	1.38838100	-0.00042100
H	1.99292800	2.73157800	-0.00039500

pre-R2

C	1.73929700	-0.43719400	-0.57817200
C	3.12422100	-0.94769500	-0.42624200
C	4.21839400	-0.09064400	-0.57700800
C	3.34431500	-2.29231900	-0.10267100
C	5.51498800	-0.57165000	-0.41072200
H	4.06253600	0.96131600	-0.80047400
C	4.63862100	-2.76856000	0.05447000
H	2.48972400	-2.94922000	0.01898100
C	5.72794300	-1.91068200	-0.09996200
H	6.35696000	0.10370600	-0.52262700
H	4.80110600	-3.81391600	0.29618200
H	6.73822000	-2.28719300	0.02356700
N	0.79806500	-1.09806000	-0.01951100
N	-0.48863300	-0.59971400	-0.16476800
H	-0.57036300	0.39568500	0.08291700
S	-1.57854000	-1.54023400	0.74494700
O	-1.38834800	-1.33949500	2.17574000

O	-1.52094400	-2.88150700	0.18848700
C	-3.08170000	-0.74025500	0.26019000
C	-3.72282400	0.09875300	1.16258400
C	-4.90563600	0.72016400	0.77207300
C	-5.44340500	0.50711300	-0.49857900
C	-4.77329800	-0.34787100	-1.38425900
C	-3.59505900	-0.97827900	-1.01423600
H	-3.29927300	0.25148600	2.14947200
H	-5.41927400	1.37817600	1.46652400
H	-5.18866900	-0.52104200	-2.37304100
H	-3.07710300	-1.65030500	-1.69096400
C	-6.73195200	1.16420500	-0.91677200
H	-6.62375900	1.65087700	-1.88976500
H	-7.52895000	0.42018900	-1.01048500
H	-7.05165800	1.91298800	-0.18987800
C	1.49327300	0.81153100	-1.40749600
C	1.31915300	2.02261100	-0.51956700
O	0.39095300	2.15315600	0.25253900
O	2.29884000	2.91003300	-0.66506500
C	2.25456200	4.06612600	0.20167000
C	2.78642100	3.71983600	1.57781300
H	1.22527200	4.42739500	0.24612600
H	2.87905400	4.80358700	-0.30332000
H	2.81487600	4.61850700	2.19855400
H	2.14140100	2.98464100	2.06250300
H	3.79860200	3.31519500	1.50561500
H	2.30097600	0.97020400	-2.11985600
H	0.55306100	0.66725400	-1.95151900

NHC

C	-4.45794700	0.71825800	-0.59464500
C	-3.60611400	0.94376900	0.48870200
C	-3.28915600	2.23159100	0.90222700
C	-3.85164500	3.30679300	0.21748100
C	-4.71280200	3.08726400	-0.85930300
C	-5.02136700	1.79273100	-1.27435200
C	-4.60708000	-0.75918100	-0.86112500
C	-4.14254400	-1.37757300	0.47610300
C	-3.12702900	-0.36489800	1.06687800
H	-2.60869900	2.38929100	1.73261000
H	-3.62114800	4.32209800	0.52329400
H	-5.14828200	3.93514200	-1.37868600
H	-5.69138600	1.62762300	-2.11298000
H	-3.95398700	-1.05911200	-1.68956800

H	-4.99744100	-1.41001800	1.15630000
H	-5.62419100	-1.06254800	-1.11958100
H	-3.12091200	-0.37905200	2.15951900
N	-1.77879500	-0.71035200	0.60777100
O	-3.66319700	-2.70451000	0.42778500
C	-0.65860200	0.04847400	0.80964800
C	-1.46949800	-1.87959500	-0.03850400
N	0.26719500	-0.74981500	0.22833700
N	-0.20042100	-1.93631600	-0.29463000
C	-2.51852900	-2.89089000	-0.37987900
H	-2.76642100	-2.83045400	-1.44800900
H	-2.14536800	-3.89638400	-0.17808800
C	1.65678600	-0.45777300	0.12833700
C	2.13145400	0.77895500	0.56650700
C	2.53611500	-1.39202800	-0.40390700
C	3.48447800	1.06203400	0.46616100
C	3.89270600	-1.08489400	-0.49689500
C	4.39950900	0.14205300	-0.06708000
H	3.83524400	2.03033700	0.81209700
H	4.55599900	-1.83259500	-0.91663900
H	2.15921500	-2.34848600	-0.74402100
H	1.43043800	1.49550500	0.97703500
C	5.88180300	0.51175000	-0.15523800
C	6.41901200	0.80190700	1.25620900
C	6.04209400	1.76723500	-1.02879000
C	6.72060700	-0.61343400	-0.76852900
H	6.31833900	-0.07934000	1.89706600
H	5.88140600	1.62798100	1.73039600
H	7.47881200	1.07391100	1.20746200
H	5.66083700	1.58770400	-2.03864100
H	7.09948600	2.04273900	-1.10254000
H	5.50114100	2.62045700	-0.60973100
H	7.76857200	-0.30252700	-0.81566800
H	6.39515400	-0.84922300	-1.78665300
H	6.66941800	-1.52687400	-0.16762900

Et₃N

N	0.00000000	0.00000000	0.17833700
C	-0.40385800	1.32965400	-0.27927300
C	0.48716300	2.45377600	0.23949200
H	-1.41860400	1.51045100	0.08343700
H	-0.44914600	1.36782800	-1.38678500
H	0.00000000	3.41754900	0.07141300
H	0.65305800	2.33308300	1.31376400

H	1.45816500	2.48760500	-0.25926300
C	1.35344300	-0.31507600	-0.27927300
C	1.88145100	-1.64878300	0.23949200
H	2.01739100	0.47332100	0.08343700
H	1.40914700	-0.29494200	-1.38678500
H	2.95968400	-1.70877400	0.07141300
H	1.69398000	-1.73210600	1.31376400
H	1.42524600	-2.50661000	-0.25926300
C	-0.94958500	-1.01457800	-0.27927300
C	-2.36861400	-0.80499300	0.23949200
H	-0.59878700	-1.98377200	0.08343700
H	-0.96000100	-1.07288600	-1.38678500
H	-2.95968400	-1.70877400	0.07141300
H	-2.34703800	-0.60097700	1.31376400
H	-2.88341100	0.01900600	-0.25926300

Et₃NH⁺

N	0.00193100	-0.00287700	0.93344700
C	-0.62669400	1.33318700	0.58084900
C	-0.32978000	1.86284400	-0.81048300
H	-0.25001200	2.03572100	1.32775000
H	-1.69908700	1.20873700	0.74736700
H	-0.86312000	2.81054400	-0.91084300
H	0.73197300	2.07417600	-0.94874900
H	-0.67281600	1.20299400	-1.60700700
C	1.47213900	-0.12818000	0.57722200
C	1.77972500	-0.64195900	-0.81768200
H	1.88685700	-0.81500700	1.31794000
H	1.90555200	0.85898900	0.75192800
H	2.86690000	-0.65508500	-0.91963300
H	1.42922800	-1.66566900	-0.96175300
H	1.38005700	-0.00960900	-1.60958700
C	-0.84211500	-1.21305800	0.57491500
C	-1.45426600	-1.21059500	-0.81437300
H	-1.63687900	-1.24105700	1.32310700
H	-0.19864000	-2.08107200	0.73406900
H	-2.00298900	-2.14851900	-0.92371400
H	-2.17341400	-0.39886200	-0.94168700
H	-0.71386000	-1.16452600	-1.61216200
H	0.00268100	-0.00504200	1.95615400

HBr

Br	0.00000000	0.00000000	0.03923800
H	0.00000000	0.00000000	-1.37332900

Re-TS1

C	5.94058300	-0.29812600	0.65600200
C	4.58181600	-0.53750500	0.84264900
C	4.04809000	-0.73182300	2.11136300
C	4.90491500	-0.68848500	3.20839700
C	6.27013500	-0.45420900	3.02815600
C	6.79701400	-0.25798100	1.75298000
C	6.25882600	-0.11609700	-0.80714500
C	4.88514000	0.02083100	-1.50718400
C	3.84051700	-0.53502700	-0.47513200
H	2.98212600	-0.90344800	2.24201800
H	4.51031900	-0.83414100	4.20860900
H	6.92614000	-0.42013000	3.89203500
H	7.85795600	-0.06840400	1.61893600
H	6.87224500	0.76609400	-1.01460300
H	4.84006300	-0.55882600	-2.42937000
H	6.79779400	-0.98553400	-1.19848800
H	3.47878600	-1.52311700	-0.77479100
N	2.66512400	0.32931700	-0.41046800
O	4.62787800	1.35575800	-1.92415700
C	1.38016100	0.01838300	-0.12632600
C	2.78712900	1.68449800	-0.52934100
N	0.79583000	1.22736700	-0.08069200
N	1.64586200	2.27449700	-0.34645300
C	4.12593800	2.21679500	-0.91976800
H	4.79487600	2.26259800	-0.04843100
H	4.03096800	3.21395700	-1.34950400
C	-0.57774100	1.50651300	0.17730300
C	-1.24261600	0.81405200	1.17629900
C	-1.23608600	2.46150300	-0.59082500
C	-2.59866800	1.05494800	1.38655800
C	-2.57890800	2.70645600	-0.34976700
C	-3.29297200	2.00393200	0.63307900
H	-3.10742100	0.48716100	2.15700000
H	-3.08427000	3.45503400	-0.95279900
H	-0.69574900	2.98908200	-1.36870300
H	-0.70487600	0.08875200	1.77764400
C	-4.77770800	2.30432200	0.84684400
C	-5.52977000	2.11466200	-0.48093000
C	-5.40550200	1.37960400	1.89457700
C	-4.93524600	3.75976300	1.31786600
H	-5.18173400	2.81094600	-1.24878500
H	-5.39063500	1.09748000	-0.85849900

H	-6.60104200	2.28632100	-0.33391000
H	-5.99505600	3.99449000	1.46236700
H	-4.41510000	3.91870000	2.26738000
H	-4.52930000	4.46437200	0.58632100
C	-1.45111200	-2.27261400	0.24105000
C	-0.60565100	-1.69532100	-0.61722100
H	-0.94034000	-2.78389700	1.05911800
C	-2.91533200	-2.38427400	0.30284200
C	-3.43660500	-3.36676000	1.15980900
C	-3.81797400	-1.57193600	-0.40141300
C	-4.80558300	-3.56084200	1.29103300
H	-2.74913300	-3.99212200	1.72321300
C	-5.18942700	-1.77349100	-0.27229700
H	-3.44983700	-0.78118200	-1.04291600
C	-5.69050700	-2.76509100	0.56810200
H	-5.18067200	-4.33174500	1.95639800
H	-5.87572000	-1.14786700	-0.83511100
H	-6.76162100	-2.91339700	0.66047900
Br	-1.09060200	-0.78936200	-2.19835600
C	0.90075000	-1.80173800	-0.44950600
H	-6.46910100	1.61549000	1.99584100
H	-5.31763300	0.32726200	1.60421200
H	-4.94148300	1.51121000	2.87712700
H	1.11610900	-2.18356200	0.57342200
O	1.59775400	-2.16348500	-1.42694200

Si-TS1

C	4.36933500	-2.81618900	-0.09896900
C	3.20137800	-2.26735000	-0.62154200
C	2.61134700	-2.77410700	-1.77565500
C	3.22837500	-3.84628100	-2.41612900
C	4.40619100	-4.39526600	-1.90343100
C	4.98353100	-3.88682900	-0.74211700
C	4.78977300	-2.10620200	1.16299100
C	3.58875000	-1.20998800	1.54606300
C	2.71090000	-1.12688500	0.24306100
H	1.68489900	-2.35611800	-2.16329600
H	2.78813800	-4.26042000	-3.31686600
H	4.87240900	-5.23285200	-2.41215400
H	5.89260600	-4.32443300	-0.34056400
H	5.02183900	-2.78710100	1.98747100
H	3.90861000	-0.20993500	1.84127500
H	5.68059200	-1.49364400	0.98825200
H	2.85322400	-0.15267700	-0.22773000

N	1.29261800	-1.26520800	0.55496600
O	2.88762200	-1.69787900	2.67904300
C	0.20631300	-0.76476800	-0.08194200
C	0.88691300	-2.10379800	1.55499400
N	-0.81170700	-1.32506100	0.59878200
N	-0.40475800	-2.15293400	1.61731400
C	1.94291500	-2.71813100	2.41192000
H	2.40334100	-3.57851800	1.90517600
H	1.52397700	-3.04535700	3.36337100
C	-2.22184300	-1.13120700	0.42427300
C	-2.71661300	-0.66969200	-0.79155500
C	-3.07585900	-1.42753300	1.47888100
C	-4.08742700	-0.49922100	-0.92607400
C	-4.44784100	-1.25556900	1.31272300
C	-4.98491800	-0.78846900	0.11125200
H	-4.46230600	-0.13021800	-1.87643100
H	-5.09537900	-1.49529200	2.14813900
H	-2.67418100	-1.79135000	2.41637900
H	-2.03581900	-0.42926800	-1.60704000
C	-6.48555300	-0.58108800	-0.10543500
C	-6.75010000	0.90200600	-0.41448800
C	-6.95159700	-1.44163300	-1.29194600
C	-7.30718600	-0.97310100	1.12670400
H	-6.43464200	1.53340400	0.42174000
H	-6.20934800	1.22776500	-1.30701200
H	-7.81903900	1.06625800	-0.58699500
H	-8.36946800	-0.80990100	0.92238000
H	-7.17239100	-2.02951100	1.38019100
H	-7.03849100	-0.36991900	1.99956800
C	1.78058300	2.30422300	-0.88694600
C	0.61629600	1.64892500	-0.91537900
H	2.57829700	1.79806600	-1.43548400
C	2.17254300	3.60218000	-0.31369100
C	3.24428900	4.27615800	-0.91650800
C	1.57474200	4.17309300	0.81803400
C	3.68716900	5.49963600	-0.42980000
H	3.72471400	3.83335900	-1.78488600
C	2.02568700	5.39408700	1.30939600
H	0.76342900	3.65765500	1.31698500
C	3.07658400	6.06444100	0.68738700
H	4.51113300	6.00906600	-0.91898600
H	1.55564100	5.82135600	2.18946000
H	3.42201200	7.01733500	1.07512200
Br	-1.01227100	2.30267800	-0.21962800

C	0.45096400	0.31484000	-1.63514100
H	1.47004400	-0.09492000	-1.83382600
O	-0.43494000	0.17727700	-2.50540400
H	-8.02385800	-1.29832100	-1.46155800
H	-6.42656500	-1.17580100	-2.21343700
H	-6.77229800	-2.50288600	-1.09441200

Re-M1

C	5.82648600	0.05993000	0.47117000
C	4.52642700	-0.22098100	0.88122500
C	4.14208300	-0.11016600	2.21521100
C	5.08659900	0.33288700	3.13657400
C	6.38792300	0.64170500	2.72950600
C	6.77003200	0.49607200	1.39878500
C	6.01880700	-0.21152100	-0.99728800
C	4.62913600	-0.66246200	-1.51671900
C	3.65919900	-0.66019000	-0.27392100
H	3.13754600	-0.41922600	2.49435200
H	4.81627800	0.42629600	4.18362400
H	7.11266900	0.98486400	3.46142100
H	7.78817000	0.71576300	1.09047300
H	6.36778800	0.66605200	-1.55270600
H	4.67255200	-1.67812200	-1.91037400
H	6.76169200	-0.99731400	-1.16223100
H	3.17695300	-1.61898500	-0.08434300
N	2.53863400	0.28433500	-0.49519300
O	4.18338800	0.11471400	-2.61817900
C	1.32386200	0.32655500	0.07647100
C	2.59540300	1.30712600	-1.40290200
N	0.71509700	1.37014800	-0.49093600
N	1.48518200	1.98344800	-1.43652400
C	3.80796400	1.42697400	-2.26059300
H	4.61081500	1.95304500	-1.72563900
H	3.57000800	1.97689800	-3.17114500
C	-0.66932600	1.69880500	-0.33257100
C	-1.14372600	2.15493200	0.88977600
C	-1.52544400	1.43553100	-1.39083600
C	-2.51371900	2.31037000	1.05507200
C	-2.89306700	1.60954700	-1.20828400
C	-3.41631000	2.02672500	0.01969500
H	-2.88578500	2.64965700	2.01702900
H	-3.55578800	1.38401100	-2.03542400
H	-1.12318900	1.05475500	-2.32391800
H	-0.45171500	2.35992800	1.70040200

C	-4.91978200	2.16382600	0.26860600
C	-5.74126300	1.83591400	-0.98182300
C	-5.33236300	1.18376100	1.37979600
C	-5.23666700	3.60467000	0.70170700
H	-5.50053900	2.50567500	-1.81369100
H	-5.57809500	0.80099200	-1.30099400
H	-6.80521700	1.95184100	-0.75591000
H	-6.31181800	3.71322000	0.87707500
H	-4.71872700	3.87221100	1.62687900
H	-4.94040900	4.31900400	-0.07264800
C	-1.73084300	-1.24220300	1.10809100
C	-0.56074600	-1.22068500	0.47008900
H	-1.68333500	-0.81752800	2.11210300
C	-3.05933700	-1.74830700	0.72106800
C	-3.89802900	-2.22856400	1.73631700
C	-3.55485700	-1.70461900	-0.58937800
C	-5.18389900	-2.67535600	1.45363500
H	-3.52894100	-2.25144200	2.75809300
C	-4.84647800	-2.14079900	-0.86949900
H	-2.93022600	-1.31717500	-1.38539500
C	-5.66488600	-2.62973000	0.14705800
H	-5.81343900	-3.05034900	2.25424900
H	-5.21694000	-2.09460300	-1.88921500
H	-6.67104300	-2.96893900	-0.07747200
Br	-0.28438400	-1.96409700	-1.26052300
C	0.75657500	-0.71450800	1.10135600
H	-6.40045000	1.29510000	1.59507000
H	-5.14642700	0.15027000	1.07134200
H	-4.78077500	1.36812600	2.30685900
H	0.40324600	-0.07562600	1.95518200
O	1.63756800	-1.64621100	1.36936000

Si-M1

C	5.90648700	0.02001900	-0.07060900
C	4.59866200	0.02261800	-0.54671900
C	4.20963900	-0.72199600	-1.65752500
C	5.18507700	-1.48881200	-2.29146100
C	6.50200900	-1.50161400	-1.82375800
C	6.87419200	-0.74770700	-0.71284600
C	6.05831000	0.91832900	1.13027200
C	4.61807400	1.32158000	1.52677500
C	3.71671200	0.91361000	0.29920300
H	3.17087700	-0.70254900	-1.99858100
H	4.91810600	-2.08402000	-3.15857000

H	7.24540100	-2.10827000	-2.33152300
H	7.89837700	-0.76335100	-0.35211000
H	6.55267000	0.43283800	1.97772600
H	4.53452000	2.39377100	1.70670800
H	6.64633500	1.80805100	0.88301700
H	3.37756300	1.79932200	-0.24249700
N	2.52397000	0.19777800	0.75939700
O	4.20950300	0.73338000	2.75249200
C	1.29511200	0.09367100	0.21433400
C	2.57603700	-0.64396000	1.83649900
N	0.66313600	-0.80044100	0.98458900
N	1.44679900	-1.25799900	2.00940700
C	3.82357700	-0.62528800	2.65465300
H	4.60519300	-1.24155800	2.18885200
H	3.62634300	-0.99565800	3.66035700
C	-0.67451800	-1.29471600	0.84754200
C	-1.14075300	-1.65910400	-0.40962800
C	-1.47351900	-1.38557200	1.97849700
C	-2.46042900	-2.07510100	-0.52359100
C	-2.78463600	-1.83009000	1.83980200
C	-3.30842300	-2.17021000	0.58792800
H	-2.83247900	-2.32015700	-1.51412700
H	-3.40255100	-1.89032600	2.72789900
H	-1.07758500	-1.10159200	2.94748700
H	-0.48299200	-1.55633800	-1.27292800
C	-4.76566600	-2.59148400	0.38852100
C	-5.47409400	-1.50477400	-0.43877100
C	-4.82526400	-3.93183800	-0.36251500
C	-5.50995500	-2.75118300	1.71759500
H	-5.47425600	-0.55507200	0.10628100
H	-4.97770800	-1.34397000	-1.40082000
H	-6.51330200	-1.79099600	-0.63248600
H	-6.53872000	-3.06747900	1.52190000
H	-5.03981300	-3.50856000	2.35305000
H	-5.55271400	-1.80921100	2.27300100
C	-0.98474500	1.96229700	0.00321900
C	-0.56309700	1.23274300	-1.03057500
H	-0.22347400	2.16384100	0.76222300
C	-2.31361300	2.53583800	0.28421800
C	-2.39627600	3.80358000	0.87189100
C	-3.49715500	1.82658500	0.04079400
C	-3.62984400	4.37143800	1.17176100
H	-1.48125400	4.35016400	1.08430600
C	-4.72957600	2.39528900	0.34377100

H	-3.44260800	0.82593900	-0.37802800
C	-4.80217200	3.66944500	0.90350600
H	-3.67628900	5.36076400	1.61592000
H	-5.64134500	1.84055500	0.14303100
H	-5.76701900	4.10951200	1.13456700
Br	-1.64630000	0.84922500	-2.52760000
C	0.87966300	0.65509300	-1.16335100
H	1.51940500	1.56665500	-1.28749300
O	1.07761600	-0.30901200	-2.04375900
H	-5.86792900	-4.23816100	-0.49573700
H	-4.36951000	-3.86456300	-1.35369500
H	-4.30591800	-4.71489900	0.19807700

M02

C	4.81285600	-2.54625000	-0.18920700
C	3.61002100	-2.06427500	0.31844000
C	3.11483400	-2.48132700	1.54990400
C	3.86382300	-3.39406700	2.28627400
C	5.08231400	-3.86894200	1.79313000
C	5.56338300	-3.45344100	0.55398100
C	5.10617000	-1.96562700	-1.54945300
C	3.80378800	-1.25110900	-1.97839400
C	2.97727900	-1.09115400	-0.64801600
H	2.15660000	-2.12344000	1.91939600
H	3.49915700	-3.74244300	3.24634500
H	5.65462300	-4.58035600	2.37912400
H	6.50248000	-3.83923400	0.16989700
H	5.37749300	-2.71990900	-2.29431500
H	4.00002600	-0.26978100	-2.41058400
H	5.93204000	-1.24876200	-1.50076900
H	3.03150700	-0.06061800	-0.30197800
N	1.56216200	-1.43374100	-0.86437100
O	3.10315600	-1.94616500	-2.99580100
C	0.41698100	-1.03539300	-0.27982200
C	1.24366100	-2.46798400	-1.70549500
N	-0.52889600	-1.83046900	-0.78554600
N	-0.03112600	-2.71998100	-1.68460900
C	2.33719800	-3.04392400	-2.54458900
H	2.93532400	-3.76134000	-1.96623500
H	1.91471200	-3.54618000	-3.41458800
C	-1.94286600	-1.81711600	-0.51935000
C	-2.41864900	-2.11983000	0.74719700
C	-2.80485100	-1.55194500	-1.58041800
C	-3.79715000	-2.13401000	0.95594700

C	-4.17149900	-1.57113600	-1.34836600
C	-4.69735000	-1.86017100	-0.07768000
H	-4.16090400	-2.36922800	1.94884300
H	-4.84113200	-1.36188400	-2.17678300
H	-2.40248700	-1.34280400	-2.56631500
H	-1.72752400	-2.33229500	1.55430700
C	-6.21391300	-1.87932900	0.11945800
C	-6.79786700	-0.52015600	-0.30150500
C	-6.60098500	-2.14290200	1.57737400
C	-6.81492200	-2.99049800	-0.75880000
H	-6.60369500	-0.30055200	-1.35543500
H	-6.37371600	0.28930000	0.30166600
H	-7.88253600	-0.52145300	-0.15732500
H	-7.90173100	-3.01485300	-0.63359000
H	-6.41421400	-3.96875900	-0.47735500
H	-6.60202000	-2.82634400	-1.81891600
C	1.06024000	2.19166700	-0.13720600
C	1.13845600	1.17825000	0.73248900
H	0.16175000	2.13505000	-0.75584800
C	1.90106500	3.35736100	-0.43071900
C	1.37599100	4.28139800	-1.35018800
C	3.17229600	3.60538900	0.11116400
C	2.08183600	5.42300500	-1.70575000
H	0.39812500	4.09606600	-1.78803000
C	3.87848600	4.74624200	-0.25107600
H	3.62026800	2.91744000	0.81350400
C	3.33840400	5.65932600	-1.15406700
H	1.65415200	6.12451100	-2.41379000
H	4.85923300	4.92210100	0.17804500
H	3.89606300	6.54853200	-1.42820000
Br	2.49103700	0.96023500	2.04694200
C	0.10610500	0.06863700	0.72109800
H	-7.69016700	-2.12831700	1.67031400
H	-6.19862500	-1.37520100	2.24655200
H	-6.25233200	-3.12213800	1.91960700
H	-0.81924800	0.54227500	0.35725800
O	-0.16336800	-0.51906900	1.96738200
N	-2.28734900	2.23553600	0.16037900
C	-3.06917900	1.32854400	0.99720800
C	-4.36036700	1.86180000	1.62256400
H	-3.30315200	0.45355500	0.38063500
H	-2.42266100	0.96518700	1.81091500
H	-4.85105900	1.05595300	2.17916700
H	-5.06025300	2.23471900	0.87002700

H	-4.15577100	2.67171000	2.32852800
C	-2.58089300	2.19081500	-1.26743700
C	-4.04820800	2.28908400	-1.69352500
H	-2.00511900	2.99515300	-1.74434900
H	-2.18044100	1.24488500	-1.66830100
H	-4.12164500	2.25566400	-2.78464900
H	-4.51481700	3.21386900	-1.34595500
H	-4.62267300	1.44487100	-1.29776700
C	-1.99706100	3.54934000	0.72440100
C	-3.01320900	4.66829800	0.47328800
H	-1.85325100	3.40984400	1.80251500
H	-1.02608700	3.88556600	0.33310300
H	-2.67953900	5.58535400	0.96728400
H	-4.00775200	4.41996500	0.85061100
H	-3.09930200	4.88507000	-0.59575700
H	0.53484900	-0.27793200	2.59549700

TS2

C	4.26030500	-2.98670500	0.12209900
C	3.13956700	-2.26002000	0.51333900
C	2.49088800	-2.49845400	1.72143100
C	2.99193100	-3.50222100	2.54537400
C	4.11603100	-4.23928500	2.16230700
C	4.75871200	-3.98766600	0.95245900
C	4.77703900	-2.51962800	-1.21624500
C	3.69603500	-1.55514000	-1.76241100
C	2.76991800	-1.23514900	-0.53240700
H	1.61629300	-1.92018400	2.01538400
H	2.50772000	-3.71400600	3.49278400
H	4.49192400	-5.01908700	2.81660900
H	5.63019900	-4.56581200	0.66103400
H	4.94523800	-3.33379400	-1.92830200
H	4.13000500	-0.63068700	-2.14406600
H	5.72926300	-1.99211000	-1.10276900
H	2.94614800	-0.21928900	-0.18520800
N	1.35033800	-1.37137400	-0.90370700
O	2.99186600	-2.08897000	-2.87233000
C	0.22397400	-0.89693400	-0.30788000
C	0.97231200	-2.38455100	-1.74454100
N	-0.76341900	-1.64823500	-0.82684500
N	-0.31021700	-2.57234800	-1.72622800
C	2.03849200	-3.07220500	-2.53364200
H	2.47893500	-3.89104500	-1.94732000
H	1.62381900	-3.48051600	-3.45533700

C	-2.17444800	-1.52691000	-0.62243000
C	-2.74962600	-1.88005800	0.58831200
C	-2.95628100	-1.11458800	-1.70041200
C	-4.13521400	-1.79051000	0.72814300
C	-4.33193100	-1.03722700	-1.54323100
C	-4.95121600	-1.36654800	-0.32564900
H	-4.57331000	-2.06526500	1.68048300
H	-4.93458000	-0.71923400	-2.38810700
H	-2.48444100	-0.87832800	-2.64927600
H	-2.11886400	-2.20242900	1.40935400
C	-6.47210100	-1.25396600	-0.20783200
C	-6.89903800	0.18368000	-0.55259800
C	-6.96551800	-1.58475500	1.20359000
C	-7.12535000	-2.23276200	-1.19924700
H	-6.62986400	0.45399700	-1.57772000
H	-6.42971200	0.90587900	0.12401200
H	-7.98433300	0.28331100	-0.45650700
H	-8.21494000	-2.16261200	-1.12631900
H	-6.83158200	-3.26308200	-0.97859100
H	-6.84298000	-2.01142200	-2.23240100
C	1.48834700	1.90131000	-0.39133300
C	1.22386900	1.11944700	0.67260200
H	0.73093800	1.79541100	-1.17065400
C	2.58288300	2.79757600	-0.78177500
C	2.48134000	3.36302000	-2.06579400
C	3.70009900	3.13683700	0.00034600
C	3.45024400	4.22593400	-2.55782900
H	1.62269400	3.11317000	-2.68407000
C	4.66798600	4.00447000	-0.49550900
H	3.81760700	2.73180900	0.99516800
C	4.55245500	4.55177000	-1.77075300
H	3.34475200	4.64504600	-3.55302100
H	5.52134400	4.25616200	0.12576900
H	5.31302600	5.22760900	-2.14717400
Br	2.29051200	1.08682700	2.24567600
C	0.06644000	0.18524500	0.66714300
H	-8.05291900	-1.47889100	1.24258000
H	-6.53758700	-0.90693100	1.94998600
H	-6.72255500	-2.61342400	1.48696300
H	-1.05713900	1.24852700	0.42793300
O	-0.26736600	-0.40401300	1.91900000
N	-1.89110300	2.10955800	0.45560200
C	-3.08702900	1.38081000	0.97608400
C	-4.20266500	2.20716400	1.59686900

H	-3.46482800	0.77782400	0.14807000
H	-2.70761100	0.67668600	1.72279500
H	-4.98098600	1.51131500	1.92376300
H	-4.65337500	2.91154300	0.89576700
H	-3.86700600	2.75311100	2.48166900
C	-1.98457900	2.50949700	-0.97896200
C	-3.31710100	3.08016200	-1.44099600
H	-1.16882100	3.21584300	-1.16118800
H	-1.76185900	1.59903200	-1.55121900
H	-3.23523300	3.32753400	-2.50186500
H	-3.58896600	3.98979500	-0.90310000
H	-4.12367000	2.34896800	-1.33421400
C	-1.35579600	3.16108800	1.37500200
C	-1.95918600	4.55269100	1.23419100
H	-1.48991400	2.77838300	2.39217900
H	-0.28014800	3.21052700	1.18969600
H	-1.47265900	5.20798600	1.96018900
H	-3.03227000	4.57650400	1.42694000
H	-1.77094800	4.97190100	0.24294200
H	-0.79066100	0.21947900	2.43568700

TS2'

C	3.18310700	-3.19020800	-0.21940000
C	2.27358000	-2.26307000	0.28066800
C	1.62551300	-2.44395100	1.50142300
C	1.92611600	-3.59450800	2.22683300
C	2.84554600	-4.52847700	1.74001700
C	3.47945500	-4.33574500	0.51522600
C	3.73003100	-2.76576600	-1.55903300
C	2.91961300	-1.50683200	-1.95812400
C	2.09835600	-1.10934800	-0.67898000
H	0.90269500	-1.71676400	1.88142700
H	1.44089300	-3.76669100	3.18195000
H	3.06482800	-5.41792600	2.32234200
H	4.18690000	-5.06804100	0.13743100
H	3.62504600	-3.53699500	-2.32970900
H	3.57496500	-0.68178900	-2.23756000
H	4.79587600	-2.52581100	-1.49452700
H	2.46712600	-0.17102300	-0.26598200
N	0.67928100	-0.93822800	-1.00761600
O	2.11427200	-1.70763900	-3.10971300
C	-0.30256500	-0.38309900	-0.24480100
C	0.08076700	-1.72379100	-1.95034400
N	-1.44721900	-0.85794800	-0.79105200

N	-1.21032200	-1.68760100	-1.85728900
C	0.96346700	-2.49075900	-2.87998900
H	1.21409800	-3.46604900	-2.43697700
H	0.46564300	-2.65496500	-3.83588700
C	-2.79941500	-0.49935700	-0.50234300
C	-3.25400900	-0.40498300	0.80527300
C	-3.65655700	-0.26550800	-1.57823500
C	-4.58109200	-0.03758500	1.03125900
C	-4.97230500	0.08501900	-1.32699900
C	-5.46436500	0.21567100	-0.01827800
H	-4.91654200	0.03779800	2.05886700
H	-5.62930600	0.26986900	-2.17169200
H	-3.28426700	-0.35959600	-2.59193900
H	-2.57555500	-0.61435000	1.62710900
C	-6.92299200	0.62300500	0.20105400
C	-7.16453500	1.99842900	-0.44396400
C	-7.27723700	0.71649200	1.68815300
C	-7.84587500	-0.41831200	-0.45415200
H	-6.97311000	1.97825100	-1.52057200
H	-6.51312100	2.75551300	0.00287800
H	-8.20448000	2.30559500	-0.29269500
H	-8.89318400	-0.13349700	-0.30947900
H	-7.69308900	-1.40614000	-0.00924200
H	-7.66545200	-0.49896400	-1.52978300
C	1.25081600	2.33079400	-0.03133000
C	1.04328700	1.35721400	0.87238300
H	0.38059100	2.50556300	-0.66430300
C	2.39037700	3.20516700	-0.34173600
C	2.11811200	4.33943500	-1.12562100
C	3.72282700	2.97446300	0.03666900
C	3.12253300	5.22385300	-1.49547500
H	1.09484600	4.52604900	-1.44068300
C	4.72858700	3.85851100	-0.34019500
H	3.97764800	2.10596800	0.62863700
C	4.43760600	4.98732100	-1.10172500
H	2.87872500	6.09565000	-2.09426800
H	5.75166900	3.65825000	-0.03721000
H	5.22816900	5.67263900	-1.38989100
Br	2.30794100	0.93204200	2.25591300
C	-0.15297300	0.50495300	0.89011500
H	-8.32561200	1.01035000	1.79398400
H	-6.66624400	1.46524300	2.20175700
H	-7.14710700	-0.24511300	2.19427800
H	-1.13216200	0.86753500	1.45263900

0	-0.56868000	-0.03983100	2.18142900
TS2''			
C	-3.96437900	-3.25401300	-0.60097200
C	-2.93953100	-2.32681300	-0.77142100
C	-2.23008600	-2.21185100	-1.96607300
C	-2.58803400	-3.06732600	-3.00660800
C	-3.61828700	-3.99914200	-2.85252700
C	-4.31346000	-4.10102000	-1.64986300
C	-4.56520200	-3.17308800	0.78020200
C	-3.69975000	-2.14328900	1.55087200
C	-2.72980300	-1.51588000	0.48588300
H	-1.40315100	-1.49848800	-2.08301200
H	-2.05623700	-3.00879900	-3.95111600
H	-3.87661300	-4.65493700	-3.67839200
H	-5.10850500	-4.83153700	-1.53107100
H	-4.56148800	-4.13440000	1.30591800
H	-4.31554000	-1.35312300	1.98136800
H	-5.60686100	-2.83965300	0.74268600
H	-2.96455200	-0.46222600	0.33849500
N	-1.33355300	-1.60225200	0.93263500
O	-3.03434200	-2.70451500	2.67299600
C	-0.23033000	-1.00041800	0.39014200
C	-0.90915100	-2.66228700	1.68127700
N	0.79747000	-1.75132900	0.86055400
N	0.38012300	-2.77442300	1.67489900
C	-1.93893600	-3.52511300	2.33365800
H	-2.23303800	-4.33504500	1.64945200
H	-1.54491400	-3.96582900	3.24995500
C	2.19909800	-1.57440700	0.67296700
C	2.70883700	-1.24104800	-0.57421400
C	3.04134000	-1.74798200	1.77194000
C	4.08825200	-1.07195800	-0.70931700
C	4.40714600	-1.57262700	1.60919000
C	4.96458100	-1.23312300	0.36605000
H	4.47270800	-0.81589400	-1.69102600
H	5.05382600	-1.71142500	2.47088300
H	2.62148700	-2.01791200	2.73463300
H	2.00512600	-1.07265400	-1.39376100
C	6.48318300	-1.09302400	0.23267700
C	7.00043000	-0.03211900	1.21806200
C	6.90209800	-0.67933700	-1.18129400
C	7.13662500	-2.44776300	0.55717400
H	6.74609500	-0.27776300	2.25295300

H	6.57835000	0.95053300	0.98670400
H	8.09079200	0.04055900	1.14967000
H	8.22467500	-2.37274100	0.45853100
H	6.78016700	-3.22320100	-0.12737600
H	6.91107900	-2.76707200	1.57862200
C	-1.73190400	1.56162900	0.76520500
C	-1.29379600	1.04243100	-0.41103600
H	-1.12348100	1.23884200	1.61378700
C	-2.78595500	2.49977200	1.13978600
C	-2.69092000	3.07950100	2.42140800
C	-3.89722100	2.85825800	0.35242600
C	-3.63218200	3.98674800	2.88663200
H	-1.85109500	2.80599600	3.05577800
C	-4.83857100	3.76800600	0.82250100
H	-4.02653200	2.42019700	-0.62806700
C	-4.71551200	4.34314400	2.08545600
H	-3.52060200	4.41657400	3.87757600
H	-5.68540300	4.02435600	0.19272600
H	-5.45523800	5.05194700	2.44301800
Br	-1.97881800	1.64238200	-2.08859100
C	-0.15619500	0.10812800	-0.57746300
H	7.99048400	-0.57750100	-1.22347200
H	6.46414200	0.28361100	-1.46466600
H	6.60732600	-1.42590000	-1.92510100
H	0.84996900	1.18679300	-0.23444500
O	0.24304400	-0.27963000	-1.80851400
N	1.65640900	2.18015800	-0.35031800
C	2.67609400	1.97668800	0.71042900
C	4.06165700	2.55959400	0.46295400
H	2.24896400	2.38153300	1.63380200
H	2.77539700	0.89658100	0.85134100
H	4.68361500	2.33931500	1.33505400
H	4.05046100	3.64141300	0.31661300
H	4.53597900	2.09155600	-0.40526400
C	0.82086500	3.39722100	-0.14282500
C	1.55373900	4.71390300	0.10020500
H	0.14430800	3.45755600	-1.00202200
H	0.19416600	3.19042000	0.72699500
H	0.80296700	5.50066700	0.21158000
H	2.22347900	5.00038100	-0.71024000
H	2.12804900	4.68168200	1.02997500
C	2.12777100	1.99384800	-1.75913700
C	2.71881800	3.20152400	-2.47611700
H	2.84828200	1.17262100	-1.72565400

H	1. 25941700	1. 60745200	-2. 29919200
H	3. 04847400	2. 86974600	-3. 46448900
H	3. 58020900	3. 63687200	-1. 96530600
H	1. 97112900	3. 98300400	-2. 63335500

M2

C	2. 16095600	-3. 42314100	1. 05874400
C	2. 06942100	-2. 03094200	0. 95654700
C	2. 07449400	-1. 23871500	2. 10204800
C	2. 15651500	-1. 85980900	3. 34747800
C	2. 24388200	-3. 24757000	3. 44826200
C	2. 25120800	-4. 03899400	2. 30142100
C	2. 14541800	-4. 07569900	-0. 29735500
C	2. 47213900	-2. 89740400	-1. 23765100
C	2. 00137800	-1. 60899300	-0. 50011900
H	2. 01353400	-0. 15911400	2. 04682500
H	2. 15879100	-1. 25197600	4. 24632400
H	2. 31541600	-3. 71390900	4. 42586800
H	2. 33081100	-5. 11963200	2. 37590900
H	1. 15519600	-4. 49861800	-0. 50149200
H	3. 55655800	-2. 82184400	-1. 34450200
H	2. 87107600	-4. 88607600	-0. 39971400
H	2. 64847700	-0. 75844000	-0. 72963000
N	0. 63659900	-1. 29317300	-0. 95147300
O	1. 97614400	-3. 00114400	-2. 55421900
C	-0. 26424400	-0. 39002800	-0. 38922400
C	-0. 10084500	-2. 15378600	-1. 73489900
N	-1. 49903100	-0. 89292000	-0. 76200300
N	-1. 36718800	-1. 94667500	-1. 65018900
C	0. 57666300	-3. 15442700	-2. 62408600
H	0. 25739900	-4. 17191200	-2. 36865700
H	0. 29082600	-2. 96475200	-3. 66120000
C	-2. 81166300	-0. 39992600	-0. 52992300
C	-3. 31104000	-0. 25615100	0. 76007900
C	-3. 63265800	-0. 13943700	-1. 62635100
C	-4. 61942600	0. 18007800	0. 94659300
C	-4. 93959200	0. 28034200	-1. 42259000
C	-5. 46224200	0. 45576100	-0. 13426700
H	-4. 98083400	0. 28883600	1. 96250700
H	-5. 56224900	0. 47982100	-2. 29015400
H	-3. 23879400	-0. 27664300	-2. 62764700
H	-2. 67257100	-0. 47398500	1. 60757000
C	-6. 90780200	0. 92882100	0. 03737900
C	-7. 07328100	2. 30556000	-0. 62815200

C	-7.30250600	1.05429800	1.51216700
C	-7.85692900	-0.07863600	-0.63320800
H	-6.84626100	2.26531400	-1.69730400
H	-6.40663000	3.04087900	-0.16741200
H	-8.10435000	2.65670800	-0.51551900
H	-8.89537200	0.24947900	-0.51816600
H	-7.75527600	-1.06831800	-0.17778200
H	-7.65163100	-0.17573900	-1.70292600
C	2.07535200	1.51662200	-0.89265400
C	1.27413300	1.46460200	0.19499200
H	1.62448400	1.10221300	-1.79481300
C	3.43444100	2.03864500	-1.07217000
C	3.80463100	2.47566900	-2.35438100
C	4.40526000	2.07059600	-0.05825000
C	5.08051000	2.96259600	-2.60924300
H	3.07101800	2.43649000	-3.15536300
C	5.68210500	2.55595100	-0.31594800
H	4.15856600	1.70927300	0.93284600
C	6.02638100	3.00925900	-1.58757100
H	5.33788800	3.30261600	-3.60743700
H	6.41775800	2.56978500	0.48237900
H	7.02496900	3.38705900	-1.78196600
Br	1.71396800	2.49411400	1.77416000
C	0.02060300	0.77302000	0.29652000
H	-8.34073700	1.39153000	1.58436200
H	-6.67638200	1.78304500	2.03643100
H	-7.22604500	0.09401400	2.03187100
O	-0.98779400	1.32011800	1.07173500
H	-1.20353700	2.19848800	0.73359800

TS3

C	2.88771100	2.96587700	-1.17493700
C	2.39847900	1.67095100	-0.98020000
C	2.30803900	0.77955300	-2.04888000
C	2.70472000	1.21149800	-3.31326100
C	3.18915200	2.50483800	-3.50867700
C	3.28767400	3.38923400	-2.43779300
C	2.90508100	3.75849700	0.10344300
C	2.68692400	2.68415300	1.18913800
C	2.05123500	1.44513400	0.47987700
H	1.95353900	-0.23814600	-1.92320800
H	2.64276500	0.52426000	-4.15067300
H	3.49983300	2.82091600	-4.49944600
H	3.67506900	4.39331000	-2.58331000

H	2. 10775200	4. 50938800	0. 10248600
H	3. 65742800	2. 35721400	1. 56696500
H	3. 84410700	4. 29388700	0. 26296100
H	2. 44999300	0. 51402700	0. 88388900
N	0. 59540500	1. 43864600	0. 73029400
O	1. 97905500	3. 11425800	2. 33412100
C	-0. 34733700	0. 55692700	0. 27785600
C	-0. 07617900	2. 45910000	1. 34810400
N	-1. 53044900	1. 14916900	0. 56523200
N	-1. 36034200	2. 31978700	1. 25863400
C	0. 66498400	3. 54360000	2. 06673700
H	0. 63780900	4. 47449700	1. 48782400
H	0. 18145900	3. 72968400	3. 02708600
C	-2. 86702000	0. 66607400	0. 38590800
C	-3. 38523200	0. 46393100	-0. 88435100
C	-3. 65381300	0. 47520100	1. 51777000
C	-4. 70379200	0. 03790300	-1. 01782800
C	-4. 96783600	0. 05907200	1. 36422000
C	-5. 52012700	-0. 17325500	0. 09637900
H	-5. 09041400	-0. 12223100	-2. 01710900
H	-5. 57232200	-0. 09100700	2. 25373000
H	-3. 23275600	0. 65559700	2. 50112000
H	-2. 75807400	0. 62164300	-1. 75332600
C	-6. 97302800	-0. 63993700	-0. 01806700
C	-7. 13836300	-1. 97000300	0. 73672600
C	-7. 39716400	-0. 85504200	-1. 47412000
C	-7. 89629200	0. 42031700	0. 60568100
H	-6. 90147700	-1. 86418100	1. 79913000
H	-6. 48191700	-2. 73812800	0. 31728900
H	-8. 17311700	-2. 31871300	0. 65655900
H	-8. 94024600	0. 09950200	0. 52800000
H	-7. 79109400	1. 37909500	0. 08904400
H	-7. 67147600	0. 57891200	1. 66409900
C	1. 60466800	-1. 69814500	1. 28594100
C	0. 90709300	-1. 49671600	0. 15535100
H	1. 02417400	-1. 64600000	2. 20685800
C	3. 02035300	-2. 03060100	1. 43797000
C	3. 46865700	-2. 54216700	2. 66638600
C	3. 96420300	-1. 82592200	0. 41755400
C	4. 80564000	-2. 86236900	2. 86389600
H	2. 74975000	-2. 69512600	3. 46702200
C	5. 30054500	-2. 15325200	0. 61664800
H	3. 64229400	-1. 41285900	-0. 53274600
C	5. 72856900	-2. 67335600	1. 83661000

H	5.12946000	-3.26134600	3.82017900
H	6.01527800	-1.99255800	-0.18445400
H	6.77379500	-2.92277000	1.98847400
Br	1.48214400	-2.83942000	-1.62701900
C	-0.14719400	-0.74879400	-0.26817400
H	-8.43774800	-1.19090300	-1.50252300
H	-6.78538800	-1.61931700	-1.96340700
H	-7.32932900	0.07015400	-2.05491000
O	-1.07952900	-1.17125700	-1.17790500
H	-0.68477400	-1.96010600	-1.59620400

NTS2

C	3.68959800	-3.06937900	-0.13250300
C	2.71252900	-2.23144000	0.39661400
C	2.26731400	-2.35510500	1.71018300
C	2.80032300	-3.38331500	2.48211700
C	3.76277300	-4.24792400	1.95293300
C	4.22165700	-4.09304700	0.64738400
C	4.06356900	-2.66496400	-1.53511900
C	3.05789500	-1.55564700	-1.92878100
C	2.28126300	-1.19155500	-0.60766300
H	1.53804400	-1.65799700	2.11604200
H	2.47311900	-3.50751100	3.50903200
H	4.16677100	-5.04262700	2.57232100
H	4.98362100	-4.75529700	0.24720600
H	4.01228400	-3.48713800	-2.25703300
H	3.56379800	-0.66710100	-2.30660100
H	5.08604700	-2.27701200	-1.56807100
H	2.50908400	-0.18498000	-0.23951200
N	0.82460300	-1.25670600	-0.84517300
O	2.21181300	-1.95402000	-2.99997700
C	-0.19844000	-0.63424700	-0.23922500
C	0.28098400	-2.14289900	-1.73202400
N	-1.30572600	-1.17237800	-0.75777100
N	-1.01876300	-2.10397000	-1.70959400
C	1.21927700	-2.88501900	-2.62392400
H	1.64287200	-3.75546500	-2.10373100
H	0.70094400	-3.22005300	-3.52227600
C	-2.67570700	-0.86819700	-0.45871500
C	-3.06961600	-0.63326800	0.85202900
C	-3.58900400	-0.84427900	-1.50928800
C	-4.41023800	-0.34490400	1.10195600
C	-4.91820600	-0.57003500	-1.22902500
C	-5.35875400	-0.31020100	0.07802900

H	-4.70505100	-0.15995500	2.12783000
H	-5.62741600	-0.55521400	-2.05095200
H	-3.25543200	-1.04331000	-2.52138200
H	-2.34621500	-0.68507500	1.66096800
C	-6.83833200	-0.01250100	0.32917100
C	-7.24508000	1.23723800	-0.47033900
C	-7.13069200	0.24199600	1.81091100
C	-7.68015200	-1.21356600	-0.13454800
H	-7.10157100	1.09446900	-1.54512100
H	-6.65638800	2.10581800	-0.16036000
H	-8.30303400	1.46016600	-0.29941800
H	-8.74210800	-1.01233500	0.03847700
H	-7.40604000	-2.11648100	0.41913300
H	-7.54521400	-1.41435400	-1.20110300
C	0.22189300	2.85556600	0.05099200
C	0.31769700	1.63862600	0.57917800
H	-0.79209400	3.21756700	-0.11277400
C	1.24275600	3.84621800	-0.33364400
C	0.82073200	5.18133100	-0.39392900
C	2.55335000	3.53138100	-0.71113400
C	1.69672100	6.18950800	-0.77761600
H	-0.20234800	5.42918800	-0.12347000
C	3.42375300	4.54061400	-1.10479100
H	2.89174000	2.50536700	-0.66149100
C	3.00366200	5.86899800	-1.13484600
H	1.35757900	7.21979900	-0.80359700
H	4.43939600	4.28686100	-1.39039200
H	3.69148900	6.65088800	-1.44094100
Br	2.69786600	1.34274400	1.71266400
C	-0.11631600	0.33213000	0.93734100
H	-8.19682900	0.44900200	1.93978500
H	-6.57478500	1.10537200	2.18965300
H	-6.88326300	-0.62862400	2.42613700
H	-1.04064800	1.23037300	0.55284000
O	-0.21777900	-0.18619200	2.06535300

M3

C	4.13635200	-1.29620900	0.63846500
C	3.47261000	-0.11803800	0.29050700
C	3.42641600	0.97156300	1.15288900
C	4.02262500	0.85349900	2.40449000
C	4.66142400	-0.33228700	2.76987400
C	4.72961200	-1.41040800	1.88993200
C	4.10132900	-2.29646400	-0.48373800

C	3.73212800	-1.43515700	-1.69838800
C	2.93570200	-0.21580800	-1.11263800
H	2.91576200	1.88875000	0.87309900
H	3.98701500	1.68578300	3.09888200
H	5.11934300	-0.41273900	3.75074100
H	5.24130400	-2.32407900	2.17522200
H	3.30091000	-3.02455400	-0.31009900
H	4.63341800	-1.00739400	-2.15910700
H	5.04750100	-2.82304500	-0.62669400
H	3.10527800	0.69479300	-1.69647500
N	1.48863700	-0.50303100	-1.23750100
O	3.04433400	-2.22378700	-2.65223600
C	0.41424500	-0.26753500	-0.46441700
C	1.02798200	-1.08579900	-2.38477100
N	-0.63316800	-0.67970800	-1.17899500
N	-0.26664700	-1.20535700	-2.37726600
C	2.04120600	-1.54913200	-3.37785500
H	1.58991600	-2.25700800	-4.07226300
H	2.44629900	-0.69742600	-3.94406900
C	-2.00761900	-0.69229600	-0.77148600
C	-2.35756900	-1.33033900	0.41353500
C	-2.95165200	-0.08512200	-1.58417000
C	-3.69463200	-1.33297500	0.78425000
C	-4.28799200	-0.11075200	-1.19416300
C	-4.68467400	-0.72904300	-0.00464700
H	-3.97128300	-1.83517100	1.70601300
H	-5.02024000	0.36399000	-1.83609200
H	-2.64440600	0.39720600	-2.50619000
H	-1.59284400	-1.83928800	0.99554200
C	-6.14456200	-0.78146800	0.45204700
C	-6.26967500	-0.11552700	1.83265000
C	-6.58703000	-2.25169500	0.55014500
C	-7.08070100	-0.05809300	-0.52094000
H	-5.95674200	0.93212200	1.78854500
H	-5.65625300	-0.62147100	2.58309300
H	-7.31059300	-0.15005300	2.17016800
H	-8.10753300	-0.11910900	-0.14912800
H	-7.05926100	-0.51324900	-1.51619800
H	-6.82242100	1.00140000	-0.61713900
C	-0.83427900	2.82039300	0.52147500
C	-0.24220200	1.66480100	0.70473600
H	-1.91631800	2.87178700	0.65781800
C	-0.15847000	4.08101700	0.15361800
C	-0.82512000	5.29687200	0.32976600

C	1.13374900	4.08712600	-0.38332400
C	-0.20363900	6.49720300	-0.00157900
H	-1.83250700	5.29782800	0.73672800
C	1.75411200	5.28404300	-0.71588200
H	1.63532500	3.13743500	-0.55161400
C	1.08721600	6.49420000	-0.52248600
H	-0.72845000	7.43549800	0.14576100
H	2.75627800	5.27652100	-1.13245100
H	1.57137200	7.42941900	-0.78393700
Br	0.90846100	-2.94447600	0.96800400
C	0.31204700	0.47642000	0.82291000
O	0.77643900	-0.06431000	1.95599600
H	-7.63192000	-2.30700200	0.87230700
H	-5.98214600	-2.80847800	1.27106500
H	-6.49896300	-2.74812000	-0.42093300
H	0.94444400	-1.04415700	1.79873300

NM2

C	4.41420100	-1.87550300	-0.46289300
C	3.17572400	-1.84128700	0.17671900
C	2.67672100	-2.94357800	0.85981400
C	3.44128100	-4.10907500	0.88141700
C	4.67958000	-4.15424000	0.23894100
C	5.17742800	-3.03795300	-0.43171000
C	4.72468600	-0.54050500	-1.09197600
C	3.37723500	0.20068400	-1.13498400
C	2.54235100	-0.47874100	0.00358700
H	1.72008600	-2.89013400	1.37128800
H	3.07361300	-4.98581700	1.40445600
H	5.26272300	-5.06931900	0.26333600
H	6.14321800	-3.07773400	-0.92650600
H	5.16989800	-0.60473800	-2.08827400
H	3.49911000	1.25688700	-0.89945800
H	5.39791400	0.03376300	-0.44448100
H	2.61163900	0.15011300	0.90118500
N	1.13870900	-0.59366300	-0.40635300
O	2.75404900	0.15642300	-2.41958800
C	-0.00479400	-0.43575900	0.26574600
C	0.80807300	-0.88446100	-1.69787900
N	-0.97978700	-0.67827800	-0.61262000
N	-0.48533000	-0.94203400	-1.85283700
C	1.93135300	-0.95859100	-2.68039100
H	2.46618200	-1.91219700	-2.57573800
H	1.54583600	-0.86873100	-3.69605400

C	-2.39283000	-0.71243800	-0.39043200
C	-2.90326600	-1.39073800	0.70611200
C	-3.22622900	-0.07226800	-1.30110700
C	-4.27940000	-1.39447800	0.91496300
C	-4.59500100	-0.09824600	-1.07886800
C	-5.15098900	-0.74826800	0.03366700
H	-4.66492000	-1.92479700	1.77734700
H	-5.24386100	0.40353300	-1.79018900
H	-2.79708400	0.43896300	-2.15608200
H	-2.24088500	-1.92215500	1.38365200
C	-6.66722600	-0.73152900	0.23539000
C	-7.13699500	0.72618000	0.38127000
C	-7.09020900	-1.50585100	1.48725400
C	-7.34806100	-1.37054000	-0.98696700
H	-6.89909800	1.31895700	-0.50646300
H	-6.66471100	1.20205700	1.24601400
H	-8.22181000	0.75535300	0.52313800
H	-8.43406500	-1.36502500	-0.85168800
H	-7.02225600	-2.40696000	-1.11588100
H	-7.12246900	-0.82568900	-1.90784100
C	-1.50614100	1.89227800	1.57995100
C	-1.08420000	0.80859400	2.25489500
H	-2.33748500	2.45893400	1.99625800
C	-0.89403500	2.40281400	0.34566600
C	-1.68909800	2.80534200	-0.73727700
C	0.50079300	2.51475200	0.25936900
C	-1.08889000	3.23961800	-1.91302600
H	-2.77166900	2.75099000	-0.65801700
C	1.09542800	2.98042600	-0.91035800
H	1.14392800	2.29893000	1.11273500
C	0.30294700	3.32360000	-2.00255500
H	-1.70522500	3.52963200	-2.75807300
H	2.17541400	3.09574400	-0.92025200
H	0.76333400	3.68338400	-2.91714400
Br	3.81928000	2.33010900	1.48465500
C	-0.10113500	-0.16444100	1.75988700
H	-8.17806600	-1.46245800	1.58877100
H	-6.65405700	-1.07684300	2.39479200
H	-6.80326800	-2.56034800	1.42652800
H	-1.48294800	0.56765900	3.23522700
O	0.58910500	-0.87176100	2.46231200

***E*-TS4**

C	4.74636200	0.20081700	0.69204100
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C	3. 60100700	0. 98684500	0. 54240800
C	3. 07619100	1. 71608600	1. 60138400
C	3. 69161100	1. 61103600	2. 84637400
C	4. 81921000	0. 80428100	3. 00692000
C	5. 36199200	0. 10314300	1. 93172500
C	5. 11637700	-0. 45620800	-0. 61244400
C	4. 40979500	0. 47090000	-1. 62437200
C	3. 12656000	0. 91706600	-0. 88300900
H	2. 20635600	2. 35305700	1. 46207000
H	3. 29887000	2. 16333000	3. 69339300
H	5. 28582900	0. 72940300	3. 98359000
H	6. 24492600	-0. 51352500	2. 06451900
H	4. 69365300	-1. 46989500	-0. 61649900
H	5. 01672500	1. 36725600	-1. 77104600
H	6. 19039200	-0. 52375700	-0. 79300700
H	2. 69819200	1. 84118100	-1. 27930600
N	2. 11875600	-0. 16268800	-1. 10712500
O	4. 15530100	-0. 02150400	-2. 92059100
C	0. 99476600	-0. 43336500	-0. 43260300
C	2. 22436000	-1. 13178300	-2. 07123400
N	0. 44404200	-1. 48909600	-1. 01902800
N	1. 20088900	-1. 93879400	-2. 04547000
C	3. 42408100	-1. 22351800	-2. 96207700
H	4. 02615600	-2. 08528000	-2. 64809300
H	3. 10788100	-1. 38134800	-3. 99464900
C	-0. 79408100	-2. 13239800	-0. 66881900
C	-0. 92208900	-2. 73447200	0. 57793500
C	-1. 82168800	-2. 14915800	-1. 60106000
C	-2. 13672000	-3. 32644000	0. 89641800
C	-3. 02639600	-2. 75549500	-1. 25818500
C	-3. 21246200	-3. 34456400	-0. 00234600
H	-2. 23706900	-3. 80144600	1. 86723600
H	-3. 82352200	-2. 76856300	-1. 99184300
H	-1. 67757500	-1. 71317400	-2. 58484500
H	-0. 07019000	-2. 78068600	1. 24957600
C	-4. 52374500	-4. 01656700	0. 40877700
C	-5. 06364200	-3. 33451500	1. 67754100
C	-4. 25570900	-5. 50338800	0. 69945900
C	-5. 59028300	-3. 91902900	-0. 68612900
H	-5. 26045700	-2. 27336100	1. 49573200
H	-4. 36045500	-3. 41303100	2. 51110700
H	-6. 00077800	-3. 80941600	1. 98367300
H	-6. 50827900	-4. 40207100	-0. 34061300
H	-5. 27502900	-4. 42415100	-1. 60435900

H	-5.83135800	-2.87793900	-0.92457600
C	-0.74599300	2.09188600	1.69464000
C	-0.50794100	1.29316400	0.60147900
H	0.04732700	2.23934700	2.43633300
C	-1.97708500	2.81976100	1.92861900
C	-1.97649400	3.99522600	2.69577700
C	-3.18515900	2.34169500	1.39194600
C	-3.15323000	4.71175200	2.87104300
H	-1.04658300	4.35119100	3.13031900
C	-4.36312800	3.04615000	1.58977000
H	-3.17992200	1.39894700	0.85110600
C	-4.34287100	4.24015100	2.31572400
H	-3.14939300	5.63003000	3.44757500
H	-5.29879500	2.66820000	1.19139200
H	-5.26361500	4.79469200	2.46464900
Br	2.64590200	-2.39791400	1.32347900
C	0.42062100	0.27513600	0.76031600
O	0.72180100	-0.22997600	1.90860900
H	-5.18495000	-5.99563400	1.00247200
H	-3.52840000	-5.63358800	1.50529200
H	-3.87159000	-6.01023700	-0.19066300
H	1.46397500	-0.99189600	1.83598500
H	-1.08447000	1.84408500	-0.64406400
N	-1.44099500	2.56832600	-1.62291200
C	-0.34962300	2.40366700	-2.61768900
C	-0.29163200	1.01109700	-3.22300600
H	-0.45416000	3.15061600	-3.40798900
H	0.57520300	2.63598800	-2.07607000
H	0.66639700	0.87601400	-3.73132100
H	-1.08272700	0.85200000	-3.95958800
H	-0.39273200	0.24306100	-2.45459500
C	-1.46182600	3.95674000	-1.06600300
C	-1.19390000	5.10029400	-2.03890500
H	-2.43209300	4.08455800	-0.57962300
H	-0.70090300	3.97411800	-0.27613400
H	-1.36830600	6.03832700	-1.50745900
H	-1.85379300	5.08260500	-2.90788800
H	-0.15969900	5.11157600	-2.38817200
C	-2.76762000	2.07588400	-2.08406200
C	-3.31157200	2.72919700	-3.34724100
H	-2.67304200	0.99316200	-2.21160100
H	-3.45796000	2.23864600	-1.25358000
H	-4.22318500	2.20725200	-3.64619100
H	-2.60956000	2.67239000	-4.18330400

H	-3.57177900	3.77611300	-3.17977700
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Z-TS4

C	-4.09344000	-1.65211200	-1.23915200
C	-3.72740400	-0.41086300	-0.71351800
C	-3.61345500	0.71842700	-1.51747700
C	-3.80613600	0.57916200	-2.88782300
C	-4.12131900	-0.66980500	-3.42759000
C	-4.28158100	-1.78715000	-2.61053500
C	-4.24508300	-2.68612800	-0.15590500
C	-4.27859200	-1.84379300	1.12844800
C	-3.51931100	-0.52164200	0.76885500
H	-3.38047100	1.69078900	-1.09145700
H	-3.71716300	1.44209700	-3.53885600
H	-4.26366000	-0.76659500	-4.49890500
H	-4.55565300	-2.74691800	-3.03644900
H	-3.37112300	-3.34451200	-0.12815400
H	-5.30592500	-1.53842300	1.36743000
H	-5.14551500	-3.29331400	-0.26858700
H	-3.89590000	0.33231700	1.34079700
N	-2.09869500	-0.68288900	1.17566000
O	-3.74179000	-2.58614300	2.20680900
C	-0.91378700	-0.37713500	0.62846700
C	-1.82573800	-1.27550100	2.37935100
N	0.00843900	-0.72297700	1.52588300
N	-0.54526400	-1.31618600	2.61088700
C	-2.97687200	-1.85281900	3.13654800
H	-2.61149000	-2.54441300	3.89503700
H	-3.56062800	-1.05816900	3.62274400
C	1.44062200	-0.73246100	1.35564300
C	2.06455600	-1.95941600	1.15339500
C	2.15686300	0.45222800	1.41888200
C	3.44483200	-1.97755800	1.00870800
C	3.53807200	0.40880700	1.25117900
C	4.20973700	-0.80162300	1.05066300
H	3.93209600	-2.93598400	0.86326500
H	4.08976700	1.34008400	1.28825800
H	1.64686300	1.39357400	1.59343000
H	1.46575700	-2.86081100	1.08127900
C	5.73427900	-0.87999200	0.93876900
C	6.14432200	-1.72992000	-0.27495800
C	6.27308300	-1.53608200	2.22261400
C	6.36732000	0.50646000	0.78295000
H	5.78425100	-1.27779700	-1.20309800

H	5.75900300	-2.75108200	-0.21686000
H	7.23554300	-1.79243600	-0.32465600
H	7.44847300	0.39959800	0.65904700
H	6.19860200	1.13372200	1.66353100
H	5.97393600	1.02379900	-0.09904700
C	0.93146100	2.04605000	-1.45232700
C	-0.09617500	1.52995500	-0.73183500
H	0.97269700	3.13455800	-1.54295600
C	2.09382500	1.37159400	-2.02026300
C	3.04693800	2.17780200	-2.66453000
C	2.31729000	-0.01508300	-1.94245300
C	4.18313300	1.62071600	-3.23674000
H	2.88498100	3.25098200	-2.71739300
C	3.44993100	-0.56802800	-2.51746000
H	1.61943000	-0.67578800	-1.43948200
C	4.38433800	0.24460400	-3.16459000
H	4.90736000	2.25522300	-3.73564800
H	3.60994600	-1.63940200	-2.45382200
H	5.27067800	-0.19796600	-3.60846400
Br	-0.74737000	-3.16765200	-0.66468000
C	-0.57275000	0.23087900	-0.70827400
O	-0.80852500	-0.46520400	-1.75607600
H	7.36429200	-1.60804500	2.17543900
H	5.87010800	-2.54491100	2.35136900
H	6.00370300	-0.94673800	3.10418900
H	-0.95701600	-1.49583400	-1.50911900
H	-0.64673900	2.49200200	0.05680500
N	-1.14572500	3.60728700	0.61582400
C	-2.19914400	3.14141200	1.54334300
C	-1.65691400	2.36083800	2.73333700
H	-2.79591800	3.98925100	1.89436300
H	-2.87126400	2.51243200	0.94601200
H	-2.48738300	1.87468300	3.25203800
H	-1.16258400	3.01291000	3.45687600
H	-0.93887800	1.59051600	2.43193700
C	-1.69131700	4.31964400	-0.57644900
C	-2.90938900	5.20867600	-0.35208100
H	-0.86716000	4.90630800	-0.99305800
H	-1.93349200	3.54501800	-1.31539900
H	-3.12674600	5.73197200	-1.28564100
H	-2.74299000	5.95978900	0.42264500
H	-3.79634900	4.62810600	-0.08889100
C	-0.01263600	4.30640500	1.26471400
C	-0.36151300	5.63179500	1.92827600

H	0.42046900	3.61666700	1.99392400
H	0.74362200	4.45770700	0.48834800
H	0.52750700	6.03016300	2.42176000
H	-1.13955200	5.51585900	2.68830600
H	-0.69455100	6.37091200	1.19621100

E-M4

C	-3.50357300	-2.78686900	-1.01052700
C	-3.14734200	-1.46862100	-0.70500700
C	-3.26448300	-0.45280600	-1.64846700
C	-3.71151900	-0.78294400	-2.92594000
C	-4.04578000	-2.10044200	-3.24075000
C	-3.95423300	-3.11031200	-2.28391700
C	-3.35270000	-3.68359400	0.19160800
C	-3.34029900	-2.66095700	1.34702100
C	-2.71119700	-1.38064300	0.73735800
H	-3.03329400	0.57757700	-1.39723300
H	-3.81253300	-0.00743800	-3.67707500
H	-4.39804200	-2.33861200	-4.23894000
H	-4.24077300	-4.12865800	-2.52698600
H	-2.41366600	-4.24682400	0.13271200
H	-4.37023500	-2.40796800	1.60632400
H	-4.16132500	-4.40841300	0.30220700
H	-3.00824700	-0.46950600	1.26075500
N	-1.23017100	-1.51698300	0.89157600
O	-2.73504500	-3.05663400	2.55611500
C	-0.24979200	-0.80031500	0.31401600
C	-0.61430100	-2.48803400	1.63626200
N	0.89476200	-1.35896000	0.69449400
N	0.68232300	-2.40778800	1.52940600
C	-1.40015000	-3.48466800	2.43355800
H	-1.32014600	-4.47404700	1.96745800
H	-0.98305900	-3.54829400	3.43999300
C	2.24187400	-0.95640000	0.39067600
C	2.62614900	-0.74361900	-0.92917800
C	3.13807300	-0.83269800	1.44306000
C	3.93971600	-0.37182300	-1.17803800
C	4.45003500	-0.46665200	1.16439900
C	4.87734900	-0.22546400	-0.14586400
H	4.24055900	-0.20602900	-2.20753700
H	5.14224100	-0.36972200	1.99173900
H	2.81327400	-1.02212900	2.46032000
H	1.91533500	-0.87036100	-1.73678600
C	6.31379600	0.17670100	-0.48477400

C	6.30074800	1.54376900	-1.18976200
C	6.92302200	-0.87995800	-1.42259500
C	7.19244300	0.28242700	0.76526800
H	5.87315700	2.31271600	-0.53936800
H	5.71968400	1.51779800	-2.11581700
H	7.32349400	1.83848400	-1.44386400
H	8.20469000	0.57279300	0.47171600
H	7.26154700	-0.67374500	1.29348400
H	6.81761600	1.04034500	1.46030400
C	-1.21966500	2.75386400	-0.42918700
C	-1.03032800	1.58181100	0.21792000
H	-0.91629700	2.77964500	-1.47614300
C	-1.77405200	3.98538400	0.10817300
C	-1.85094300	5.10090600	-0.73935300
C	-2.22844800	4.10068000	1.43276900
C	-2.36749600	6.30510500	-0.27746500
H	-1.49868000	5.01584400	-1.76333200
C	-2.74556000	5.30185800	1.89087300
H	-2.17829400	3.25005300	2.10501900
C	-2.81523900	6.40549800	1.03706600
H	-2.41998600	7.16229800	-0.93949600
H	-3.09577400	5.38511800	2.91386700
H	-3.21954200	7.34410500	1.40145100
C	-0.42025300	0.47077000	-0.50608800
O	-0.03789200	0.47663800	-1.65670500
H	7.95172000	-0.60344800	-1.67308000
H	6.36221700	-0.96505400	-2.35762500
H	6.93865100	-1.86325100	-0.94306900
H	-1.27432400	1.44110000	1.26669300

Z-M4

C	-4.27404400	0.62217700	-1.23529000
C	-4.00140300	0.80169000	0.12419300
C	-3.83299900	2.06617100	0.67691600
C	-3.87946400	3.16809700	-0.17480100
C	-4.11090700	2.99364500	-1.53992900
C	-4.32562200	1.72442900	-2.07861900
C	-4.50142000	-0.83605500	-1.54485000
C	-4.78021400	-1.43539100	-0.15379900
C	-3.94937800	-0.53435300	0.80967800
H	-3.68466900	2.19894200	1.74459700
H	-3.74829500	4.16634900	0.22784700
H	-4.14612700	3.86231600	-2.18887700
H	-4.53861100	1.60335000	-3.13571800

H	-3.60199300	-1.30452200	-1.96283600
H	-5.83193600	-1.29067500	0.11974600
H	-5.32208500	-1.01116500	-2.24286700
H	-4.31372200	-0.53826900	1.83980400
N	-2.57928300	-1.10720100	0.82975200
O	-4.47523600	-2.81937900	-0.13427600
C	-1.35767300	-0.59602100	0.62670000
C	-2.42833300	-2.46824300	0.92471800
N	-0.52364100	-1.63504700	0.63807700
N	-1.17846700	-2.81335800	0.81030000
C	-3.68199400	-3.28117400	0.94281600
H	-3.45359000	-4.33066400	0.76260700
H	-4.19705400	-3.18339000	1.90692000
C	0.89234300	-1.60633000	0.38999800
C	1.40950000	-2.45248400	-0.58551900
C	1.69898000	-0.72278400	1.08996800
C	2.76613200	-2.38876200	-0.86168300
C	3.05650000	-0.66652800	0.78355200
C	3.61646800	-1.49358200	-0.19275900
H	3.16697800	-3.04341100	-1.62840900
H	3.67290200	0.03959900	1.32757900
H	1.28577300	-0.09315600	1.87102600
H	0.75592000	-3.13468600	-1.11779100
C	5.09812600	-1.43570100	-0.56695100
C	5.21458400	-0.90799600	-2.00753500
C	5.71388800	-2.84221300	-0.47967700
C	5.88707400	-0.50585400	0.35985600
H	4.78266000	0.09506700	-2.08536000
H	4.69549500	-1.55890800	-2.71732400
H	6.26738000	-0.85702200	-2.30268000
H	6.93976300	-0.50902600	0.06402400
H	5.83004900	-0.83475100	1.40249900
H	5.52544200	0.52538900	0.29877900
C	0.38802700	2.52240800	1.56523900
C	-0.69007700	1.73406900	1.36455400
H	0.40519500	3.02583800	2.53108500
C	1.62692000	2.68123200	0.79896100
C	2.78886400	2.91115100	1.55836000
C	1.73729300	2.58148500	-0.59640300
C	4.03446000	2.97637900	0.94953600
H	2.70794300	3.01993900	2.63677800
C	2.98729200	2.65655300	-1.20204000
H	0.84802300	2.47203100	-1.20115800
C	4.13544700	2.84058200	-0.43535500

H	4.92374100	3.14228400	1.54884400
H	3.06274300	2.58370100	-2.28194700
H	5.10685300	2.90063800	-0.91673300
C	-0.90676900	0.81978900	0.24170100
O	-0.69917500	0.98662500	-0.93583400
H	6.77820500	-2.79317900	-0.72863000
H	5.24457400	-3.54185000	-1.17632800
H	5.61668400	-3.24877500	0.53132600
H	-1.40282100	1.63096500	2.17794200

TS5RR

C	2.36950200	0.93920500	1.15007200
C	1.77600000	-0.04927900	0.39667900
H	2.32252900	0.84238400	2.23239000
C	3.46758400	1.75401800	0.60133400
C	4.47524700	2.21643900	1.45573200
C	3.55759100	2.04435200	-0.76925500
C	5.56945400	2.91327100	0.95280000
H	4.39782600	2.02010000	2.52187200
C	4.65042800	2.74188700	-1.26873800
H	2.75561300	1.74708300	-1.44006300
C	5.66415000	3.17325900	-0.41245400
H	6.34856100	3.25398800	1.62796100
H	4.70465200	2.96145400	-2.33026700
H	6.51668900	3.71746500	-0.80661600
C	0.95813200	-1.08153600	0.93815100
O	0.53421500	-1.24310400	2.07839500
H	1.90034500	-0.04797100	-0.67865800
C	-0.38756400	2.07036300	1.22158100
C	-1.29509700	1.79278300	2.37894700
C	-2.04815800	0.61680700	2.44639400
C	-1.42642400	2.73586900	3.40439500
C	-2.88692500	0.38506800	3.53066100
H	-1.94940800	-0.11750500	1.65402600
C	-2.28083800	2.50951800	4.47985100
H	-0.86850300	3.66511400	3.34652100
C	-3.01036300	1.32737600	4.55032600
H	-3.44054500	-0.54617300	3.58449800
H	-2.37636900	3.25890300	5.25941900
H	-3.66975400	1.13798100	5.39189100
N	-0.77798100	1.56002400	0.09216900
N	0.05886700	1.81794200	-0.99420300
H	0.42662600	2.79324200	-1.09067900
S	-0.37700400	1.05970500	-2.37881400

O	-0.46167300	-0.37646900	-2.09602900
O	0.56453300	1.52867900	-3.39116800
C	-2.00798400	1.60042400	-2.83973700
C	-3.08703300	1.38797500	-1.97759200
C	-4.34792300	1.81015600	-2.37533100
C	-4.55069300	2.43121100	-3.61488000
C	-3.45199700	2.63279300	-4.45030300
C	-2.17578500	2.22535900	-4.06897900
H	-2.92577200	0.92828600	-1.00804700
H	-5.19432800	1.66243300	-1.70890900
H	-3.59359500	3.11628200	-5.41255400
H	-1.31577300	2.38527300	-4.71019700
C	-5.93156600	2.87462400	-4.02171400
H	-6.62442800	2.02807100	-4.03494500
H	-6.32737200	3.60938000	-3.31454500
H	-5.92695800	3.32681500	-5.01535000
C	0.82259500	2.80092000	1.50860400
H	1.06727600	2.89760300	2.55950100
C	1.38610600	3.84454900	0.70874000
O	1.11461900	4.16046700	-0.45908700
O	2.33858200	4.52910900	1.38563200
C	3.04167300	5.52363100	0.63825800
C	4.02569500	6.17800500	1.58352300
H	2.32637900	6.24507300	0.23126000
H	3.54914800	5.04306700	-0.20436600
H	4.60140700	6.94188700	1.05474900
H	3.50379400	6.65248700	2.41820100
H	4.71783800	5.43301800	1.98308700
C	3.89116100	-4.52257700	0.02947200
C	3.58340800	-3.16955700	0.20969800
C	3.87347200	-2.52379600	1.40768300
C	4.44992100	-3.26276100	2.43906700
C	4.73880300	-4.61654400	2.26889500
C	4.46947300	-5.25455900	1.05918100
C	3.53930600	-4.97938200	-1.36256100
C	3.44510600	-3.63766600	-2.11933400
C	2.98057000	-2.60406800	-1.05913000
H	3.66645600	-1.46703300	1.53107800
H	4.68168300	-2.77585500	3.38026600
H	5.19158300	-5.17486000	3.08206000
H	4.71584300	-6.30275100	0.91983900
H	2.58227800	-5.51501100	-1.35925100
H	4.44902200	-3.33595700	-2.42620600
H	4.28339800	-5.64442600	-1.80603500

H	3.29093900	-1.58761900	-1.30082300
N	1.49119100	-2.63959400	-1.03707600
O	2.67323800	-3.62344400	-3.29640300
C	0.63424000	-2.13029900	-0.12560200
C	0.73746100	-3.35818100	-1.92473300
N	-0.55799000	-2.61260700	-0.45095000
N	-0.51710500	-3.36200100	-1.58171000
C	1.33719300	-4.03120600	-3.12097900
H	1.24790400	-5.12008300	-3.02016100
H	0.78580200	-3.72360900	-4.01136800
C	-1.83229700	-2.36931200	0.15647600
C	-2.06930800	-2.78225200	1.45765600
C	-2.82769600	-1.79453100	-0.62567000
C	-3.34833200	-2.61656200	1.98545000
C	-4.08569400	-1.61933300	-0.06921400
C	-4.37639500	-2.03142700	1.24014500
H	-3.52918800	-2.94924200	3.00117000
H	-4.85792900	-1.15292200	-0.67450400
H	-2.59236500	-1.47649500	-1.63592300
H	-1.26669700	-3.20963400	2.04744800
C	-5.79012200	-1.82876500	1.79086300
C	-5.93008300	-2.32874300	3.23226100
C	-6.78638800	-2.60694100	0.91397100
C	-6.13774800	-0.33028500	1.75535200
H	-5.27164900	-1.78740100	3.91933900
H	-5.71210300	-3.39831200	3.31264400
H	-6.95836200	-2.17161200	3.57031700
H	-6.76725100	-2.26078000	-0.12311300
H	-7.80342000	-2.47161400	1.29594500
H	-6.55570100	-3.67662100	0.91951500
H	-7.14305000	-0.17230500	2.15937000
H	-6.12160700	0.06153600	0.73406000
H	-5.42753900	0.25153100	2.35077700

TS5'RR

C	-1.19720400	2.22382900	0.09918100
C	-1.91175300	1.09729800	0.45155700
H	-0.68030200	2.17817400	-0.85938800
C	-1.38162000	3.56267300	0.67519100
C	-0.80542600	4.65928400	0.01909300
C	-2.09104200	3.78299200	1.86245000
C	-0.92691800	5.94175900	0.53810800
H	-0.23838700	4.49082600	-0.89303400
C	-2.21559600	5.06744900	2.37915400

H	-2.52751600	2.94533400	2.39753500
C	-1.63467700	6.15029200	1.72069400
H	-0.46028800	6.77607100	0.02446400
H	-2.76182100	5.22511000	3.30384400
H	-1.72972600	7.15045000	2.13096700
C	-1.81359200	-0.07622200	-0.35846500
O	-1.28891900	-0.20770800	-1.45785700
H	-2.46554500	1.03703400	1.38447500
C	1.89515400	2.47980800	0.07634500
C	2.53640400	3.83206300	0.18573800
C	2.78678600	4.57723700	-0.97351100
C	2.87951700	4.38401900	1.42323300
C	3.35320400	5.84375700	-0.89428400
H	2.52666300	4.14250900	-1.93297700
C	3.45057900	5.65179900	1.50241600
H	2.71335700	3.81235700	2.33082700
C	3.68387700	6.38891100	0.34555700
H	3.53428000	6.40957000	-1.80309900
H	3.71522400	6.06186700	2.47224600
H	4.12262800	7.37990600	0.40886600
N	2.15045700	1.88755400	-1.05002700
N	1.47540500	0.72485100	-1.35638800
H	1.10137600	0.14628200	-0.58096400
S	2.26750800	-0.18614300	-2.49507100
O	2.57448900	0.62569800	-3.66037200
O	1.45696900	-1.38915000	-2.66440600
C	3.81501000	-0.63818800	-1.72636800
C	4.87699600	-1.00050400	-2.54795600
C	6.07711400	-1.40037900	-1.96790200
C	6.23450900	-1.41341000	-0.58026800
C	5.15696600	-1.02013800	0.22008400
C	3.93846600	-0.65026600	-0.33741500
H	4.76666700	-0.95456300	-3.62672200
H	6.90831600	-1.69257700	-2.60310600
H	5.27533200	-1.00648200	1.30037400
H	3.10148000	-0.37495800	0.29949200
C	7.52402000	-1.86172800	0.05522000
H	8.31945700	-1.96403500	-0.68555000
H	7.85333900	-1.15283200	0.81962500
H	7.39043600	-2.83259500	0.54420200
C	1.02427600	2.10067300	1.16805300
H	0.82286400	2.88330300	1.88640300
C	0.68056400	0.81098100	1.63649200
O	0.85566700	-0.29868100	1.10547600

O	-0.02072700	0.87953300	2.80523700
C	-0.44811800	-0.36732000	3.34444400
C	-1.19132100	-0.06798600	4.62893900
H	0.41765700	-1.01719000	3.51175100
H	-1.09162000	-0.87843400	2.61828700
H	-1.54964600	-0.99487300	5.08396600
H	-0.53789500	0.44010100	5.34160500
H	-2.05056200	0.57914200	4.43218300
C	-5.94129100	-0.74585500	-2.07905300
C	-4.94430400	0.01704200	-1.46257400
C	-4.17321200	0.91650300	-2.19260600
C	-4.39450100	1.01815200	-3.56407900
C	-5.37609700	0.24585300	-4.18469900
C	-6.16334200	-0.63593500	-3.44596800
C	-6.67171400	-1.60060300	-1.07553600
C	-6.32365000	-0.89713300	0.25274700
C	-4.92489300	-0.26377800	0.02320400
H	-3.41895100	1.52835700	-1.70985800
H	-3.79740800	1.70658800	-4.15182500
H	-5.53582100	0.34081300	-5.25390200
H	-6.94086600	-1.22005900	-3.92852300
H	-6.29463600	-2.62971500	-1.10434100
H	-7.01936700	-0.06923800	0.40506800
H	-7.75050800	-1.64394800	-1.23912800
H	-4.74657800	0.61396600	0.64665100
N	-3.91249000	-1.28838700	0.40696500
O	-6.40681300	-1.67430600	1.42731700
C	-2.57759800	-1.26889500	0.21208500
C	-4.20678200	-2.48069000	1.01061700
N	-2.12921400	-2.44207400	0.65340900
N	-3.13573500	-3.20240100	1.16696300
C	-5.60498000	-2.83207600	1.41822500
H	-6.00448200	-3.60767100	0.75369200
H	-5.59363200	-3.22868700	2.43483200
C	-0.78689400	-2.95626700	0.68749800
C	0.05512700	-2.78849400	-0.39823600
C	-0.38616000	-3.64586700	1.82928800
C	1.33637800	-3.33344000	-0.33262600
C	0.89051200	-4.18182700	1.86615500
C	1.77535400	-4.04556100	0.78400600
H	1.97883600	-3.18376200	-1.19170100
H	1.20158700	-4.72006500	2.75666300
H	-1.06989900	-3.76026800	2.66363700
H	-0.25532600	-2.23398000	-1.27730800

C	3.17089000	-4.66706500	0.86716500
C	3.96705000	-4.46824900	-0.42743100
C	3.04475200	-6.17708000	1.13011500
C	3.93704500	-4.00915200	2.02688700
H	4.10962700	-3.40904300	-0.66184800
H	3.47099800	-4.94783400	-1.27719700
H	4.95713200	-4.92219300	-0.31633600
H	2.52179900	-6.38469500	2.06813400
H	4.04060200	-6.62769900	1.19550900
H	2.49826500	-6.66835400	0.31939200
H	4.95275100	-4.41543800	2.08558400
H	3.44529400	-4.18917100	2.98770300
H	4.00319900	-2.92860600	1.87457800

TS5''RR

C	0.02836300	-1.88907800	-0.53260900
C	1.00363200	-1.26306800	0.22543000
H	0.20654100	-1.93490000	-1.60651500
C	-1.02624200	-2.74072800	-0.00399000
C	-1.74548300	-3.55659600	-0.89289800
C	-1.37903300	-2.73465400	1.35440000
C	-2.79647000	-4.33819700	-0.43923000
H	-1.48138800	-3.54433400	-1.94793000
C	-2.43479100	-3.51384600	1.80495200
H	-0.85392500	-2.08711100	2.05004900
C	-3.15024200	-4.30674800	0.91080900
H	-3.36227800	-4.94715300	-1.13501300
H	-2.73491300	-3.47000000	2.84595100
H	-3.99924300	-4.88513500	1.26071900
C	2.04596200	-0.56705900	-0.43934400
O	2.15342300	-0.32850700	-1.64288000
H	0.98231400	-1.26258200	1.31000500
C	-2.06349400	0.24742900	-0.00506500
C	-1.23704500	1.20731600	0.79717800
C	-1.15361600	1.05752100	2.18771400
C	-0.52347000	2.24789100	0.19446100
C	-0.37114100	1.91797300	2.95053000
H	-1.71904300	0.25547500	2.65112100
C	0.24896600	3.11706900	0.95925700
H	-0.59043700	2.39705200	-0.87864600
C	0.33780400	2.95106600	2.33850300
H	-0.31497400	1.78205700	4.02669200
H	0.78471900	3.92544700	0.47138900
H	0.94965000	3.62570700	2.93073500

N	-3.06833800	-0.22289600	0.67283800
N	-3.84473600	-1.21532800	0.12663700
H	-3.87483700	-1.33920800	-0.90571600
S	-5.25930900	-1.48553600	0.92791800
O	-4.97111600	-1.66723300	2.34549400
O	-5.93294300	-2.53060900	0.16473800
C	-6.21808000	0.00651800	0.78766800
C	-5.87394700	1.10786500	1.57012700
C	-6.59650700	2.28390900	1.42617500
C	-7.65986300	2.37246900	0.51800200
C	-7.98199400	1.25300500	-0.24875800
C	-7.26342100	0.06669800	-0.12506300
H	-5.05235600	1.03010600	2.27349600
H	-6.33793200	3.15008300	2.02781600
H	-8.80882900	1.30804800	-0.95269200
H	-7.50843800	-0.80932000	-0.71708400
C	-8.43212400	3.65974100	0.38164500
H	-8.86530600	3.95941500	1.34283800
H	-7.77620800	4.47439600	0.05137100
H	-9.24436800	3.55921600	-0.34382000
C	-1.53586000	-0.07166100	-1.30667500
H	-0.60668800	0.41087500	-1.58003100
C	-2.13137300	-0.79851400	-2.37720600
O	-3.26617500	-1.28043700	-2.48202000
O	-1.23883300	-0.98437400	-3.39621000
C	-1.74104900	-1.67577300	-4.53879800
C	-0.59518500	-1.80962100	-5.51932100
H	-2.57864200	-1.11458600	-4.96630300
H	-2.13096200	-2.65261400	-4.23382900
H	-0.92596500	-2.34132800	-6.41479500
H	-0.22444700	-0.82548500	-5.81463900
H	0.23106500	-2.36568700	-5.06873700
C	5.50263700	-3.53638400	-0.09730300
C	4.16108000	-3.13993000	-0.10503700
C	3.36392700	-3.34279900	-1.22803700
C	3.93947800	-3.92263400	-2.35743200
C	5.28188600	-4.30182900	-2.35641600
C	6.07132800	-4.11923600	-1.22305700
C	6.14597000	-3.26405500	1.23660600
C	4.92027900	-3.08937300	2.15629500
C	3.78250500	-2.55955400	1.24094000
H	2.31557200	-3.06858800	-1.22635700
H	3.33294500	-4.08668800	-3.24046600
H	5.71190300	-4.75557900	-3.24346900

H	7.11015700	-4.43469700	-1.21562900
H	6.75676900	-2.35514800	1.18869900
H	4.60013200	-4.07193800	2.50919200
H	6.79462300	-4.07232900	1.58086600
H	2.78957700	-2.84035200	1.59250600
N	3.85504300	-1.06818000	1.26213100
O	5.11011000	-2.31843300	3.32316600
C	3.19614300	-0.17728300	0.48927100
C	4.72571700	-0.35544100	2.03743900
N	3.72617900	1.01191400	0.78157300
N	4.67049300	0.91295300	1.75667200
C	5.57409000	-1.01164700	3.08365200
H	6.62807100	-0.99012000	2.78266400
H	5.47684200	-0.45648400	4.01837200
C	3.44672000	2.31882600	0.25272400
C	3.09694500	2.48619800	-1.07839300
C	3.59939000	3.40969200	1.10620100
C	2.87212900	3.77859100	-1.55091000
C	3.38644100	4.68371100	0.60746500
C	3.01279600	4.89922900	-0.72898800
H	2.59540400	3.89388600	-2.59197000
H	3.50108700	5.52764300	1.28096100
H	3.87795800	3.25338600	2.14147200
H	3.00596100	1.62920100	-1.73538300
C	2.75565500	6.32495200	-1.21972500
C	2.42045600	6.36832900	-2.71357000
C	4.00719900	7.18495300	-0.97671200
C	1.56867500	6.91034600	-0.43525500
H	1.51004200	5.80526200	-2.94168700
H	3.23818200	5.96976000	-3.32160300
H	2.25341300	7.40574000	-3.01692700
H	4.26327400	7.24083100	0.08484500
H	3.83118700	8.20534300	-1.33155900
H	4.86908400	6.77814200	-1.51427000
H	1.37689900	7.93848800	-0.75874400
H	1.76460300	6.92590500	0.64090800
H	0.66147700	6.32246900	-0.60875400

TS5'''RR

C	0.52763900	-1.27958600	-0.60452600
C	-0.80984400	-1.23678800	-0.90024700
H	0.85998400	-0.74332300	0.28293400
C	1.48491900	-2.21991800	-1.18605600
C	2.58663900	-2.60478500	-0.40928800

C	1. 32291000	-2. 76838600	-2. 46749500
C	3. 48559500	-3. 55088600	-0. 89399500
H	2. 74339000	-2. 15086800	0. 56611700
C	2. 23907000	-3. 68835200	-2. 95634400
H	0. 49580800	-2. 44173300	-3. 09243000
C	3. 31713900	-4. 09089400	-2. 16497200
H	4. 33331200	-3. 84357600	-0. 28257200
H	2. 12021200	-4. 09115000	-3. 95705900
H	4. 03271100	-4. 81022300	-2. 55066700
C	-1. 70110400	-0. 51705900	-0. 03671900
O	-1. 43165200	0. 34186600	0. 79058800
H	-1. 23645600	-1. 82926700	-1. 70411400
C	3. 09189500	0. 33598300	-1. 46660500
C	3. 96701000	-0. 17061400	-2. 57212700
C	5. 03639500	-1. 02707900	-2. 28391000
C	3. 73261700	0. 17912700	-3. 90565300
C	5. 83650100	-1. 53155400	-3. 30166800
H	5. 21091700	-1. 29718100	-1. 24797300
C	4. 53331500	-0. 32638600	-4. 92652000
H	2. 92765600	0. 86722700	-4. 14253200
C	5. 58519400	-1. 18795400	-4. 62931400
H	6. 65608000	-2. 20201600	-3. 05998000
H	4. 33686600	-0. 04111600	-5. 95568700
H	6. 20824700	-1. 58555800	-5. 42472500
N	3. 65283500	0. 28710500	-0. 29390200
N	2. 80927500	0. 52878100	0. 78953200
H	2. 21119600	1. 38524000	0. 72105300
S	3. 59679600	0. 34842000	2. 23714600
O	4. 16052900	-0. 99752100	2. 26562700
O	2. 63537600	0. 76252800	3. 25439500
C	4. 95507300	1. 49292000	2. 24978000
C	6. 10775900	1. 18849700	1. 52697800
C	7. 14783400	2. 10702900	1. 50927300
C	7. 05270700	3. 32015100	2. 20162600
C	5. 88706600	3. 59524200	2. 91935800
C	4. 83028600	2. 68977000	2. 94481400
H	6. 17319200	0. 24769700	0. 99262200
H	8. 05197400	1. 88177800	0. 95026900
H	5. 80509100	4. 53029100	3. 46609200
H	3. 92169400	2. 89485800	3. 50086700
C	8. 18652200	4. 31081800	2. 15342000
H	9. 14625000	3. 81895800	2. 33343000
H	8. 24240700	4. 78551900	1. 16861700
H	8. 05802700	5. 09776300	2. 89936200

C	1. 74425900	0. 69261000	-1. 80536000
H	1. 35793700	0. 32140800	-2. 74570400
C	0. 93185800	1. 65677400	-1. 16274200
O	1. 19996700	2. 38679200	-0. 19335100
O	-0. 28804700	1. 75422300	-1. 76959300
C	-1. 14982100	2. 77213000	-1. 27560300
C	-2. 31215800	2. 85034600	-2. 24210400
H	-0. 60592700	3. 72011000	-1. 21472300
H	-1. 47506400	2. 51079200	-0. 26174200
H	-3. 05787000	3. 56992700	-1. 89566100
H	-1. 96575000	3. 14889200	-3. 23480900
H	-2. 79538300	1. 87263600	-2. 33002200
C	-3. 01438400	-4. 07276700	2. 60873000
C	-2. 16442400	-3. 38144900	1. 73934100
C	-1. 03190200	-2. 72937300	2. 21942800
C	-0. 77748500	-2. 75105800	3. 58885900
C	-1. 63429500	-3. 42610000	4. 45826800
C	-2. 75353500	-4. 09994100	3. 97327000
C	-4. 14368500	-4. 73339400	1. 86338000
C	-3. 61869400	-4. 73462400	0. 41273900
C	-2. 65684300	-3. 51826300	0. 31353400
H	-0. 34462600	-2. 22839000	1. 54950300
H	0. 10069200	-2. 24334000	3. 97320700
H	-1. 41865100	-3. 43789200	5. 52169900
H	-3. 40709800	-4. 64426700	4. 64816200
H	-5. 06395200	-4. 14677400	1. 96723900
H	-3. 00746600	-5. 62607200	0. 25673000
H	-4. 36374400	-5. 74490200	2. 21132400
H	-1. 87088200	-3. 65766200	-0. 42832600
N	-3. 47825900	-2. 34144400	-0. 11451800
O	-4. 59096100	-4. 76415000	-0. 60975600
C	-3. 14269400	-1. 03147100	-0. 12348800
C	-4. 81684800	-2. 40781000	-0. 38311000
N	-4. 28289800	-0. 37020700	-0. 32493300
N	-5. 33030700	-1. 21833700	-0. 50928200
C	-5. 52795300	-3. 71738900	-0. 54446700
H	-6. 25597200	-3. 85424400	0. 26372500
H	-6. 07142800	-3. 70895000	-1. 49138900
C	-4. 55556500	1. 04095800	-0. 33117700
C	-3. 99527000	1. 86747000	0. 63084200
C	-5. 47164000	1. 52333900	-1. 26392900
C	-4. 35235400	3. 21527400	0. 64065300
C	-5. 81643700	2. 86385400	-1. 22558800
C	-5. 26838700	3. 73946600	-0. 27384700

H	-3.90378400	3.85176900	1.39394100
H	-6.52957100	3.23593700	-1.95444800
H	-5.90493300	0.85105300	-1.99568100
H	-3.29205700	1.47066300	1.35320700
C	-5.68986800	5.21006100	-0.27245900
C	-4.98900700	6.00762700	0.83133500
C	-7.20940000	5.29644600	-0.04951100
C	-5.33417800	5.84067400	-1.62960900
H	-3.90165200	5.99684700	0.70796000
H	-5.23081300	5.61914300	1.82555500
H	-5.31950900	7.04930200	0.79083600
H	-7.76407100	4.78098100	-0.83864000
H	-7.52547600	6.34435100	-0.04605100
H	-7.48721600	4.84980700	0.90993200
H	-5.64730700	6.88950600	-1.64459800
H	-5.83187800	5.32944500	-2.45846600
H	-4.25460600	5.80457700	-1.80545700

TS5RS

C	-1.10699500	2.11648800	-1.31797500
C	-1.55995400	1.07079800	-0.52510500
H	-1.17425400	1.97948300	-2.39646400
C	-1.03859600	3.50859600	-0.83741700
C	-1.08403300	4.55075300	-1.77238500
C	-0.91532100	3.82538200	0.52304900
C	-1.02737600	5.87727300	-1.36379200
H	-1.16242000	4.30969900	-2.82960400
C	-0.85790000	5.15465200	0.92862800
H	-0.82405300	3.03446100	1.26224200
C	-0.91678900	6.18368200	-0.00895800
H	-1.06671500	6.67219900	-2.10173400
H	-0.75238300	5.38568800	1.98410800
H	-0.86699900	7.21871300	0.31373000
C	-1.83614600	-0.22313600	-1.03173100
O	-1.87970400	-0.62978300	-2.19493300
H	-1.57266700	1.18838500	0.55138900
C	1.85130600	2.53142900	-0.38814800
C	2.61645200	3.80933800	-0.52166600
C	2.60831500	4.73307000	0.52967800
C	3.33783200	4.11210100	-1.68061600
C	3.30079500	5.93298500	0.42087000
H	2.04244700	4.49362100	1.42339700
C	4.03569200	5.31226700	-1.78710700
H	3.36753400	3.39557500	-2.49590100

C	4. 01569200	6. 22790200	-0. 73895700
H	3. 27771200	6. 64401000	1. 24101300
H	4. 59729500	5. 53046300	-2. 69012600
H	4. 55330800	7. 16718800	-0. 82481500
N	1. 76339800	2. 09870100	0. 82951400
N	0. 88117800	1. 05166900	1. 02520700
S	0. 86873700	0. 37132200	2. 51850700
O	-0. 15721000	-0. 67346300	2. 40178100
O	0. 71974400	1. 39602000	3. 53999200
C	2. 45224300	-0. 40505300	2. 74293500
C	3. 09960200	-0. 96463500	1. 64327300
C	4. 30328800	-1. 62979200	1. 84898700
C	4. 86391100	-1. 73798900	3. 12561300
C	4. 19317000	-1. 15728500	4. 20601200
C	2. 99039900	-0. 48472200	4. 02288700
H	2. 67817400	-0. 87642800	0. 64329000
H	4. 82413400	-2. 06403000	0. 99952100
H	4. 62174300	-1. 22943300	5. 20162700
H	2. 47376500	-0. 01703200	4. 85441000
C	6. 18523500	-2. 43270500	3. 32571100
H	6. 33866900	-3. 21277200	2. 57656300
H	7. 01064100	-1. 71917900	3. 23505500
H	6. 24816300	-2. 88674400	4. 31722800
C	1. 24416300	1. 99835400	-1. 60314400
H	1. 27365900	2. 67153400	-2. 45158800
C	1. 19295000	0. 62352700	-1. 97615700
O	1. 22857400	-0. 36901700	-1. 22740100
O	1. 02614700	0. 47347100	-3. 31074100
C	0. 86944500	-0. 86841000	-3. 77431500
C	0. 92355400	-0. 83421200	-5. 28638200
H	-0. 08635300	-1. 25049900	-3. 40460000
H	1. 66456000	-1. 48947900	-3. 35026800
H	0. 80109300	-1. 84460500	-5. 68652300
H	0. 12357200	-0. 20667900	-5. 68651700
H	1. 88141400	-0. 43853200	-5. 63312100
C	-6. 14702700	-0. 86828900	0. 26912600
C	-5. 04330500	-0. 05334400	-0. 00538600
C	-4. 93057500	0. 61889500	-1. 21833300
C	-5. 93552200	0. 44477600	-2. 16852500
C	-7. 03001400	-0. 37821100	-1. 90346700
C	-7. 14766800	-1. 03599000	-0. 67993200
C	-6. 06158700	-1. 44600200	1. 65862700
C	-5. 05919300	-0. 48767300	2. 33487900
C	-4. 11893100	-0. 02223000	1. 19205000

H	-4.08419100	1.26773900	-1.41803200
H	-5.86603400	0.95966300	-3.12072400
H	-7.80419200	-0.49917700	-2.65434200
H	-8.01016900	-1.66059200	-0.46829200
H	-5.67598900	-2.47222400	1.62257300
H	-5.59611500	0.39957400	2.67820000
H	-7.01850900	-1.47301500	2.18398900
H	-3.65685500	0.94528600	1.39126400
N	-3.03383200	-1.03252600	1.08696600
O	-4.37491700	-0.97262800	3.46520700
C	-2.12757000	-1.20109600	0.10362700
C	-2.83830000	-2.04659500	1.98451400
N	-1.47091300	-2.31458500	0.41328700
N	-1.89733400	-2.85020300	1.58604500
C	-3.63688700	-2.15279400	3.24670500
H	-4.28185500	-3.03963700	3.20822500
H	-2.94904500	-2.26216200	4.08718300
C	-0.34440300	-2.90353900	-0.24810600
C	-0.42546500	-3.23697300	-1.59317200
C	0.79547200	-3.14947000	0.50138900
C	0.67831000	-3.82731800	-2.19146300
C	1.89009300	-3.73878100	-0.12332700
C	1.85529200	-4.08806200	-1.47682200
H	0.61807200	-4.08428800	-3.24565700
H	2.78179900	-3.91369500	0.46832300
H	0.82100900	-2.86135900	1.54766200
H	-1.32671400	-3.01491700	-2.15297200
C	3.03999900	-4.73953900	-2.19423000
C	3.48934900	-3.83585900	-3.35455600
C	2.60674800	-6.10771300	-2.74765700
C	4.23405800	-4.95300400	-1.25911600
H	3.79788300	-2.85356500	-2.98281100
H	2.68835600	-3.68660800	-4.08520400
H	4.33836300	-4.29049600	-3.87554700
H	2.27526800	-6.76590200	-1.93879700
H	3.44674800	-6.58751200	-3.26026800
H	1.78646500	-6.01203700	-3.46469300
H	5.05114900	-5.42319300	-1.81399200
H	3.97819000	-5.60754500	-0.42007100
H	4.60545300	-4.00412000	-0.85913300
H	0.80767700	0.34376600	0.26267200

TS5'RS

C	-0.52927100	-0.69014300	2.36661900
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C	-0.05421500	0.31455400	1.54255100
H	0.21274200	-1.25923100	2.92521600
C	-1.90198500	-0.70421200	2.89994200
C	-2.23281400	-1.61174100	3.91463900
C	-2.88702300	0.18013600	2.43778100
C	-3.50749100	-1.63122900	4.46564700
H	-1.47661400	-2.30975300	4.26592300
C	-4.16044000	0.16364300	2.99686100
H	-2.67055300	0.87081400	1.62804200
C	-4.47593700	-0.73848300	4.00944000
H	-3.74751000	-2.34467900	5.24751000
H	-4.91426600	0.85236200	2.62783000
H	-5.47407100	-0.75349600	4.43585000
C	1.33588000	0.49844600	1.32295900
O	2.29151000	-0.03528000	1.88771300
H	-0.75057400	0.90531800	0.96263300
C	-2.06989500	-2.28589600	0.33824800
C	-3.26199900	-2.99261300	0.91877800
C	-4.51492800	-2.37017700	0.91880600
C	-3.16047300	-4.28687100	1.44085200
C	-5.62581200	-3.01136400	1.45302700
H	-4.59700600	-1.37151200	0.50492400
C	-4.27528200	-4.93304600	1.96852500
H	-2.20830300	-4.80671600	1.41598300
C	-5.51129200	-4.29487200	1.98477700
H	-6.58584700	-2.50362900	1.45999800
H	-4.17485400	-5.93915300	2.36380100
H	-6.37986600	-4.79370300	2.40358600
N	-2.39021300	-1.45065500	-0.60101200
N	-1.36232100	-0.79145300	-1.26244800
S	-1.67815800	0.73814800	-1.73193800
O	-0.42040600	1.19301800	-2.34014900
O	-2.24986500	1.58539900	-0.67435600
C	-2.93542100	0.55438000	-2.96661800
C	-2.83053000	-0.47723600	-3.89309300
C	-3.78213600	-0.57332700	-4.90149200
C	-4.82878800	0.34792400	-4.99366000
C	-4.90803200	1.37429300	-4.04647600
C	-3.96824100	1.48483600	-3.02935200
H	-2.02617200	-1.20032900	-3.80822100
H	-3.71483500	-1.38011700	-5.62522000
H	-5.72156100	2.09221600	-4.10492400
H	-4.03014800	2.26914600	-2.28307200
C	-5.86458600	0.24238400	-6.08214700

H	-5.65452300	-0.59456000	-6.75048500
H	-6.86126100	0.09651700	-5.65555200
H	-5.89551200	1.15822900	-6.67945600
C	-0.79520600	-2.59346000	0.97007800
H	-0.85922800	-3.30258300	1.78434100
C	0.53178500	-2.45017300	0.47329900
O	0.92657900	-1.74840600	-0.47537500
O	1.42369200	-3.11748100	1.23994200
C	2.80993100	-2.93183300	0.93459000
C	3.58759000	-3.16029700	2.21173800
H	2.96471100	-1.91952000	0.56445500
H	3.09340900	-3.63853800	0.14363100
H	4.65577700	-3.02098600	2.02334100
H	3.27014200	-2.43015100	2.95997800
H	3.42945200	-4.16822100	2.60435900
C	1.18125800	5.10749200	1.84887900
C	0.59074200	3.84329400	1.96890900
C	0.55514200	3.18245900	3.19256600
C	1.15187300	3.79328200	4.29495300
C	1.75993800	5.04267200	4.17332200
C	1.77125900	5.71329300	2.95108800
C	1.03488700	5.64320900	0.44675700
C	-0.12393300	4.77863900	-0.09382200
C	0.01503200	3.41967600	0.63604000
H	0.07004200	2.21666600	3.28786800
H	1.13447400	3.29329500	5.25755100
H	2.21649300	5.50408400	5.04321000
H	2.22428500	6.69628100	2.86406800
H	1.95768400	5.48535300	-0.12558200
H	-1.07028600	5.21037300	0.24006600
H	0.80341200	6.70980400	0.40781100
H	-0.93032000	2.87865100	0.66447200
N	0.98357500	2.60458600	-0.15018300
O	-0.23794400	4.65807900	-1.49001300
C	1.62550600	1.46458100	0.18265900
C	1.46435300	2.98107700	-1.37351800
N	2.49628900	1.24628000	-0.79965400
N	2.40314500	2.17917000	-1.78264700
C	0.90649100	4.14509800	-2.12986800
H	1.67973400	4.91186000	-2.26524700
H	0.59048400	3.78545200	-3.11097800
C	3.44874300	0.18208600	-0.94818700
C	4.52509100	0.09207200	-0.07391300
C	3.29162500	-0.70076000	-2.00327100

C	5.45543600	-0.91949400	-0.26868600
C	4.23519000	-1.70838500	-2.17972900
C	5.33219400	-1.83763100	-1.32237400
H	6.29436800	-0.99064200	0.41710500
H	4.09527000	-2.40282900	-2.99897100
H	2.42616100	-0.61180600	-2.65109000
H	4.61085500	0.78562200	0.75411400
C	6.39348900	-2.92603900	-1.50450200
C	6.48062800	-3.77857300	-0.22810000
C	7.75459600	-2.25881100	-1.76683300
C	6.07127900	-3.85339100	-2.68066900
H	5.51963800	-4.25761300	-0.01393400
H	6.76345400	-3.17900300	0.64210200
H	7.23446100	-4.56257000	-0.35354800
H	7.71741300	-1.64382300	-2.67103200
H	8.52681300	-3.02314200	-1.90150300
H	8.05547000	-1.61867300	-0.93259600
H	6.84904900	-4.61784200	-2.76513500
H	6.03690900	-3.30704800	-3.62834500
H	5.11330000	-4.36397800	-2.53915600
H	-0.35927000	-0.99149800	-1.00332900

TS5''RS

C	1.57377600	1.80688000	-0.29615400
C	1.74819800	0.47494600	-0.67888600
H	1.34410300	1.94544900	0.76058900
C	2.27556400	2.93275000	-0.93837000
C	2.68239700	4.00787300	-0.14044000
C	2.58040600	2.95549700	-2.30554500
C	3.38598800	5.07627900	-0.68887500
H	2.44176900	3.99972800	0.92043400
C	3.27303800	4.02599600	-2.85526100
H	2.24876900	2.14000200	-2.94279300
C	3.68299100	5.08916900	-2.04900600
H	3.69651800	5.90070600	-0.05406100
H	3.49409000	4.03570300	-3.91793800
H	4.22564000	5.92318400	-2.48249000
C	1.64159400	-0.55622000	0.28626100
O	1.39279500	-0.49771500	1.48947900
H	2.05003100	0.20825200	-1.68784100
C	-1.29674600	1.30547400	-0.87026300
C	-1.74295000	0.70127900	-2.16299900
C	-1.51100000	-0.64493600	-2.44577200
C	-2.40611600	1.48890200	-3.11005300

C	-1.94133000	-1.19814200	-3.64931700
H	-0.98391700	-1.24268500	-1.71160500
C	-2.85143900	0.93373300	-4.30537800
H	-2.58400700	2.53905600	-2.89550900
C	-2.61884200	-0.41317000	-4.57937600
H	-1.74542100	-2.24598500	-3.85739500
H	-3.37964700	1.55238900	-5.02421800
H	-2.95910000	-0.84502000	-5.51558300
N	-1.54881100	0.59523900	0.18372500
N	-1.10483500	1.10710900	1.38675600
S	-1.83120900	0.45598800	2.72962200
O	-1.52978900	1.40495100	3.79488300
O	-1.46881500	-0.94517200	2.90319100
C	-3.57320200	0.47389300	2.35254600
C	-4.11752100	1.54801400	1.65196600
C	-5.47613800	1.53957700	1.36490700
C	-6.29605300	0.48008100	1.77153800
C	-5.72583000	-0.57489400	2.48642900
C	-4.36410100	-0.58778800	2.77618600
H	-3.48191400	2.36766700	1.32430300
H	-5.91100500	2.36561300	0.80906700
H	-6.35063700	-1.40322400	2.80925100
H	-3.90851400	-1.41476200	3.31259700
C	-7.75915800	0.46992700	1.41453000
H	-8.03077800	1.35663000	0.83640900
H	-7.99890900	-0.40704200	0.80420100
H	-8.38517500	0.43623800	2.30880400
C	-0.54992400	2.54442200	-0.98960100
H	-0.27369800	2.79948500	-2.00640200
C	-0.67708000	3.70333900	-0.14943400
O	-1.12675000	3.76821100	1.00270900
O	-0.19878100	4.81054200	-0.75678300
C	-0.14155100	5.99663300	0.04059800
C	0.30823600	7.11871200	-0.86950300
H	0.56228400	5.83750800	0.86520700
H	-1.12543100	6.18844300	0.47771100
H	0.39172800	8.05013500	-0.30418900
H	1.28088100	6.88246300	-1.30833300
H	-0.41102400	7.26617400	-1.67854700
C	5.75929200	-1.66171700	1.78113800
C	4.84320200	-0.85287200	1.10165600
C	4.33328900	0.30174800	1.68566300
C	4.72735800	0.61838600	2.98309400
C	5.62416900	-0.19819900	3.67206400

C	6.15522100	-1.33939000	3.07331800
C	6.21319900	-2.80936200	0.91665000
C	5.85642000	-2.29796900	-0.49470400
C	4.61455800	-1.38711100	-0.29413000
H	3.65055500	0.94458600	1.14081800
H	4.33252100	1.50946900	3.45875500
H	5.92042900	0.06500300	4.68239700
H	6.87094900	-1.95987500	3.60381000
H	5.66075800	-3.72093600	1.17332700
H	6.66233200	-1.64993200	-0.84624700
H	7.27787400	-3.03454600	1.00758800
H	4.52290700	-0.61189200	-1.05752800
N	3.40814700	-2.25316500	-0.41864000
O	5.69512200	-3.27118700	-1.50302500
C	2.11467800	-1.92902300	-0.21622500
C	3.42942900	-3.55471300	-0.84571100
N	1.42420200	-3.03579500	-0.48081400
N	2.22881200	-4.05437600	-0.88728300
C	4.70763000	-4.23631300	-1.22407500
H	5.01710400	-4.92630900	-0.42956000
H	4.54847500	-4.81474600	-2.13546100
C	-0.00164600	-3.19824500	-0.47793700
C	-0.75327200	-2.59236000	0.51913500
C	-0.59525100	-3.90271000	-1.52037900
C	-2.13606300	-2.63175800	0.40897500
C	-1.98431000	-3.93747100	-1.59420000
C	-2.77958200	-3.26383200	-0.65874900
H	-2.70788500	-2.10659700	1.16588300
H	-2.44215500	-4.46505600	-2.42355900
H	0.02017500	-4.38352100	-2.27294400
H	-0.29085100	-2.05566000	1.34063100
C	-4.29981400	-3.14424700	-0.77727700
C	-4.66488500	-1.65233600	-0.90646600
C	-4.95949200	-3.72523400	0.48401300
C	-4.84092500	-3.88506900	-2.00283600
H	-4.26916100	-1.23801900	-1.83941900
H	-4.25959200	-1.05893000	-0.08025800
H	-5.75529600	-1.53780600	-0.90725600
H	-4.70792000	-4.78339800	0.60704700
H	-6.04872600	-3.63502200	0.40966200
H	-4.64085700	-3.18963800	1.38256400
H	-5.92699000	-3.76255900	-2.05308700
H	-4.62607900	-4.95799900	-1.95647500
H	-4.41727800	-3.48269100	-2.92923700

H	-1. 05990400	2. 14345400	1. 47062800
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TS5'''RS

C	0. 09396900	-0. 96779600	-1. 71572800
C	-1. 26487400	-0. 81307800	-1. 50380200
H	0. 68740300	-1. 24047000	-0. 84946500
C	0. 69124700	-1. 22726600	-3. 02622400
C	1. 89994200	-1. 93654600	-3. 09387200
C	0. 07038700	-0. 82605700	-4. 21987700
C	2. 44997700	-2. 27300200	-4. 32734100
H	2. 39897500	-2. 24040900	-2. 17729300
C	0. 62367600	-1. 15982400	-5. 44803300
H	-0. 83938700	-0. 23408400	-4. 17874900
C	1. 81311100	-1. 89036700	-5. 50477400
H	3. 37967500	-2. 83089800	-4. 36322300
H	0. 13497000	-0. 84525100	-6. 36509900
H	2. 24415800	-2. 15037300	-6. 46660100
C	-1. 70804700	-0. 72940500	-0. 16214400
O	-1. 03069400	-0. 60025400	0. 85679900
H	-1. 98791900	-0. 76512900	-2. 31139000
C	1. 51315800	1. 01716100	0. 35467100
C	0. 98107700	1. 99353000	1. 35714100
C	0. 45857200	1. 55441100	2. 57796500
C	1. 07898800	3. 36693200	1. 11291400
C	0. 04843300	2. 47576700	3. 53804300
H	0. 38030200	0. 48570700	2. 74945500
C	0. 70098300	4. 28878000	2. 08790400
H	1. 48585200	3. 70668600	0. 16444300
C	0. 18105400	3. 84481800	3. 30281800
H	-0. 36324900	2. 12509900	4. 47954000
H	0. 81290800	5. 35289400	1. 89902800
H	-0. 12091100	4. 56080400	4. 06160200
N	2. 24332000	0. 08739900	0. 88125300
N	2. 71669800	-0. 87256800	-0. 01607000
S	3. 80994800	-1. 92155400	0. 65745400
O	4. 31338700	-2. 68159000	-0. 48576600
O	3. 20001900	-2. 63584700	1. 77262600
C	5. 11199600	-0. 89887900	1. 30947100
C	5. 51046900	0. 22259800	0. 58274700
C	6. 55853500	0. 99232500	1. 06651000
C	7. 21064000	0. 65960400	2. 25989200
C	6. 78486100	-0. 46615400	2. 96646100
C	5. 73201600	-1. 24971800	2. 50077500
H	4. 99471800	0. 50269600	-0. 33341100

H	6.87392800	1.87293000	0.51360500
H	7.27901100	-0.73086200	3.89685500
H	5.38512400	-2.11567400	3.05454600
C	8.33411600	1.52114200	2.77461200
H	7.95536700	2.49273600	3.10680200
H	8.84041100	1.04993400	3.61955500
H	9.07417600	1.70854000	1.99177300
C	1.16448500	1.23563100	-1.04061400
H	0.28458700	1.84287400	-1.22210100
C	2.10958500	1.20169100	-2.09618600
O	3.26401300	0.73011500	-2.06841600
O	1.62931100	1.73219000	-3.25051200
C	2.48843500	1.61450800	-4.38533900
C	1.76542500	2.24414700	-5.55636600
H	2.70516700	0.55649000	-4.56486700
H	3.43822900	2.11817600	-4.17819000
H	2.37768000	2.17436800	-6.45909600
H	0.81846400	1.72908200	-5.73704300
H	1.55476900	3.29829300	-5.35908300
C	-2.82936300	-4.56073000	1.86023500
C	-2.25210500	-3.83158000	0.81625900
C	-0.88241500	-3.59490700	0.77325600
C	-0.08993300	-4.05824400	1.82092000
C	-0.66778200	-4.77111800	2.87288300
C	-2.03654100	-5.03906000	2.89588900
C	-4.31292300	-4.72963000	1.64796800
C	-4.44942800	-4.44618100	0.13650400
C	-3.31189700	-3.44292600	-0.18636800
H	-0.43303400	-3.06125100	-0.05696000
H	0.97632000	-3.85140900	1.81576900
H	-0.03886700	-5.13034300	3.68114800
H	-2.47416800	-5.61400400	3.70645400
H	-4.87260300	-4.00344100	2.24994400
H	-4.22331100	-5.36109100	-0.41527100
H	-4.68422500	-5.72340400	1.90702200
H	-2.98696600	-3.47683400	-1.22855200
N	-3.86294800	-2.07577900	0.04308800
O	-5.71813100	-4.03686000	-0.32928100
C	-3.20841100	-0.90174700	0.03812600
C	-5.18796200	-1.78683200	0.23585500
N	-4.13002100	0.03056700	0.25365800
N	-5.37531300	-0.50433500	0.37000700
C	-6.22180800	-2.86954800	0.27638600
H	-6.53590400	-3.04371200	1.31304500

H	-7.09600800	-2.55548000	-0.29584400
C	-3.92544300	1.44845700	0.31746800
C	-2.80339000	1.94298300	0.97348600
C	-4.84672200	2.28952900	-0.28997700
C	-2.59203800	3.31276100	0.97489000
C	-4.62092800	3.66283000	-0.25601200
C	-3.48648200	4.19972400	0.36148800
H	-1.70371700	3.68314100	1.47532500
H	-5.34481800	4.31315900	-0.73298100
H	-5.71939000	1.87498100	-0.78251500
H	-2.10441700	1.27994900	1.47151100
C	-3.17470100	5.69650300	0.37743500
C	-1.88448100	5.93426500	-0.42674200
C	-2.95852800	6.16164600	1.82779600
C	-4.30248700	6.52810700	-0.23960200
H	-2.01143800	5.62273200	-1.46803500
H	-1.04561500	5.37234000	-0.00435200
H	-1.62556600	6.99826900	-0.41331900
H	-3.84999800	5.97552200	2.43467600
H	-2.74880200	7.23595600	1.84431200
H	-2.11258000	5.64790600	2.29462500
H	-4.04275300	7.58930100	-0.18733300
H	-5.24654500	6.38621300	0.29646400
H	-4.46020700	6.27734600	-1.29333000
H	3.08696400	-0.46968200	-0.90841900

TS5SR

C	5.85228900	-0.93736000	0.87160900
C	4.59638300	-1.48372400	1.12238100
C	4.43932300	-2.63726700	1.88386700
C	5.58243900	-3.25583500	2.38397300
C	6.84760500	-2.72007400	2.12987500
C	6.99200000	-1.55601500	1.37831400
C	5.74372300	0.32964500	0.06082600
C	4.27289800	0.38521300	-0.41633600
C	3.50892700	-0.65243500	0.48542500
H	3.44410900	-3.02324900	2.08571400
H	5.49153800	-4.15903900	2.97852700
H	7.72858800	-3.21529300	2.52582100
H	7.97746100	-1.14060800	1.18903600
H	6.41523400	0.35495700	-0.80300200
H	3.82912400	1.37287400	-0.27972300
H	5.97615600	1.20471000	0.67662900
H	2.88085000	-0.13069500	1.21110000

N	2.61478600	-1.46833400	-0.33761300
O	4.16086200	0.14049100	-1.81297900
C	1.38468900	-1.93706000	-0.08953000
C	2.93108100	-1.82113800	-1.61713800
N	1.02336300	-2.57753500	-1.20319800
N	1.97450100	-2.50724100	-2.17171900
C	4.17181600	-1.22378500	-2.19138600
H	5.06962100	-1.74039400	-1.82470500
H	4.14114500	-1.27137600	-3.27921000
C	-0.27902600	-3.11491900	-1.47062000
C	-1.07680100	-2.45891200	-2.39643100
C	-0.75973300	-4.16512900	-0.69947300
C	-2.40717400	-2.84966000	-2.52275900
C	-2.08742400	-4.53987400	-0.84661900
C	-2.94250500	-3.87756000	-1.73963600
H	-3.03117700	-2.30932200	-3.22416200
H	-2.46917700	-5.35078600	-0.23445400
H	-0.11217800	-4.65581200	0.02020700
H	-0.67315900	-1.62403800	-2.96049700
C	-4.41627400	-4.28372300	-1.80579700
C	-4.51893400	-5.75580200	-2.23884500
C	-5.20421100	-3.42613600	-2.80045900
C	-5.04624300	-4.11086800	-0.41224900
H	-4.00609100	-6.41980600	-1.53699500
H	-4.07755500	-5.90195500	-3.22938300
H	-5.56983900	-6.05983500	-2.28178600
H	-6.10617200	-4.38325300	-0.44793600
H	-4.96579800	-3.07297600	-0.07343400
H	-4.56201300	-4.74847200	0.33280400
C	-1.45936300	-0.79160700	2.08644100
C	-0.71467700	-1.33518500	1.05736100
H	-1.06038800	-0.86150500	3.09704000
C	-2.91223800	-0.58115900	1.95462000
C	-3.72582600	-0.67781800	3.08966700
C	-3.50217100	-0.29114600	0.71497300
C	-5.10332100	-0.50342200	2.99170300
H	-3.26998800	-0.89345600	4.05266000
C	-4.87632200	-0.10121400	0.62458600
H	-2.88083300	-0.17529300	-0.17034200
C	-5.68141300	-0.21232300	1.75859200
H	-5.72303800	-0.58829600	3.87885300
H	-5.32033900	0.14372000	-0.33517600
H	-6.75371700	-0.06405400	1.68087500
C	0.63805800	-1.71420700	1.21307300

O	1. 31184200	-1. 83258900	2. 24591300
H	-6. 24906800	-3. 74954100	-2. 80914700
H	-4. 81501600	-3. 52620600	-3. 81846600
H	-5. 18300700	-2. 36763000	-2. 52188200
H	-1. 13125800	-1. 34938100	0. 05991700
C	-1. 59436300	2. 21262600	1. 06791600
C	-2. 67831900	3. 19804900	1. 37763600
C	-2. 73535200	4. 40293500	0. 67036300
C	-3. 66137900	2. 92498200	2. 33261200
C	-3. 74930200	5. 32108900	0. 91893600
H	-1. 97079000	4. 60574800	-0. 07293200
C	-4. 68503700	3. 83869600	2. 56934600
H	-3. 64726700	1. 98115800	2. 87074500
C	-4. 72941200	5. 04141600	1. 86927200
H	-3. 77527700	6. 25735100	0. 36989100
H	-5. 45219500	3. 60595600	3. 30165000
H	-5. 52317100	5. 75660000	2. 06114800
N	-1. 38551200	2. 08611700	-0. 20279100
N	-0. 47617800	1. 11577400	-0. 59208100
S	-0. 08350300	1. 15034600	-2. 19689100
O	0. 97791700	0. 14689300	-2. 31211200
O	-1. 30401200	1. 01127400	-2. 97875100
C	0. 62793000	2. 73511700	-2. 54430700
C	2. 01258000	2. 85135900	-2. 60069500
C	2. 56567400	4. 11045200	-2. 81697100
C	1. 75615500	5. 23938000	-2. 96237700
C	0. 36564400	5. 08641400	-2. 90055100
C	-0. 20932400	3. 83960700	-2. 69339600
H	2. 63337300	1. 96478600	-2. 49452900
H	3. 64504300	4. 21759700	-2. 87766000
H	-0. 27239200	5. 95759900	-3. 02233800
H	-1. 28583000	3. 71069400	-2. 65111300
C	2. 35893000	6. 60439400	-3. 16861200
H	1. 83837100	7. 14776700	-3. 96138800
H	3. 41567300	6. 53591200	-3. 43451300
H	2. 27985800	7. 20193000	-2. 25486700
C	-0. 96707100	1. 54152700	2. 20418600
H	-1. 45166000	1. 72351300	3. 15639500
C	0. 42464100	1. 28500400	2. 33155900
O	1. 27176800	1. 21328800	1. 41745500
O	0. 78956000	1. 05486300	3. 61440000
C	2. 16025800	0. 72265600	3. 84415000
C	2. 36021700	0. 67649300	5. 34428400
H	2. 36893000	-0. 24829800	3. 38309500

H	2.79925600	1.47828200	3.37425400
H	3.39640100	0.41754500	5.57492500
H	1.70749300	-0.07653300	5.79169300
H	2.13368100	1.64537400	5.79555500
H	0.36203800	1.01205500	0.02158600

TS5'SR

C	-1.76883900	5.50499800	0.79472100
C	-0.90096700	4.50687800	1.22199500
C	-0.11981200	4.65207800	2.36134400
C	-0.20111500	5.85517100	3.06793500
C	-1.05765200	6.86834600	2.62957200
C	-1.85148400	6.69440300	1.49751700
C	-2.53314900	5.05546000	-0.43736300
C	-1.82773000	3.75726900	-0.90281500
C	-0.96463300	3.29666700	0.32342500
H	0.51742200	3.83890800	2.69951800
H	0.39704600	6.00520000	3.96089400
H	-1.11884500	7.80042300	3.18202900
H	-2.52254800	7.48286500	1.16968600
H	-2.54248900	5.79243800	-1.24659200
H	-2.54078400	2.97250300	-1.15619700
H	-3.57516300	4.83654600	-0.18032600
H	-1.41368200	2.43953800	0.82326700
N	0.37977800	2.90401700	-0.12104700
O	-1.07670700	3.95664200	-2.09656300
C	1.21673300	1.94787800	0.31073900
C	1.00546400	3.57400900	-1.13775400
N	2.32189700	2.10387400	-0.42862400
N	2.19839200	3.09911900	-1.35287000
C	0.18531300	4.56872000	-1.90031000
H	0.11069400	5.50957200	-1.35312000
H	0.63526300	4.74942200	-2.87677200
C	3.53752600	1.35390100	-0.33548900
C	4.02381100	0.72617500	-1.48505300
C	4.16590500	1.20921200	0.88914000
C	5.15352200	-0.07740500	-1.38092900
C	5.29512100	0.41070300	0.97095000
C	5.79967300	-0.26054800	-0.15622900
H	5.51056300	-0.56863100	-2.27299600
H	5.78064300	0.29313000	1.93857200
H	3.77171800	1.71279200	1.77529900
H	3.49212600	0.85453100	-2.42038700
C	7.03372500	-1.16138400	0.00589900

C	8.23231100	-0.30044200	0.45238600
C	7.39507800	-1.87210200	-1.31414900
C	6.73204100	-2.24125100	1.07885400
H	8.03598900	0.20973800	1.41199600
H	8.46684000	0.46720200	-0.30402100
H	9.11728900	-0.93334500	0.58374600
H	7.59090400	-2.91778700	1.16724400
H	5.84650500	-2.84061300	0.80955400
H	6.55601000	-1.78884700	2.06729500
C	0.61563400	-1.52656800	1.50175100
C	1.30612200	-0.40582400	1.02237600
H	-0.09841800	-1.32317100	2.29725800
C	1.20135000	-2.89017300	1.50276700
C	0.61704700	-3.87020200	2.32103100
C	2.32717500	-3.23711900	0.74244100
C	1.11490500	-5.15665900	2.35524200
H	-0.23700900	-3.58870300	2.92839400
C	2.82194100	-4.53658000	0.77250400
H	2.81555200	-2.48632200	0.12276200
C	2.22129000	-5.49695600	1.56887100
H	0.65371300	-5.90202800	2.99225900
H	3.68989400	-4.78971200	0.16139400
H	2.61267000	-6.50742100	1.58853200
C	0.81905500	0.88756800	1.31013300
O	0.01896800	1.24128900	2.18984400
H	8.27573700	-2.51146800	-1.15885100
H	7.64848700	-1.15158900	-2.11388700
H	6.58513400	-2.51884700	-1.67416000
H	2.05389200	-0.51483400	0.24013400
C	-1.06889900	-0.67343100	-0.60416600
C	-0.12484900	-0.53483700	-1.77553400
C	-0.15881000	0.62724300	-2.55807400
C	0.82880500	-1.50973500	-2.08360300
C	0.70984500	0.77965400	-3.64243600
H	-0.86882500	1.40991200	-2.33141800
C	1.69729100	-1.35674400	-3.16210500
H	0.92171900	-2.40621500	-1.47929200
C	1.63572300	-0.21204100	-3.95492200
H	0.64851800	1.68886000	-4.23953300
H	2.42230800	-2.13141200	-3.38129100
H	2.29646700	-0.08958800	-4.80166700
N	-1.71302100	0.43110000	-0.37188800
N	-2.57440600	0.49347200	0.73812400
S	-4.18521000	0.59031700	0.28579100

O	-4.92949200	0.59127000	1.53898500
O	-4.32104600	1.68691700	-0.66615100
C	-4.49649700	-0.93014000	-0.56382300
C	-5.05327800	-1.99519300	0.12924800
C	-5.16117600	-3.23617400	-0.49732500
C	-4.70115900	-3.41844900	-1.81080500
C	-4.14883500	-2.31647500	-2.48780800
C	-4.05497600	-1.07382500	-1.87474900
H	-5.39197900	-1.85121800	1.15003400
H	-5.61357700	-4.07325100	0.02859100
H	-3.80096000	-2.45391200	-3.50455300
H	-3.62249900	-0.22405000	-2.40407200
C	-4.74845500	-4.77145000	-2.45869200
H	-5.48460100	-5.41770600	-1.97525600
H	-3.77331000	-5.26560200	-2.39319500
H	-5.00369600	-4.68718400	-3.51785300
C	-1.03202700	-1.92351400	0.10522600
H	-0.64721700	-2.73746300	-0.50135900
C	-1.97823200	-2.47601100	1.06620800
O	-2.51175200	-1.92831800	2.02942900
O	-2.13666000	-3.79743200	0.86553100
C	-2.93046300	-4.49986100	1.82682400
C	-3.09184400	-5.90807700	1.31471000
H	-2.41089100	-4.48051600	2.79689600
H	-3.88637600	-3.98371500	1.95797300
H	-3.68422600	-6.50086400	2.02537500
H	-2.11892200	-6.38878100	1.18369100
H	-3.61273600	-5.90372300	0.34851700
H	-2.46112000	-0.23712300	1.45068200

TS5''SR

C	0.74928200	5.90207300	-1.20154800
C	0.27213300	4.60779900	-1.39101400
C	-0.19245600	4.18441500	-2.63402300
C	-0.18302100	5.09141500	-3.68903300
C	0.28993700	6.39300500	-3.50375700
C	0.76334200	6.80515100	-2.26162500
C	1.22207300	6.11933600	0.21034700
C	0.81550400	4.84323400	0.98403300
C	0.33603900	3.80740600	-0.10691800
H	-0.53112300	3.16346000	-2.77317300
H	-0.53717100	4.78133000	-4.66649400
H	0.29254800	7.08691000	-4.33822000
H	1.13733800	7.81476900	-2.12025300

H	0.77628300	7.00072700	0.68369800
H	1.65600700	4.40895300	1.52349900
H	2.30734000	6.25506000	0.24471800
H	1.00982900	2.95170500	-0.16809400
N	-0.99815700	3.26814400	0.23293300
O	-0.14156800	5.11580700	1.99588800
C	-1.58906500	2.09449900	-0.06444800
C	-1.89199100	3.99591600	0.96096700
N	-2.81045900	2.17453000	0.47701200
N	-3.00875800	3.34876800	1.13450800
C	-1.44982800	5.31137600	1.50758200
H	-1.48891600	6.08526900	0.72725000
H	-2.08910400	5.60732400	2.33912500
C	-3.86403500	1.20172700	0.44660800
C	-4.28756500	0.64377700	1.64230400
C	-4.40404300	0.80929600	-0.77275300
C	-5.26067300	-0.35161200	1.61194400
C	-5.36021000	-0.19526700	-0.78212100
C	-5.80376900	-0.80086200	0.40435300
H	-5.58087000	-0.78550800	2.55128300
H	-5.76024500	-0.51887700	-1.73756100
H	-4.05600300	1.26118200	-1.69583200
H	-3.85088700	0.97281700	2.57976300
C	-6.82373600	-1.93892200	0.33342800
C	-8.05756000	-1.48541200	-0.46511500
C	-7.28712800	-2.38529000	1.72370600
C	-6.16220400	-3.13785600	-0.36919600
H	-7.80707200	-1.22149100	-1.49587900
H	-8.52766100	-0.61679200	0.00560100
H	-8.79191800	-2.29595900	-0.50049000
H	-6.87950600	-3.95938600	-0.46490500
H	-5.30530400	-3.49477300	0.21241900
H	-5.80944200	-2.87562700	-1.37198000
C	-0.62458600	-1.39520200	-1.17041300
C	-1.40020400	-0.35059000	-0.71157000
H	0.34127300	-1.13452500	-1.60212500
C	-1.09744700	-2.75350300	-1.44096300
C	-0.21104400	-3.65627900	-2.04753300
C	-2.40805500	-3.16883400	-1.16475200
C	-0.62396900	-4.94397900	-2.36703500
H	0.80748400	-3.33601000	-2.25426200
C	-2.81622100	-4.45826700	-1.48140200
H	-3.11761600	-2.47706500	-0.71649900
C	-1.92578500	-5.35064300	-2.07952700

H	0.07277200	-5.63197700	-2.83508100
H	-3.83433900	-4.77085400	-1.26808000
H	-2.24887200	-6.35731400	-2.32594500
C	-0.88695200	0.97165000	-0.81954100
O	0.10723200	1.33797200	-1.44887600
H	-8.03033400	-3.18053100	1.61871700
H	-7.75194200	-1.56239000	2.27609900
H	-6.45943200	-2.78292200	2.31879400
H	-2.33498400	-0.53489500	-0.20286700
C	1.45853500	-0.88347600	0.87482600
C	1.20784700	0.28932000	1.77452000
C	2.27344400	1.12694200	2.13286800
C	-0.06821500	0.59922900	2.26261200
C	2.06969400	2.22729400	2.95731300
H	3.26342500	0.88485600	1.76119000
C	-0.27683700	1.72052300	3.06525300
H	-0.91690700	-0.02783300	2.00741100
C	0.79088000	2.53758400	3.42234800
H	2.91514500	2.84681800	3.24343700
H	-1.27894400	1.95205100	3.41914200
H	0.62954200	3.40723800	4.05036000
N	2.45097800	-0.70201100	0.05985100
N	2.64074300	-1.69469300	-0.89228900
S	4.03586900	-1.47274900	-1.77139800
O	4.16091900	-2.68977500	-2.56709600
O	3.99022400	-0.16748400	-2.41151300
C	5.36349600	-1.43870900	-0.58810500
C	6.00146000	-2.62587300	-0.24986200
C	7.00628000	-2.59922900	0.71250500
C	7.36872300	-1.40596900	1.34082100
C	6.70803100	-0.22593500	0.97946000
C	5.70521600	-0.23219600	0.01880600
H	5.71692000	-3.54898300	-0.74408400
H	7.51883000	-3.51931800	0.97807500
H	6.99019700	0.70894700	1.45657700
H	5.19322500	0.67775200	-0.27592000
C	8.43955600	-1.38170400	2.40012600
H	9.01419100	-2.31006100	2.40506000
H	7.99670500	-1.25536600	3.39318400
H	9.13108500	-0.54987600	2.24168100
C	0.55211200	-2.00500800	0.96601200
H	-0.35335600	-1.86039700	1.53775200
C	0.88235900	-3.37692400	0.80455900
O	1.93933600	-3.88418300	0.39063900

O	-0.15436800	-4.18564600	1.15182700
C	0.09016300	-5.58733500	1.04543500
C	-1.16593100	-6.29514300	1.50616000
H	0.33435600	-5.83479700	0.00806600
H	0.95552000	-5.85411700	1.66118200
H	-1.03541300	-7.37794200	1.43420000
H	-2.01361300	-6.00255600	0.88190800
H	-1.39363200	-6.04085300	2.54445600
H	2.55460600	-2.67858100	-0.53546200

TS5'''SR

C	-5.82583600	-1.15849000	-0.89394400
C	-4.53952900	-1.60683900	-1.18233400
C	-4.31733200	-2.72569000	-1.97909600
C	-5.42315000	-3.40817200	-2.48008800
C	-6.71787900	-2.96877300	-2.19067100
C	-6.92895800	-1.84043000	-1.40107700
C	-5.79468600	0.08348900	-0.03946400
C	-4.32134800	0.23580100	0.40568500
C	-3.50179000	-0.72227800	-0.53363500
H	-3.30251700	-3.04031600	-2.20417200
H	-5.27942200	-4.28628300	-3.10125100
H	-7.56937600	-3.51303700	-2.58675900
H	-7.93704400	-1.50243000	-1.18043700
H	-6.44508300	0.02294600	0.83859500
H	-3.95444000	1.25620300	0.28253500
H	-6.10912300	0.95992000	-0.61487400
H	-2.91560100	-0.14284700	-1.24723500
N	-2.54807100	-1.50421300	0.25716700
O	-4.15207800	-0.03339800	1.79202100
C	-1.30421700	-1.91745600	-0.02433000
C	-2.84063700	-1.93035100	1.51969500
N	-0.90892100	-2.59499000	1.05550200
N	-1.85471000	-2.60862500	2.03137300
C	-4.09707000	-1.40755200	2.13328400
H	-4.97772800	-1.95347800	1.76944100
H	-4.04474900	-1.48468100	3.21847900
C	0.39340900	-3.14752700	1.28479100
C	1.17808200	-2.58896100	2.28286900
C	0.87379400	-4.14346700	0.44350200
C	2.49198600	-3.02994100	2.42149300
C	2.18662000	-4.56464000	0.59904600
C	3.02592800	-4.00832000	1.57605400
H	3.10492200	-2.57574500	3.19058700

H	2.56571500	-5.33466300	-0.06521800
H	0.23524500	-4.56374000	-0.32686900
H	0.77180700	-1.80087500	2.90919300
C	4.48021400	-4.47491200	1.66968000
C	4.51059300	-5.98060700	1.98154700
C	5.25337600	-3.73415200	2.76514600
C	5.17655800	-4.21400400	0.32247800
H	4.00439700	-6.56352300	1.20685200
H	4.02298900	-6.18803800	2.93898900
H	5.54710000	-6.32771700	2.04107500
H	6.22373100	-4.52816300	0.37875700
H	5.14737300	-3.14950300	0.06892800
H	4.70276800	-4.76936500	-0.49182800
C	1.46156600	-0.56830800	-2.17729600
C	0.77586300	-1.22238500	-1.16873900
H	1.00743300	-0.55397700	-3.16681200
C	2.91868700	-0.35250600	-2.12295600
C	3.64613200	-0.29199800	-3.31782500
C	3.59752400	-0.21033100	-0.90411000
C	5.02518900	-0.10188000	-3.29930700
H	3.12293300	-0.39619900	-4.26476500
C	4.97307500	-0.00744100	-0.88939900
H	3.04198500	-0.22461000	0.03019700
C	5.69141000	0.04391300	-2.08445600
H	5.57764600	-0.06363700	-4.23270200
H	5.48610500	0.11660000	0.05906300
H	6.76494000	0.20141000	-2.06744300
C	-0.57960500	-1.59639400	-1.31742600
O	-1.27025700	-1.63389600	-2.34601800
H	6.28409600	-4.09911400	2.78908400
H	4.81595200	-3.90281400	3.75414000
H	5.28355300	-2.65616700	2.57712700
H	1.22957700	-1.32166700	-0.19224100
C	1.59282700	2.27987200	-0.83582200
C	2.65481700	3.30812600	-1.08234900
C	2.72514300	4.43643600	-0.25871100
C	3.60339100	3.14896300	-2.09651000
C	3.72010900	5.38971900	-0.44824600
H	1.98512200	4.55720900	0.52622700
C	4.60795100	4.09694300	-2.27619000
H	3.57876000	2.26542300	-2.72788100
C	4.66711300	5.22204500	-1.45733200
H	3.75530000	6.26630200	0.19109100
H	5.34866700	3.95101300	-3.05638100

H	5.44545200	5.96411600	-1.60389700
N	1.43214000	2.02877900	0.42392300
N	0.54805900	1.01717000	0.77415900
S	0.06538000	1.07822500	2.36115600
O	-0.94824900	0.02581100	2.45366000
O	1.24882100	1.02077100	3.20927300
C	-0.73379300	2.63722400	2.61267300
C	-2.12138100	2.70118200	2.53038900
C	-2.73809900	3.94271200	2.65535800
C	-1.98788200	5.10637200	2.84697700
C	-0.59341400	5.00569900	2.92896200
C	0.04333300	3.77678800	2.81302400
H	-2.69847200	1.78983300	2.39206800
H	-3.82124400	4.00871200	2.60614500
H	-0.00252200	5.90278000	3.09166100
H	1.12248300	3.69082600	2.88588900
C	-2.65892000	6.45069800	2.94766100
H	-2.19471600	7.06493900	3.72299300
H	-3.72156900	6.34720400	3.17542200
H	-2.56959000	6.99372200	2.00138900
C	0.93342000	1.72513900	-2.01700300
H	1.37877600	2.02736600	-2.95793400
C	-0.46289500	1.47185300	-2.12010900
O	-1.26622200	1.27038100	-1.18776700
O	-0.87649300	1.40688600	-3.40694500
C	-2.24850100	1.07054700	-3.63271000
C	-2.51869800	1.26937700	-5.10906300
H	-2.40646200	0.02917400	-3.33195400
H	-2.88535800	1.71311500	-3.01582700
H	-3.55883100	1.02222400	-5.33372500
H	-1.87273600	0.62293800	-5.70770800
H	-2.33701700	2.30717100	-5.39846900
H	-0.27590800	0.91601500	0.14258200

TS5SS

C	-0.28165300	0.48425000	-2.27169000
C	0.35838400	1.00994400	-1.15096100
H	0.36239800	0.00170800	-3.00108200
C	-1.56217200	0.99093400	-2.78740300
C	-1.87448200	0.77934200	-4.13705500
C	-2.49015000	1.67211700	-1.98328000
C	-3.07308900	1.23353600	-4.67509600
H	-1.16014300	0.25871800	-4.77035500
C	-3.69282800	2.11477600	-2.51903700

H	-2.28722600	1.82835300	-0.92694800
C	-3.98819200	1.89977400	-3.86511400
H	-3.29480500	1.06011000	-5.72330000
H	-4.40946000	2.61542800	-1.87487900
H	-4.93210100	2.24292900	-4.27648400
C	1.60445300	0.44386900	-0.82465000
O	2.17849100	-0.45216800	-1.47703400
H	-0.15742600	1.69580900	-0.49972500
C	-0.40618100	-1.75259000	-0.18823100
C	0.75812000	-2.56106300	0.29901400
C	1.40360000	-2.21959100	1.49553100
C	1.19675000	-3.69184800	-0.39479900
C	2.45116200	-2.99136700	1.98476400
H	1.05474300	-1.34980000	2.04477000
C	2.25070300	-4.46275500	0.08930900
H	0.69156000	-3.99123000	-1.30736300
C	2.88011300	-4.11870900	1.28152300
H	2.94677100	-2.70215800	2.90732800
H	2.56840000	-5.34288800	-0.46099800
H	3.69405100	-4.72670000	1.66591600
N	-0.99470100	-1.09882700	0.76353300
N	-2.02129700	-0.24525800	0.41713800
S	-3.13756900	-0.03918000	1.64703500
O	-2.43201200	0.29860500	2.87781500
O	-4.11374900	0.88785300	1.08226700
C	-3.91348400	-1.61459500	1.89092500
C	-3.51934100	-2.40135600	2.96653600
C	-4.10363900	-3.65322600	3.12973600
C	-5.06216600	-4.12121500	2.22808900
C	-5.42433500	-3.31116300	1.14506300
C	-4.85529500	-2.05781700	0.96475700
H	-2.77441900	-2.02584100	3.65915600
H	-3.80896200	-4.27668400	3.96887100
H	-6.15914900	-3.67240400	0.43130600
H	-5.12493100	-1.43580600	0.11767400
C	-5.71378000	-5.46538800	2.42164900
H	-5.11254400	-6.10807600	3.06800700
H	-5.85749100	-5.97323200	1.46480900
H	-6.69925100	-5.35172400	2.88496500
C	-0.67181800	-1.74033800	-1.62133700
H	0.14931100	-2.14293000	-2.19652600
C	-1.98201700	-1.85251300	-2.19836200
O	-3.05282100	-1.61307500	-1.63297100
O	-2.09220800	-2.19909100	-3.50837100

C	-0.96225000	-2.59741200	-4.27535700
C	-1.45637200	-2.84935200	-5.68463500
H	-0.19838000	-1.80976600	-4.27103000
H	-0.51622800	-3.50247000	-3.84404400
H	-2.21891200	-3.63101100	-5.68512200
H	-0.62942200	-3.16154600	-6.32654300
H	-1.89851200	-1.93813200	-6.09556100
C	6.65962500	-0.33299600	-0.29664500
C	5.34483700	-0.09131500	-0.68847900
C	5.06140500	0.65341800	-1.83202100
C	6.12256500	1.16823200	-2.57035500
C	7.44266500	0.93453100	-2.17717800
C	7.71917000	0.17823100	-1.04238200
C	6.72920500	-1.18428400	0.94165600
C	5.25904500	-1.41184100	1.36713100
C	4.35728000	-0.72920300	0.26619300
H	4.03424300	0.80465200	-2.14563300
H	5.92180600	1.74943200	-3.46441700
H	8.25909500	1.34200900	-2.76496400
H	8.74549400	-0.01071800	-0.74148700
H	7.29255100	-0.71025400	1.75286700
H	5.01460300	-2.47279200	1.38355700
H	7.21953000	-2.14109700	0.74008600
H	3.69688900	-1.44907900	-0.21706000
N	3.47500800	0.29552700	0.87454800
O	5.00012400	-0.97321700	2.69030500
C	2.32749600	0.86144200	0.43453000
C	3.80106200	0.91743100	2.04457300
N	2.03106700	1.79413400	1.34722600
N	2.93292400	1.83361100	2.36210600
C	4.98260300	0.43209300	2.81359200
H	5.90660600	0.88945300	2.43272500
H	4.86967600	0.68536500	3.86772000
C	0.90203600	2.68437800	1.35223600
C	1.01334100	3.91759600	0.72019100
C	-0.28870000	2.24894900	1.90728600
C	-0.11926300	4.71195400	0.61691100
C	-1.41516600	3.05967500	1.78618200
C	-1.35873600	4.28908700	1.12241900
H	-0.03891300	5.66963300	0.11190000
H	-2.34708800	2.68934800	2.19533500
H	-0.37020500	1.26908300	2.36800000
H	1.96175800	4.23013700	0.29557400
C	-2.59594500	5.16557800	0.92248200

C	-2.76970600	5.45885000	-0.57757500
C	-2.40560200	6.48833400	1.68322300
C	-3.86739700	4.47880100	1.43181900
H	-2.86545900	4.52975400	-1.14799400
H	-1.92349700	6.01947300	-0.98493100
H	-3.67295800	6.05691700	-0.73600700
H	-2.28282600	6.30558900	2.75504300
H	-3.28163400	7.12987000	1.54180000
H	-1.52637900	7.03452500	1.32782600
H	-4.73063100	5.11789500	1.22341600
H	-3.83007000	4.31353200	2.51322800
H	-4.03106000	3.50972600	0.94826400
H	-2.54307200	-0.53292100	-0.44224000

TS5'SS

C	1.44217100	-0.53015900	-2.07606500
C	0.76059200	-1.25510800	-1.10440600
H	0.82029700	-0.07340300	-2.84457100
C	2.82830200	-0.83092600	-2.48441000
C	3.28462400	-0.38381700	-3.73212700
C	3.70020300	-1.57268700	-1.67624900
C	4.58448000	-0.64174600	-4.15288500
H	2.60413300	0.16608500	-4.37792500
C	5.00199100	-1.82580100	-2.09491600
H	3.36367500	-1.93963000	-0.71000100
C	5.45184700	-1.35644400	-3.32860100
H	4.92032600	-0.28774100	-5.12222300
H	5.67132800	-2.39383800	-1.45534300
H	6.46898900	-1.55703900	-3.64956500
C	-0.65339200	-1.25055300	-1.13443500
O	-1.37367500	-0.85035000	-2.05674800
H	1.29675400	-1.71386300	-0.28963200
C	0.60344900	2.25015800	-1.27652200
C	0.52966300	3.30160800	-2.34554400
C	-0.21454900	4.46486300	-2.12067800
C	1.17341000	3.14831600	-3.57708800
C	-0.30794700	5.44875600	-3.09758200
H	-0.70843200	4.58512300	-1.16233100
C	1.07054600	4.12840400	-4.56117800
H	1.74644900	2.24863000	-3.78170100
C	0.33320000	5.28422700	-4.32417600
H	-0.88064000	6.34968600	-2.90009000
H	1.56599900	3.98453100	-5.51626300
H	0.25745300	6.05122600	-5.08835300

N	-0.49909100	2.14634600	-0.61289200
N	-0.60436900	1.17984900	0.37195200
S	-1.84973600	1.42562400	1.42170400
O	-3.08076900	1.57106700	0.65438200
O	-1.71135200	0.33586300	2.39092500
C	-1.56078700	2.96588300	2.25067100
C	-1.93854400	4.14965800	1.61968500
C	-1.63706100	5.35911900	2.23196200
C	-0.97043200	5.39879800	3.46213200
C	-0.60620400	4.19478100	4.06981000
C	-0.89181200	2.97300100	3.46909600
H	-2.46586600	4.10776200	0.67227200
H	-1.92521600	6.29016200	1.75147900
H	-0.08951100	4.21414000	5.02501800
H	-0.61028300	2.03483600	3.93573700
C	-0.67637000	6.71972200	4.12353100
H	-0.32098300	7.45251900	3.39472500
H	0.08067600	6.61319200	4.90296900
H	-1.58036200	7.12846200	4.58627900
C	1.88652600	1.53339500	-1.18700700
H	2.60060300	1.88928600	-1.91562900
C	2.47270800	1.04439800	0.02477500
O	1.86733900	0.68143400	1.04379300
O	3.81575600	0.84572400	0.07964300
C	4.70507400	1.45837200	-0.85461200
C	6.11091600	1.18210100	-0.36537500
H	4.56083800	1.03533500	-1.85414500
H	4.50218500	2.53516700	-0.89709800
H	6.83882400	1.63637700	-1.04210800
H	6.29020200	0.10422700	-0.33669900
H	6.25705700	1.59009700	0.63736900
C	-5.73854200	-2.27686100	-1.43355400
C	-4.35763400	-2.16405900	-1.57452600
C	-3.65404100	-2.97827600	-2.45854500
C	-4.35930100	-3.92497200	-3.19564800
C	-5.74382600	-4.04743400	-3.05355500
C	-6.44198900	-3.22215300	-2.17684500
C	-6.27930800	-1.27608000	-0.44764300
C	-5.03805000	-0.58338400	0.16743200
C	-3.79950600	-1.08764300	-0.66992100
H	-2.58256500	-2.85644300	-2.57831800
H	-3.83042600	-4.56881600	-3.89090400
H	-6.27992200	-4.79127800	-3.63451300
H	-7.51902300	-3.31524300	-2.07121100

H	-6.88283300	-1.73689700	0.34200800
H	-5.08197700	0.49990400	0.08143600
H	-6.91879400	-0.54016000	-0.94472300
H	-3.33222300	-0.26778400	-1.21138100
N	-2.75811400	-1.64639400	0.21886600
O	-4.93529000	-0.81472400	1.56201600
C	-1.42350500	-1.77608300	0.07122800
C	-3.08462600	-2.21248400	1.41507100
N	-1.01597600	-2.41690100	1.17265300
N	-2.03769100	-2.68881900	2.02259500
C	-4.49480200	-2.11179800	1.88783500
H	-5.11795000	-2.88929900	1.42118600
H	-4.52998900	-2.22674200	2.97106300
C	0.33023200	-2.67946900	1.60270100
C	1.02455900	-3.78173600	1.11749400
C	0.91737400	-1.75994200	2.45300200
C	2.35800900	-3.92786100	1.47309800
C	2.25412400	-1.92916500	2.80187100
C	3.00255600	-2.99827700	2.30822000
H	2.91125300	-4.77355400	1.07614400
H	2.71327200	-1.18083700	3.43503800
H	0.34092900	-0.90397900	2.78959400
H	0.53867800	-4.48356000	0.44773300
C	4.49647000	-3.15268600	2.60183000
C	5.26715100	-2.95146100	1.28561900
C	4.78153600	-4.55388700	3.16511200
C	4.99615000	-2.11183400	3.60886600
H	5.08504900	-1.94468800	0.89267000
H	4.95922600	-3.67886300	0.52620700
H	6.34310300	-3.07013100	1.45400300
H	4.23020000	-4.71817800	4.09590700
H	5.85050000	-4.65858700	3.37642800
H	4.50380400	-5.34359400	2.46175900
H	6.06092300	-2.27564900	3.79880700
H	4.46786100	-2.18975700	4.56436500
H	4.87774700	-1.09438700	3.22407500
H	0.30124600	0.87188100	0.81718700

TS5''SS

C	-0.78483300	1.59149800	1.12536300
C	-1.62723600	0.53279600	0.75290100
H	0.05954300	1.28886900	1.74424700
C	-1.26028900	2.97263800	1.37016200
C	-0.42246700	3.86404100	2.05111900

C	-2.53782400	3.40720400	0.99278500
C	-0.83569300	5.16369500	2.32348500
H	0.56671200	3.53020600	2.35541300
C	-2.94894300	4.70914300	1.25803800
H	-3.22397800	2.71507500	0.51109100
C	-2.09827900	5.59303500	1.92051000
H	-0.16852700	5.84142600	2.84641600
H	-3.94169700	5.03109000	0.95921200
H	-2.42314800	6.60682700	2.13147500
C	-1.16820400	-0.77339700	1.01256100
O	-0.31999900	-1.14033300	1.83917700
H	-2.47220000	0.68001000	0.08834100
C	1.86650600	2.33507900	0.00398400
C	2.36925300	3.74111100	-0.15687800
C	3.75168700	3.97178300	-0.13686600
C	1.51851600	4.83739400	-0.33931500
C	4.26408500	5.25441200	-0.28675800
H	4.41735600	3.12423900	-0.01401200
C	2.03275600	6.12416100	-0.48023400
H	0.44133700	4.70846300	-0.34204300
C	3.40672700	6.33961900	-0.45723500
H	5.33903200	5.40657300	-0.27661900
H	1.35014000	6.95884300	-0.60598900
H	3.80695600	7.34158900	-0.57505700
N	2.66446200	1.57604700	0.68015200
N	2.32259900	0.25648600	0.85325300
S	3.61856100	-0.68943500	1.31830200
O	3.99687400	-0.34746000	2.67819100
O	3.21174800	-2.05252200	0.97307000
C	4.97283100	-0.23146000	0.26208200
C	5.80521500	0.81364500	0.65034800
C	6.84005000	1.19769400	-0.19431100
C	7.05094900	0.54991500	-1.41566300
C	6.20378100	-0.50316400	-1.77421000
C	5.15977100	-0.89710000	-0.94471700
H	5.63808700	1.30533800	1.60264100
H	7.49799000	2.01047000	0.10038900
H	6.36646700	-1.02157300	-2.71487400
H	4.50401700	-1.71810200	-1.21653600
C	8.15496000	0.99131200	-2.34020100
H	8.95469100	1.49290000	-1.79130800
H	7.77104400	1.69469400	-3.08622000
H	8.58387100	0.14232100	-2.87760300
C	0.55308500	2.01694600	-0.57723300

H	0.07358900	2.89827100	-0.97406300
C	0.23620700	0.82594700	-1.32116300
O	0.78539500	-0.28019600	-1.23732600
O	-0.86471700	0.83259400	-2.10476800
C	-1.60752100	2.02672300	-2.35670700
C	-2.82713800	1.62700300	-3.15925000
H	-1.90407800	2.49311800	-1.41136500
H	-0.98120900	2.73613100	-2.91033900
H	-3.41231800	2.51292500	-3.41655800
H	-3.45714500	0.94925100	-2.57669500
H	-2.52989600	1.12183000	-4.08089400
C	1.74313500	-5.10628500	0.45226100
C	0.76301000	-4.23232000	0.91419700
C	0.08690100	-4.45376100	2.10697700
C	0.39563500	-5.60122200	2.83468900
C	1.36813100	-6.49127200	2.37344800
C	2.05331300	-6.24799400	1.18417200
C	2.35646500	-4.59426600	-0.82746600
C	1.38898300	-3.49600300	-1.31656600
C	0.60922700	-3.06785600	-0.03390100
H	-0.64418200	-3.73327400	2.46233800
H	-0.11605200	-5.80116600	3.77043500
H	1.59818800	-7.38020100	2.95228600
H	2.81553700	-6.93870100	0.83581500
H	2.48745600	-5.35886700	-1.59843100
H	1.90390600	-2.63030600	-1.73491000
H	3.33393200	-4.14924300	-0.61227600
H	1.02409600	-2.16105100	0.39583100
N	-0.79560800	-2.81473300	-0.35400600
O	0.54808600	-3.95753100	-2.37565200
C	-1.64177200	-1.86936400	0.07866200
C	-1.46064700	-3.58280300	-1.26044300
N	-2.79424500	-2.12197600	-0.55203000
N	-2.69178400	-3.18439900	-1.40619200
C	-0.64831800	-4.60369800	-1.98935100
H	-0.46204000	-5.47596400	-1.34847000
H	-1.16562200	-4.92335900	-2.89389400
C	-4.04267600	-1.43696500	-0.42725500
C	-4.48129600	-1.00826300	0.82232200
C	-4.80012200	-1.21886900	-1.56840700
C	-5.68001700	-0.31609400	0.90655200
C	-6.00761100	-0.53303600	-1.45810700
C	-6.46636200	-0.05840600	-0.22620800
H	-6.01079900	0.02371600	1.88285600

H	-6.58465400	-0.36477000	-2.35967000
H	-4.44187700	-1.57692000	-2.52730300
H	-3.89163300	-1.20566300	1.71130700
C	-7.77518400	0.71774300	-0.07135500
C	-7.46871600	2.10725800	0.51357600
C	-8.70791700	-0.04658500	0.88346600
C	-8.49650700	0.90314200	-1.40970300
H	-6.80384400	2.66980600	-0.14960800
H	-6.99052700	2.03698900	1.49467100
H	-8.39715300	2.67516700	0.63149400
H	-8.93211900	-1.04308600	0.49121800
H	-9.65037300	0.49790100	0.99961100
H	-8.26368400	-0.16392300	1.87571900
H	-9.42205400	1.46278700	-1.24785800
H	-8.76246700	-0.05751300	-1.86179000
H	-7.88590100	1.46664300	-2.12233100
H	1.77757800	-0.17376200	0.07634900

TS5'''SS

C	0.75437300	-1.52330700	-0.63013800
C	1.50623700	-0.37692300	-0.47066200
H	1.03294200	-2.41001100	-0.06764800
C	-0.17949800	-1.69833000	-1.73258800
C	-0.65564400	-2.98566100	-2.02337600
C	-0.63226700	-0.61065500	-2.50045600
C	-1.58305600	-3.17887300	-3.03871500
H	-0.32253000	-3.82335300	-1.41683200
C	-1.54937300	-0.81009500	-3.51818000
H	-0.31269400	0.40139600	-2.26484700
C	-2.03768700	-2.09192300	-3.77947800
H	-1.97282200	-4.17243800	-3.23199600
H	-1.92241900	0.03639200	-4.08559800
H	-2.79182700	-2.23597300	-4.54557800
C	2.48095000	-0.26500900	0.55006200
O	2.70377600	-1.03346900	1.49216400
H	1.38615900	0.44665000	-1.16056500
C	-1.85544600	-0.51651600	1.13527400
C	-1.63499400	0.60308200	2.11246000
C	-2.69359800	1.47251600	2.41457400
C	-0.40662800	0.81535700	2.74816500
C	-2.52208600	2.53212200	3.29776300
H	-3.65449400	1.29623000	1.94270200
C	-0.23684700	1.87400400	3.63949600
H	0.44300100	0.17283200	2.53217500

C	-1.28847400	2.74280600	3.91352900
H	-3.35794500	3.19023700	3.51560300
H	0.72798400	2.02098600	4.11709600
H	-1.15387300	3.56483000	4.60921400
N	-2.78562600	-0.24247800	0.27350300
N	-3.11404700	-1.17656400	-0.68244600
S	-4.50661400	-0.80513100	-1.48830900
O	-4.34770200	0.49828500	-2.12410000
O	-4.82014900	-1.98549700	-2.28641600
C	-5.77434800	-0.61801300	-0.25446000
C	-5.94626000	0.61721100	0.36513100
C	-6.90322600	0.74133900	1.36529000
C	-7.68890100	-0.35049300	1.75056500
C	-7.49942700	-1.57537800	1.10525900
C	-6.54155800	-1.71978600	0.10665400
H	-5.34373700	1.46251400	0.04686000
H	-7.05050800	1.70230700	1.85109400
H	-8.11136000	-2.42746000	1.38737200
H	-6.39222700	-2.66805500	-0.39905100
C	-8.70488800	-0.20980100	2.85411300
H	-8.23062800	-0.33705300	3.83270300
H	-9.49108200	-0.96274900	2.76581000
H	-9.16997800	0.77894500	2.83935100
C	-1.01538400	-1.68558900	1.30111500
H	-0.21691200	-1.56365800	2.01543800
C	-1.32903900	-3.02421600	0.96338100
O	-2.31810100	-3.45548800	0.35093000
O	-0.40635600	-3.99640400	1.27383100
C	0.57987800	-3.77758300	2.28078000
C	1.28173200	-5.10150700	2.50599700
H	1.29525200	-3.00646600	1.96866300
H	0.09096900	-3.43149900	3.20008100
H	0.56611400	-5.86330500	2.82263700
H	2.04866000	-4.99517300	3.27710600
H	1.75969200	-5.43942300	1.58329100
C	7.47048500	-1.22241700	-0.09477800
C	6.08548900	-1.08831600	-0.12547000
C	5.32449900	-1.60814500	-1.16861900
C	5.98333700	-2.27159000	-2.19963700
C	7.37360800	-2.41130900	-2.17595100
C	8.12573200	-1.89122800	-1.12610800
C	8.05859600	-0.58988000	1.14006300
C	6.88771900	0.16168400	1.81831200
C	5.58433400	-0.33517700	1.08491900

H	4. 24250700	-1. 49781200	-1. 18846200
H	5. 41382000	-2. 68528600	-3. 02495500
H	7. 87263200	-2. 93104000	-2. 98728800
H	9. 20572900	-2. 00198900	-1. 11383900
H	8. 87234000	0. 10937200	0. 92204100
H	6. 81888200	-0. 07334200	2. 88015300
H	8. 46325700	-1. 34927100	1. 81601700
H	4. 95383400	-0. 94433800	1. 73277500
N	4. 76689900	0. 81695800	0. 67006100
O	7. 05339300	1. 57078900	1. 78812200
C	3. 45253500	0. 89855000	0. 40097900
C	5. 33192200	1. 99980100	0. 28670300
N	3. 27327600	2. 12665300	-0. 09455300
N	4. 43620300	2. 82774600	-0. 17135300
C	6. 79530000	2. 16696100	0. 53387200
H	7. 37740300	1. 70145000	-0. 27421400
H	7. 05208200	3. 22410100	0. 59758900
C	2. 01329400	2. 70125100	-0. 46771600
C	1. 78899500	3. 09365700	-1. 78280600
C	1. 00292700	2. 71024300	0. 47734800
C	0. 49670800	3. 44854700	-2. 14664400
C	-0. 28833200	3. 04815100	0. 08857500
C	-0. 57355700	3. 39346500	-1. 23564700
H	0. 31269400	3. 74319000	-3. 17487000
H	-1. 07313500	3. 00516700	0. 83561000
H	1. 20910700	2. 41619200	1. 49997000
H	2. 59884800	3. 08298100	-2. 50476300
C	-1. 99381400	3. 70733300	-1. 70815900
C	-2. 32734500	2. 84576700	-2. 93715300
C	-2. 07166900	5. 19813000	-2. 07701500
C	-3. 03430000	3. 38985100	-0. 62749500
H	-2. 32892500	1. 78614700	-2. 66799400
H	-1. 63036000	3. 01477400	-3. 76384000
H	-3. 33424500	3. 08693100	-3. 29142300
H	-1. 83707700	5. 82760000	-1. 21278800
H	-3. 08212000	5. 44386500	-2. 41870000
H	-1. 37228200	5. 44917900	-2. 88105800
H	-4. 03284900	3. 58928300	-1. 02944200
H	-2. 90131700	4. 00923300	0. 26666400
H	-2. 99298200	2. 33136600	-0. 34170400
H	-2. 97961700	-2. 18893000	-0. 43510300

NTS5

C	4. 84437300	-2. 08590800	0. 66068500
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C	3. 63076000	-1. 43771400	0. 44929500
C	3. 34260600	-0. 81639300	-0. 75951500
C	4. 28095300	-0. 88082100	-1. 78379000
C	5. 49319900	-1. 54799800	-1. 58742500
C	5. 78766400	-2. 14535500	-0. 36323500
C	4. 94124600	-2. 61891900	2. 06718300
C	3. 52016100	-2. 47083400	2. 66200500
C	2. 75539900	-1. 50268900	1. 67846000
H	2. 41089900	-0. 28837000	-0. 90395200
H	4. 05932600	-0. 39918200	-2. 73124400
H	6. 21819700	-1. 59497700	-2. 39451000
H	6. 73745400	-2. 64999700	-0. 21051400
H	5. 26081100	-3. 66430100	2. 12318300
H	3. 54541400	-2. 02930500	3. 65881200
H	5. 65731100	-2. 03310400	2. 65401600
H	2. 61206200	-0. 52024500	2. 12320100
N	1. 41048300	-2. 03546000	1. 36067100
O	2. 88885100	-3. 72656700	2. 85817600
C	0. 22470200	-1. 44407400	1. 08632600
C	1. 21244400	-3. 38436600	1. 29643700
N	-0. 63555200	-2. 45951400	0. 91822300
N	-0. 02577500	-3. 67249100	1. 03529000
C	2. 33688400	-4. 28445400	1. 68317800
H	3. 07796100	-4. 36702700	0. 87577500
H	1. 95353400	-5. 27635300	1. 92224600
C	-2. 02527400	-2. 48441200	0. 54537700
C	-2. 34776300	-3. 03071100	-0. 69442300
C	-3. 01277100	-2. 07981300	1. 42973200
C	-3. 68251700	-3. 14390400	-1. 04964100
C	-4. 34991700	-2. 18133500	1. 04343900
C	-4. 71241200	-2. 71988000	-0. 19447200
H	-3. 92415300	-3. 57452300	-2. 01603900
H	-5. 11020700	-1. 84718700	1. 73965700
H	-2. 74735300	-1. 70071900	2. 41157100
H	-1. 54896500	-3. 33273500	-1. 36317400
C	-6. 16907200	-2. 91119100	-0. 62248400
C	-6. 38945500	-2. 32424900	-2. 02800400
C	-6. 46789700	-4. 42088800	-0. 65612000
C	-7. 14805700	-2. 24459500	0. 34968100
H	-6. 10071000	-1. 27028900	-2. 07330700
H	-5. 81708700	-2. 86096800	-2. 78900000
H	-7. 44713500	-2. 40309700	-2. 29722400
H	-8. 16971300	-2. 38114300	-0. 01523600
H	-7. 09177000	-2. 68909600	1. 34806900

H	-6.96525500	-1.16889400	0.44053500
C	-1.12134100	2.03876600	1.68804400
C	-1.15208900	0.71955400	1.43642500
H	-0.15542100	2.53800200	1.63872800
C	-2.28335900	2.89643900	1.92444600
C	-2.09873900	4.28421700	1.85236400
C	-3.57002300	2.39463400	2.16226800
C	-3.17559200	5.14924300	2.01196400
H	-1.10348500	4.66736000	1.64047500
C	-4.64249900	3.26023000	2.32708800
H	-3.73490600	1.32101600	2.20603400
C	-4.44948200	4.63984300	2.25327500
H	-3.02114500	6.22150600	1.94467500
H	-5.63609500	2.85931000	2.50329100
H	-5.29083700	5.31419900	2.37954900
C	0.09822200	0.07014300	1.01939100
O	1.19821900	0.65707300	1.04580500
H	-7.50123100	-4.58947500	-0.97621800
H	-5.80695500	-4.94160100	-1.35527100
H	-6.33571400	-4.86680600	0.33426600
H	-2.07935100	0.16480600	1.36985200
C	-1.10961200	1.41208600	-1.38167900
C	-2.57440100	1.73488700	-1.28795200
C	-2.98749400	3.07615100	-1.32457500
C	-3.54891500	0.75495000	-1.06852400
C	-4.31960800	3.42210100	-1.15129000
H	-2.23631600	3.84392500	-1.46675500
C	-4.88410600	1.10695400	-0.87172800
H	-3.29469400	-0.30022100	-1.04477500
C	-5.27876800	2.43759600	-0.91633700
H	-4.60727500	4.46877500	-1.17257300
H	-5.61376300	0.32654100	-0.67540900
H	-6.31800800	2.70870400	-0.75716400
N	-0.35160400	2.45629400	-1.46557100
N	1.01748900	2.26745100	-1.38223700
H	1.27769400	1.46118600	-0.80788400
S	1.78012000	3.61990000	-0.71055900
O	1.21571200	3.99939400	0.58660700
O	1.87832600	4.64241200	-1.74233900
C	3.36840400	2.87536300	-0.43442100
C	3.66456300	2.34375200	0.81663600
C	4.89745500	1.72780100	1.00455200
C	5.83061000	1.64906900	-0.03241600
C	5.50482300	2.20120400	-1.27624300

C	4. 27552800	2. 81274300	-1. 48859700
H	2. 92901500	2. 40335300	1. 61109400
H	5. 14235100	1. 30192800	1. 97475300
H	6. 22229800	2. 14026600	-2. 09003800
H	4. 01432200	3. 24091000	-2. 45104900
C	7. 17487500	1. 00780100	0. 19011800
H	7. 12768700	0. 26263700	0. 98843500
H	7. 52661200	0. 51127100	-0. 71745100
H	7. 91880000	1. 76050100	0. 47219900
C	-0. 67885900	0. 02443800	-1. 21125400
C	0. 33042900	-0. 57334900	-2. 05607300
O	1. 03501700	-0. 03790800	-2. 89280900
O	0. 46021800	-1. 92631800	-1. 78327600
C	1. 26322000	-2. 67776200	-2. 69948200
C	1. 87834300	-3. 84626700	-1. 95885600
H	2. 03254600	-2. 02904200	-3. 12067400
H	0. 61994100	-3. 02127300	-3. 51882600
H	2. 42886400	-4. 48199000	-2. 65708500
H	2. 58248800	-3. 47500400	-1. 20706100
H	1. 11247600	-4. 45291200	-1. 46547000
H	-1. 46950300	-0. 67592600	-0. 99452400

M5RR

C	-1. 11653800	2. 13523100	0. 29583300
C	-1. 85061100	0. 87182900	0. 64915200
H	-0. 89471400	2. 05911500	-0. 77670100
C	-1. 92753800	3. 41309400	0. 48189900
C	-1. 30414600	4. 66514300	0. 40498400
C	-3. 31041100	3. 37902700	0. 67215600
C	-2. 03783900	5. 84006000	0. 52646000
H	-0. 23130600	4. 72851900	0. 24086600
C	-4. 04923200	4. 55475200	0. 79622700
H	-3. 81774700	2. 42050000	0. 71706300
C	-3. 41606000	5. 79057400	0. 72678700
H	-1. 52992200	6. 79708500	0. 46190300
H	-5. 12295500	4. 50043300	0. 94710100
H	-3. 98898400	6. 70702000	0. 82396500
C	-1. 69404600	-0. 20469700	-0. 16730700
O	-1. 06356500	-0. 27729900	-1. 27994200
H	-2. 37633300	0. 78844700	1. 59571500
C	1. 44606600	2. 61251800	0. 13010300
C	2. 23787100	3. 83184800	0. 46885400
C	2. 87350400	4. 55436600	-0. 54982100
C	2. 38193100	4. 26797000	1. 79128400

C	3. 62914600	5. 68133800	-0. 25197700
H	2. 76212800	4. 21345600	-1. 57337500
C	3. 14406900	5. 39512500	2. 08794200
H	1. 92271700	3. 71431400	2. 60511100
C	3. 76643100	6. 10842300	1. 06829300
H	4. 10850600	6. 23293500	-1. 05444300
H	3. 25226200	5. 71216400	3. 12025800
H	4. 35378200	6. 99123900	1. 29918500
N	1. 85625100	1. 98669100	-0. 91216700
N	1. 30975900	0. 84218500	-1. 37211800
S	2. 17716800	0. 14471400	-2. 59773100
O	2. 43275800	1. 06252700	-3. 70048000
O	1. 47529200	-1. 10572800	-2. 88022700
C	3. 75572800	-0. 19431200	-1. 84132400
C	4. 83374300	-0. 42328300	-2. 69153000
C	6. 07653200	-0. 72557100	-2. 14422100
C	6. 25922100	-0. 76863700	-0. 75987600
C	5. 16225400	-0. 51078300	0. 06829100
C	3. 90155800	-0. 24652400	-0. 45656100
H	4. 70209100	-0. 34906400	-3. 76612500
H	6. 92001400	-0. 91407900	-2. 80198000
H	5. 29791600	-0. 51917100	1. 14658500
H	3. 04988800	-0. 07037000	0. 19333200
C	7. 59712900	-1. 11292100	-0. 16047000
H	7. 58282400	-2. 13121700	0. 24295000
H	8. 39422900	-1. 05730200	-0. 90443500
H	7. 84493700	-0. 43820800	0. 66300000
C	0. 28425000	2. 24098400	1. 03532200
H	0. 17066200	3. 02257800	1. 78748200
C	0. 56331200	0. 96525500	1. 80934500
O	1. 26753700	0. 04811100	1. 46042600
O	-0. 10543800	0. 96806600	2. 97320300
C	-0. 08845300	-0. 27806400	3. 68481600
C	-0. 94721000	-0. 10488200	4. 91738100
H	0. 94520000	-0. 53677700	3. 93045300
H	-0. 47123200	-1. 05858900	3. 01638200
H	-0. 96689500	-1. 03384400	5. 49176300
H	-0. 55053500	0. 68835500	5. 55466800
H	-1. 97139600	0. 15552700	4. 63981600
C	-5. 79903700	-1. 13288500	-1. 95306700
C	-4. 84593100	-0. 33933400	-1. 30598600
C	-4. 12931200	0. 63219000	-1. 99992900
C	-4. 37383400	0. 78741200	-3. 36268200
C	-5. 31827500	-0. 00764300	-4. 01210500

C	-6.04235400	-0.97056700	-3.31124700
C	-6.45213100	-2.09503900	-0.99447200
C	-6.12963600	-1.45571100	0.37136600
C	-4.79267900	-0.69363600	0.16377400
H	-3.39803700	1.25426700	-1.49596000
H	-3.82181800	1.53517900	-3.92121800
H	-5.49496900	0.12933000	-5.07399400
H	-6.78549500	-1.58015100	-3.81594600
H	-6.00480300	-3.09093000	-1.09371100
H	-6.88762300	-0.70193700	0.59478500
H	-7.52811400	-2.20426300	-1.14542400
H	-4.68914100	0.16161200	0.83257100
N	-3.69127400	-1.63644500	0.48807600
O	-6.12210100	-2.31573300	1.49110100
C	-2.36762400	-1.46370700	0.30100200
C	-3.86249800	-2.88705900	1.01584300
N	-1.80218300	-2.61318100	0.67136000
N	-2.72360900	-3.50540600	1.13232100
C	-5.22004100	-3.39401200	1.39526900
H	-5.55371700	-4.15030300	0.67465400
H	-5.16848200	-3.86272400	2.37918900
C	-0.41119100	-2.98112000	0.66852800
C	0.38739800	-2.69687500	-0.42876300
C	0.08242400	-3.67622100	1.77065400
C	1.71314300	-3.12621000	-0.41503100
C	1.40293400	-4.09758200	1.75488000
C	2.24290200	-3.84440300	0.65827700
H	2.31400500	-2.89077400	-1.28585200
H	1.78240600	-4.64375000	2.61326500
H	-0.56691600	-3.89269400	2.61232400
H	0.00052000	-2.14598600	-1.27837300
C	3.68124900	-4.36711400	0.66997800
C	4.41412700	-4.05720200	-0.64016800
C	3.66768000	-5.89293400	0.86558400
C	4.44343300	-3.71034200	1.83254800
H	4.46936600	-2.98168300	-0.83214700
H	3.92399100	-4.53664900	-1.49335200
H	5.43778400	-4.44074400	-0.58164300
H	3.20268700	-6.17837100	1.81345500
H	4.69296200	-6.27721200	0.86663400
H	3.11824600	-6.38266000	0.05601000
H	5.48154700	-4.05968700	1.84710600
H	3.99167600	-3.95445000	2.79874500
H	4.44420900	-2.62287800	1.72080400

H	0.33297300	0.41528700	-1.21147200
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M5RS

C	-0.61426600	-0.40293300	2.32140500
C	-0.14457000	0.56028200	1.28334300
H	0.17512600	-0.48004200	3.07921900
C	-1.92402300	-0.04514000	3.00423100
C	-2.27524100	-0.70916300	4.18441200
C	-2.82433800	0.87794900	2.46888500
C	-3.49431000	-0.47244700	4.80732100
H	-1.58226500	-1.43035600	4.61332300
C	-4.04528800	1.12585100	3.09675600
H	-2.58800800	1.39729900	1.54514600
C	-4.38722600	0.44954400	4.26228100
H	-3.74885100	-1.00645300	5.71751900
H	-4.73345300	1.84592700	2.66427000
H	-5.34141600	0.63657600	4.74472800
C	1.20106100	0.79573400	1.14023000
O	2.17957700	0.37971900	1.81981300
H	-0.85086200	0.95401700	0.56607100
C	-1.95420400	-1.99648700	0.83399200
C	-3.17560400	-2.53987500	1.50853800
C	-4.40378700	-1.89364000	1.34005300
C	-3.11468400	-3.68244300	2.31132600
C	-5.54231000	-2.36796500	1.97944200
H	-4.43905900	-0.99979400	0.72583100
C	-4.25973200	-4.16884900	2.93577500
H	-2.17335200	-4.20991500	2.43806200
C	-5.47436800	-3.50757600	2.77902500
H	-6.48501600	-1.84305200	1.86039100
H	-4.20098900	-5.06338300	3.54755500
H	-6.36434300	-3.87672400	3.27882600
N	-2.16630700	-1.58083300	-0.36019900
N	-1.15523500	-1.09805300	-1.15468000
S	-1.58499100	0.21624500	-2.07788700
O	-0.33010300	0.62245700	-2.71193400
O	-2.33998400	1.19594400	-1.29527000
C	-2.68160100	-0.46126200	-3.28549600
C	-2.16339200	-0.87295000	-4.50732800
C	-3.02808800	-1.42738200	-5.44532400
C	-4.38857900	-1.57946400	-5.16750100
C	-4.87721500	-1.15493000	-3.92606900
C	-4.03380800	-0.59230700	-2.97835400
H	-1.10585000	-0.74995000	-4.71532900

H	-2.64023200	-1.74802500	-6.40752700
H	-5.93464800	-1.26644200	-3.70342200
H	-4.40668800	-0.25320400	-2.01843200
C	-5.32428400	-2.19061500	-6.17695300
H	-4.80756300	-2.41897700	-7.11087200
H	-5.75554700	-3.11856000	-5.78996300
H	-6.15313900	-1.51286400	-6.39994800
C	-0.72646600	-1.88174200	1.73371000
H	-0.89549600	-2.53022200	2.59620100
C	0.63602000	-2.25474100	1.19494200
O	0.97659300	-2.24256700	0.02836400
O	1.45927400	-2.55017100	2.19351500
C	2.86511900	-2.58503600	1.86478900
C	3.62164500	-2.18168000	3.10827100
H	3.04064200	-1.87736300	1.05405700
H	3.10812600	-3.59759300	1.52313100
H	4.69579800	-2.20278800	2.90372500
H	3.33031900	-1.16250500	3.37042300
H	3.41164700	-2.85614900	3.94251400
C	0.70563000	5.43956700	0.65720400
C	0.19475100	4.18120600	0.99666800
C	0.06532300	3.79506900	2.32705200
C	0.48172400	4.68248200	3.31851600
C	1.00818600	5.92967500	2.98277300
C	1.11733500	6.32089500	1.64908700
C	0.68800400	5.64502500	-0.83641200
C	-0.35151700	4.59283600	-1.27650000
C	-0.20465700	3.43461300	-0.25727100
H	-0.34892100	2.82485600	2.58088900
H	0.38920700	4.39993600	4.36187800
H	1.32445300	6.60825200	3.76882100
H	1.50707700	7.30101100	1.39062100
H	1.67712100	5.43883100	-1.26427100
H	-1.35201000	5.00708600	-1.13202200
H	0.40343600	6.65542400	-1.13797800
H	-1.11568500	2.84094800	-0.19037200
N	0.88066200	2.55108100	-0.75892800
O	-0.31068100	4.17348800	-2.61906500
C	1.52580700	1.53890500	-0.13633600
C	1.45240300	2.68355000	-1.99689200
N	2.48426700	1.16308400	-0.98428900
N	2.44452300	1.86095000	-2.15448800
C	0.92559600	3.63577700	-3.02377500
H	1.66650000	4.41979900	-3.22651000

H	0.74624000	3.07810600	-3.94488000
C	3.44762500	0.10654500	-0.84507100
C	4.48688900	0.22784500	0.07113600
C	3.34178500	-0.99439800	-1.67701700
C	5.43619400	-0.78017800	0.13650500
C	4.30262700	-2.00077900	-1.59155600
C	5.36786700	-1.91208700	-0.69289500
H	6.24700800	-0.68154900	0.85218000
H	4.20266600	-2.86154500	-2.24132800
H	2.50877400	-1.06586100	-2.36869300
H	4.51940900	1.08270000	0.73513600
C	6.45573200	-2.98512900	-0.59585100
C	6.53544900	-3.51442200	0.84545800
C	7.80733400	-2.36125800	-0.98342300
C	6.18265700	-4.16929200	-1.52817700
H	5.58084000	-3.95360400	1.15354600
H	6.79151200	-2.72241600	1.55518800
H	7.30683700	-4.28814500	0.91784500
H	7.77744400	-1.98006700	-2.00863400
H	8.60064200	-3.11329300	-0.91770100
H	8.07181100	-1.53206200	-0.32095800
H	6.97725800	-4.91234100	-1.41391100
H	6.16393900	-3.86025100	-2.57783500
H	5.23063000	-4.65563600	-1.29264700
H	-0.19924000	-1.04720300	-0.78254700

M5SR

C	5.44638500	-2.05652500	1.01596500
C	4.09603100	-2.14169500	1.34342900
C	3.64217000	-2.97995300	2.35865400
C	4.57802000	-3.75992700	3.03293400
C	5.93414100	-3.69055000	2.70209500
C	6.37883500	-2.83491300	1.69730900
C	5.68762900	-1.04844900	-0.07746700
C	4.28060800	-0.62075500	-0.56177900
C	3.26352500	-1.22068900	0.48117600
H	2.58553600	-2.98418600	2.61252100
H	4.25314600	-4.42353200	3.82786900
H	6.64941400	-4.30664800	3.23804300
H	7.43453700	-2.77769200	1.44841600
H	6.26238600	-1.45143300	-0.91826100
H	4.16973700	0.46530700	-0.57785100
H	6.24112000	-0.18318700	0.30099500
H	2.77865100	-0.43149400	1.05727800

N	2.19211700	-1.94698800	-0.21090900
O	4.04229900	-1.01241500	-1.90705300
C	0.89397300	-2.09819900	0.11495100
C	2.38747600	-2.56694200	-1.41229500
N	0.37742900	-2.82429400	-0.88316700
N	1.29462900	-3.11211500	-1.85255700
C	3.71247400	-2.38072000	-2.06836600
H	4.47452400	-3.03407500	-1.62064200
H	3.63727200	-2.58750100	-3.13532200
C	-1.00482900	-3.14448800	-1.07701800
C	-1.66818200	-2.56249900	-2.14664100
C	-1.66777200	-3.94020800	-0.15155700
C	-3.04026000	-2.76707200	-2.27426300
C	-3.03344000	-4.13058100	-0.29847500
C	-3.75034000	-3.53602500	-1.34771900
H	-3.55310100	-2.29100800	-3.10117800
H	-3.55413900	-4.74256800	0.43123600
H	-1.12418000	-4.37807500	0.67909200
H	-1.11566600	-1.93229300	-2.83684600
C	-5.26536400	-3.73622900	-1.42520400
C	-5.57194600	-5.23338800	-1.59632000
C	-5.88785700	-2.97388300	-2.59886800
C	-5.90543200	-3.22581100	-0.12234700
H	-5.18165200	-5.82187400	-0.76097400
H	-5.12886100	-5.61819900	-2.51989500
H	-6.65458100	-5.39052600	-1.64217000
H	-6.99367400	-3.33620200	-0.17448000
H	-5.67007500	-2.16941300	0.04118900
H	-5.55348600	-3.78681900	0.74788800
C	-1.51635100	0.15697100	2.00152800
C	-0.93992400	-0.85307700	1.06120400
H	-1.26274400	-0.14545300	3.02509900
C	-3.01863800	0.30072700	1.87677600
C	-3.82416800	0.32783700	3.01727100
C	-3.61987400	0.46741900	0.62351900
C	-5.20047400	0.52245800	2.91492500
H	-3.36600900	0.19580500	3.99452800
C	-4.99335300	0.66699500	0.52006900
H	-3.00945200	0.45408800	-0.27689600
C	-5.78846300	0.69535100	1.66497500
H	-5.81178000	0.53643800	3.81193700
H	-5.44357200	0.80290400	-0.45868100
H	-6.85948000	0.85045800	1.58167700
C	0.27098600	-1.43302300	1.31459500

O	1. 01698300	-1. 34693600	2. 34423600
H	-6. 96934200	-3. 13843600	-2. 60458500
H	-5. 49342300	-3. 31731300	-3. 56038900
H	-5. 71249700	-1. 89646000	-2. 51541200
H	-1. 44210500	-1. 02660900	0. 12048000
C	-1. 23530900	2. 47351600	0. 68052500
C	-1. 92451500	3. 76730500	0. 96296000
C	-1. 56927600	4. 91047800	0. 23941400
C	-2. 94887100	3. 85227800	1. 91170700
C	-2. 22086400	6. 11763500	0. 46387000
H	-0. 77014700	4. 83608500	-0. 49162200
C	-3. 60685600	5. 05993000	2. 12653000
H	-3. 25803800	2. 96654100	2. 46106500
C	-3. 24246800	6. 19578400	1. 40831200
H	-1. 92966900	7. 00024400	-0. 09680500
H	-4. 41019700	5. 11060800	2. 85453400
H	-3. 75160400	7. 13814700	1. 58341200
N	-1. 01343600	2. 26009700	-0. 56403600
N	-0. 42369300	1. 08865900	-0. 94785600
S	0. 10738700	1. 02111400	-2. 52906400
O	0. 77378400	-0. 27889700	-2. 58610600
O	-1. 01865100	1. 32897800	-3. 39217700
C	1. 33048600	2. 28521500	-2. 71498500
C	2. 67384800	1. 92697100	-2. 70639300
C	3. 62978300	2. 93425300	-2. 80026100
C	3. 25742600	4. 27786800	-2. 89011200
C	1. 89505100	4. 60161900	-2. 90399800
C	0. 92271300	3. 61372000	-2. 82143000
H	2. 95506000	0. 87851600	-2. 64728000
H	4. 68377600	2. 66997200	-2. 80995900
H	1. 59536200	5. 64234000	-2. 99030400
H	-0. 13501100	3. 85562500	-2. 84720500
C	4. 29687800	5. 36555800	-2. 95566000
H	3. 98120800	6. 17237200	-3. 62135700
H	5. 25425900	4. 97880900	-3. 31053300
H	4. 45837100	5. 80124900	-1. 96432200
C	-0. 86426400	1. 60925700	1. 88759700
H	-1. 22204600	2. 14607300	2. 76929900
C	0. 63835800	1. 48665800	2. 06680700
O	1. 44528200	1. 40512200	1. 15802100
O	0. 96495000	1. 46989200	3. 35164700
C	2. 32879100	1. 11732200	3. 65388900
C	2. 46304300	1. 12407000	5. 15983100
H	2. 50370600	0. 12485700	3. 22912900

H	2.99197200	1.84452700	3.17595800
H	3.48449400	0.85682500	5.44035800
H	1.78008200	0.39586300	5.60212700
H	2.23715900	2.11197100	5.56825800
H	0.26283900	0.68454500	-0.30321200

M5SS

C	1.65754400	-0.04050800	-1.63297300
C	0.84970100	-0.80138500	-0.63182200
H	1.00911400	0.14965400	-2.49757700
C	2.90192100	-0.76357400	-2.12761700
C	3.29437800	-0.65106000	-3.46387400
C	3.72968100	-1.45788600	-1.23976000
C	4.50259500	-1.18983100	-3.90210800
H	2.64200900	-0.14004800	-4.16857700
C	4.94287000	-1.98696400	-1.67229100
H	3.42165300	-1.57469300	-0.20276800
C	5.33746000	-1.84799800	-3.00250100
H	4.79031100	-1.09608100	-4.94460900
H	5.58524800	-2.51023500	-0.97014800
H	6.28285200	-2.26239100	-3.33748100
C	-0.31774000	-1.41305100	-1.01274300
O	-0.85192000	-1.50302900	-2.15625600
H	1.21907300	-0.87942700	0.37971900
C	0.96990500	2.39209600	-1.07837200
C	0.95814300	3.40043600	-2.18607900
C	0.35618200	4.64787700	-1.97549500
C	1.50550000	3.12584700	-3.44462700
C	0.30825200	5.59303100	-2.99241900
H	-0.06683400	4.86211300	-1.00005900
C	1.44886500	4.07084700	-4.46569300
H	1.95744900	2.16015700	-3.65114400
C	0.85508900	5.30890500	-4.24276000
H	-0.15214900	6.55828000	-2.80719100
H	1.86735600	3.83345900	-5.43827700
H	0.81865000	6.04781400	-5.03655900
N	-0.03298400	2.49222000	-0.28937900
N	-0.20062600	1.72407700	0.82485200
S	-1.81102600	1.33558900	1.08954500
O	-2.49263600	1.00960300	-0.15756800
O	-1.75946400	0.34614600	2.16396400
C	-2.48933100	2.85209900	1.69102900
C	-2.91068400	3.81181100	0.77453000
C	-3.41339300	5.01388800	1.25740700

C	-3.50611200	5.25765700	2.63190400
C	-3.07572100	4.27035100	3.52391200
C	-2.56157100	3.06410700	3.06323600
H	-2.84012000	3.61154300	-0.28911500
H	-3.74338000	5.77581300	0.55723600
H	-3.14406900	4.45012800	4.59272400
H	-2.22685000	2.29179800	3.74736700
C	-4.08825100	6.54953600	3.14212600
H	-5.17344500	6.46128400	3.25667400
H	-3.89473000	7.37110000	2.44905500
H	-3.67267000	6.81277100	4.11711000
C	2.12174400	1.38292900	-1.11199000
H	2.80641200	1.76809600	-1.86415800
C	2.91188800	1.23616600	0.18389700
O	2.39623500	1.01321900	1.25762300
O	4.25087400	1.29140400	0.14623600
C	5.01888800	1.62448200	-1.02317100
C	6.47017200	1.41841700	-0.64809700
H	4.74775200	0.96957700	-1.85499100
H	4.81662900	2.66548200	-1.29828200
H	7.11116500	1.67723200	-1.49374900
H	6.63781600	0.36948700	-0.39085200
H	6.74244100	2.04079000	0.20669600
C	-5.25879800	-2.98115400	-1.80561800
C	-3.87240000	-2.85985700	-1.77458000
C	-3.04444500	-3.77671100	-2.41538100
C	-3.63738900	-4.84968500	-3.07547600
C	-5.02819900	-4.98865700	-3.09859100
C	-5.84817100	-4.05319900	-2.47192100
C	-5.92459100	-1.83470900	-1.08779300
C	-4.77821400	-1.06352500	-0.38700000
C	-3.44588900	-1.63654900	-0.99718900
H	-1.96959000	-3.61932800	-2.40905400
H	-3.01653900	-5.58077200	-3.58320800
H	-5.47436400	-5.83166200	-3.61692300
H	-6.92869700	-4.15955200	-2.50162000
H	-6.66519700	-2.15614700	-0.34796600
H	-4.81901800	0.00771700	-0.57778800
H	-6.44455600	-1.18212600	-1.79642200
H	-2.93017100	-0.90771600	-1.61926400
N	-2.50837500	-1.99732200	0.07525700
O	-4.86213500	-1.16585200	1.02785200
C	-1.16389400	-1.96322000	0.11843200
C	-2.94727500	-2.44862600	1.28611900

N	-0.85471600	-2.43342200	1.33579400
N	-1.95853500	-2.71820800	2.08452300
C	-4.41564000	-2.40436000	1.54174100
H	-4.92727600	-3.25313900	1.06580000
H	-4.61043100	-2.42060200	2.61370300
C	0.44616000	-2.46863400	1.93342200
C	1.41403800	-3.33638500	1.44324700
C	0.73779200	-1.53488600	2.91640300
C	2.71209400	-3.22146800	1.92192900
C	2.04728900	-1.43157500	3.37625500
C	3.06310200	-2.24490600	2.86775600
H	3.47267100	-3.88555400	1.52171400
H	2.27309500	-0.66703500	4.10890000
H	-0.04211900	-0.86286600	3.25859800
H	1.16023400	-4.05390300	0.67022400
C	4.52759100	-2.08224500	3.28089000
C	5.37386600	-1.82119000	2.02214800
C	5.01093800	-3.36784600	3.97098600
C	4.72431800	-0.89906600	4.23334600
H	5.03316900	-0.91656600	1.50556700
H	5.31877500	-2.66189700	1.32373700
H	6.42481100	-1.68699500	2.29991400
H	4.42284000	-3.56956100	4.87133900
H	6.06169100	-3.26609100	4.26142900
H	4.92645400	-4.23491500	3.30923100
H	5.78626600	-0.80268700	4.47735200
H	4.17848400	-1.03759100	5.17181100
H	4.39542800	0.03574400	3.76849300
H	0.42626200	0.92813000	0.98189300

TS6RR

C	-0.98937300	-0.21865200	-2.49135600
C	-1.32856200	-0.53330200	-1.03814300
H	-0.22198200	-0.94833500	-2.77579400
C	-2.10348500	-0.37052500	-3.51561500
C	-1.75812700	-0.75385700	-4.81570100
C	-3.45400800	-0.15851700	-3.22630500
C	-2.72710500	-0.92247700	-5.80052200
H	-0.71100300	-0.93021400	-5.05313400
C	-4.42865500	-0.33634600	-4.20544000
H	-3.74448200	0.17818500	-2.23705500
C	-4.07038200	-0.71802600	-5.49581000
H	-2.43358300	-1.22341600	-6.80141700
H	-5.47234000	-0.16698200	-3.95913800

H	-4.83151400	-0.85441900	-6.25746000
C	-0.62987900	-1.65718900	-0.49266900
O	0.16824000	-2.40153900	-1.05700000
H	-2.34435100	-0.35218700	-0.69996000
C	1.02330100	1.08151900	-1.73350200
C	2.24103300	0.56793400	-2.41082200
C	2.91038500	-0.53194400	-1.86432300
C	2.69142900	1.11442000	-3.61760600
C	4.00884600	-1.07766200	-2.52152800
H	2.53901300	-0.97483600	-0.94541400
C	3.80661100	0.58305300	-4.25723000
H	2.17845300	1.97279100	-4.04369800
C	4.46436100	-0.51955700	-3.71355500
H	4.49414100	-1.95468600	-2.10323700
H	4.15888100	1.02478700	-5.18386500
H	5.32158600	-0.94716900	-4.22400400
N	1.08780800	1.30068400	-0.46718700
N	-0.15512700	1.54843400	0.08946200
H	-0.84194900	0.53354300	-0.28399100
S	-0.17028700	1.81934800	1.70664600
O	0.91240000	1.13605300	2.41934800
O	-1.55066100	1.52488800	2.11330100
C	0.10357900	3.56324100	1.91187200
C	1.40962200	4.04248300	1.96243900
C	1.61785500	5.41168300	2.08919700
C	0.54113900	6.30149400	2.16081400
C	-0.75937800	5.78889800	2.11635600
C	-0.98746200	4.42293500	1.98966800
H	2.24139500	3.34739700	1.91468100
H	2.63237500	5.79738800	2.13402300
H	-1.60357800	6.46946600	2.18534100
H	-1.99278100	4.01475400	1.96657000
C	0.77657300	7.78645900	2.24732400
H	1.72296500	8.01030500	2.74433800
H	0.81791500	8.22429600	1.24405700
H	-0.02801500	8.28477500	2.79263800
C	-0.26132400	1.15144800	-2.57092800
H	0.03310100	1.32867900	-3.61280400
C	-1.14624100	2.32179000	-2.17325600
O	-2.33111500	2.26127700	-1.94539500
O	-0.44144800	3.45975400	-2.15039000
C	-1.13000200	4.59867700	-1.61567400
C	-0.08790300	5.65455500	-1.32402900
H	-1.65389200	4.28745700	-0.70708100

H	-1.87685200	4.93676100	-2.34122100
H	-0.56479300	6.54269500	-0.90085500
H	0.63537800	5.27227200	-0.59865700
H	0.44182000	5.94125900	-2.23577400
C	-4.25004400	-3.30239200	1.95237800
C	-3.71707000	-2.45183400	0.97427800
C	-3.83023400	-2.76832600	-0.37739000
C	-4.46660500	-3.95658700	-0.73476100
C	-4.98484600	-4.80887200	0.23907100
C	-4.88527600	-4.48360800	1.59081500
C	-4.05058900	-2.73587100	3.33393800
C	-3.80067500	-1.24634700	3.02378000
C	-3.09578200	-1.23918700	1.64211100
H	-3.44375200	-2.11550200	-1.15178700
H	-4.56287700	-4.21187600	-1.78457500
H	-5.48010700	-5.72751300	-0.05841800
H	-5.30465700	-5.13749400	2.34928600
H	-3.18044200	-3.19685200	3.81810800
H	-4.76324300	-0.75081600	2.87810300
H	-4.90802000	-2.87833800	3.99486200
H	-3.20987700	-0.27890500	1.13848100
N	-1.64421100	-1.43334800	1.89307100
O	-3.13734100	-0.49564800	4.00648600
C	-0.65295200	-1.73565100	1.03087700
C	-1.08412400	-1.37469800	3.13801100
N	0.43998800	-1.89643400	1.78560300
N	0.18047400	-1.67505100	3.09921600
C	-1.86024400	-0.97276500	4.35316100
H	-1.91345700	-1.81427500	5.05600200
H	-1.32934900	-0.14856300	4.83341800
C	1.81201000	-2.14606200	1.41752400
C	2.16923400	-3.27341300	0.69223800
C	2.76944900	-1.25142000	1.88597300
C	3.51619900	-3.48976100	0.41038300
C	4.10533000	-1.49643600	1.60328600
C	4.51075400	-2.61535900	0.86287000
H	3.77966800	-4.36795900	-0.16708100
H	4.84501400	-0.79427200	1.97353200
H	2.45160400	-0.37480800	2.43666100
H	1.40903000	-3.95376500	0.33244000
C	6.00339400	-2.87416200	0.63741200
C	6.24880300	-4.01366200	-0.35777400
C	6.62978600	-3.26326800	1.98894700
C	6.69974100	-1.60831400	0.10940600

H	5.79156600	-3.80886000	-1.33161100
H	5.85882700	-4.96673000	0.01167400
H	7.32481800	-4.13530400	-0.51180200
H	6.50878000	-2.46288300	2.72477900
H	7.70079400	-3.45576700	1.86618400
H	6.15965200	-4.16666300	2.38914000
H	7.75854200	-1.82040000	-0.06995000
H	6.64633000	-0.78383000	0.82461700
H	6.25208700	-1.26829500	-0.82858400

TS6RS

S	0.19870200	-0.87333700	2.68385500
O	-1.09942100	-3.88829400	-0.60232600
O	-1.55169900	-2.07295500	-1.84963700
O	0.13670700	-1.76952800	3.83483600
O	-0.78135300	0.22188600	2.58161300
N	0.08527700	-1.66283100	1.24550700
N	1.14987700	-2.51697900	1.10464900
C	-0.81159700	0.79800500	-1.18054300
C	0.31268800	-0.00027200	-0.79308100
C	0.91361600	-0.99129000	-1.78597800
H	0.36730400	-0.88775500	-2.73002800
C	0.72562000	-2.47787600	-1.34112100
H	1.09518900	-3.10313900	-2.16328800
C	1.47623400	-2.89601100	-0.07785700
C	2.38345500	-0.71674900	-2.04835200
C	3.27852700	-0.48042700	-0.99689000
H	2.92268200	-0.46344300	0.03151700
C	4.63507500	-0.30231000	-1.24661700
H	5.31282400	-0.13654100	-0.41398600
C	5.12182300	-0.34809400	-2.55191200
H	6.18073800	-0.21028200	-2.74563700
C	4.23996100	-0.56862100	-3.60622300
H	4.60762900	-0.59939900	-4.62714700
C	2.88093900	-0.75125300	-3.35332600
H	2.19539000	-0.93181400	-4.17806100
C	-0.73812800	-2.89890700	-1.19093700
C	-2.96042300	-2.35025800	-1.79864900
H	-3.35044300	-1.94621800	-0.85698000
H	-3.10835100	-3.43307500	-1.79678600
C	-3.58679900	-1.68556900	-3.00482300
H	-3.37778200	-0.61405300	-2.99113800
H	-3.18129200	-2.11285800	-3.92559900
H	-4.66827700	-1.84348200	-2.99565900

C	1. 81229400	-0. 09617900	2. 70158700
C	1. 88537400	1. 29084000	2. 63743100
H	0. 97260800	1. 87739000	2. 63847200
C	3. 13061400	1. 91369400	2. 59434900
H	3. 17926400	2. 99984500	2. 56387900
C	4. 30786300	1. 16305900	2. 60608800
C	4. 20988900	-0. 23156800	2. 69563900
H	5. 11773100	-0. 82828700	2. 72345500
C	2. 97565400	-0. 86780500	2. 75444300
H	2. 90806900	-1. 94779900	2. 81960600
C	5. 65611100	1. 83006800	2. 53125800
H	6. 19929100	1. 50852500	1. 63694700
H	5. 55897300	2. 91691500	2. 49248100
H	6. 27014500	1. 57022100	3. 39755600
C	2. 63323800	-3. 82510900	-0. 16871000
C	3. 43859900	-3. 89046100	-1. 31197800
C	2. 95711100	-4. 63891500	0. 92663400
C	4. 54042600	-4. 74112500	-1. 35599600
H	3. 23224300	-3. 25326800	-2. 16706500
C	4. 05470600	-5. 48904300	0. 87882900
H	2. 32434700	-4. 59951300	1. 80681400
C	4. 85248100	-5. 54459000	-0. 26373800
H	5. 15811500	-4. 76856800	-2. 24820400
H	4. 28433200	-6. 11821500	1. 73320100
H	5. 70826400	-6. 21109400	-0. 30141000
O	-1. 54467800	0. 74775100	-2. 15746600
C	0. 64791600	5. 06591300	-1. 44593400
C	0. 89736900	3. 69030800	-1. 39131900
C	1. 13958600	2. 94866800	-2. 54206100
C	1. 09656400	3. 60559500	-3. 77037700
C	0. 82852300	4. 97343700	-3. 83351800
C	0. 61099800	5. 71629600	-2. 67293700
C	0. 48292900	5. 64018900	-0. 05901300
C	1. 16065100	4. 55449600	0. 80563900
C	0. 91022200	3. 23207400	0. 04511800
H	1. 37610100	1. 88933700	-2. 48846100
H	1. 28455200	3. 04952100	-4. 68250900
H	0. 80329800	5. 46964100	-4. 79840600
H	0. 42668600	6. 78472500	-2. 72843800
H	-0. 58067900	5. 74983200	0. 18585500
H	2. 24066400	4. 72177900	0. 79652400
H	0. 95214200	6. 61742200	0. 07009700
H	1. 65774600	2. 47218000	0. 27961000
N	-0. 41717300	2. 72614900	0. 48847800

O	0.80596500	4.48342100	2.16914200
C	-1.18455500	1.77174600	-0.06647800
C	-1.12963600	3.23310200	1.54551800
N	-2.31436200	1.76101600	0.62727900
N	-2.29284800	2.65959800	1.64626800
C	-0.57440100	4.31997000	2.41502200
H	-1.13046600	5.25122200	2.25207700
H	-0.68361100	4.03227100	3.46236400
C	-3.43343800	0.86845700	0.48978500
C	-4.22355300	0.91698700	-0.65348700
C	-3.72277900	0.01739800	1.54595100
C	-5.33877400	0.09217200	-0.71962600
C	-4.84345400	-0.80307900	1.45231200
C	-5.67594800	-0.77765300	0.32833400
H	-5.95838500	0.13314100	-1.61052700
H	-5.05702600	-1.47099900	2.27793200
H	-3.06532000	-0.00378100	2.40801800
H	-3.95867200	1.57858200	-1.47049100
C	-6.92698700	-1.65132900	0.21171800
C	-6.82877300	-2.52069800	-1.05285400
C	-8.16364500	-0.74208900	0.11057300
C	-7.09877900	-2.57484600	1.42134500
H	-5.93077700	-3.14713600	-1.02738600
H	-6.79767400	-1.91034600	-1.96018800
H	-7.70245500	-3.17648500	-1.12342700
H	-8.25655200	-0.11427500	1.00195100
H	-9.06917000	-1.35124300	0.02243700
H	-8.11127000	-0.08680200	-0.76368000
H	-8.00005300	-3.18026000	1.28881700
H	-7.21295000	-2.00720900	2.34992700
H	-6.24934300	-3.25593400	1.53219200
H	-0.04278300	-0.74092300	0.23100200
H	1.04587900	0.57603500	-0.22388200

TS6SR

C	-1.67229500	-0.35162500	1.82269400
C	-0.92496000	-1.02957900	0.68344600
H	-1.69125200	-1.00536800	2.70366800
C	-3.09825800	-0.03013700	1.41302100
C	-4.14161400	-0.17757300	2.32846100
C	-3.38737600	0.46776500	0.13533700
C	-5.44849800	0.16196700	1.98413000
H	-3.92686200	-0.56326000	3.32239300
C	-4.69184400	0.81706000	-0.20509700

H	-2.59402800	0.60537800	-0.59773800
C	-5.72701200	0.66321600	0.71577900
H	-6.24665400	0.03472500	2.70875000
H	-4.89460900	1.21716000	-1.19422800
H	-6.74322800	0.93286300	0.44600300
C	0.24372200	-1.80635600	0.94980400
O	0.83576100	-2.00346100	2.00806300
H	-1.55627400	-1.42184000	-0.11263700
C	-1.04858500	2.15942900	1.34504900
C	-1.82734400	3.34981900	1.78684200
C	-2.60898500	4.04313200	0.85437400
C	-1.79612100	3.80497400	3.10899000
C	-3.33482400	5.16511400	1.23464700
H	-2.64211300	3.67243500	-0.16574000
C	-2.51807100	4.93382800	3.48799600
H	-1.18417400	3.29250800	3.84680000
C	-3.29135800	5.61609200	2.55337600
H	-3.94423400	5.68569500	0.50232500
H	-2.47268000	5.28110700	4.51547400
H	-3.86085900	6.49112000	2.85015000
N	-0.56258700	2.23888800	0.15981300
N	0.13337400	1.18200900	-0.35259800
S	0.20632400	1.25098500	-1.98824000
O	0.94538200	0.03294900	-2.36571800
O	-1.11214200	1.46170900	-2.60031800
C	1.20946100	2.65395600	-2.41204100
C	2.53368400	2.45401200	-2.78467600
C	3.32347600	3.56393200	-3.07529200
C	2.80678600	4.85836000	-2.99398900
C	1.46946500	5.02607300	-2.61522400
C	0.66278400	3.93370300	-2.32715200
H	2.92752400	1.44311300	-2.84960900
H	4.35857400	3.42031200	-3.37331000
H	1.05714600	6.02916200	-2.54633900
H	-0.37329200	4.06022900	-2.03276500
C	3.65713800	6.05734100	-3.32522100
H	3.54406100	6.83893200	-2.56921200
H	3.36175300	6.48782800	-4.28743000
H	4.71391700	5.78939000	-3.38753400
C	-0.98020800	0.97639000	2.31459200
H	-1.56053000	1.25696400	3.19842000
C	0.42528700	0.69891400	2.82572300
O	1.45655000	1.05302500	2.30196100
O	0.37227000	-0.00185400	3.96326300

C	1. 62362700	-0. 50901500	4. 45566700
C	1. 30791400	-1. 69940300	5. 33230000
H	2. 24290100	-0. 79638400	3. 60333800
H	2. 13116300	0. 29178900	5. 00296700
H	2. 23252400	-2. 12059400	5. 73486100
H	0. 80217800	-2. 46197700	4. 73590200
H	0. 66274500	-1. 41496500	6. 16694500
H	-0. 34014700	-0. 06531700	0. 08799600
C	5. 46785100	-1. 30565100	0. 90008000
C	4. 18189600	-1. 80651100	1. 08586100
C	3. 93916100	-2. 91017800	1. 89798000
C	5. 02521300	-3. 52384500	2. 51795300
C	6. 31972200	-3. 03380700	2. 32903700
C	6. 54995700	-1. 92011400	1. 52431900
C	5. 45435400	-0. 08458900	0. 01559300
C	4. 03353500	-0. 03719700	-0. 59220300
C	3. 17128800	-0. 98357500	0. 32089900
H	2. 92365600	-3. 26573400	2. 04604400
H	4. 86450300	-4. 38810700	3. 15425400
H	7. 15510900	-3. 52543000	2. 81734700
H	7. 55720600	-1. 53914600	1. 38457200
H	6. 19931500	-0. 11608400	-0. 78504600
H	3. 60469300	0. 96690600	-0. 57289200
H	5. 64446800	0. 81928000	0. 60363100
H	2. 53179200	-0. 38490400	0. 97750100
N	2. 29273600	-1. 81812100	-0. 50167000
O	4. 04390700	-0. 38724100	-1. 97092300
C	1. 02016000	-2. 17524800	-0. 30851600
C	2. 63301600	-2. 22176800	-1. 76028900
N	0. 64371000	-2. 78723700	-1. 42757800
N	1. 63948200	-2. 82084200	-2. 35334800
C	3. 95879800	-1. 76702800	-2. 26988800
H	4. 77421100	-2. 33706300	-1. 80367000
H	4. 00692700	-1. 87889000	-3. 35233500
C	-0. 72560100	-3. 09460100	-1. 72863500
C	-1. 40430300	-2. 22914800	-2. 57536100
C	-1. 38287300	-4. 06882100	-0. 98891000
C	-2. 79273500	-2. 31278100	-2. 63275900
C	-2. 76706000	-4. 13555700	-1. 06737600
C	-3. 50062900	-3. 23603600	-1. 85493400
H	-3. 31984700	-1. 59945800	-3. 25487400
H	-3. 28659100	-4. 87780800	-0. 46957600
H	-0. 82270600	-4. 72679200	-0. 33205400
H	-0. 85743300	-1. 44860300	-3. 09579300

C	-5.02816200	-3.25455400	-1.78345300
C	-5.65669700	-2.16626600	-2.65836200
C	-5.44472300	-2.99695500	-0.32337200
C	-5.55302200	-4.62422400	-2.24234700
H	-5.39987600	-2.29389200	-3.71473500
H	-5.34065400	-1.16908800	-2.33575800
H	-6.74587100	-2.21713500	-2.57064500
H	-5.10543900	-3.79794200	0.34015800
H	-6.53612500	-2.94159700	-0.25130700
H	-5.02628600	-2.05160900	0.03795300
H	-6.64495400	-4.64856900	-2.16801100
H	-5.15737000	-5.43664500	-1.62588900
H	-5.27512000	-4.81996600	-3.28253800

TS6SS

C	-1.47381700	-0.54239800	1.57710100
C	-0.54433900	-0.97312100	0.46181100
H	-0.85374800	-0.22080500	2.42180800
C	-2.41514500	-1.62871500	2.06971500
C	-2.73036800	-1.71535900	3.42834100
C	-3.08227700	-2.46752200	1.17160800
C	-3.70351800	-2.60333000	3.88106300
H	-2.21046000	-1.07228200	4.13503200
C	-4.06463800	-3.34710500	1.61948600
H	-2.84774500	-2.42323800	0.11011300
C	-4.38183100	-3.41496000	2.97475500
H	-3.93384300	-2.65847400	4.94049300
H	-4.58641000	-3.97907000	0.90660200
H	-5.14693900	-4.10115400	3.32341000
C	0.72705500	-1.49883800	0.85194100
O	1.20021300	-1.58841500	1.98359200
H	-1.01739600	-1.41820400	-0.40757500
C	-1.59209500	2.04302200	1.10405800
C	-2.10341900	3.15753800	1.95823900
C	-1.93986700	4.48162400	1.52511200
C	-2.71854600	2.93827900	3.19755400
C	-2.38375400	5.54552500	2.29983500
H	-1.45953500	4.65473100	0.56785300
C	-3.16131500	4.00615800	3.97479700
H	-2.82747100	1.93136300	3.59114100
C	-3.00160600	5.31349800	3.52799500
H	-2.25582300	6.56146000	1.93911200
H	-3.62573700	3.81211600	4.93654300
H	-3.35274300	6.14494600	4.13067100

N	-0.56308600	2.34371900	0.39700900
N	-0.05110600	1.45898500	-0.50325200
S	1.54616000	1.74189300	-0.77118400
O	2.33790400	1.58965500	0.46309700
O	1.90737100	0.85991800	-1.89159900
C	1.69532400	3.43078100	-1.29178200
C	1.71305700	4.44102100	-0.33341100
C	1.77942200	5.76308100	-0.75589300
C	1.83442200	6.08398200	-2.11647300
C	1.81410100	5.04770800	-3.05409100
C	1.73993500	3.71888300	-2.65148100
H	1.67390400	4.18520500	0.71962800
H	1.79039700	6.56156200	-0.01896400
H	1.85577000	5.28576200	-4.11329800
H	1.72233100	2.90782200	-3.37169600
C	1.94680800	7.51912800	-2.56113600
H	2.99996800	7.82224200	-2.61906400
H	1.44697200	8.19145400	-1.85633200
H	1.50400800	7.66158600	-3.55186500
C	-2.34400300	0.70571500	1.19036300
H	-3.04180700	0.82179500	2.01491200
C	-3.16490000	0.40955200	-0.06789700
O	-2.68537100	0.36108500	-1.17331300
O	-4.48004000	0.13491000	0.05679300
C	-5.19772400	0.21681400	1.29640300
C	-6.61292600	-0.22967000	0.99937400
H	-4.74048700	-0.44289800	2.04032600
H	-5.17160200	1.24913300	1.66481900
H	-7.21793500	-0.17992800	1.90749000
H	-6.60682200	-1.26159900	0.63944800
H	-7.06654200	0.40635600	0.23650200
C	5.91378400	-1.86247700	1.75217700
C	4.54580700	-2.10253000	1.65508700
C	3.96987600	-3.25458000	2.18181100
C	4.79914600	-4.18364300	2.80398600
C	6.17397600	-3.95321400	2.90029000
C	6.73950000	-2.79156700	2.38055400
C	6.28437600	-0.53767300	1.13692700
C	5.00466600	-0.03857600	0.42224000
C	3.84512100	-0.96742800	0.94535100
H	2.89654900	-3.40550900	2.11766700
H	4.37531900	-5.09082400	3.22204500
H	6.80777200	-4.68714200	3.38804100
H	7.80799800	-2.61469100	2.46155800

H	7.10759400	-0.60995200	0.41863500
H	4.75665900	0.99207500	0.66943600
H	6.59348300	0.17656900	1.90685800
H	3.17010800	-0.40858600	1.59146500
N	3.03673200	-1.46190500	-0.17832500
O	5.15640100	-0.03002200	-0.98894200
C	1.72544600	-1.73043600	-0.27863200
C	3.58334800	-1.68024000	-1.40864500
N	1.54161600	-2.12134000	-1.54008300
N	2.68840800	-2.08619300	-2.26389700
C	5.01001100	-1.29133100	-1.60390800
H	5.68556200	-2.04356400	-1.17155800
H	5.22443600	-1.18053500	-2.66651000
C	0.27047500	-2.36161400	-2.16243700
C	-0.42715400	-3.52868300	-1.87918000
C	-0.29038600	-1.32506400	-2.89291000
C	-1.74430900	-3.62904400	-2.30902200
C	-1.61149800	-1.44809600	-3.30849200
C	-2.37210600	-2.57928700	-2.99829200
H	-2.30190200	-4.52997100	-2.07086500
H	-2.06468100	-0.60961900	-3.82046800
H	0.27579200	-0.41027600	-3.04092800
H	0.03959000	-4.31847700	-1.29950800
C	-3.85512100	-2.69024600	-3.35985200
C	-4.67356400	-2.92441200	-2.07812900
C	-4.05408500	-3.87108200	-4.32345400
C	-4.37740100	-1.40882200	-4.01717400
H	-4.57782400	-2.07033900	-1.39868800
H	-4.35374500	-3.82989200	-1.55169600
H	-5.73243000	-3.04299800	-2.33208600
H	-3.47631100	-3.72565100	-5.24135200
H	-5.11150600	-3.96025800	-4.59319000
H	-3.74068900	-4.81691600	-3.87108600
H	-5.44517900	-1.52041900	-4.22806000
H	-3.87069400	-1.20317200	-4.96550800
H	-4.24633900	-0.55058000	-3.35014800
H	-0.21183200	0.15318100	-0.11347600

M6RR

C	-1.81223700	1.83322900	-1.16090300
C	-1.79628500	0.69053900	-0.13091600
H	-1.40486400	1.41954000	-2.08921800
C	-3.19023500	2.35811600	-1.53040100
C	-3.43272400	2.67122700	-2.87231600

C	-4. 22783800	2. 53691800	-0. 60923900
C	-4. 67276600	3. 14634500	-3. 28887900
H	-2. 63465200	2. 53356100	-3. 59885900
C	-5. 47348600	3. 00189200	-1. 02541300
H	-4. 04823800	2. 34269600	0. 44277400
C	-5. 70159700	3. 30769900	-2. 36461600
H	-4. 83764000	3. 38040100	-4. 33603400
H	-6. 26573700	3. 13343400	-0. 29503400
H	-6. 67272800	3. 67090000	-2. 68559300
C	-1. 43053800	-0. 63367200	-0. 73906800
O	-1. 23830400	-0. 86282300	-1. 90824800
H	-2. 75110800	0. 59984600	0. 39203300
C	0. 58868600	2. 26155800	-0. 81059600
C	1. 14341500	2. 01589200	-2. 16820100
C	1. 76066100	0. 79145100	-2. 46320300
C	1. 02519600	2. 96441700	-3. 19162200
C	2. 23985100	0. 53177700	-3. 74147600
H	1. 83819700	0. 04015500	-1. 68064700
C	1. 51779800	2. 70627500	-4. 46825700
H	0. 56663000	3. 92768500	-2. 98925000
C	2. 12497000	1. 48692100	-4. 75078600
H	2. 68806100	-0. 43446400	-3. 95206200
H	1. 42484800	3. 46223500	-5. 24183500
H	2. 49842800	1. 27818700	-5. 74831900
N	1. 19895100	1. 71741000	0. 18286800
N	0. 67172900	1. 92804400	1. 42426100
H	-1. 06517200	0. 87615600	0. 67079000
S	1. 16924200	0. 79582600	2. 45855800
O	0. 79021000	-0. 56409700	1. 99516200
O	0. 68690500	1. 17905000	3. 78942300
C	2. 95937400	0. 79283600	2. 53775900
C	3. 73549300	0. 47657100	1. 42032100
C	5. 12037600	0. 48545200	1. 53452100
C	5. 74881600	0. 79826800	2. 74515700
C	4. 95090200	1. 11739800	3. 84471500
C	3. 56178400	1. 11937100	3. 74741800
H	3. 25711000	0. 25776800	0. 47258700
H	5. 72934900	0. 25499800	0. 66320900
H	5. 42267700	1. 37089700	4. 79036800
H	2. 93581200	1. 37181600	4. 59634200
C	7. 25138500	0. 77485000	2. 85718000
H	7. 61651800	-0. 24894000	2. 99052000
H	7. 72009800	1. 17533200	1. 95459000
H	7. 59316500	1. 36278600	3. 71187500

C	-0.79124400	2.92063400	-0.74019500
H	-0.83815400	3.73627600	-1.47055800
C	-1.10959900	3.54910300	0.60308200
O	-2.06893500	3.27872500	1.29057000
O	-0.22442600	4.50337000	0.89889900
C	-0.20642700	4.89923000	2.27888100
C	1.06228000	5.69307600	2.49428500
H	-0.21917600	3.98674200	2.88261300
H	-1.10567000	5.48406000	2.49701500
H	1.12436000	6.02306300	3.53412500
H	1.92960200	5.06737600	2.27244300
H	1.08827000	6.57359100	1.84735600
C	-4.84793100	-3.23234900	0.81544600
C	-4.27336400	-1.97531100	0.58781300
C	-4.64671500	-1.21414600	-0.51756900
C	-5.58489600	-1.73864800	-1.40536400
C	-6.14576300	-2.99587700	-1.18655900
C	-5.78653800	-3.74825900	-0.06936400
C	-4.33070500	-3.84685500	2.09040700
C	-3.76939100	-2.61470200	2.82819800
C	-3.29829600	-1.65433400	1.70366000
H	-4.25298100	-0.21994300	-0.69957400
H	-5.88496400	-1.15127100	-2.26646500
H	-6.87864300	-3.38652300	-1.88492000
H	-6.23925400	-4.71828300	0.11164100
H	-3.54488300	-4.58040900	1.87173500
H	-4.58699900	-2.10749900	3.34463700
H	-5.10022000	-4.35554000	2.67446600
H	-3.27077500	-0.61642000	2.03682400
N	-1.90638400	-2.05489700	1.34991000
O	-2.79118700	-2.84808500	3.81030600
C	-1.17877400	-1.74839100	0.26029700
C	-1.18049700	-2.97734900	2.05027400
N	-0.09562400	-2.51802600	0.30983700
N	-0.07718700	-3.27854300	1.42802200
C	-1.65180000	-3.53915600	3.35534300
H	-1.83694500	-4.61552500	3.25082300
H	-0.86811800	-3.39341200	4.10094100
C	1.06894700	-2.52317600	-0.53281800
C	0.96445700	-2.79188500	-1.88902700
C	2.30067400	-2.31446500	0.08111300
C	2.13070400	-2.83635500	-2.65170900
C	3.44399900	-2.36262100	-0.70071800
C	3.38801800	-2.62521200	-2.07817900

H	2.03880400	-3.04386000	-3.71145900
H	4.40112100	-2.18379200	-0.21892600
H	2.33328400	-2.08414100	1.13992500
H	-0.00521900	-2.95312200	-2.34332300
C	4.69051400	-2.68647600	-2.87942000
C	4.44601800	-2.95431900	-4.36782200
C	5.56302100	-3.82501200	-2.32190400
C	5.44378900	-1.35256200	-2.73495000
H	3.84269400	-2.16825100	-4.83344100
H	3.94643000	-3.91481000	-4.52808600
H	5.40593000	-2.98645400	-4.89104800
H	5.80990000	-3.66336900	-1.26892400
H	6.50116700	-3.88496200	-2.88299100
H	5.04870900	-4.78708100	-2.40675000
H	6.37229000	-1.38529500	-3.31393400
H	5.70721600	-1.15140000	-1.69279700
H	4.84021900	-0.51447500	-3.09595300

M6RS

S	0.17125300	-0.38518800	2.63269000
O	-2.98915300	-0.57169800	-0.56782600
O	-2.57187200	-0.65170400	-2.77593100
O	-0.56050900	-1.00915200	3.73758700
O	0.46291000	1.05532500	2.75051000
N	-0.49292100	-0.60420700	1.14893400
N	-0.69532300	-1.93909600	1.05526300
C	0.00239900	1.05873500	-1.08078100
C	0.89990400	-0.12680100	-1.30761200
C	0.20091600	-1.28207200	-2.04598000
H	-0.10391800	-0.89943000	-3.02606800
C	-1.10007100	-1.87492700	-1.41279900
H	-1.37420800	-2.66394600	-2.12206300
C	-0.95603500	-2.53254300	-0.05335400
C	1.19753600	-2.40730200	-2.26077500
C	1.94842200	-2.91933500	-1.19682500
H	1.84656000	-2.49749100	-0.19965300
C	2.79822400	-4.00373100	-1.38889800
H	3.35848900	-4.39589700	-0.54455800
C	2.91499900	-4.59092800	-2.64696200
H	3.57542100	-5.43937500	-2.79530100
C	2.17815100	-4.08332600	-3.71361400
H	2.26524000	-4.53179000	-4.69836700
C	1.32621800	-2.99781000	-3.51962000
H	0.74480000	-2.60947900	-4.35266300

C	-2.30960900	-0.94640900	-1.48788800
C	-3.61731300	0.30502500	-2.98719300
H	-3.49744200	1.11608900	-2.26335500
H	-4.58231000	-0.17707900	-2.79623000
C	-3.49753100	0.79203100	-4.41434900
H	-2.52523200	1.26714600	-4.56586400
H	-3.59452100	-0.03667400	-5.11972800
H	-4.28141900	1.52277900	-4.62876100
C	1.76004500	-1.20525700	2.51531900
C	2.89646600	-0.43447100	2.28579400
H	2.81474700	0.64842000	2.34960300
C	4.10926500	-1.06857900	2.02815300
H	5.00905200	-0.47859100	1.86601400
C	4.20089800	-2.46317500	1.99370900
C	3.05174800	-3.21415700	2.26335800
H	3.11241800	-4.29953700	2.26530200
C	1.83141700	-2.59767500	2.52265000
H	0.93622500	-3.18120700	2.71080200
C	5.50300100	-3.14171400	1.65565700
H	6.35862900	-2.54789600	1.98644500
H	5.56848800	-4.12819700	2.12035400
H	5.59582100	-3.27894400	0.57249200
C	-1.12398600	-4.00942000	0.05886600
C	-0.87859000	-4.88384000	-1.00797900
C	-1.50304900	-4.56548200	1.29210600
C	-1.00876000	-6.26193900	-0.84905400
H	-0.54521800	-4.50229300	-1.96861500
C	-1.63138000	-5.93916500	1.44843300
H	-1.69635600	-3.89118200	2.12018600
C	-1.38759700	-6.79820700	0.37670300
H	-0.80192200	-6.91662800	-1.69039900
H	-1.93413700	-6.34210600	2.41037900
H	-1.49316100	-7.87179400	0.49788500
O	-0.89818500	1.37384100	-1.82395200
C	4.22343500	3.92805600	-1.08107500
C	3.11749800	3.10824900	-1.29277300
C	2.39677300	3.16482900	-2.48404200
C	2.81058200	4.05155700	-3.47309700
C	3.92604100	4.86717300	-3.26948800
C	4.63680000	4.81250900	-2.07441400
C	4.83216600	3.71358500	0.27834300
C	3.95275900	2.63675400	0.95875200
C	2.84805300	2.22921500	-0.09116400
H	1.51834400	2.54702600	-2.65144800

H	2. 26253500	4. 10888800	-4. 40730800
H	4. 23800400	5. 55315600	-4. 05020000
H	5. 49884400	5. 45334900	-1. 91549000
H	4. 84654000	4. 62939200	0. 87875600
H	4. 54210800	1. 74858000	1. 18835000
H	5. 86806000	3. 37075000	0. 20727600
H	2. 92023100	1. 16171400	-0. 30847700
N	1. 50241000	2. 46955400	0. 45549500
O	3. 43016000	3. 03703500	2. 20807700
C	0. 30475400	2. 01981300	0. 04696000
C	1. 25565700	3. 40358900	1. 42112100
N	-0. 60050900	2. 71150300	0. 73211800
N	-0. 02014100	3. 56445500	1. 61015800
C	2. 41623100	4. 01786500	2. 12867900
H	2. 76025000	4. 91935400	1. 60278200
H	2. 12863800	4. 28487200	3. 14509800
C	-2. 02735400	2. 51317800	0. 75986700
C	-2. 81081100	2. 99350300	-0. 28098300
C	-2. 57404000	1. 85563400	1. 84935800
C	-4. 17838900	2. 76926700	-0. 23422300
C	-3. 94770300	1. 63589000	1. 86881900
C	-4. 76932300	2. 06560500	0. 82474100
H	-4. 79233400	3. 12953500	-1. 05464100
H	-4. 36492800	1. 09557200	2. 70957600
H	-1. 92936300	1. 51218200	2. 65052400
H	-2. 35072700	3. 50843000	-1. 11666700
C	-6. 26548000	1. 75468700	0. 77131000
C	-6. 52146500	0. 86400300	-0. 45784500
C	-7. 07023600	3. 05790000	0. 64439100
C	-6. 74439500	1. 00925900	2. 02042200
H	-5. 89775500	-0. 03409600	-0. 41460500
H	-6. 28518300	1. 39312200	-1. 38692800
H	-7. 57474100	0. 56628200	-0. 49649900
H	-6. 89960800	3. 70582800	1. 50967300
H	-8. 14008200	2. 83134400	0. 59050500
H	-6. 80194500	3. 61719800	-0. 25638800
H	-7. 81865400	0. 81875700	1. 93952700
H	-6. 57524500	1. 59691500	2. 92837200
H	-6. 24058700	0. 04466300	2. 13181300
H	1. 32961400	-0. 44351600	-0. 35776700
H	1. 71705200	0. 21629100	-1. 96254500

M6SR

C	-6. 35810500	1. 75206500	-0. 05738500
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C	-5.01713800	1.83861500	-0.42468200
C	-4.59317300	2.70304900	-1.42812600
C	-5.54631500	3.48331600	-2.07748900
C	-6.89333600	3.39839600	-1.71808700
C	-7.30795900	2.53726700	-0.70442600
C	-6.55094000	0.76830600	1.06950700
C	-5.21227300	0.00371600	1.17422000
C	-4.17397000	0.90561100	0.41216500
H	-3.54158100	2.77196200	-1.69014700
H	-5.24055400	4.16402200	-2.86504900
H	-7.62508700	4.01166600	-2.23408200
H	-8.35608900	2.47675700	-0.42699200
H	-7.37182000	0.06463500	0.90189700
H	-4.87201400	-0.13770300	2.19883100
H	-6.75875900	1.29237100	2.00811400
H	-3.52953000	1.41579200	1.12432900
N	-3.30238500	0.07177800	-0.43147600
O	-5.32116500	-1.31856100	0.65423600
C	-1.98966000	0.12758600	-0.71021800
C	-3.79982500	-1.03030700	-1.06075800
N	-1.75071400	-0.93353000	-1.48942500
N	-2.86780200	-1.66971700	-1.71236800
C	-5.20653900	-1.42012900	-0.75032100
H	-5.92386700	-0.77479200	-1.27507700
H	-5.37825700	-2.45919200	-1.03211500
C	-0.47939400	-1.37202900	-2.00239600
C	0.31959000	-2.16600300	-1.19440200
C	-0.05280300	-0.91901600	-3.24527200
C	1.60862700	-2.46601400	-1.62735300
C	1.23495200	-1.23222800	-3.65536100
C	2.09902600	-1.98688000	-2.84584500
H	2.24186700	-3.05175200	-0.97174600
H	1.58106200	-0.86041500	-4.61486800
H	-0.70668700	-0.30682800	-3.85806400
H	-0.03272400	-2.49446000	-0.22125900
C	3.53926100	-2.22651300	-3.29998500
C	3.53850000	-2.94379300	-4.65946900
C	4.32174700	-3.07147400	-2.29161200
C	4.24528900	-0.86530900	-3.42783300
H	3.03713600	-2.35499400	-5.43300900
H	3.03232900	-3.91125100	-4.58672700
H	4.56800500	-3.11936200	-4.98730900
H	5.27665100	-1.01091500	-3.76509200
H	4.27082700	-0.35823600	-2.45710700

H	3.74379700	-0.21162700	-4.14773600
C	1.17989500	2.10880300	0.27099200
C	0.35123000	1.31790200	-0.75563000
H	0.59029700	2.20771100	1.18333400
C	1.58674600	3.49551500	-0.19088100
C	1.45018300	4.57923800	0.67848600
C	2.19179300	3.70549400	-1.43354800
C	1.90479500	5.84575300	0.31564300
H	0.99088600	4.42232700	1.65106500
C	2.64124300	4.96913200	-1.80273200
H	2.32978400	2.86964600	-2.11700000
C	2.49930900	6.04505800	-0.92766000
H	1.78891100	6.67673200	1.00451500
H	3.10772800	5.11465300	-2.77221100
H	2.85005100	7.03135500	-1.21458200
C	-1.09758900	1.30820900	-0.35615200
O	-1.66537500	2.27064400	0.10624100
H	5.34382300	-3.21429800	-2.65518600
H	3.87287200	-4.06123100	-2.15721800
H	4.37903800	-2.57794500	-1.31650500
H	0.40107700	1.77383900	-1.75374100
C	2.23751700	-0.14527000	1.11625100
C	3.44400200	-1.02282400	1.09383500
C	3.32658500	-2.39467600	1.38190800
C	4.72445700	-0.53070900	0.80002700
C	4.43610600	-3.22733600	1.39715900
H	2.33937200	-2.79175100	1.58808300
C	5.83923200	-1.37089500	0.81303300
H	4.88124600	0.51998800	0.57999600
C	5.70596500	-2.72021000	1.11449300
H	4.31044300	-4.28146200	1.62674900
H	6.81768000	-0.95629600	0.59019100
H	6.57443700	-3.37070800	1.12472600
N	1.16532700	-0.68408300	1.59079600
N	-0.02276200	-0.03339100	1.59875300
S	-1.06976800	-0.79670400	2.59701500
O	-0.61807800	-0.83980800	3.98842300
O	-2.38028600	-0.18113800	2.31353400
C	-1.18429100	-2.49560800	2.05819800
C	-0.14747400	-3.38446000	2.34037200
C	-0.16815000	-4.65207400	1.76962900
C	-1.22122900	-5.05594800	0.93891500
C	-2.27166100	-4.16372900	0.71227900
C	-2.25920200	-2.88759200	1.26924100

H	0.65867500	-3.07270600	2.99506800
H	0.64401500	-5.34562400	1.97356300
H	-3.10932200	-4.46876200	0.09008800
H	-3.08804400	-2.20216200	1.12296000
C	-1.23816500	-6.43980400	0.34383600
H	-1.62588700	-7.16580400	1.06575500
H	-0.23197800	-6.76096100	0.06343800
H	-1.87339400	-6.48083300	-0.54368900
C	2.44719800	1.28677600	0.62689200
H	3.07254700	1.25504800	-0.27439500
C	3.19026700	2.10671200	1.67485400
O	2.85919500	2.19636600	2.83060700
O	4.20443400	2.79889000	1.13244200
C	4.79973600	3.79570400	1.97845300
C	5.68700100	4.64823300	1.09940800
H	3.99735300	4.38110100	2.43773900
H	5.35487300	3.29645300	2.77821900
H	6.16348500	5.42987600	1.69573900
H	5.09011400	5.11934600	0.31391900
H	6.46773000	4.04304800	0.63252300
H	0.73595800	0.30471300	-0.84304400

M6SS

C	-1.40845400	-0.94121600	1.84442900
C	-0.52092300	-1.52841500	0.74771300
H	-0.78979300	-0.74907700	2.72751500
C	-2.52289200	-1.89365100	2.23410900
C	-2.92027400	-1.99774100	3.56940800
C	-3.24452000	-2.59191500	1.26040200
C	-4.02403700	-2.76868300	3.92641000
H	-2.36190100	-1.46183700	4.33380800
C	-4.35616200	-3.35320800	1.61328500
H	-2.94418400	-2.52486000	0.21597000
C	-4.75104800	-3.44143400	2.94654200
H	-4.31810100	-2.84072100	4.96883000
H	-4.91654100	-3.87504100	0.84315900
H	-5.61710500	-4.03487300	3.22098900
C	0.91363400	-1.09308300	0.88093400
O	1.42500400	-0.75118600	1.92662400
H	-0.50556400	-2.62499200	0.83662000
C	-1.19555000	1.66755400	1.38436900
C	-1.59707200	2.81199200	2.25778500
C	-1.45704600	4.12492000	1.78495400
C	-2.09895000	2.62896000	3.55335500

C	-1.80673600	5.21097400	2.57746100
H	-1.07286100	4.27181200	0.78073600
C	-2.44712900	3.71818900	4.34907600
H	-2.19186600	1.62824500	3.96872100
C	-2.30622100	5.01460100	3.86445000
H	-1.69762500	6.21751200	2.18455400
H	-2.82301900	3.54981600	5.35362900
H	-2.58334000	5.86349200	4.48122000
N	-0.19932200	1.91338300	0.60984300
N	0.26353900	1.03483800	-0.30806600
S	1.58052700	1.73295600	-1.00915000
O	2.66487000	2.01826800	-0.04987200
O	1.93053100	0.87192600	-2.15373100
C	1.07005700	3.30955000	-1.66347900
C	1.13078300	4.44113400	-0.85550000
C	0.68275000	5.65635100	-1.36222100
C	0.18231000	5.75397800	-2.66427500
C	0.13676600	4.60147900	-3.45423700
C	0.57560400	3.37750500	-2.96111300
H	1.52286800	4.35720500	0.15236300
H	0.72146700	6.54531100	-0.73801300
H	-0.24818800	4.66566300	-4.46832200
H	0.54791000	2.48047000	-3.57103700
C	-0.26863900	7.08132800	-3.21657900
H	0.56221700	7.59701400	-3.70932200
H	-0.63860100	7.73498700	-2.42327200
H	-1.06216100	6.95309900	-3.95641300
C	-2.07867700	0.42008800	1.48272700
H	-2.72975800	0.61128700	2.33161600
C	-2.97720300	0.27789200	0.24845700
O	-2.55131100	0.08648700	-0.86448800
O	-4.31589700	0.34367400	0.39691900
C	-4.96693800	0.50461500	1.66406300
C	-6.45522100	0.47707600	1.38898300
H	-4.68513500	-0.31747700	2.33147200
H	-4.66546300	1.45617900	2.11750400
H	-7.00829400	0.59736700	2.32331000
H	-6.73394700	-0.47748600	0.93650400
H	-6.73530000	1.28317300	0.70777100
C	6.11652900	-1.30576400	1.61657600
C	4.74191600	-1.52734700	1.58119100
C	4.16406700	-2.60109000	2.25101300
C	4.99320500	-3.46756900	2.95818900
C	6.37292800	-3.25248300	2.99598900

C	6.94274400	-2.16997500	2.33005500
C	6.49116700	-0.07389000	0.83317900
C	5.21252100	0.33027400	0.06094500
C	4.04767600	-0.47082000	0.75253700
H	3.08899900	-2.75312700	2.22798800
H	4.56482500	-4.31314300	3.48626300
H	7.00690500	-3.93603400	3.55172800
H	8.01576400	-2.00587600	2.36223300
H	7.31398400	-0.23981800	0.13075200
H	4.98818500	1.39253200	0.13344700
H	6.79863500	0.73386700	1.50528900
H	3.42756800	0.20484900	1.33831900
N	3.17305300	-1.08873100	-0.25759600
O	5.34055600	0.09514000	-1.33338300
C	1.85527600	-1.34988500	-0.27778200
C	3.67827700	-1.52278900	-1.44591400
N	1.62732600	-1.94916100	-1.44961400
N	2.75352100	-2.05024100	-2.19603800
C	5.11291900	-1.23652200	-1.73541200
H	5.76603400	-1.94728500	-1.20826800
H	5.29616200	-1.30607500	-2.80744500
C	0.35184700	-2.27664500	-2.03472100
C	-0.21784800	-3.52637100	-1.82049300
C	-0.30385100	-1.27897700	-2.73672100
C	-1.50944400	-3.74785200	-2.27947200
C	-1.59233700	-1.52971900	-3.19646700
C	-2.23008000	-2.74763700	-2.95382400
H	-1.97108500	-4.71243500	-2.09006900
H	-2.11410500	-0.72891500	-3.70423000
H	0.17552600	-0.31313400	-2.85490900
H	0.32592300	-4.29240600	-1.27665600
C	-3.68522900	-3.00121800	-3.35429100
C	-4.51520500	-3.21190500	-2.07573200
C	-3.77138600	-4.25369200	-4.24079300
C	-4.28414400	-1.81527900	-4.11628800
H	-4.49362400	-2.31130300	-1.45156200
H	-4.13437000	-4.05373100	-1.48683900
H	-5.55737800	-3.42586900	-2.33591500
H	-3.17863900	-4.12587700	-5.15168400
H	-4.81157000	-4.43477000	-4.53016100
H	-3.40981700	-5.14631400	-3.72230300
H	-5.32235800	-2.04021200	-4.37777600
H	-3.73984200	-1.61516200	-5.04473200
H	-4.27931900	-0.90896700	-3.50320900

H	-0.90596200	-1.27956300	-0.23966700
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TS7RR

C	-3.81116100	-3.18784900	1.84402600
C	-3.00488700	-2.80531800	0.77108500
C	-3.41219900	-2.99238500	-0.54361700
C	-4.66968000	-3.55085300	-0.77728300
C	-5.48883500	-3.91707600	0.29089300
C	-5.06318300	-3.74263000	1.60854800
C	-3.11330000	-2.89842500	3.15300100
C	-1.63420000	-2.74368200	2.75398800
C	-1.72792700	-2.19182000	1.30258300
H	-2.76610200	-2.72422200	-1.37531000
H	-5.00700600	-3.70827200	-1.79676900
H	-6.46196400	-4.35603400	0.09523900
H	-5.69662700	-4.04645200	2.43658400
H	-3.23023000	-3.68423900	3.90257000
H	-1.08482500	-2.04745500	3.39136500
H	-3.47962900	-1.95822800	3.58183400
H	-1.79498100	-1.09939300	1.34730200
N	-0.53626200	-2.54926300	0.53843500
O	-0.95243500	-3.99476700	2.85816400
C	0.33450500	-1.80360900	-0.16216600
C	0.04889400	-3.76534500	0.74333600
N	1.36060900	-2.60825900	-0.41874500
N	1.21280800	-3.83401100	0.16811700
C	-0.65025500	-4.70198200	1.66956500
H	-1.55288700	-5.10432800	1.19072200
H	0.01251600	-5.52440000	1.93881500
C	2.63836500	-2.26154100	-0.98314600
C	2.79739800	-2.13681500	-2.35168900
C	3.69511600	-2.06759200	-0.10318500
C	4.05002300	-1.79459000	-2.85189700
C	4.93573400	-1.72408600	-0.62240300
C	5.13897900	-1.57749400	-2.00132200
H	4.16449000	-1.69056100	-3.92422300
H	5.75625300	-1.55396600	0.06831400
H	3.52377200	-2.15484700	0.96504500
H	1.95049400	-2.28074200	-3.01358900
C	6.52390300	-1.17749800	-2.51626800
C	6.89049700	0.20396700	-1.94674600
C	6.57232100	-1.09818600	-4.04530300
C	7.56085800	-2.21393500	-2.05156300
H	6.89601700	0.19940400	-0.85238200

H	6.17349400	0.96057500	-2.28147100
H	7.88770000	0.49977100	-2.28910900
H	8.55437700	-1.94067600	-2.42178000
H	7.31261800	-3.20867400	-2.43379000
H	7.61411400	-2.27320200	-0.96106000
C	-1.63096600	1.10695200	-1.79918000
C	-1.24749600	-0.27265600	-1.28294900
C	0.15994000	-0.35582100	-0.67079100
O	1.10873500	0.13823000	-1.31335300
H	7.57939700	-0.81247800	-4.36276800
H	5.87508600	-0.34911500	-4.43297500
H	6.33770300	-2.06319000	-4.50576300
C	-0.88504700	2.53226100	0.25909900
C	-0.72243200	4.00235800	0.48852900
C	-0.27673200	4.45629300	1.73770100
C	-0.97013700	4.94327200	-0.51599900
C	-0.10160100	5.81268500	1.97631300
H	-0.07304100	3.72269100	2.51102200
C	-0.78387500	6.30328700	-0.27839700
H	-1.28262300	4.62288000	-1.50549000
C	-0.35625300	6.74363200	0.96944700
H	0.23289900	6.14714100	2.95329700
H	-0.97093500	7.01740800	-1.07408600
H	-0.21912100	7.80378500	1.15721800
N	-0.09996900	1.80758900	0.95842200
N	-0.05574500	0.44280500	0.95837800
H	-1.20429400	-0.95239100	-2.14518200
S	0.97368100	0.07925900	2.25098700
O	0.32780600	0.47557400	3.50037100
O	1.34245000	-1.33789200	2.12015100
C	2.45309800	1.05835300	2.07402900
C	2.96465900	1.68534500	3.20424200
C	4.18009100	2.35467600	3.10679200
C	4.87823100	2.40418700	1.89707300
C	4.32986000	1.76912500	0.77831500
C	3.11659500	1.09451300	0.85182400
H	2.41323600	1.64346500	4.13733000
H	4.59389100	2.84527900	3.98353500
H	4.85934000	1.80572700	-0.17032000
H	2.67852400	0.62722500	-0.02945200
C	6.17873500	3.15739900	1.79056100
H	5.99497100	4.20913600	1.54772600
H	6.81203700	2.74291200	1.00224600
H	6.73258800	3.12816500	2.73181600

C	-2.01053400	2.10181100	-0.66896700
C	-3.18845300	1.55913300	0.13156700
O	-3.14152700	0.65847000	0.94038700
O	-4.32545200	2.16285700	-0.22197100
C	-5.53113100	1.59785700	0.32120000
C	-6.68798400	2.26246600	-0.39031300
H	-5.51165600	0.51554400	0.15571300
H	-5.54632500	1.77193800	1.40098100
H	-7.63378400	1.86306900	-0.01718900
H	-6.62514900	2.07460500	-1.46505000
H	-6.67541500	3.34161300	-0.22293900
H	-2.00892400	-0.64966500	-0.60219000
H	-2.39130700	2.99461700	-1.16453400
H	-0.75347300	1.52738500	-2.30325200
C	-2.78143600	1.02036400	-2.78780700
C	-2.79685600	1.83172200	-3.92366700
C	-3.86988700	0.17088200	-2.55909500
C	-3.86832600	1.79510800	-4.81301300
H	-1.95687400	2.49579800	-4.11401600
C	-4.94267100	0.13199700	-3.44459300
H	-3.88853900	-0.46748400	-1.67775000
C	-4.94529800	0.94525000	-4.57608600
H	-3.85958100	2.42913800	-5.69394400
H	-5.77659700	-0.53568100	-3.24856800
H	-5.77959400	0.91425700	-5.26937400

TS7RS

S	0.07076900	0.52054300	2.33529800
O	0.88799600	2.42561600	-2.86501000
O	0.70922300	2.76277600	-0.64748300
O	1.08548100	-0.53905500	2.40087400
O	-1.03022800	0.47492700	3.29919300
N	-0.50126400	0.49466400	0.78557300
N	-1.51751500	1.39691000	0.66835900
C	0.22378300	-0.53973200	-0.56544600
C	-1.05609100	-0.73376000	-1.39576900
H	-0.93771100	-1.67627600	-1.94599800
H	-1.94876300	-0.82873300	-0.76821800
C	-1.22337500	0.38454700	-2.41993600
H	-0.37225800	0.33797400	-3.10566600
C	-1.16444000	1.80267300	-1.78871200
H	-1.69027500	2.43963700	-2.50368200
C	-1.84369100	1.95912100	-0.44004400
C	-2.49409500	0.16784600	-3.21745000

C	-3.75566300	0.25371300	-2.61763000
H	-3.83740300	0.49535900	-1.55983500
C	-4.91111300	0.04262900	-3.36340300
H	-5.88194200	0.11882300	-2.88390800
C	-4.82364900	-0.26228200	-4.72062600
H	-5.72569500	-0.42741800	-5.30123100
C	-3.57411100	-0.35129100	-5.32624400
H	-3.49594300	-0.58520300	-6.38344700
C	-2.41904000	-0.13622100	-4.57760400
H	-1.44404600	-0.20159000	-5.05335200
C	0.26954900	2.33924100	-1.83041500
C	2.09063900	3.15139100	-0.59490900
H	2.65897500	2.48167800	-1.24457800
H	2.38258500	2.98633000	0.44322700
C	2.25564700	4.60643700	-0.98792600
H	1.96812700	4.75671900	-2.03067700
H	1.63251800	5.23885600	-0.34906300
H	3.29881100	4.91153700	-0.86543500
C	0.92270300	2.06876500	2.55293700
C	0.24794300	3.27590600	2.36644100
H	-0.80144100	3.27850600	2.09009900
C	0.95183500	4.46180400	2.52183400
H	0.44206000	5.40920400	2.36787400
C	2.30843600	4.46312400	2.87428600
C	2.94800500	3.24030500	3.08213700
H	3.99550800	3.22587000	3.36939700
C	2.26348300	2.03737100	2.91721600
H	2.75481300	1.08171500	3.06582400
C	3.05340100	5.76556800	3.00601000
H	3.19764800	6.22636600	2.02320600
H	2.49471100	6.47618700	3.62097500
H	4.03657500	5.61805300	3.45723400
C	-2.96700300	2.93508600	-0.32025200
C	-3.06224800	4.05202100	-1.15868900
C	-3.93578200	2.76606200	0.67977900
C	-4.09797100	4.96977000	-1.00674300
H	-2.31219800	4.23536600	-1.92110600
C	-4.97174000	3.68027200	0.82650000
H	-3.85815400	1.90638700	1.33715800
C	-5.05995800	4.78533100	-0.01878300
H	-4.14730200	5.83338900	-1.66212800
H	-5.71710000	3.52745500	1.60066500
H	-5.87136300	5.49711500	0.09354000
O	1.21603700	-0.02488900	-1.10168600

C	-3.67722300	-3.64087600	1.88449600
C	-2.80754400	-3.21185700	0.88027500
C	-3.00435200	-3.57394800	-0.44650700
C	-4.10316200	-4.37329000	-0.76216000
C	-4.98173800	-4.79472500	0.23548200
C	-4.77430100	-4.43221200	1.56620000
C	-3.23025300	-3.12513900	3.23116300
C	-1.76066800	-2.72989500	3.00763700
C	-1.72226700	-2.34760900	1.49268900
H	-2.31800100	-3.25491900	-1.22412700
H	-4.27289000	-4.66938100	-1.79194300
H	-5.83065500	-5.41805900	-0.02615200
H	-5.45228400	-4.77326200	2.34282900
H	-3.31002700	-3.85997500	4.03552700
H	-1.44463400	-1.88165900	3.61614600
H	-3.81231300	-2.24241400	3.52036700
H	-1.93892900	-1.28045000	1.39464200
N	-0.38628700	-2.58958300	0.94587000
O	-0.88794800	-3.80573500	3.35069900
C	0.48416600	-1.82223000	0.25752200
C	0.28677800	-3.71350900	1.33689000
N	1.61483600	-2.52766800	0.22244600
N	1.51123400	-3.70677000	0.90665700
C	-0.40206500	-4.62074400	2.30030800
H	-1.20360900	-5.18210000	1.80381900
H	0.31666700	-5.31781900	2.73067900
C	2.90546900	-2.18100900	-0.30841000
C	3.52250200	-3.07529200	-1.17251400
C	3.53949000	-1.02269700	0.11241500
C	4.79504300	-2.78128900	-1.64205400
C	4.81389500	-0.74700300	-0.37160700
C	5.46502300	-1.61212200	-1.25697000
H	5.27098500	-3.47834400	-2.32490800
H	5.29862700	0.16482100	-0.04343500
H	3.02954200	-0.35320900	0.79616100
H	3.00942400	-3.98429400	-1.46813600
C	6.86283900	-1.32827700	-1.81309500
C	6.78299200	-1.22747300	-3.34581900
C	7.80838300	-2.47718200	-1.42434400
C	7.44509700	-0.01868500	-1.27237000
H	6.11047300	-0.41865500	-3.64626800
H	6.41637800	-2.15665600	-3.79113200
H	7.77598600	-1.02395700	-3.76012700
H	7.87512000	-2.57434300	-0.33652100

H	8.81253500	-2.28393100	-1.81572600
H	7.46839600	-3.43412600	-1.83009600
H	8.44007700	0.13850500	-1.69901200
H	7.54818200	-0.04239400	-0.18287200
H	6.82502300	0.84082700	-1.54508600

TS7SR

C	6.56980600	-0.66379300	0.62691800
C	5.21637200	-0.98252100	0.55475200
C	4.77675800	-2.30172400	0.60056400
C	5.72954100	-3.31321800	0.69033100
C	7.09084700	-3.00219200	0.74629300
C	7.51987400	-1.67732700	0.72341000
C	6.78011800	0.82927600	0.61728900
C	5.39884900	1.43733700	0.27090000
C	4.37017400	0.26509900	0.46353000
H	3.71212900	-2.51691900	0.59430400
H	5.41327100	-4.35070200	0.72640700
H	7.82126300	-3.80210700	0.81657800
H	8.57822800	-1.43958500	0.77857700
H	7.52496900	1.15985700	-0.11399000
H	5.12640700	2.25924600	0.93194200
H	7.11604500	1.18018700	1.59833400
H	3.74957400	0.41724200	1.34229500
N	3.45253500	0.19526100	-0.68948300
O	5.39156100	2.01620500	-1.02679600
C	2.16656600	-0.18524600	-0.80321400
C	3.89500100	0.50137200	-1.94346500
N	1.89772300	-0.10429100	-2.10954400
N	2.96500700	0.32912700	-2.83566600
C	5.26392600	1.08010700	-2.07505200
H	6.03050900	0.29360600	-2.02347400
H	5.35549100	1.61069700	-3.02267500
C	0.65461900	-0.34950400	-2.78778100
C	0.45117200	-1.57668100	-3.40153900
C	-0.30609000	0.65310800	-2.81600600
C	-0.77128400	-1.82570200	-4.01903900
C	-1.51515300	0.38438500	-3.44414400
C	-1.78072800	-0.85690300	-4.03792400
H	-0.92972100	-2.79306200	-4.48106300
H	-2.27722500	1.15754700	-3.45106100
H	-0.10454200	1.60484200	-2.33347800
H	1.22988900	-2.33232500	-3.37260800
C	-3.15592500	-1.10055400	-4.66138300

C	-3.28539500	-2.51088300	-5.24384100
C	-3.39110100	-0.08237800	-5.78985700
C	-4.22686700	-0.91475600	-3.57242000
H	-3.15117900	-3.27839200	-4.47496400
H	-2.55707900	-2.68660600	-6.04197300
H	-4.28445300	-2.63762000	-5.67061800
H	-5.22367900	-1.08669100	-3.99268300
H	-4.20711200	0.09416900	-3.14901200
H	-4.07229700	-1.62212500	-2.75086000
C	-0.72417400	-1.70640600	1.31355400
C	0.20288100	-1.65211500	0.09061400
H	-0.21964100	-1.17283100	2.12428400
C	-1.04757800	-3.10143600	1.80943300
C	-1.05800500	-3.36257900	3.18118800
C	-1.42670000	-4.11727600	0.92888300
C	-1.44492900	-4.60973100	3.66603200
H	-0.76194600	-2.57592200	3.87158700
C	-1.81055200	-5.36619400	1.40831100
H	-1.42709800	-3.92629300	-0.14261500
C	-1.82445800	-5.61491400	2.77958500
H	-1.44568100	-4.79707800	4.73547400
H	-2.10217000	-6.14639600	0.71202300
H	-2.12493200	-6.58846900	3.15366800
C	1.30545600	-0.63146200	0.40182000
O	2.00450500	-0.86243100	1.41055200
H	-4.37580300	-0.24530000	-6.23978400
H	-2.63304500	-0.18673300	-6.57206400
H	-3.35770300	0.94541800	-5.41815900
H	0.73564400	-2.59953400	-0.04556500
C	-1.98239400	0.34222100	0.26989400
C	-3.25663600	0.86309900	-0.31526900
C	-3.25475200	2.07650600	-1.02303800
C	-4.47451500	0.18954900	-0.16009300
C	-4.42616600	2.58817500	-1.56352300
H	-2.31510600	2.60865200	-1.13215500
C	-5.65161900	0.71002800	-0.69768100
H	-4.53181700	-0.74422300	0.38883100
C	-5.63424300	1.90606300	-1.40417500
H	-4.39973300	3.52756700	-2.10711600
H	-6.58376800	0.17097000	-0.56117000
H	-6.55042100	2.30786700	-1.82492500
N	-0.96401700	1.09697300	0.09469700
N	0.26525500	0.86432300	0.65589100
H	-0.36061300	-1.44640400	-0.82254100

S	1. 10627200	2. 30977400	0. 52329100
O	2. 32504100	2. 15369400	1. 31872300
O	1. 28201400	2. 73756200	-0. 87261600
C	0. 01017600	3. 46935800	1. 31140200
C	-0. 71230300	3. 08710000	2. 44081700
C	-1. 51703500	4. 03010700	3. 06413300
C	-1. 60343800	5. 34259500	2. 58304400
C	-0. 87204200	5. 69099100	1. 44641300
C	-0. 06408000	4. 75866300	0. 80087300
H	-0. 67736900	2. 06036600	2. 79360800
H	-2. 10075500	3. 74030300	3. 93330100
H	-0. 94102600	6. 70199300	1. 05506400
H	0. 49304500	5. 01781100	-0. 09322500
C	-2. 46753900	6. 35359400	3. 29020600
H	-2. 13786700	6. 48560700	4. 32573600
H	-3. 51023700	6. 02657500	3. 31846800
H	-2. 42514400	7. 32735400	2. 79791100
C	-2. 06218700	-0. 98959100	0. 99370000
H	-2. 64190500	-1. 67198700	0. 36094600
C	-2. 79803900	-0. 82354000	2. 31418500
O	-2. 51921400	0. 00685400	3. 14657500
O	-3. 72827600	-1. 76962500	2. 48302300
C	-4. 29638300	-1. 86845100	3. 79966100
C	-5. 09926400	-3. 14926300	3. 83376300
H	-3. 47766400	-1. 87813900	4. 52567200
H	-4. 90814400	-0. 98160000	3. 98983900
H	-5. 54385400	-3. 28588100	4. 82213500
H	-4. 44888400	-4. 00067900	3. 61662500
H	-5. 90114900	-3. 12284300	3. 09224400

NTS7SR

C	-0. 26043700	1. 63095600	-1. 21913500
C	0. 46858000	0. 45474800	-1. 89927100
H	-1. 18102300	1. 81022500	-1. 78162300
C	0. 48943600	2. 95078200	-1. 26424100
C	0. 50076700	3. 85564600	-0. 20211600
C	1. 11055700	3. 33439700	-2. 46048700
C	1. 09965600	5. 10653400	-0. 33306900
H	0. 00969000	3. 60935600	0. 73299300
C	1. 71626800	4. 57873600	-2. 59380100
H	1. 10014400	2. 65397700	-3. 30836500
C	1. 70699400	5. 47684500	-1. 52831500
H	1. 07525200	5. 79764300	0. 50440100
H	2. 18268400	4. 85407700	-3. 53526000

H	2.16103800	6.45818100	-1.63368700
C	0.42836600	-0.87749700	-1.11579100
O	0.13700100	-1.91253600	-1.78784700
H	1.50298900	0.70433700	-2.14210000
C	-0.86694700	-0.36625200	0.19280600
C	-0.69174200	-1.09162600	1.49436100
C	-1.25242200	-2.36786900	1.67527800
C	0.07805300	-0.56774100	2.54105300
C	-1.03418300	-3.08281500	2.84871300
H	-1.87694400	-2.78340000	0.89196500
C	0.31312600	-1.29520000	3.70432200
H	0.49970900	0.42817900	2.46516100
C	-0.23864100	-2.56156000	3.86564600
H	-1.49227100	-4.06084300	2.96800500
H	0.92313100	-0.85978300	4.49034200
H	-0.05704100	-3.13113700	4.77081400
N	-2.02074100	-0.87076200	-0.45264400
N	-2.58820800	-0.11055700	-1.24499600
S	-3.98941800	-0.89454600	-1.96967700
O	-3.95922600	-0.48837800	-3.36759000
O	-4.08228300	-2.29690600	-1.59043400
C	-5.26049400	0.00772100	-1.12384600
C	-5.55025500	1.31237500	-1.51869300
C	-6.51665800	2.02104900	-0.81597300
C	-7.18487800	1.44620000	0.27258800
C	-6.87449900	0.13374500	0.63937000
C	-5.90897500	-0.59273500	-0.05039400
H	-5.03112500	1.75374100	-2.36311500
H	-6.75570700	3.03862400	-1.11124700
H	-7.39326800	-0.32512600	1.47634600
H	-5.66213600	-1.61343200	0.22297400
C	-8.19534000	2.24588000	1.05175000
H	-8.81886400	2.84942900	0.38792400
H	-7.68890300	2.93179500	1.73919600
H	-8.84464300	1.59746700	1.64328000
C	-0.71058200	1.15508100	0.17580500
H	0.06028700	1.43323000	0.90457800
C	-2.00021500	1.85325200	0.60418900
O	-2.42542500	2.87808400	0.12690800
O	-2.61262300	1.19215800	1.59327900
C	-3.89409200	1.70360900	1.99015500
C	-4.44790600	0.74600700	3.02123100
H	-3.76700700	2.71559300	2.38717900
H	-4.53231500	1.76666500	1.10313000

H	-5.45039100	1.06242500	3.32218200
H	-3.80699900	0.71307900	3.90539900
H	-4.51245100	-0.26031700	2.59999300
H	-0.02464800	0.19126800	-2.83706000
C	2.52730700	-5.64434400	-0.79228700
C	2.12674000	-4.36092300	-1.15350100
C	2.52003300	-3.79145400	-2.36116400
C	3.35286600	-4.52886400	-3.19842600
C	3.77110300	-5.81212300	-2.83545200
C	3.35558300	-6.38139700	-1.63500200
C	1.92714300	-6.05725200	0.52530800
C	1.26960900	-4.77809400	1.09695400
C	1.24270200	-3.74453800	-0.09097800
H	2.14888900	-2.80920300	-2.63755800
H	3.67354800	-4.10839400	-4.14614100
H	4.41971100	-6.37394700	-3.50028800
H	3.67181600	-7.38331900	-1.35981600
H	2.66216700	-6.44802800	1.23665100
H	0.24776300	-4.96067200	1.42835600
H	1.17489000	-6.83920700	0.38075600
H	0.23549100	-3.56032900	-0.45793100
N	1.78595800	-2.43530300	0.33201000
O	1.93350700	-4.32084900	2.26480400
C	1.59122900	-1.17825000	-0.13262400
C	2.76501300	-2.37822900	1.27808200
N	2.48151500	-0.43201800	0.54096600
N	3.21105400	-1.17095900	1.43448800
C	3.13193200	-3.62740400	2.00574100
H	3.83452200	-4.22704300	1.40830600
H	3.59743600	-3.37765400	2.95949400
C	2.89014200	0.94287400	0.42456800
C	3.46818000	1.40811100	-0.74660000
C	2.91142900	1.71859900	1.58178400
C	4.05971700	2.66860000	-0.76186300
C	3.52889900	2.95987000	1.55446300
C	4.13789300	3.45406000	0.39119600
H	4.50403600	3.01095900	-1.68866900
H	3.57072900	3.53423000	2.47435800
H	2.50696400	1.31821900	2.50546700
H	3.50851500	0.77422500	-1.62585800
C	4.98669300	4.72787500	0.45097100
C	5.39586900	5.20964500	-0.94534300
C	6.26088800	4.38951900	1.24854600
C	4.24916000	5.87426100	1.15838900

H	4. 51851200	5. 37286600	-1. 57949900
H	6. 05933500	4. 49563700	-1. 44270000
H	5. 93809800	6. 15575400	-0. 85904300
H	6. 01894900	4. 09428900	2. 27409900
H	6. 91914500	5. 26364200	1. 29019100
H	6. 80675700	3. 56662500	0. 77723200
H	4. 91959900	6. 73475300	1. 24916900
H	3. 92636200	5. 60244400	2. 16694400
H	3. 37161100	6. 18138100	0. 58679400

TS7SS

C	-1. 15459500	-1. 23861100	1. 72216800
C	-0. 32701400	-1. 45248700	0. 46211900
H	-0. 45655200	-1. 11706200	2. 55652100
C	-2. 05815800	-2. 42034100	2. 00639700
C	-2. 25879000	-2. 84898700	3. 32068200
C	-2. 77569800	-3. 04047700	0. 97791000
C	-3. 17885300	-3. 85416800	3. 60927500
H	-1. 69949500	-2. 37570600	4. 12407500
C	-3. 70287800	-4. 03876200	1. 26476700
H	-2. 61919800	-2. 72836500	-0. 05289000
C	-3. 91285500	-4. 44323600	2. 58196900
H	-3. 32570000	-4. 17426400	4. 63606800
H	-4. 26553600	-4. 49996600	0. 45809000
H	-4. 63754500	-5. 21989600	2. 80445200
C	0. 97603200	-0. 64443300	0. 51612700
O	1. 56408800	-0. 52871700	1. 61670100
H	-0. 02956500	-2. 50902400	0. 42230300
C	-1. 20956400	1. 36434500	1. 62751500
C	-1. 65353200	2. 44154800	2. 56316200
C	-0. 70346400	3. 27461900	3. 16507700
C	-3. 00865100	2. 66399000	2. 82528700
C	-1. 10210700	4. 30032600	4. 01460900
H	0. 34709300	3. 09007600	2. 96057900
C	-3. 40833600	3. 69622300	3. 66945400
H	-3. 76240900	2. 05284300	2. 33522900
C	-2. 45582800	4. 51365600	4. 27150100
H	-0. 35397700	4. 93155500	4. 48400700
H	-4. 46509300	3. 86518700	3. 85062700
H	-2. 76606200	5. 31353800	4. 93613200
N	-0. 23423300	1. 71569100	0. 88031800
N	0. 35190400	0. 97208900	-0. 10095900
S	1. 54448400	2. 00084300	-0. 73089000
O	2. 52444400	2. 40440800	0. 28362500

O	2.05250200	1.33670200	-1.93952900
C	0.66612100	3.45616100	-1.25457800
C	0.33021400	4.44121000	-0.33039500
C	-0.33002400	5.57902700	-0.77677300
C	-0.65228700	5.74504400	-2.12745600
C	-0.29155800	4.74365100	-3.03293600
C	0.36572100	3.59555800	-2.60543600
H	0.57934900	4.30779700	0.71597500
H	-0.59952400	6.35374500	-0.06457400
H	-0.52266400	4.86824300	-4.08716000
H	0.66690100	2.82358700	-3.30553500
C	-1.39062000	6.97062800	-2.59834300
H	-1.29056400	7.79133700	-1.88503900
H	-2.45811200	6.75597600	-2.71275200
H	-1.01729100	7.30803200	-3.56844500
C	-2.01247300	0.06232300	1.68575800
H	-2.55300500	0.08555100	2.63513900
C	-3.02304600	0.02500700	0.53418600
O	-2.70485100	0.25537000	-0.60719500
O	-4.31242700	-0.28580000	0.77561600
C	-4.84322100	-0.64081900	2.06267000
C	-6.24194900	-1.16424700	1.81631900
H	-4.22697000	-1.41011300	2.53216400
H	-4.86091200	0.24471100	2.70789300
H	-6.70545200	-1.44206000	2.76582100
H	-6.19890200	-2.04890700	1.17618400
H	-6.85981600	-0.40653100	1.32967300
C	6.16913100	-1.15081200	1.36554500
C	4.79300200	-1.35017000	1.29487500
C	4.17159200	-2.40127300	1.96015000
C	4.96690000	-3.28014200	2.69141500
C	6.35024600	-3.09526300	2.75863800
C	6.96017800	-2.02731600	2.10315200
C	6.57733100	0.08136100	0.59665400
C	5.33270400	0.47346100	-0.23510100
C	4.13912700	-0.28604000	0.44719700
H	3.09117900	-2.50487100	1.91621000
H	4.50899800	-4.11127100	3.21794200
H	6.95640900	-3.78901000	3.33274900
H	8.03507400	-1.88435400	2.16459700
H	7.43252800	-0.07824900	-0.06716000
H	5.13021900	1.54447000	-0.21338900
H	6.84487600	0.89189900	1.28279400
H	3.52716500	0.39724800	1.03457400

N	3.26223500	-0.87885900	-0.57225700
O	5.51144800	0.17521700	-1.61456600
C	1.92944200	-1.00525700	-0.64185300
C	3.77327100	-1.35314400	-1.74547600
N	1.69247600	-1.57445300	-1.82574700
N	2.83505800	-1.78367100	-2.53746900
C	5.23377600	-1.16118900	-1.98001600
H	5.82533900	-1.88130800	-1.39748200
H	5.46202200	-1.27774000	-3.03925800
C	0.40158300	-1.78678800	-2.42084300
C	-0.29238800	-0.67904800	-2.87910100
C	-0.17130600	-3.05289200	-2.40513700
C	-1.62133300	-0.83144800	-3.26116600
C	-1.49919200	-3.18211500	-2.78934100
C	-2.26076800	-2.07016100	-3.18669800
H	-2.16907400	0.05165900	-3.56379900
H	-1.96148600	-4.16393100	-2.74266100
H	0.39829800	-3.90527300	-2.04886600
H	0.19207400	0.29075600	-2.86843900
C	-3.75247400	-2.23870400	-3.48263900
C	-3.94290000	-3.25929300	-4.61604900
C	-4.40740700	-0.91478000	-3.88779500
C	-4.45522100	-2.73950500	-2.20833500
H	-3.53528100	-4.23965100	-4.35201100
H	-3.44712500	-2.92105900	-5.53107400
H	-5.00922800	-3.38643900	-4.82916700
H	-4.31189900	-0.17191300	-3.08976500
H	-5.47289800	-1.08015000	-4.07320000
H	-3.96792600	-0.50906900	-4.80476300
H	-5.52206100	-2.89043600	-2.40546400
H	-4.35357200	-2.00519800	-1.40094600
H	-4.03869300	-3.69442100	-1.86948300
H	-0.90667800	-1.22586800	-0.43129900

M7RR

C	-3.94900700	-2.82772800	1.96067000
C	-2.99825800	-2.59592000	0.96539200
C	-3.22603200	-2.96392100	-0.35551700
C	-4.45792200	-3.53161200	-0.68456500
C	-5.43161300	-3.72170200	0.29697900
C	-5.18026600	-3.38012600	1.62743600
C	-3.41226800	-2.40146700	3.30861000
C	-1.89192300	-2.30218400	3.08079800
C	-1.80008600	-1.90962300	1.58520000

H	-2.45867500	-2.83238900	-1.11396100
H	-4.65720900	-3.83044200	-1.70881300
H	-6.38655400	-4.16090100	0.02626600
H	-5.93075600	-3.55841100	2.39168700
H	-3.63943500	-3.10135700	4.11588300
H	-1.41627200	-1.54287400	3.70638100
H	-3.80600300	-1.41619300	3.58502300
H	-1.87894900	-0.82207900	1.50347600
N	-0.52351600	-2.32372400	1.02734600
O	-1.23932500	-3.53451400	3.39212800
C	0.39287600	-1.67366100	0.28949900
C	0.00527800	-3.53080500	1.38042100
N	1.39591500	-2.53862700	0.15347600
N	1.18362500	-3.69408400	0.85954800
C	-0.79173100	-4.36140100	2.33213600
H	-1.62928200	-4.83691900	1.80478900
H	-0.16005500	-5.13481100	2.76960000
C	2.69924100	-2.32830400	-0.41179100
C	2.85548800	-2.07431700	-1.76368800
C	3.79330600	-2.42124400	0.43988200
C	4.13923200	-1.90530400	-2.27183900
C	5.06650600	-2.24631500	-0.08630700
C	5.26721700	-1.98847400	-1.44946900
H	4.24770500	-1.70262000	-3.33042400
H	5.91756500	-2.30742100	0.58512600
H	3.63332400	-2.60230800	1.49712700
H	1.98570700	-1.98186000	-2.40289100
C	6.69117500	-1.79733700	-1.97844400
C	7.30674300	-0.55179600	-1.31836500
C	6.72203000	-1.60577400	-3.49787100
C	7.53852400	-3.03275900	-1.62961500
H	7.32783300	-0.64327100	-0.22845100
H	6.73038700	0.34238900	-1.57508600
H	8.33498300	-0.40992800	-1.66736600
H	8.55650900	-2.90740000	-2.01239600
H	7.11133700	-3.93528900	-2.07708900
H	7.60430300	-3.18826200	-0.54935700
C	-1.35624300	1.00199100	-1.86661400
C	-0.97852300	-0.32272500	-1.22415100
C	0.28806400	-0.23060200	-0.32339900
O	1.34058000	0.19610100	-0.88725700
H	7.75814200	-1.48837700	-3.82871500
H	6.17136300	-0.71090200	-3.80361800
H	6.29855200	-2.46977800	-4.01985600

C	-1.26363400	2.52343400	0.18638900
C	-1.43237800	3.98385200	0.45106700
C	-1.27418700	4.45963300	1.75914900
C	-1.72883700	4.89410600	-0.56743100
C	-1.41287800	5.81284300	2.03909100
H	-1.05387800	3.74287800	2.54432200
C	-1.85888200	6.25235500	-0.28637400
H	-1.83290700	4.55480900	-1.59433100
C	-1.70558200	6.71499500	1.01654800
H	-1.30053600	6.16614100	3.05931400
H	-2.07733100	6.94840300	-1.08997900
H	-1.81566800	7.77229000	1.23560100
N	-0.41953600	1.94994600	0.94998300
N	-0.12631800	0.61078200	1.01981600
H	-0.68616500	-1.03090900	-2.00946000
S	1.06502500	0.57483200	2.26261100
O	0.41938300	1.07082000	3.47144000
O	1.62190300	-0.77910800	2.27646300
C	2.35269900	1.71332400	1.81610400
C	2.30525600	3.00764500	2.31955600
C	3.33132600	3.88928300	1.99687300
C	4.39444800	3.48525300	1.18612300
C	4.40675600	2.17665800	0.68990600
C	3.38916800	1.28207200	0.99156800
H	1.47711100	3.30718800	2.95210100
H	3.30486800	4.90561700	2.37888100
H	5.22520500	1.85575700	0.05124900
H	3.37331600	0.28105000	0.57441000
C	5.52042900	4.43075900	0.85824600
H	5.78617800	4.37191300	-0.20048500
H	6.41613300	4.17917400	1.43531700
H	5.25204800	5.46369100	1.08916100
C	-2.14853700	1.88534400	-0.86090100
C	-3.25955600	1.10763200	-0.15709300
O	-3.26503100	0.80408400	1.01499800
O	-4.23315000	0.77608500	-1.00544600
C	-5.31430600	-0.00592600	-0.46023400
C	-6.12345000	-0.52232300	-1.62773700
H	-4.89803900	-0.81904600	0.14066400
H	-5.90397400	0.63746600	0.19985800
H	-6.96611500	-1.11221400	-1.25858300
H	-5.50525500	-1.16128200	-2.26348900
H	-6.50592600	0.30254200	-2.23326700
H	-1.83628100	-0.75753400	-0.70032200

H	-2.65063200	2.67082200	-1.43075700
H	-0.41383700	1.52652400	-2.06671100
C	-2.09128700	0.85690000	-3.18671200
C	-1.98146500	1.87781100	-4.13457500
C	-2.88589300	-0.25007500	-3.49220100
C	-2.65080000	1.80216400	-5.35230200
H	-1.35266700	2.73829800	-3.91522600
C	-3.55696900	-0.33199700	-4.70928300
H	-2.99651900	-1.05122000	-2.76561200
C	-3.44292400	0.69431900	-5.64333600
H	-2.54637900	2.60328400	-6.07714700
H	-4.17189300	-1.19994100	-4.92816600
H	-3.96379000	0.62887900	-6.59320500

M7RS

S	0.08174300	0.64684900	2.32186900
O	0.86664400	2.37562700	-2.93564600
O	0.55721700	2.89051800	-0.76549200
O	1.18810700	-0.30478600	2.43978100
O	-1.03179000	0.54345700	3.26186900
N	-0.50885200	0.46576700	0.76980700
N	-1.54989700	1.33149200	0.58275200
C	0.25088100	-0.41804000	-0.37350700
C	-0.92310300	-0.80252600	-1.32212900
H	-0.66144400	-1.75622500	-1.79607200
H	-1.86101000	-0.95088200	-0.77357500
C	-1.10466100	0.22943500	-2.42955000
H	-0.21600900	0.20060300	-3.06597300
C	-1.17380500	1.67833800	-1.88238400
H	-1.73955200	2.24205900	-2.62869300
C	-1.87304800	1.84689100	-0.54767600
C	-2.31695000	-0.12853800	-3.26630100
C	-3.60947600	-0.06017900	-2.73344900
H	-3.75539100	0.27438400	-1.70795900
C	-4.71484200	-0.40772900	-3.50311600
H	-5.71024700	-0.34313100	-3.07503400
C	-4.54550600	-0.83491800	-4.81909000
H	-5.40783300	-1.10622500	-5.41966200
C	-3.26490700	-0.90797600	-5.35840900
H	-3.12292400	-1.23662000	-6.38330100
C	-2.15987700	-0.55608000	-4.58543200
H	-1.16105200	-0.60957900	-5.01053200
C	0.21520700	2.32026100	-1.92023000
C	1.89313600	3.41254900	-0.70585500

H	2. 53921400	2. 76946600	-1. 30639000
H	2. 17540600	3. 33337100	0. 34399200
C	1. 92179000	4. 85228100	-1. 18023800
H	1. 63779400	4. 91283700	-2. 23336400
H	1. 22850100	5. 45637900	-0. 58758200
H	2. 92737400	5. 26689400	-1. 06622200
C	0. 76845100	2. 28055500	2. 45552300
C	-0. 03531700	3. 40490300	2. 26561800
H	-1. 08722900	3. 29266300	2. 02502200
C	0. 54351500	4. 66109700	2. 37857300
H	-0. 06770900	5. 54503000	2. 21717600
C	1. 89851500	4. 81263600	2. 70246200
C	2. 66708100	3. 66859400	2. 92158600
H	3. 71507600	3. 76970800	3. 18826000
C	2. 11256100	2. 39709800	2. 79060600
H	2. 70671000	1. 50314100	2. 94616100
C	2. 50579300	6. 18775300	2. 79189200
H	2. 60602000	6. 62787300	1. 79434600
H	1. 87593300	6. 85720600	3. 38347100
H	3. 49762300	6. 15518900	3. 24700600
C	-3. 02437900	2. 79308500	-0. 46985400
C	-3. 10077600	3. 91301800	-1. 30584800
C	-4. 02990000	2. 59677200	0. 48615300
C	-4. 15772800	4. 81132700	-1. 19123100
H	-2. 31990400	4. 11071700	-2. 03356700
C	-5. 08780200	3. 49150300	0. 59441400
H	-3. 96573000	1. 73200700	1. 13842300
C	-5. 15756900	4. 60110500	-0. 24622900
H	-4. 19530100	5. 67943300	-1. 84130900
H	-5. 86323600	3. 32020200	1. 33425800
H	-5. 98575400	5. 29755700	-0. 16425200
O	1. 26199600	0. 11799200	-0. 91358600
C	-3. 61042600	-3. 66982800	1. 94353100
C	-2. 72507700	-3. 21631000	0. 96323200
C	-2. 87687300	-3. 58468400	-0. 36806800
C	-3. 94602400	-4. 41186400	-0. 71252000
C	-4. 83982800	-4. 85701900	0. 26091300
C	-4. 67692100	-4. 49019200	1. 59658600
C	-3. 21345600	-3. 14612400	3. 30291900
C	-1. 74895300	-2. 71604700	3. 11660400
C	-1. 68150700	-2. 32187000	1. 60815200
H	-2. 17983100	-3. 24875800	-1. 12852500
H	-4. 07981300	-4. 71095400	-1. 74673000
H	-5. 66507700	-5. 50208900	-0. 02285700

H	-5.36548800	-4.84997300	2.35527700
H	-3.29716300	-3.88428700	4.10381400
H	-1.46532100	-1.86652100	3.73975100
H	-3.82399600	-2.27797800	3.57752900
H	-1.93349500	-1.26336500	1.50677300
N	-0.32308600	-2.52082700	1.10257300
O	-0.85932200	-3.77535700	3.46894700
C	0.54229200	-1.73711500	0.42126500
C	0.35282700	-3.64976100	1.47485600
N	1.67311100	-2.44155100	0.37098300
N	1.57401200	-3.63384900	1.04010600
C	-0.33538700	-4.57441500	2.42297400
H	-1.11536500	-5.15152200	1.91062800
H	0.38944000	-5.25789900	2.86496000
C	2.96322800	-2.10597000	-0.16879800
C	3.59362000	-3.04936500	-0.97006600
C	3.59178100	-0.92308400	0.18711200
C	4.87267100	-2.78581500	-1.43880800
C	4.87300700	-0.67812900	-0.29704800
C	5.53836800	-1.59579200	-1.11554400
H	5.35786100	-3.52489200	-2.06922500
H	5.35297000	0.25270900	-0.01925500
H	3.07263700	-0.21089000	0.81609200
H	3.08581100	-3.97612400	-1.21478800
C	6.94802600	-1.35016600	-1.65950800
C	6.90605100	-1.36603300	-3.19681600
C	7.88582800	-2.46263000	-1.16099200
C	7.51546300	-0.00140000	-1.20645000
H	6.23700400	-0.58685600	-3.57377500
H	6.55490300	-2.32816400	-3.58018900
H	7.90786500	-1.18740900	-3.60128900
H	7.92764300	-2.47322100	-0.06760400
H	8.89862400	-2.29827400	-1.54349600
H	7.55530400	-3.44936200	-1.49716900
H	8.51755400	0.12986300	-1.62531300
H	7.59858100	0.05567600	-0.11650100
H	6.89632200	0.83218200	-1.55212700

M7SR

C	6.18130400	-0.19577700	-0.96734700
C	4.79383800	-0.08941900	-1.08537600
C	4.11742700	-0.69927300	-2.13265900
C	4.85973300	-1.39293100	-3.08850200
C	6.24682000	-1.49062600	-2.98104500

C	6. 91786200	-0. 89922700	-1. 91088400
C	6. 66249000	0. 51620200	0. 27585800
C	5. 51069200	1. 47813700	0. 56627700
C	4. 26182100	0. 69733500	0. 09555100
H	3. 03509300	-0. 67077900	-2. 17433900
H	4. 34949100	-1. 87172200	-3. 91811700
H	6. 80769500	-2. 03551900	-3. 73394400
H	7. 99736800	-0. 97974900	-1. 82192300
H	7. 59754100	1. 06528700	0. 14299900
H	5. 43145800	1. 79696000	1. 61390600
H	6. 78851100	-0. 18603700	1. 10757000
H	3. 87449100	0. 03685000	0. 87272200
N	3. 17607500	1. 65697500	-0. 19565100
O	5. 73084800	2. 60529200	-0. 27572200
C	1. 84415000	1. 46257800	-0. 24081500
C	3. 38538700	3. 00530100	-0. 29667100
N	1. 31691300	2. 67826100	-0. 40693700
N	2. 26855100	3. 65467900	-0. 44363900
C	4. 75081000	3. 59704200	-0. 12713700
C	-0. 06430400	3. 04824600	-0. 57223700
C	-0. 49927200	3. 41468700	-1. 83859100
C	-0. 92967600	3. 03545600	0. 51474000
C	-1. 84021700	3. 73475500	-2. 02831000
C	-2. 26689300	3. 34337500	0. 29965900
C	-2. 75219600	3. 68951000	-0. 96830100
H	-2. 16862700	4. 01170000	-3. 02298700
H	-2. 94657100	3. 29436200	1. 14534400
H	-0. 57792600	2. 76473200	1. 50482000
H	0. 20273700	3. 43098200	-2. 66631600
C	-4. 24161400	3. 99023600	-1. 14203900
C	-4. 59404500	4. 35122700	-2. 58810100
C	-4. 63070300	5. 17100500	-0. 23639700
C	-5. 04684900	2. 74474600	-0. 73464200
H	-4. 36348600	3. 53178200	-3. 27637400
H	-4. 06130900	5. 24723800	-2. 92262200
H	-5. 66646200	4. 55426400	-2. 66001300
H	-6. 11917800	2. 93662000	-0. 84933100
H	-4. 86284600	2. 46062700	0. 30619200
H	-4. 78163200	1. 88768300	-1. 36206800
C	-0. 53745500	-1. 42287200	-1. 21539000
C	0. 18260900	-0. 08077500	-1. 34259600
H	-0. 00806900	-2. 00696600	-0. 45404100
C	-0. 56878500	-2. 24467400	-2. 48814000
C	-0. 33811100	-3. 62094800	-2. 43502300

C	-0.90388200	-1.66634400	-3.71475200
C	-0.44258500	-4.40502300	-3.58178400
H	-0.08191200	-4.07813200	-1.48224000
C	-1.00551400	-2.44511100	-4.86374000
H	-1.09158200	-0.59597000	-3.77047300
C	-0.77567900	-3.81843400	-4.80040500
H	-0.25721600	-5.47322100	-3.52376400
H	-1.26455700	-1.98047300	-5.81012100
H	-0.85180000	-4.42612200	-5.69658800
C	1.14571100	0.06415800	-0.14267200
O	2.00190500	-0.88054100	-0.01006100
H	-5.69737500	5.39037900	-0.34881800
H	-4.06418500	6.06875400	-0.50192300
H	-4.44259200	4.94876700	0.81747200
H	0.82051200	-0.06190400	-2.23238100
C	-2.07552900	-0.36663400	0.56374200
C	-3.45777200	-0.11634500	1.09499600
C	-3.62711600	0.60367100	2.28955500
C	-4.60262800	-0.54045000	0.41109300
C	-4.89570700	0.87357700	2.78317800
H	-2.74282300	0.94451200	2.81872500
C	-5.87644900	-0.26607900	0.90937200
H	-4.52875700	-1.08119000	-0.52622500
C	-6.03067400	0.43926000	2.09554900
H	-5.00131300	1.42597300	3.71192900
H	-6.74802200	-0.60454400	0.35784900
H	-7.02189200	0.65334700	2.48242700
N	-1.15643400	0.15449200	1.28369200
N	0.18047500	0.25235700	1.12338200
H	-0.52911900	0.74670900	-1.42529100
S	0.87667100	0.56495300	2.63154100
O	2.26572000	0.93475800	2.36441500
O	0.04885200	1.50618700	3.37950000
C	0.81858500	-1.00330400	3.45788500
C	1.30747300	-2.12231800	2.78595100
C	1.29394000	-3.34062900	3.44946200
C	0.80298700	-3.45075400	4.75725900
C	0.31938000	-2.30744000	5.39566900
C	0.31997800	-1.07312800	4.75157700
H	1.67300400	-2.01554600	1.76338600
H	1.66486800	-4.22872900	2.94501800
H	-0.06813600	-2.38363500	6.40738100
H	-0.06349000	-0.18009800	5.23296900
C	0.77860900	-4.79088900	5.44418200

H	1. 73594900	-5. 30628400	5. 32961000
H	0. 00682600	-5. 43251800	5. 00762700
H	0. 56804100	-4. 68778300	6. 51052000
C	-1. 97747000	-1. 17734000	-0. 71764100
H	-2. 53811600	-0. 66859000	-1. 51256000
C	-2. 58612700	-2. 55861200	-0. 51259600
O	-2. 32538500	-3. 28345500	0. 41608400
O	-3. 35577100	-2. 91277400	-1. 54951200
C	-3. 74885600	-4. 29439900	-1. 59751600
C	-4. 28261200	-4. 54949500	-2. 98867700
H	-2. 87079200	-4. 90903200	-1. 37847200
H	-4. 49532400	-4. 47607000	-0. 81839600
H	-4. 58484300	-5. 59475100	-3. 08712900
H	-3. 50476800	-4. 33530200	-3. 72652100
H	-5. 14840100	-3. 91626100	-3. 19599900
H	4. 80281800	4. 06570100	0. 86676000
H	4. 92425100	4. 36383700	-0. 88388500

M7SS

C	-0. 98552700	-1. 38514700	1. 66280400
C	-0. 17960100	-1. 42913400	0. 37381000
H	-0. 27246800	-1. 25711900	2. 48384000
C	-1. 77570100	-2. 65820700	1. 88441400
C	-1. 91675700	-3. 17794700	3. 17374100
C	-2. 45118100	-3. 28186300	0. 82957700
C	-2. 73966400	-4. 27586100	3. 41349200
H	-1. 38767300	-2. 70336100	3. 99657800
C	-3. 28038900	-4. 37495000	1. 06770900
H	-2. 33848200	-2. 90232800	-0. 18419100
C	-3. 43414700	-4. 86969300	2. 36157900
H	-2. 84125300	-4. 66593800	4. 42134500
H	-3. 81000600	-4. 83950300	0. 24083800
H	-4. 08308700	-5. 71946100	2. 54778400
C	1. 02847300	-0. 46217000	0. 44099400
O	1. 66764500	-0. 43844200	1. 54463900
H	0. 24025400	-2. 43777600	0. 27134900
C	-1. 25932400	1. 19333600	1. 73550900
C	-1. 80856300	2. 20468400	2. 68956400
C	-0. 94471800	3. 11183900	3. 31310200
C	-3. 17998300	2. 29053300	2. 94522300
C	-1. 44496100	4. 08349700	4. 17253100
H	0. 12060700	3. 02853200	3. 11924600
C	-3. 68134000	3. 26837300	3. 80007000
H	-3. 86868900	1. 61464100	2. 44455900

C	-2.81474500	4.16472300	4.41919600
H	-0.76301500	4.77455900	4.65801600
H	-4.75025000	3.33223300	3.97689700
H	-3.20399900	4.92108200	5.09309100
N	-0.30872100	1.64748400	1.01624900
N	0.36974200	1.00037200	0.01832300
S	1.46698000	2.18961800	-0.54410100
O	2.35001100	2.68135000	0.51334200
O	2.08325500	1.62704800	-1.75164300
C	0.40320000	3.51836500	-1.05766200
C	-0.08919000	4.42560800	-0.12400500
C	-0.90342900	5.46151400	-0.56514300
C	-1.22121300	5.60547000	-1.91883400
C	-0.70046000	4.68535400	-2.83403100
C	0.11334800	3.64063900	-2.41329500
H	0.15180700	4.30704100	0.92601100
H	-1.30215600	6.16924000	0.15570000
H	-0.93282300	4.79197100	-3.88996200
H	0.53582200	2.93641700	-3.12192900
C	-2.08908200	6.74090300	-2.39458000
H	-1.48736000	7.49711100	-2.90839600
H	-2.59952800	7.22671600	-1.56099000
H	-2.84337900	6.38674000	-3.10188600
C	-1.95193000	-0.16666500	1.73594300
H	-2.47280500	-0.24414800	2.69369800
C	-2.97481900	-0.19657000	0.59412000
O	-2.69280200	0.16769300	-0.52175700
O	-4.22421600	-0.64884400	0.81085100
C	-4.71690800	-1.13249200	2.07082000
C	-6.01404500	-1.85268400	1.77077000
H	-4.00036100	-1.81703300	2.52576500
H	-4.87864400	-0.28411900	2.74600300
H	-6.44508700	-2.24144200	2.69626500
H	-5.81937400	-2.69008400	1.09598000
H	-6.73291800	-1.17828500	1.30068400
C	6.23874100	-0.91065000	1.26468900
C	4.86702800	-1.13739600	1.19132200
C	4.26708700	-2.21211500	1.83802100
C	5.08266600	-3.08858500	2.54987900
C	6.46234000	-2.87794800	2.61769900
C	7.04949000	-1.78477600	1.98317100
C	6.61741500	0.34605100	0.52071100
C	5.37174000	0.70566100	-0.32258400
C	4.19068500	-0.07580100	0.35709700

H	3.18770400	-2.32588800	1.79428900
H	4.64324000	-3.93892200	3.06146600
H	7.08361500	-3.57098200	3.17646800
H	8.12137000	-1.62107100	2.04576100
H	7.48727900	0.22854800	-0.13251600
H	5.15273400	1.77383100	-0.31359400
H	6.84381800	1.15450300	1.22425400
H	3.56669800	0.58283000	0.96217200
N	3.32292600	-0.67343900	-0.66604600
O	5.56944900	0.39596600	-1.69773400
C	1.98910600	-0.77899300	-0.75100400
C	3.84368200	-1.14271000	-1.83697900
N	1.76233100	-1.33151700	-1.94525200
N	2.91146400	-1.55465600	-2.64582100
C	5.30570400	-0.94627800	-2.05730600
H	5.89652100	-1.65746800	-1.46403600
H	5.54593900	-1.06646400	-3.11350500
C	0.47413000	-1.53825000	-2.54172800
C	-0.28367900	-0.42187200	-2.85445300
C	-0.04111600	-2.82417300	-2.65532100
C	-1.61713600	-0.59196500	-3.21136300
C	-1.37333200	-2.97224200	-3.01681000
C	-2.19831300	-1.86045400	-3.25712700
H	-2.21347100	0.29308900	-3.39281900
H	-1.78765400	-3.97482700	-3.07336800
H	0.57622800	-3.68206500	-2.40927100
H	0.15482500	0.56354500	-2.74748600
C	-3.69150600	-2.06697300	-3.52025300
C	-3.87750000	-2.92318500	-4.78262500
C	-4.42687000	-0.73609900	-3.70318300
C	-4.31534000	-2.78304600	-2.30847900
H	-3.41102600	-3.90703300	-4.67617700
H	-3.43558300	-2.43081000	-5.65425600
H	-4.94382500	-3.07676700	-4.97802800
H	-4.32293300	-0.11089300	-2.81085800
H	-5.49142200	-0.93039200	-3.86426000
H	-4.05384000	-0.18298600	-4.57120700
H	-5.37972200	-2.96548300	-2.49196500
H	-4.22230100	-2.16481800	-1.40825900
H	-3.83745500	-3.75060500	-2.12183400
H	-0.81268700	-1.23228100	-0.49016500

TS8RR

C	-3.80493800	-3.08021000	1.67896400
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C	-2.83145300	-2.78568700	0.72365100
C	-3.04325700	-3.03033500	-0.62749900
C	-4.27957900	-3.54282500	-1.02621700
C	-5.26811000	-3.81410500	-0.07860500
C	-5.03466700	-3.59336200	1.28082800
C	-3.29928600	-2.73558400	3.06109300
C	-1.77261800	-2.62262400	2.88037000
C	-1.62576400	-2.17518300	1.40133500
H	-2.25610900	-2.84462200	-1.35484400
H	-4.46851600	-3.74166700	-2.07660300
H	-6.22300500	-4.21677800	-0.40118700
H	-5.80037900	-3.82752700	2.01439000
H	-3.54688300	-3.47752700	3.82359500
H	-1.32752600	-1.88107500	3.54786600
H	-3.70240700	-1.76639600	3.37790700
H	-1.67216500	-1.08277200	1.37331000
N	-0.35404500	-2.58509900	0.84695000
O	-1.12805900	-3.85949800	3.18700700
C	0.52188400	-1.89098300	0.08048200
C	0.19383000	-3.78132900	1.21939400
N	1.55429000	-2.75098100	0.01025000
N	1.38371600	-3.91644600	0.72459500
C	-0.61720800	-4.64674800	2.12437200
H	-1.42697500	-5.12244500	1.55358900
H	0.00614400	-5.42290200	2.56869100
C	2.84821800	-2.43778000	-0.49347100
C	2.98469800	-1.62938100	-1.61176600
C	3.97195000	-2.90472400	0.18587000
C	4.26020900	-1.25645700	-2.03249400
C	5.23288100	-2.54434900	-0.26534100
C	5.40905300	-1.70422600	-1.37514200
H	4.33984000	-0.60488400	-2.89468400
H	6.09882100	-2.92025800	0.27115400
H	3.84461700	-3.52825000	1.06263200
H	2.10518800	-1.25888000	-2.12364200
C	6.82435600	-1.34756200	-1.83773600
C	7.64153300	-0.79078700	-0.65979500
C	6.81619500	-0.29947800	-2.95532900
C	7.50704100	-2.62183400	-2.36470600
H	7.75192300	-1.52345300	0.14367100
H	7.16797800	0.10037900	-0.23706600
H	8.64556400	-0.51714500	-0.99971300
H	8.52510200	-2.39556600	-2.69904600
H	6.95012700	-3.03766800	-3.20972000

H	7.56693700	-3.38949700	-1.58759900
C	-1.61862500	1.22922800	-1.78115400
C	-0.95542500	-0.06493600	-1.30337300
C	0.29007000	0.21961400	-0.47797000
O	1.30764100	0.63732500	-0.99846800
H	7.84547500	-0.04995600	-3.22912700
H	6.31740200	0.62232900	-2.63771200
H	6.31434900	-0.66998500	-3.85419700
C	-1.39214900	2.54592400	0.41542700
C	-1.62793800	3.96431600	0.82556600
C	-1.36326600	4.34158800	2.14888000
C	-2.07914800	4.93080400	-0.07770200
C	-1.55511400	5.65526600	2.55711600
H	-1.01525600	3.58286500	2.84330400
C	-2.26014000	6.24985700	0.33161400
H	-2.26606500	4.67177600	-1.11595300
C	-2.00400000	6.61452400	1.64951600
H	-1.35957600	5.93160600	3.58821800
H	-2.59952600	6.99192400	-0.38364500
H	-2.15395800	7.64044800	1.96976300
N	-0.43029400	1.98904900	1.04104400
N	-0.02831600	0.66346300	0.93456200
H	-0.61250100	-0.63973100	-2.16784900
S	1.27234400	0.55640100	2.09317800
O	0.70498700	1.06749500	3.33029000
O	1.78418700	-0.80527600	2.04690800
C	2.54622400	1.65862500	1.54723700
C	2.45115900	3.01009100	1.85512100
C	3.44959900	3.86802400	1.40145900
C	4.52383700	3.38629500	0.65151600
C	4.58566000	2.01741800	0.35870400
C	3.60509400	1.14356000	0.80112400
H	1.60901000	3.37537800	2.43263000
H	3.38978800	4.92760100	1.63134800
H	5.40967700	1.63488500	-0.23798700
H	3.64370000	0.08425400	0.56523200
C	5.61433200	4.30897800	0.17376500
H	5.87987000	4.09544800	-0.86497100
H	6.51982500	4.17979900	0.77540900
H	5.30994500	5.35482400	0.24502900
C	-2.34307300	1.94418800	-0.60403800
C	-3.32372900	1.01924900	0.11324200
O	-3.13708100	0.51474000	1.19742300
O	-4.41683600	0.81364400	-0.61835300

C	-5.36064000	-0.13643600	-0.08161700
C	-6.37065900	-0.43323200	-1.16548000
H	-4.81693900	-1.03360100	0.22301800
H	-5.82110600	0.30197400	0.80888700
H	-7.10457500	-1.15110600	-0.79095700
H	-5.87351300	-0.86611700	-2.03694300
H	-6.89226700	0.47456200	-1.47684000
H	-1.66596400	-0.67961300	-0.74566900
H	-2.94874100	2.74449700	-1.03380700
H	-0.82122000	1.91163700	-2.09905800
C	-2.53206100	1.02673400	-2.97657900
C	-2.68420000	2.06840400	-3.89488300
C	-3.23174100	-0.16197500	-3.19480500
C	-3.51489900	1.93146700	-5.00325500
H	-2.13468400	2.99494400	-3.74270600
C	-4.05928700	-0.30571500	-4.30493100
H	-3.14768600	-0.98027200	-2.48448100
C	-4.20485500	0.74029900	-5.21267700
H	-3.61536400	2.75128300	-5.70721900
H	-4.59358200	-1.23861000	-4.45918400
H	-4.84843600	0.62649200	-6.07882300

TS8RS

S	0.12129000	1.73467000	1.74330900
O	0.03512300	2.52882000	-2.88101300
O	-1.70637500	3.07939800	-1.56387100
O	1.55396200	1.98573700	1.74443700
O	-0.45754500	0.93428500	2.82125900
N	-0.27155400	1.05786400	0.24085100
N	-1.61313200	0.65858100	0.27598700
C	0.83522900	0.17033900	-0.44219200
C	0.14244100	-0.89366100	-1.29174000
H	0.92161100	-1.60275600	-1.58728900
H	-0.61767600	-1.43525200	-0.72460500
C	-0.47998600	-0.27692200	-2.54926800
H	0.31428200	0.24229300	-3.09375900
C	-1.53090200	0.80972500	-2.18660600
H	-2.29712100	0.80556200	-2.96929300
C	-2.20817800	0.55383400	-0.85642700
C	-1.05682300	-1.36579500	-3.43049000
C	-2.04858800	-2.23958000	-2.95828100
H	-2.43475400	-2.12572300	-1.94667100
C	-2.55287100	-3.24469600	-3.77102900
H	-3.32214500	-3.90777100	-3.38682700

C	-2.07396800	-3.40424500	-5.07018400
H	-2.46607800	-4.19308700	-5.70412800
C	-1.08951700	-2.54509400	-5.54969200
H	-0.70883800	-2.66144200	-6.55953500
C	-0.58654200	-1.53408900	-4.73379900
H	0.18415600	-0.86674800	-5.10979400
C	-0.93454900	2.21828100	-2.23816700
C	-1.26898100	4.45041200	-1.56154400
H	-0.18372300	4.46831800	-1.43555000
H	-1.74051900	4.88305700	-0.67744200
C	-1.69266000	5.15652500	-2.83496000
H	-1.20141800	4.70738200	-3.70017100
H	-2.77601500	5.09368900	-2.96519000
H	-1.41137600	6.21160500	-2.78584100
C	-0.72009300	3.29970000	1.73024800
C	-2.10890600	3.34941900	1.85306200
H	-2.68420400	2.43038900	1.89175100
C	-2.72444900	4.59115700	1.92519300
H	-3.80545800	4.64737100	2.01914800
C	-1.97527900	5.77623900	1.89469100
C	-0.58796800	5.69077700	1.76827900
H	0.00453000	6.60052000	1.74183300
C	0.04937100	4.45504700	1.68252700
H	1.12730400	4.37756400	1.59147300
C	-2.66682600	7.10984400	2.00435500
H	-3.46376400	7.19965200	1.26075400
H	-3.12617700	7.22654500	2.99056300
H	-1.96584500	7.93362000	1.85793300
C	-3.62801400	0.12337300	-0.81696500
C	-4.57211300	0.71287400	-1.66361200
C	-4.03671100	-0.87346600	0.07533500
C	-5.90471500	0.31799600	-1.60838800
H	-4.26959200	1.50504200	-2.34255700
C	-5.36579000	-1.27968700	0.11554400
H	-3.29924400	-1.34844700	0.71466900
C	-6.30332300	-0.68248700	-0.72437200
H	-6.63296300	0.79032900	-2.25949100
H	-5.66444200	-2.06987000	0.79735400
H	-7.34093400	-0.99898300	-0.69473100
O	1.79396200	0.78534600	-0.88420900
C	-2.48746400	-3.57087300	2.34066400
C	-1.49936700	-3.13241900	1.45484600
C	-1.28898800	-3.77528800	0.24050200
C	-2.12133000	-4.84083200	-0.10519700

C	-3.13383100	-5.25636500	0.75845100
C	-3.31740500	-4.62991500	1.99236700
C	-2.46200800	-2.74738600	3.60833700
C	-1.09028600	-2.05080700	3.56355400
C	-0.81360900	-1.91147400	2.04358400
H	-0.48929100	-3.47191000	-0.42801900
H	-1.97250700	-5.34825200	-1.05290800
H	-3.77165200	-6.08823000	0.47753800
H	-4.08591100	-4.97715500	2.67684600
H	-2.56650000	-3.34026300	4.52013700
H	-1.08954700	-1.06803500	4.03667900
H	-3.26092000	-1.99506300	3.60066400
H	-1.27646200	-0.98525800	1.69099900
N	0.61367800	-1.83425900	1.79177700
O	-0.10074700	-2.82028000	4.24955900
C	1.35922100	-1.00394800	1.01759700
C	1.43825800	-2.69266900	2.46245900
N	2.60592400	-1.44619300	1.24614000
N	2.67851700	-2.48359600	2.14688600
C	0.81032200	-3.58844400	3.48063700
H	0.31543300	-4.43615300	2.98864900
H	1.56988700	-3.96753500	4.16472600
C	3.83746000	-0.98855700	0.67242800
C	4.75511000	-1.94287600	0.24144400
C	4.11592400	0.36588000	0.58861500
C	5.96108200	-1.52255600	-0.29776100
C	5.33090800	0.76460100	0.03440700
C	6.27340500	-0.16066700	-0.41900200
H	6.66935900	-2.27312300	-0.63623100
H	5.53168400	1.82705300	-0.03505900
H	3.38555900	1.08721700	0.93474000
H	4.51925700	-2.99738300	0.33423500
C	7.61258100	0.25187700	-1.03521400
C	7.69893800	-0.29574900	-2.46993800
C	8.76150800	-0.33120800	-0.19580300
C	7.77818200	1.77352100	-1.08967600
H	6.88708200	0.10319800	-3.08537700
H	7.63364000	-1.38733700	-2.48917600
H	8.65218900	-0.00675100	-2.92512300
H	8.72289200	0.04874600	0.82963500
H	9.72578500	-0.04942000	-0.63199300
H	8.71736900	-1.42319800	-0.15429900
H	8.74568300	2.01798200	-1.53855600
H	7.75051000	2.21725700	-0.08951400

H	6.99774100	2.24109000	-1.69784000
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TS8SR

C	-6.19995900	-0.26800400	1.13457200
C	-4.83381700	0.01406600	1.18595300
C	-4.09612600	-0.21409700	2.33611300
C	-4.75009300	-0.72693900	3.45650400
C	-6.11427400	-1.01370200	3.40983100
C	-6.84987800	-0.78836200	2.24555900
C	-6.75435500	0.07657300	-0.22995000
C	-5.70006000	1.04069600	-0.77922200
C	-4.37996600	0.52399400	-0.16439900
H	-3.03366100	0.00105500	2.35369200
H	-4.19298200	-0.90824700	4.37003500
H	-6.60931500	-1.41228600	4.28985000
H	-7.91387100	-1.00452500	2.21508100
H	-7.73672400	0.55413300	-0.20247900
H	-5.65755600	1.09385100	-1.87528700
H	-6.81960100	-0.81319200	-0.86654100
H	-3.95452600	-0.28656200	-0.76097200
N	-3.38644200	1.59843000	-0.14466100
O	-6.02024900	2.31775500	-0.23775700
C	-2.03823800	1.48508900	-0.02370800
C	-3.71287900	2.91796600	-0.32210500
N	-1.63919500	2.76117700	-0.11715400
N	-2.65439500	3.66990100	-0.29903400
C	-5.12087400	3.32730800	-0.62750700
C	-0.28519900	3.21984300	-0.07463200
C	0.12142900	4.07114000	0.94356000
C	0.60870300	2.79853900	-1.05375100
C	1.44945500	4.48816500	0.99381000
C	1.93059800	3.21751000	-0.98138100
C	2.38103700	4.06310100	0.04090100
H	1.75189800	5.14788400	1.79858900
H	2.62142900	2.87321600	-1.74535100
H	0.27565300	2.15660100	-1.86358200
H	-0.59627100	4.39770900	1.68914200
C	3.84957900	4.49254400	0.06354300
C	4.18525200	5.33782600	1.29596700
C	4.14710500	5.32392900	-1.19620300
C	4.74228100	3.24085800	0.06550400
H	3.99107900	4.79066400	2.22420600
H	3.61084100	6.26932400	1.31610200
H	5.24670500	5.60195300	1.27802200

H	5.79792200	3.53205200	0.09346900
H	4.58786400	2.62950300	-0.82844100
H	4.53461900	2.61427600	0.93937900
C	0.72947600	-1.25073300	1.57239200
C	-0.22673600	-0.07149500	1.34360700
H	0.31579800	-2.12893700	1.06207100
C	0.92514700	-1.61816600	3.02948700
C	0.92329800	-2.95943800	3.41687100
C	1.18335100	-0.63832800	3.99090600
C	1.17888100	-3.31810600	4.73857700
H	0.72668300	-3.72733400	2.67213400
C	1.43639000	-0.99266300	5.31262200
H	1.19049600	0.41101400	3.70333100
C	1.43696200	-2.33434700	5.69022900
H	1.17190000	-4.36541700	5.02454200
H	1.63276000	-0.22075300	6.05002800
H	1.63365500	-2.60971900	6.72145700
C	-1.07569100	-0.40416900	0.13266700
O	-1.99237500	-1.21743000	0.18764800
H	5.19632900	5.63776000	-1.19945000
H	3.51890300	6.21930100	-1.22863200
H	3.96403100	4.74668900	-2.10712800
H	-0.91599600	0.03399500	2.18271200
C	2.05986800	-0.45288300	-0.50801500
C	3.38706300	-0.14228900	-1.14014100
C	3.43568400	0.31922100	-2.46608000
C	4.59137900	-0.26466800	-0.43765800
C	4.64726000	0.63486500	-3.06479500
H	2.50331500	0.42973900	-3.01119600
C	5.80813600	0.04503000	-1.04556000
H	4.61059500	-0.59073300	0.59607200
C	5.84368600	0.49547900	-2.35850100
H	4.65995600	0.99007100	-4.09053000
H	6.72796400	-0.05921500	-0.47886700
H	6.79005900	0.74156700	-2.82928000
N	1.06884100	-0.23751100	-1.28699900
N	-0.26417800	-0.34985300	-1.10807700
H	0.31174500	0.87298400	1.21278000
S	-1.03181800	-0.38208900	-2.63868100
O	-2.44920900	-0.14830000	-2.41495500
O	-0.29818000	0.50247600	-3.53194200
C	-0.77910200	-2.05424000	-3.16290000
C	-1.37427000	-3.07494900	-2.42205900
C	-1.18317000	-4.38358600	-2.83741200

C	-0.41113900	-4.67944000	-3.97007200
C	0.17353100	-3.63146000	-4.68184100
C	-0.00213400	-2.30838100	-4.28363000
H	-1.95140300	-2.82911800	-1.53382300
H	-1.63541800	-5.19577200	-2.27497600
H	0.77751900	-3.85167200	-5.55696600
H	0.45239900	-1.48516800	-4.82399400
C	-0.21401600	-6.11140900	-4.39249500
H	0.31807000	-6.67169200	-3.61799600
H	0.36213300	-6.17751600	-5.31722900
H	-1.17654600	-6.60597600	-4.55123900
C	2.09810000	-0.94044400	0.93062000
H	2.59713800	-0.17739200	1.54188800
C	2.89162300	-2.23722400	1.03753500
O	2.70601400	-3.20180800	0.33702500
O	3.72981300	-2.21339500	2.07955000
C	4.31810300	-3.47426800	2.44245500
C	4.97785800	-3.27899800	3.78879300
H	3.52207100	-4.22402700	2.48229000
H	5.02721800	-3.77030300	1.66355900
H	5.43554600	-4.21443700	4.11875200
H	4.23223900	-2.97139000	4.52701000
H	5.75435000	-2.51263300	3.73225100
H	-5.20118300	3.53109300	-1.70579100
H	-5.38123000	4.23590200	-0.08222300

TS8SS

C	-0.83136400	-1.73529900	1.53004300
C	0.12254000	-1.19790900	0.45654000
H	-0.31806100	-1.67242400	2.49630000
C	-1.18799200	-3.18850300	1.28490900
C	-1.19496600	-4.09489900	2.34746000
C	-1.57207100	-3.63161100	0.01394600
C	-1.61053500	-5.41031900	2.15724000
H	-0.88424100	-3.75962900	3.33361500
C	-1.99474100	-4.94428000	-0.17553000
H	-1.55735400	-2.94415500	-0.83079100
C	-2.02221300	-5.83514200	0.89561900
H	-1.61237700	-6.10238000	2.99339300
H	-2.30341100	-5.27091800	-1.16350700
H	-2.35380800	-6.85705600	0.74621500
C	0.95304200	-0.06704300	1.02638400
O	1.78856100	-0.22640500	1.90168100
H	0.81841100	-1.99142000	0.17300300

C	-1.92038500	0.61943200	1.87219300
C	-3.03016100	1.32333600	2.59615900
C	-2.71204700	2.39819400	3.43653400
C	-4.36955200	0.94394900	2.46601300
C	-3.71004800	3.07618000	4.12560000
H	-1.66775700	2.67869500	3.54645000
C	-5.36931000	1.62873500	3.15350100
H	-4.65738300	0.13265100	1.80506900
C	-5.04390600	2.69426300	3.98687300
H	-3.44511200	3.90062400	4.77985200
H	-6.40538900	1.32943000	3.03012400
H	-5.82300500	3.22259900	4.52540400
N	-0.97669900	1.41138500	1.54053000
N	0.22615600	1.22066400	0.94042800
S	1.11918400	2.67069000	1.25598100
O	0.94043900	3.07557600	2.64176900
O	2.45784800	2.48743800	0.71513700
C	0.24422400	3.79907200	0.20535500
C	-0.89367600	4.44435800	0.67561900
C	-1.57502700	5.30000900	-0.18297800
C	-1.13237700	5.51313600	-1.49128900
C	0.01857400	4.85121200	-1.93273800
C	0.71580300	3.99389100	-1.09116100
H	-1.23828700	4.26618200	1.68832800
H	-2.46947900	5.80641800	0.16709700
H	0.37316200	5.01186500	-2.94656900
H	1.61422100	3.48100300	-1.42083700
C	-1.86425400	6.45589200	-2.41054100
H	-1.93613000	6.04324000	-3.41941600
H	-1.33513600	7.41154400	-2.48309200
H	-2.87402100	6.65829500	-2.04704300
C	-2.12385200	-0.88085700	1.66584100
H	-2.65618900	-1.24273200	2.55026700
C	-3.01509200	-1.04613700	0.42811800
O	-2.78699100	-0.43803500	-0.59004600
O	-4.07174500	-1.87299900	0.45123500
C	-4.44520100	-2.66956100	1.58869800
C	-5.54714300	-3.59374400	1.11865200
H	-3.58593500	-3.24382100	1.94158100
H	-4.79226000	-2.00952500	2.39287300
H	-5.88035800	-4.22199300	1.94721300
H	-5.17380700	-4.23671700	0.31780900
H	-6.39866100	-3.02154300	0.74476700
C	6.29158200	-1.00845400	1.22317700

C	4. 91858300	-1. 07822100	0. 99612300
C	4. 20165600	-2. 24048100	1. 25405200
C	4. 88936100	-3. 35200300	1. 73585600
C	6. 26635600	-3. 29038200	1. 95986900
C	6. 97634200	-2. 11731100	1. 70998600
C	6. 81955900	0. 36481100	0. 88679100
C	5. 68941600	1. 02916600	0. 07120700
C	4. 39413100	0. 24027500	0. 46664600
H	3. 12745100	-2. 26187300	1. 09836700
H	4. 35164500	-4. 27187400	1. 94191500
H	6. 78875600	-4. 16565400	2. 33337200
H	8. 04717500	-2. 07287100	1. 88635400
H	7. 74583000	0. 35256000	0. 30461800
H	5. 57220500	2. 08816400	0. 30685200
H	7. 01277200	0. 93673000	1. 80154200
H	3. 82170600	0. 78356200	1. 21809700
N	3. 53328900	0. 06644600	-0. 69819500
O	5. 97031500	1. 00318700	-1. 32534800
C	2. 18111500	0. 11219600	-0. 81137600
C	4. 09177000	-0. 24488000	-1. 90942400
N	2. 01803500	-0. 18952200	-2. 11338500
N	3. 17924200	-0. 41253700	-2. 81756200
C	5. 57937900	-0. 17527900	-2. 01059900
H	6. 05052200	-1. 07118200	-1. 58474700
H	5. 88595300	-0. 07026700	-3. 05135700
C	0. 75327000	-0. 35161500	-2. 74831200
C	-0. 23401300	0. 60027300	-2. 53923900
C	0. 49272500	-1. 50193400	-3. 48615700
C	-1. 51593100	0. 36835200	-3. 02553200
C	-0. 79394200	-1. 71433500	-3. 96359800
C	-1. 83119500	-0. 80299500	-3. 71661600
H	-2. 28364600	1. 10102700	-2. 81175600
H	-0. 99888200	-2. 62894100	-4. 51285500
H	1. 28315600	-2. 22665000	-3. 64901600
H	-0. 00950600	1. 48906900	-1. 95725100
C	-3. 25746600	-1. 14362900	-4. 15236600
C	-3. 29873500	-1. 37914600	-5. 67022800
C	-4. 24422000	-0. 02709500	-3. 79662100
C	-3. 70145900	-2. 42125900	-3. 41651100
H	-2. 64689100	-2. 20417800	-5. 97187100
H	-2. 98136800	-0. 48252500	-6. 21183700
H	-4. 31850200	-1. 62639900	-5. 98393500
H	-4. 26246900	0. 14457600	-2. 71570900
H	-5. 25056300	-0. 31673900	-4. 11445000

H	-3.99032500	0.91088700	-4.30062400
H	-4.71790400	-2.69466400	-3.71928200
H	-3.69366800	-2.25638700	-2.33395700
H	-3.04354300	-3.26527700	-3.64706700
H	-0.42136100	-0.86997200	-0.43247900

PRR

S	2.00331800	-0.20919000	1.32076800
O	1.02739500	-2.21897100	-0.57804000
O	-1.69872300	-1.58322100	1.33959400
O	-1.39901500	0.46629900	2.22199000
O	2.02313700	1.08522200	1.97457100
O	1.75351600	-1.42064400	2.07379700
N	0.72978500	-0.08014200	0.15898400
N	0.39827400	1.24870100	-0.15137200
C	0.46368700	-1.15610900	-0.70793600
C	-0.52165600	-0.84674300	-1.81267200
H	-0.54673800	-1.72231700	-2.46119000
H	-0.09521400	-0.01666500	-2.38607000
C	-1.94746100	-0.45581000	-1.36027400
C	-1.90937300	0.40027600	-0.06757700
H	-2.88791400	0.86832300	0.07785400
C	-0.86164100	1.48796200	-0.22286200
C	-1.65095500	-0.38550200	1.22442300
C	-1.08224600	-0.12476400	3.50183200
H	-0.43366800	-0.98679000	3.33098600
H	-0.51911100	0.65216800	4.02037500
C	-2.34668200	-0.50528900	4.24598500
H	-2.88259100	-1.28953700	3.70790200
H	-3.00081800	0.36223300	4.36193300
H	-2.09034800	-0.88090700	5.23978500
C	3.46629500	-0.39384300	0.34691200
C	3.93900900	-1.67076000	0.05454100
H	3.40959600	-2.53984400	0.42803400
C	5.08137100	-1.78718900	-0.72619000
H	5.46744900	-2.77421700	-0.96410300
C	5.74305100	-0.65483000	-1.21462200
C	5.23739900	0.61118300	-0.90459600
H	5.74454600	1.49574700	-1.27812800
C	4.09827300	0.75443400	-0.12161500
H	3.70477300	1.73322100	0.13213900
C	6.99198600	-0.80533000	-2.04195100
H	7.84076300	-1.08049300	-1.40809400
H	7.24348400	0.12491600	-2.55489500

H	6.87340400	-1.59265200	-2.79056400
C	-1.25545500	2.88790600	-0.50757100
C	-2.47850100	3.19245700	-1.11198300
C	-0.38099100	3.92727000	-0.16428200
C	-2.82028100	4.51538200	-1.37805200
H	-3.16702800	2.40169300	-1.39538000
C	-0.73070800	5.24579100	-0.41996700
H	0.55897700	3.68045600	0.31754200
C	-1.94921800	5.54311600	-1.03028500
H	-3.76806200	4.74012500	-1.85559200
H	-0.05490000	6.04642600	-0.13809900
H	-2.21943500	6.57491800	-1.23034000
H	-2.32527200	0.22287300	-2.13527300
C	-2.93509800	-1.60920000	-1.29722500
C	-4.29440000	-1.33160000	-1.45210800
C	-2.53359100	-2.93344300	-1.11330200
C	-5.24034900	-2.35240400	-1.41945700
H	-4.61817100	-0.30444900	-1.61152700
C	-3.47588100	-3.95634800	-1.08857600
H	-1.48251200	-3.16322800	-0.96202200
C	-4.83090200	-3.67046300	-1.24059400
H	-6.29291300	-2.11888400	-1.54451400
H	-3.14938300	-4.98090400	-0.94187400
H	-5.56297700	-4.47144200	-1.21974300

PRS

S	2.38226500	1.11749800	0.33676500
O	1.62536200	0.52583800	-2.43092800
O	-0.93255000	2.94132600	-1.13252200
O	-0.68314600	2.54733800	1.07086200
O	2.17722400	1.20591300	1.76995900
O	2.63802400	2.30462400	-0.45282500
N	0.90980100	0.44627600	-0.26373800
N	0.22547100	-0.31825900	0.69943300
C	0.76566300	0.20579700	-1.64394800
C	-0.52273300	-0.48851900	-2.02208500
H	-0.48870200	-0.64644800	-3.10051900
H	-0.51664500	-1.46939600	-1.53451800
C	-1.79400100	0.29565700	-1.64477000
H	-1.84237300	1.18090900	-2.28563900
C	-1.73226000	0.85044000	-0.19511500
H	-2.75181600	1.03808600	0.15417800
C	-1.03939200	-0.09951500	0.75960300
C	-3.05166900	-0.52040400	-1.87668700

C	-3.17138600	-1.84662000	-1.45010300
H	-2.34147900	-2.34082400	-0.95152500
C	-4.36154000	-2.54642300	-1.63066700
H	-4.43698900	-3.57350900	-1.28823500
C	-5.45012300	-1.93174900	-2.24412400
H	-6.37637400	-2.47841900	-2.38804800
C	-5.34212500	-0.61168900	-2.67366000
H	-6.18304400	-0.12410900	-3.15628400
C	-4.15165300	0.08563100	-2.48949200
H	-4.07031500	1.11559400	-2.82724600
C	-1.05431000	2.22880700	-0.16625100
C	0.01928600	3.80034900	1.23066500
H	0.72444600	3.90584600	0.40287800
H	0.57555500	3.67286900	2.15981300
C	-0.95497400	4.95919700	1.29813200
H	-1.48534600	5.06591200	0.34985000
H	-1.68069800	4.80514000	2.10029400
H	-0.41144700	5.88618700	1.49703000
C	3.59959600	-0.11806400	0.00403800
C	4.33170500	-0.07074200	-1.18038600
H	4.15647300	0.72842300	-1.89142900
C	5.26589600	-1.07071400	-1.41644700
H	5.85018900	-1.05042400	-2.33191800
C	5.46777400	-2.10649500	-0.49638200
C	4.71151700	-2.12471200	0.67882200
H	4.86229900	-2.92198300	1.40027600
C	3.77357400	-1.13281600	0.94056200
H	3.18969500	-1.13262900	1.85466800
C	6.49806800	-3.16970300	-0.77139900
H	7.50710700	-2.74952800	-0.71796100
H	6.43178500	-3.98404400	-0.04770200
H	6.37022200	-3.58705300	-1.77369300
C	-1.79119800	-0.83121100	1.80842400
C	-3.18004400	-0.98513700	1.74691400
C	-1.08986100	-1.37704600	2.89346400
C	-3.85410200	-1.68382900	2.74531200
H	-3.74506100	-0.58593200	0.91086700
C	-1.76686900	-2.06404300	3.89048200
H	-0.01548900	-1.23797900	2.94356900
C	-3.15130900	-2.22237000	3.81769900
H	-4.93037400	-1.80407600	2.68089100
H	-1.21647900	-2.47353400	4.73123200
H	-3.67873300	-2.75994300	4.59909500

PSR

S	-2.38226500	1.11749800	0.33676500
O	-1.62536200	0.52583800	-2.43092800
O	0.93255000	2.94132600	-1.13252200
O	0.68314600	2.54733800	1.07086200
O	-2.17722400	1.20591300	1.76995900
O	-2.63802400	2.30462400	-0.45282500
N	-0.90980100	0.44627600	-0.26373800
N	-0.22547100	-0.31825900	0.69943300
C	-0.76566300	0.20579700	-1.64394800
C	0.52273300	-0.48851900	-2.02208500
H	0.48870200	-0.64644800	-3.10051900
H	0.51664500	-1.46939600	-1.53451800
C	1.79400100	0.29565700	-1.64477000
H	1.84237300	1.18090900	-2.28563900
C	1.73226000	0.85044000	-0.19511500
H	2.75181600	1.03808600	0.15417800
C	1.03939200	-0.09951500	0.75960300
C	3.05166900	-0.52040400	-1.87668700
C	3.17138600	-1.84662000	-1.45010300
H	2.34147900	-2.34082400	-0.95152500
C	4.36154000	-2.54642300	-1.63066700
H	4.43698900	-3.57350900	-1.28823500
C	5.45012300	-1.93174900	-2.24412400
H	6.37637400	-2.47841900	-2.38804800
C	5.34212500	-0.61168900	-2.67366000
H	6.18304400	-0.12410900	-3.15628400
C	4.15165300	0.08563100	-2.48949200
H	4.07031500	1.11559400	-2.82724600
C	1.05431000	2.22880700	-0.16625100
C	-0.01928600	3.80034900	1.23066500
H	-0.72444600	3.90584600	0.40287800
H	-0.57555500	3.67286900	2.15981300
C	0.95497400	4.95919700	1.29813200
H	1.48534600	5.06591200	0.34985000
H	1.68069800	4.80514000	2.10029400
H	0.41144700	5.88618700	1.49703000
C	-3.59959600	-0.11806400	0.00403800
C	-4.33170500	-0.07074200	-1.18038600
H	-4.15647300	0.72842300	-1.89142900
C	-5.26589600	-1.07071400	-1.41644700
H	-5.85018900	-1.05042400	-2.33191800
C	-5.46777400	-2.10649500	-0.49638200
C	-4.71151700	-2.12471200	0.67882200

H	-4.86229900	-2.92198300	1.40027600
C	-3.77357400	-1.13281600	0.94056200
H	-3.18969500	-1.13262900	1.85466800
C	-6.49806800	-3.16970300	-0.77139900
H	-7.50710700	-2.74952800	-0.71796100
H	-6.43178500	-3.98404400	-0.04770200
H	-6.37022200	-3.58705300	-1.77369300
C	1.79119800	-0.83121100	1.80842400
C	3.18004400	-0.98513700	1.74691400
C	1.08986100	-1.37704600	2.89346400
C	3.85410200	-1.68382900	2.74531200
H	3.74506100	-0.58593200	0.91086700
C	1.76686900	-2.06404300	3.89048200
H	0.01548900	-1.23797900	2.94356900
C	3.15130900	-2.22237000	3.81769900
H	4.93037400	-1.80407600	2.68089100
H	1.21647900	-2.47353400	4.73123200
H	3.67873300	-2.75994300	4.59909500

PSS

S	-2.00331800	-0.20919000	1.32076800
O	-1.02739400	-2.21897100	-0.57804000
O	1.69872300	-1.58322100	1.33959400
O	1.39901500	0.46629900	2.22199000
O	-2.02313700	1.08522200	1.97457100
O	-1.75351600	-1.42064400	2.07379700
N	-0.72978500	-0.08014200	0.15898400
N	-0.39827400	1.24870100	-0.15137200
C	-0.46368700	-1.15610900	-0.70793600
C	0.52165600	-0.84674300	-1.81267200
H	0.54673800	-1.72231700	-2.46119000
H	0.09521400	-0.01666500	-2.38607000
C	1.94746100	-0.45581000	-1.36027400
C	1.90937300	0.40027600	-0.06757700
H	2.88791400	0.86832300	0.07785400
C	0.86164100	1.48796200	-0.22286200
C	1.65095500	-0.38550200	1.22442300
C	1.08224600	-0.12476400	3.50183200
H	0.43366800	-0.98679000	3.33098600
H	0.51911100	0.65216800	4.02037500
C	2.34668200	-0.50528900	4.24598500
H	2.88259100	-1.28953700	3.70790200
H	3.00081800	0.36223300	4.36193300
H	2.09034800	-0.88090700	5.23978500

C	-3.46629500	-0.39384300	0.34691200
C	-3.93900900	-1.67076000	0.05454100
H	-3.40959600	-2.53984400	0.42803400
C	-5.08137100	-1.78718900	-0.72619000
H	-5.46744900	-2.77421700	-0.96410300
C	-5.74305100	-0.65483000	-1.21462200
C	-5.23739900	0.61118300	-0.90459600
H	-5.74454600	1.49574700	-1.27812800
C	-4.09827300	0.75443400	-0.12161500
H	-3.70477300	1.73322100	0.13213900
C	-6.99198600	-0.80533000	-2.04195100
H	-7.84076300	-1.08049300	-1.40809400
H	-7.24348400	0.12491600	-2.55489500
H	-6.87340400	-1.59265200	-2.79056400
C	1.25545500	2.88790600	-0.50757100
C	2.47850100	3.19245700	-1.11198300
C	0.38099100	3.92727000	-0.16428200
C	2.82028100	4.51538200	-1.37805200
H	3.16702800	2.40169300	-1.39538000
C	0.73070800	5.24579100	-0.41996700
H	-0.55897700	3.68045600	0.31754200
C	1.94921800	5.54311600	-1.03028500
H	3.76806200	4.74012500	-1.85559200
H	0.05490000	6.04642600	-0.13809900
H	2.21943500	6.57491800	-1.23034000
H	2.32527200	0.22287300	-2.13527300
C	2.93509800	-1.60920000	-1.29722500
C	4.29440000	-1.33160000	-1.45210800
C	2.53359100	-2.93344300	-1.11330200
C	5.24034900	-2.35240400	-1.41945700
H	4.61817100	-0.30444900	-1.61152700
C	3.47588100	-3.95634800	-1.08857600
H	1.48251200	-3.16322800	-0.96202200
C	4.83090200	-3.67046300	-1.24059400
H	6.29291300	-2.11888400	-1.54451400
H	3.14938300	-4.98090400	-0.94187400
H	5.56297700	-4.47144100	-1.21974300

NHC1

C	-3.79446700	0.55956500	-0.37645300
C	-2.93247900	0.63033100	0.71979000
C	-2.72821800	1.82374100	1.40156300
C	-3.41901600	2.95748800	0.97827200
C	-4.29336200	2.88894900	-0.10821800

C	-4.48574000	1.69135600	-0.79517000
C	-3.80117800	-0.82941800	-0.96430300
C	-3.22677300	-1.67584800	0.19313600
C	-2.30394700	-0.71538900	0.98816900
H	-2.03561600	1.86653000	2.23577500
H	-3.27890200	3.90045700	1.49660400
H	-4.82916900	3.77949200	-0.42163100
H	-5.16369300	1.64480800	-1.64232100
H	-3.15051300	-0.86560400	-1.84632100
H	-4.04904400	-1.95670700	0.85621600
H	-4.79006200	-1.17653200	-1.27248600
H	-2.26465100	-0.96898800	2.05041400
N	-0.94281000	-0.80044400	0.45517700
O	-2.61148600	-2.89577400	-0.16283100
C	0.09880500	0.01720800	0.81516200
C	-0.53436400	-1.74560200	-0.44983100
N	1.07711900	-0.51465400	0.05327100
N	0.72311600	-1.59648400	-0.73078700
C	-1.48200300	-2.76431300	-1.00311900
H	-1.77314100	-2.49206900	-2.02632300
H	-0.99767600	-3.74161100	-1.04126000
C	2.42860100	-0.04764500	-0.00020800
C	2.68999100	1.19840800	-0.57685600
C	3.44091200	-0.85636900	0.52263500
C	4.01545700	1.62930700	-0.61778200
C	4.75169200	-0.38683800	0.45279000
C	5.05760600	0.84947200	-0.11594300
H	4.23830600	2.59805100	-1.05928800
H	5.55193200	-1.00051000	0.86022000
C	6.48603300	1.32139000	-0.21091100
H	6.54775800	2.41087600	-0.15579600
H	6.93367300	1.01284600	-1.16149000
H	7.09594000	0.90116600	0.59229200
C	1.57424900	2.04311700	-1.13222300
H	0.87170700	2.32627700	-0.34394000
H	1.00355100	1.48610000	-1.88219800
H	1.97195000	2.94616400	-1.59893200
C	3.11455700	-2.18213300	1.15649200
H	2.74383600	-2.89098800	0.41122400
H	2.32798200	-2.06634500	1.90887200
H	3.99759900	-2.60681000	1.63744100

NHC2

C	-3.31130000	0.84969900	0.66242000
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C	-2.56284400	0.39595900	-0.42778300
C	-2.65274200	-0.91402300	-0.87321400
C	-3.53816400	-1.74377500	-0.19625600
C	-4.30840200	-1.31985500	0.88335400
C	-4.19195800	-0.00512900	1.31996000
C	-2.98455000	2.28768300	0.97092700
C	-2.31781500	2.76609000	-0.33941900
C	-1.68092900	1.49675100	-0.96412200
H	-2.05741000	-1.28896100	-1.69677500
H	-4.98148000	-2.02117300	1.36028700
H	-4.78102100	0.34238100	2.16223100
H	-2.28556500	2.33060000	1.81483000
H	-3.10065100	3.10645700	-1.02188900
H	-3.85587500	2.89028700	1.23539200
H	-1.66107000	1.53917100	-2.05548500
N	-0.30721000	1.35945700	-0.48526300
O	-1.42767800	3.85339300	-0.23157000
C	0.49543000	0.26842200	-0.70445800
C	0.36154900	2.32984900	0.21609800
N	1.61609000	0.68404000	-0.08001500
N	1.56785700	1.94234900	0.49078400
C	-0.29730700	3.62154800	0.58784100
H	-0.56914600	3.61549000	1.65148600
H	0.38978900	4.45267300	0.42176400
C	2.82731800	-0.07086900	0.03009400
C	2.82524900	-1.24006900	0.79982700
C	3.96849600	0.38690100	-0.63032700
C	4.01592800	-1.95578700	0.89311900
C	5.13994800	-0.36090300	-0.50150500
C	5.18227700	-1.53139600	0.25265000
H	4.03516400	-2.86720800	1.48652800
H	6.03791000	-0.02152700	-1.01241900
C	6.45139300	-2.33529600	0.37531300
H	6.32627400	-3.33136100	-0.05957100
H	6.72915500	-2.47065800	1.42470700
H	7.28227600	-1.84503300	-0.13545300
C	1.57723400	-1.70570000	1.50176100
H	0.80369700	-1.97650100	0.77826500
H	1.16394200	-0.90971700	2.12933300
H	1.79323500	-2.56961400	2.13284800
C	3.93146700	1.64014400	-1.46398700
H	3.86973600	2.53008900	-0.83170400
H	3.05263200	1.64618000	-2.11579100
H	4.82663300	1.71372900	-2.08428400

N	-3.67292700	-3.13727200	-0.64344300
O	-4.42805000	-3.86318300	-0.02064000
O	-3.02259100	-3.48605900	-1.61185400

*E-M4*_{NHC1}

C	-4.59071500	-0.98555800	0.46936700
C	-3.34682900	-1.46132800	0.04238900
C	-2.77754600	-2.59716500	0.60625600
C	-3.44701300	-3.22486500	1.65308800
C	-4.67033200	-2.73022800	2.10821400
C	-5.25798700	-1.61526200	1.51316200
C	-5.04497500	0.17380200	-0.38081800
C	-4.18882200	-0.03032100	-1.64937300
C	-2.86279700	-0.64900300	-1.13216600
H	-1.83513200	-2.99340500	0.24254700
H	-3.01994700	-4.11039400	2.11050200
H	-5.18110700	-3.23438100	2.92193300
H	-6.22615000	-1.25648300	1.84755300
H	-4.82799400	1.12707000	0.11617200
H	-4.66058600	-0.79598500	-2.26923000
H	-6.11262500	0.15792100	-0.60733600
H	-2.33370900	-1.22210500	-1.89652600
N	-1.95932600	0.49255000	-0.77092200
O	-4.00885400	1.07799100	-2.49815400
C	-0.74518300	0.48255600	-0.19527200
C	-2.18481500	1.79494000	-1.15379600
N	-0.30361200	1.73204100	-0.22395100
N	-1.18988300	2.56801200	-0.81774600
C	-3.43291400	2.20031000	-1.87612100
H	-4.12390600	2.68754300	-1.17740100
H	-3.17614900	2.91668200	-2.65772900
C	0.95485500	2.19457300	0.30560700
C	1.08711100	2.30075800	1.69110000
C	1.97706900	2.48594600	-0.60362600
C	2.33526000	2.69753900	2.17127000
C	3.20017000	2.87326800	-0.06775300
C	3.39718000	2.98081500	1.31297700
H	2.47621000	2.79148500	3.24450000
H	4.02156100	3.10019400	-0.74256900
C	2.08198700	-1.96882100	0.23598100
C	1.29256300	-0.99316100	-0.26272100
H	1.72037500	-2.48247100	1.12689300
C	3.36221700	-2.41348100	-0.29193900
C	3.96759400	-3.53647100	0.29010000

C	4.00939000	-1.76213500	-1.35557800
C	5.18215600	-4.01246500	-0.18845700
H	3.47452800	-4.03607600	1.11881900
C	5.22230600	-2.23655400	-1.82962200
H	3.56974100	-0.87469400	-1.80112900
C	5.80819600	-3.36453500	-1.25012600
H	5.64006500	-4.88422700	0.26561300
H	5.71893500	-1.72899200	-2.64934700
H	6.75705200	-3.73289800	-1.62565500
C	0.04743100	-0.66772500	0.41723700
O	-0.40051000	-1.18683500	1.41851400
H	1.54855800	-0.42807700	-1.15308800
C	4.73057300	3.42441700	1.85246400
H	5.54916400	2.91857100	1.33493700
H	4.86280700	4.50052800	1.70387700
H	4.81594800	3.21873200	2.92067600
C	1.75444700	2.40343300	-2.09066700
H	1.23709300	1.48245200	-2.38157900
H	1.13572900	3.23785200	-2.43429000
H	2.70605100	2.44252300	-2.62221100
C	-0.06259300	2.01701500	2.62294000
H	-0.98426200	2.48768900	2.26758500
H	-0.25094300	0.94291500	2.72021800
H	0.15546100	2.40880900	3.61702100

E-M4_{NHC2}

C	4.43594900	-0.36813100	-0.00386100
C	3.28931800	0.28080200	-0.47707800
C	3.02896400	1.60528600	-0.16109600
C	3.92020200	2.22858800	0.70004200
C	5.04563600	1.59865700	1.22167500
C	5.31525400	0.28475100	0.85394400
C	4.55434400	-1.74532000	-0.60068600
C	3.65299500	-1.61534000	-1.84866000
C	2.53826300	-0.61862100	-1.42760800
H	2.17971500	2.15395800	-0.54797800
H	5.70017700	2.14991200	1.88547400
H	6.20694500	-0.21249900	1.21970100
H	4.18065300	-2.49822500	0.10310400
H	4.22066400	-1.12026800	-2.63973700
H	5.57781600	-2.01842400	-0.86289700
H	2.08920200	-0.09931200	-2.27676100
N	1.44254700	-1.42069900	-0.79565500
O	3.16773400	-2.80260400	-2.42155000

C	0.29715800	-1.01453200	-0.21804700
C	1.35018500	-2.79107500	-0.89335800
N	-0.40665800	-2.10932200	0.03369500
N	0.23484600	-3.22934200	-0.38069700
C	2.42387000	-3.61018700	-1.54142200
H	3.05367300	-4.07635000	-0.77386500
H	1.96124800	-4.40233300	-2.13094600
C	-1.70409700	-2.15810200	0.66155800
C	-1.78842900	-1.90699400	2.03177800
C	-2.80799100	-2.42714400	-0.15503700
C	-3.06766300	-1.90556500	2.58855000
C	-4.05744300	-2.40980300	0.45422500
C	-4.20573800	-2.14776200	1.82053800
H	-3.17316900	-1.71413800	3.65270700
H	-4.93942500	-2.60756100	-0.14974400
C	-1.89873700	2.04579100	-0.22326900
C	-1.41264400	0.81134500	-0.48095800
H	-1.30408900	2.68106000	0.43289800
C	-3.12940300	2.61816900	-0.74369200
C	-3.36926000	3.98471300	-0.53620000
C	-4.08070800	1.85336300	-1.44044100
C	-4.52156100	4.58198900	-1.03213300
H	-2.64000300	4.57565100	0.01062800
C	-5.23218200	2.45040200	-1.92821800
H	-3.92893600	0.78688000	-1.58097200
C	-5.45190600	3.81562800	-1.72916900
H	-4.69559700	5.64031200	-0.87234800
H	-5.96643400	1.85612600	-2.46115500
H	-6.35504200	4.27753700	-2.11420700
C	-0.16839000	0.39135700	0.14009800
O	0.51834300	1.02386200	0.91779100
H	-1.91202500	0.11192700	-1.14298600
C	-5.57487000	-2.15329900	2.44536100
H	-6.28035300	-1.57588300	1.84275400
H	-5.95997100	-3.17520600	2.51259400
H	-5.55402200	-1.73269400	3.45185900
C	-2.64446500	-2.72594100	-1.62181500
H	-1.98200300	-2.00566700	-2.11541200
H	-2.20499600	-3.71679600	-1.76897100
H	-3.61037100	-2.70123800	-2.12753300
C	-0.56440000	-1.66546500	2.87705000
H	0.20983200	-2.41174300	2.67529800
H	-0.13125000	-0.67589300	2.69915600
H	-0.82325200	-1.72673600	3.93456000

N	3.66331400	3.63013900	1.06707800
O	4.43523700	4.15931700	1.84334700
O	2.69233300	4.17152700	0.57058700

TS5SR_{NHC1}

C	-5.66939600	-1.79670900	-0.78803500
C	-4.74406300	-1.19735000	0.06409300
C	-5.01197400	-1.00994600	1.41638000
C	-6.24827900	-1.42686800	1.90642200
C	-7.18410100	-2.02277900	1.05803000
C	-6.90054700	-2.21556200	-0.29299400
C	-5.11902800	-1.90968900	-2.18850800
C	-3.88311200	-0.98517700	-2.20315700
C	-3.48280800	-0.84396000	-0.69291800
H	-4.26209700	-0.56417700	2.06369800
H	-6.48470100	-1.28957900	2.95655800
H	-8.14278000	-2.34073300	1.45546200
H	-7.63042000	-2.68008700	-0.94937200
H	-5.82362600	-1.60400100	-2.96698700
H	-3.05153100	-1.40351400	-2.77169800
H	-4.81962400	-2.94168700	-2.40154700
H	-2.65096000	-1.51403700	-0.45231200
N	-3.04430800	0.52449900	-0.42596800
O	-4.16397500	0.25455400	-2.84548200
C	-2.03272300	1.00002400	0.30991200
C	-3.65873900	1.58880200	-1.01549300
N	-2.08602300	2.32737400	0.16978500
N	-3.10143600	2.70907900	-0.66149900
C	-4.70677400	1.27546500	-2.03231500
H	-5.64330600	0.96970000	-1.54660300
H	-4.89166900	2.14373100	-2.66428700
C	-1.22842800	3.32583600	0.74871300
C	-0.62463100	4.24927800	-0.12267100
C	-1.05352100	3.36477100	2.13585600
C	0.23113500	5.18901600	0.44409000
C	-0.17915100	4.33043000	2.64169500
C	0.48020200	5.23621400	1.81850800
H	0.71779800	5.90767500	-0.21150300
H	-0.02346900	4.37352600	3.71660500
C	0.99079800	-0.67621800	1.85272200
C	0.21054700	0.21733600	1.14049900
H	0.46808700	-1.29879500	2.57771400
C	2.44411100	-0.54508100	2.03845900
C	3.01367400	-1.00536000	3.23334700

C	3.27727200	0.01183800	1.05868000
C	4.38315800	-0.90014700	3.45376600
H	2.37184100	-1.44909000	3.99010400
C	4.64787800	0.09897500	1.27504700
H	2.85821100	0.33483900	0.11064100
C	5.20485200	-0.35065600	2.47159500
H	4.80883000	-1.25606500	4.38666800
H	5.28436600	0.50453900	0.49415300
H	6.27591700	-0.28250900	2.63334300
C	-1.19738900	0.10612400	1.20903400
O	-1.87619200	-0.64594900	1.92228700
H	0.64591700	0.93920800	0.45909000
C	2.12506000	-2.52785000	-0.51713100
C	3.44840800	-3.22499000	-0.50029700
C	4.01121800	-3.67970400	-1.69739200
C	4.16631800	-3.38821400	0.68807200
C	5.25743400	-4.29655000	-1.70374600
H	3.45525100	-3.54295600	-2.61883900
C	5.41974700	-3.99308500	0.67824800
H	3.76418800	-3.00817600	1.62269400
C	5.96717400	-4.45633200	-0.51516500
H	5.67463400	-4.65627100	-2.63933900
H	5.97031100	-4.09589200	1.60854200
H	6.94026800	-4.93759200	-0.52001700
N	1.97398900	-1.74815300	-1.54197000
N	0.82966000	-0.97625500	-1.52884500
S	0.72056400	0.22246800	-2.63652000
O	0.90193500	-0.21137700	-4.01622200
O	-0.52051200	0.91521500	-2.25686700
C	2.11390100	1.23436700	-2.20829700
C	3.38958700	0.84165700	-2.60207200
C	4.48311300	1.56658100	-2.13789800
C	4.31858600	2.66947800	-1.29352700
C	3.02259700	3.05222300	-0.93251300
C	1.92140400	2.33496500	-1.38094800
H	3.51722200	-0.02748000	-3.23767200
H	5.48500200	1.26354600	-2.42860400
H	2.87069800	3.90766000	-0.27821500
H	0.91845800	2.60681800	-1.07821500
C	5.51036300	3.40974600	-0.74643800
H	5.35232700	4.49080300	-0.77621200
H	6.41683200	3.17708200	-1.30884600
H	5.68146200	3.13168200	0.29932300
C	1.22442100	-2.76755500	0.60369800

H	1. 65488200	-3. 32886000	1. 42437200
C	-0. 18477300	-2. 91231200	0. 51728700
O	-0. 93183300	-2. 55630300	-0. 41917400
O	-0. 71689500	-3. 48288200	1. 62317900
C	-2. 13608000	-3. 65023500	1. 63223100
C	-2. 52243200	-4. 11664300	3. 01869700
H	-2. 61365800	-2. 69548100	1. 40092700
H	-2. 41673400	-4. 37722300	0. 86145000
H	-3. 60419400	-4. 26332800	3. 07261600
H	-2. 23726300	-3. 36223000	3. 75635600
H	-2. 02765700	-5. 05776200	3. 27047500
H	-0. 06467200	-1. 41097100	-1. 20534100
C	-1. 76991300	2. 45222100	3. 09850700
H	-2. 70078500	2. 05466000	2. 68801800
H	-1. 14206800	1. 60091700	3. 37746100
H	-2. 01030600	3. 00455600	4. 00924000
C	-0. 87245800	4. 26287400	-1. 61121500
H	-0. 94679400	3. 25557600	-2. 02938200
H	-1. 80810600	4. 78151700	-1. 83570000
H	-0. 05597600	4. 78747900	-2. 11234400
C	1. 44096700	6. 25006800	2. 38155100
H	2. 46832100	6. 01135700	2. 08433300
H	1. 21569300	7. 25364800	2. 00752800
H	1. 40181800	6. 27069500	3. 47323300

TS5SR_{NHC2}

C	4. 14145800	2. 84657300	0. 93411500
C	3. 63651700	1. 54832300	0. 88815900
C	4. 31328000	0. 47791600	1. 45829600
C	5. 53014400	0. 76736400	2. 06123600
C	6. 07218700	2. 04930600	2. 11518000
C	5. 36647800	3. 10334900	1. 54759200
C	3. 18997800	3. 82103900	0. 29226200
C	2. 11868200	2. 95249600	-0. 41092100
C	2. 29597600	1. 51099500	0. 19173200
H	3. 90270900	-0. 52751000	1. 45341200
H	7. 02875400	2. 20015700	2. 59935700
H	5. 76925800	4. 11012400	1. 58466700
H	3. 67175600	4. 48371500	-0. 43290300
H	1. 10573000	3. 30324400	-0. 20426300
H	2. 72655200	4. 45535500	1. 05468900
H	1. 48159700	1. 28801600	0. 89046900
N	2. 26203900	0. 50763200	-0. 86508000
O	2. 23177800	3. 02103500	-1. 82442900

C	1. 72006200	-0. 71478700	-0. 86997600
C	2. 70219600	0. 75807600	-2. 13107000
N	1. 89415800	-1. 18000100	-2. 10263300
N	2. 50413700	-0. 26452900	-2. 91199000
C	3. 17563900	2. 14546500	-2. 41217100
H	4. 18468300	2. 30247100	-2. 00519300
H	3. 18584300	2. 33380600	-3. 48489900
C	1. 60992500	-2. 51495100	-2. 55725700
C	0. 61817500	-2. 69080500	-3. 52553200
C	2. 35123700	-3. 56534300	-2. 00643700
C	0. 35693200	-3. 99921500	-3. 92751900
C	2. 04596800	-4. 85153800	-2. 44580900
C	1. 04982900	-5. 08678400	-3. 39480300
H	-0. 41373600	-4. 17008500	-4. 67453800
H	2. 60497000	-5. 69015400	-2. 03835700
C	-1. 04415200	-2. 21750400	1. 18283000
C	-0. 25425400	-1. 79756000	0. 12508700
H	-0. 54328600	-2. 40803100	2. 13070800
C	-2. 35391700	-2. 85121300	0. 97081900
C	-2. 78383300	-3. 85582400	1. 84672100
C	-3. 18361500	-2. 46636800	-0. 09219300
C	-4. 01413000	-4. 47802400	1. 65755000
H	-2. 14506200	-4. 14873600	2. 67597100
C	-4. 41999500	-3. 07711000	-0. 26465500
H	-2. 87801500	-1. 66064300	-0. 75587100
C	-4. 83676900	-4. 08531000	0. 60377800
H	-4. 33354900	-5. 26243700	2. 33642700
H	-5. 06477600	-2. 75805300	-1. 07685200
H	-5. 80331800	-4. 55846800	0. 46290200
C	1. 06487900	-1. 34722800	0. 33598700
O	1. 74118400	-1. 33493400	1. 37693100
H	-0. 66735000	-1. 71627300	-0. 87519300
C	-3. 07297100	0. 22092000	1. 56554000
C	-4. 47032300	0. 10543400	2. 08555100
C	-5. 37974900	1. 14831100	1. 88090300
C	-4. 90482600	-1. 05163500	2. 73787500
C	-6. 69133700	1. 04035500	2. 33023400
H	-5. 04113400	2. 04255500	1. 36775400
C	-6. 22179900	-1. 16470000	3. 17330000
H	-4. 22300200	-1. 88522600	2. 87523400
C	-7. 11772700	-0. 11713900	2. 97844000
H	-7. 38373000	1. 86204500	2. 17497900
H	-6. 54709000	-2. 07803100	3. 66210900
H	-8. 14207500	-0. 20205900	3. 32736900

N	-3.00517100	0.78102900	0.39887200
N	-1.73796000	0.79530400	-0.16106200
S	-1.62507200	1.27254800	-1.72280000
O	-0.18614400	1.19453500	-2.00152800
O	-2.56507100	0.48450500	-2.50859600
C	-2.09875600	2.97650300	-1.84931400
C	-1.11917600	3.93569500	-2.08040200
C	-1.50058200	5.27327500	-2.15285700
C	-2.83422300	5.65258500	-1.99185100
C	-3.79594700	4.65985300	-1.76194900
C	-3.44148500	3.32011300	-1.69245300
H	-0.08538500	3.62905000	-2.22153100
H	-0.74905300	6.03401400	-2.34347500
H	-4.83763400	4.94536600	-1.64336800
H	-4.18271200	2.54599500	-1.52461300
C	-3.24620700	7.09951000	-2.06618200
H	-4.01640400	7.24624800	-2.82867400
H	-2.39785500	7.74208100	-2.30955900
H	-3.66402300	7.43386800	-1.11187800
C	-1.99644100	-0.34174600	2.37295700
H	-2.31663100	-0.95195300	3.20894700
C	-0.73474000	0.27623300	2.59289200
O	-0.23187800	1.22426500	1.95211900
O	-0.04890000	-0.29849900	3.60692100
C	1.26780000	0.19379900	3.86475900
C	2.01519900	-0.88436500	4.61801500
H	1.76600000	0.40803400	2.91776900
H	1.19145500	1.12496400	4.43836300
H	3.03110000	-0.54730400	4.84196600
H	2.07594700	-1.78020000	3.99605800
H	1.51459400	-1.13171200	5.55730800
H	-0.95473900	1.08724300	0.46180200
C	3.44234100	-3.32815200	-0.99277700
H	4.06492500	-2.47184300	-1.27073600
H	3.03763900	-3.13252700	0.00580100
H	4.08671700	-4.20582100	-0.92478600
C	-0.12651800	-1.52256600	-4.11061200
H	-0.48722400	-0.83899700	-3.33787600
H	0.52573400	-0.94136600	-4.76943200
H	-0.98327900	-1.87012500	-4.68955600
C	0.71547900	-6.49298000	-3.81830300
H	0.27654100	-6.51172700	-4.81806300
H	1.60425100	-7.12813600	-3.81727300
H	-0.00930100	-6.93623600	-3.12800100

N	6.28274800	-0.33556000	2.67725600
O	7.33754000	-0.06620800	3.22454000
O	5.80821400	-1.45425200	2.60397800

***Re*-TS1 (L2)**

C	5.95511400	-0.27229700	0.63516700
C	4.60046100	-0.51724000	0.84692800
C	4.09468200	-0.71977600	2.12624300
C	4.97231500	-0.67319500	3.20646900
C	6.33204300	-0.42938100	3.00069700
C	6.83213700	-0.22787600	1.71586500
C	6.24802300	-0.09008900	-0.83288500
C	4.86334800	0.01777400	-1.51585400
C	3.83581800	-0.52400900	-0.45793300
H	3.03374300	-0.90228100	2.27923200
H	4.59817000	-0.82522400	4.21379500
H	7.00513800	-0.39290700	3.85151800
H	7.88934200	-0.03253100	1.56062000
H	6.84255500	0.80248900	-1.05164000
H	4.81145200	-0.58641100	-2.42202300
H	6.79871400	-0.95012100	-1.22876700
H	3.46962900	-1.51563900	-0.74011800
N	2.65755200	0.33837100	-0.38929900
O	4.58880300	1.33884700	-1.96445100
C	1.37332700	0.02372300	-0.10265800
C	2.76645000	1.69006100	-0.55214800
N	0.77837800	1.22826000	-0.09065200
N	1.61982100	2.27339100	-0.38719800
C	4.09699000	2.22049000	-0.97379400
H	4.77916100	2.29554000	-0.11502000
H	3.98878500	3.20760700	-1.42448400
C	-0.59475600	1.51452800	0.16490000
C	-1.26582400	0.84041900	1.17280600
C	-1.24539200	2.46720200	-0.61329000
C	-2.61834000	1.10132000	1.38449100
C	-2.58429300	2.73163000	-0.37151200
C	-3.30343800	2.05073900	0.62300000
H	-3.13043000	0.55257600	2.16663100
H	-3.08291800	3.47925500	-0.98160000
H	-0.70163300	2.98156600	-1.39798400
H	-0.73813500	0.11801800	1.78578600
C	-4.78370700	2.37345800	0.83823700
C	-5.54559100	2.16487200	-0.48007800
C	-5.41711800	1.47884100	1.90714500

C	-4.92184700	3.83952300	1.27916100
H	-5.18930500	2.83371800	-1.26884700
H	-5.43157500	1.13534800	-0.83385100
H	-6.61303600	2.36133100	-0.33397200
H	-5.97729000	4.09002100	1.43186800
H	-4.38935800	4.01580100	2.21915700
H	-4.51861500	4.52671500	0.52918400
C	-1.44793800	-2.30047900	0.27901100
C	-0.60242800	-1.71211400	-0.57165200
H	-0.94081000	-2.80242500	1.10507500
C	-2.91146400	-2.43532100	0.31745200
C	-3.43299400	-3.45459300	1.12974400
C	-3.81303200	-1.60103500	-0.36166200
C	-4.80179000	-3.66200000	1.24020800
H	-2.74550500	-4.09711200	1.67372000
C	-5.18470300	-1.81304900	-0.25048200
H	-3.44356900	-0.78537100	-0.97060700
C	-5.68586000	-2.84087000	0.54498500
H	-5.17732700	-4.46239700	1.86999200
H	-5.86994100	-1.16707300	-0.79154300
H	-6.75692800	-2.99840300	0.62389400
Br	-1.08838400	-0.83533500	-2.17031600
C	0.90415300	-1.80067300	-0.38892500
H	-6.47759900	1.72921900	2.01101800
H	-5.34756200	0.41924600	1.63780600
H	-4.94753300	1.62046400	2.88593000
H	1.11151200	-2.16105600	0.64366700
O	1.60719600	-2.18596000	-1.35243800

Si-TS1 (L2)

C	4.39025500	-2.81891300	-0.10118300
C	3.22910300	-2.25515900	-0.62453700
C	2.67975500	-2.70595300	-1.82183300
C	3.32967400	-3.73295600	-2.50294200
C	4.50134800	-4.29374900	-1.98946500
C	5.03814100	-3.84320700	-0.78592500
C	4.76915000	-2.18008400	1.21010200
C	3.56614500	-1.28857100	1.59659400
C	2.70972100	-1.15839500	0.28093200
H	1.75981300	-2.27853500	-2.21435100
H	2.92032100	-4.10227300	-3.43750900
H	4.99456700	-5.09521300	-2.53049900
H	5.94305500	-4.28912600	-0.38342600
H	4.96209400	-2.90832900	2.00414200

H	3.88926400	-0.29897200	1.92171400
H	5.67383700	-1.57192900	1.10407000
H	2.85542000	-0.16550700	-0.14853200
N	1.28524300	-1.30930400	0.56411700
O	2.84570800	-1.80011700	2.70685500
C	0.20991300	-0.76559600	-0.05742800
C	0.86045500	-2.16377300	1.54222500
N	-0.82131500	-1.32740800	0.60235300
N	-0.43172800	-2.18898500	1.59846700
C	1.89931500	-2.80688000	2.39700900
H	2.36026500	-3.65822500	1.87656800
H	1.46279200	-3.15761900	3.33258700
C	-2.23039000	-1.13029600	0.42158300
C	-2.71998000	-0.62421700	-0.77875600
C	-3.09125300	-1.47535100	1.45624400
C	-4.09161200	-0.46148600	-0.91785000
C	-4.46310600	-1.30906900	1.28592900
C	-4.99475200	-0.80009800	0.09901300
H	-4.46367600	-0.06265000	-1.85726900
H	-5.11443800	-1.58670800	2.10666700
H	-2.69516900	-1.87172200	2.38301100
H	-2.03573400	-0.34838800	-1.58055500
C	-6.49641700	-0.60521700	-0.12607100
C	-6.77796300	0.88066000	-0.40250600
C	-6.93997600	-1.44125900	-1.33806400
C	-7.32427500	-1.03670600	1.08806100
H	-6.47551100	1.49978400	0.44804400
H	-6.23956900	1.23634400	-1.28572400
H	-7.84825000	1.03748900	-0.57627400
H	-8.38709100	-0.87873400	0.88009100
H	-7.18463100	-2.09812200	1.31788600
H	-7.07119000	-0.45348900	1.97945600
C	1.77906700	2.32229400	-0.84420100
C	0.61386100	1.66928000	-0.88897800
H	2.58665300	1.80478500	-1.36671500
C	2.16701900	3.62505100	-0.27832300
C	3.25369500	4.28587200	-0.86926000
C	1.55450700	4.21239000	0.83711300
C	3.69814900	5.51015200	-0.38629300
H	3.74530100	3.83133400	-1.72538200
C	2.00725200	5.43406200	1.32537800
H	0.73081400	3.70848600	1.32769200
C	3.07415400	6.08991600	0.71559500
H	4.53435700	6.00840200	-0.86665300

H	1.52618900	5.87342100	2.19378800
H	3.42159700	7.04353500	1.10044800
Br	-1.02592100	2.33761800	-0.23167400
C	0.46526600	0.32729000	-1.59890300
H	1.49089400	-0.06994100	-1.78290100
O	-0.40621900	0.17702600	-2.48088800
H	-8.01332300	-1.31188600	-1.51434600
H	-6.41356900	-1.14300700	-2.24926000
H	-6.74647100	-2.50543200	-1.17003800

Re-M1 (L2)

C	5.80890300	0.13641500	0.47481000
C	4.52538400	-0.21100300	0.89110500
C	4.16783600	-0.18626300	2.23742800
C	5.11554700	0.23915900	3.16409700
C	6.39679500	0.61463000	2.75139900
C	6.75545500	0.55446700	1.40756900
C	5.98363700	-0.03835600	-1.00950200
C	4.63334900	-0.61171500	-1.50710200
C	3.65608900	-0.62853100	-0.27314100
H	3.17741600	-0.53949000	2.51641200
H	4.86254500	0.26579800	4.21959800
H	7.12506600	0.94222200	3.48738800
H	7.75949700	0.82488700	1.09266600
H	6.21822500	0.90417600	-1.51658600
H	4.75979700	-1.64442700	-1.83399900
H	6.80147800	-0.72589400	-1.24322300
H	3.17684200	-1.59156000	-0.09947800
N	2.52779800	0.31146800	-0.49655600
O	4.13425500	0.05699800	-2.65397800
C	1.32753700	0.36605600	0.10860500
C	2.53766200	1.28096100	-1.46237100
N	0.68849100	1.37340100	-0.48980200
N	1.41853500	1.94193700	-1.49119600
C	3.70014700	1.37209900	-2.39213000
H	4.49720000	1.99511900	-1.96488100
H	3.37914500	1.81856500	-3.33442800
C	-0.69401900	1.70036700	-0.31786100
C	-1.16323300	2.14725200	0.90999800
C	-1.55514000	1.44823900	-1.37523500
C	-2.53242000	2.30531700	1.08077800
C	-2.92152600	1.62728400	-1.18802900
C	-3.43945600	2.03898700	0.04455600
H	-2.89885600	2.63546300	2.04794000

H	-3.58636200	1.41430500	-2.01716900
H	-1.15701400	1.07712700	-2.31412300
H	-0.46987200	2.34712900	1.72063400
C	-4.94295700	2.17091800	0.30076900
C	-5.76376300	1.95462900	-0.97346100
C	-5.36082700	1.10127400	1.32287500
C	-5.25986400	3.56961900	0.85312200
H	-5.49947100	2.67281900	-1.75679900
H	-5.63248600	0.94116400	-1.36697700
H	-6.82670500	2.08339600	-0.74766200
H	-6.33842400	3.66995600	1.01346200
H	-4.76830200	3.75461500	1.81264700
H	-4.94459000	4.35114600	0.15446400
C	-1.71353700	-1.24838600	1.10431100
C	-0.53499100	-1.20890700	0.48209700
H	-1.68598300	-0.82443900	2.10944100
C	-3.03012300	-1.77316900	0.70086500
C	-3.88290100	-2.24649300	1.70812200
C	-3.50438200	-1.75310200	-0.61825200
C	-5.15751600	-2.71409300	1.40897600
H	-3.53239500	-2.24919000	2.73680700
C	-4.78425100	-2.21185500	-0.91559500
H	-2.87185400	-1.36813600	-1.40909200
C	-5.61460300	-2.69662600	0.09315700
H	-5.79715600	-3.08422300	2.20415900
H	-5.13586100	-2.18647800	-1.94278000
H	-6.61166400	-3.05362800	-0.14497800
Br	-0.22492900	-1.94946000	-1.24555000
C	0.76961500	-0.68916600	1.13320300
H	-6.42762300	1.19907800	1.55332600
H	-5.18648400	0.09772100	0.92214100
H	-4.80313700	1.19357300	2.26042900
H	0.39978500	-0.06623700	1.99028200
O	1.65466000	-1.61589100	1.39354500

Si-M1 (L2)

C	-5.90745800	0.05181600	0.06751000
C	-4.59855200	0.06950600	0.54144500
C	-4.22900000	-0.57204200	1.72166500
C	-5.22341100	-1.24402600	2.42959100
C	-6.54183900	-1.26606900	1.96675900
C	-6.89457200	-0.61909500	0.78488800
C	-6.04174300	0.81856700	-1.22258300
C	-4.59730600	1.18515500	-1.63860100

C	-3.69897300	0.85814200	-0.38460300
H	-3.18871900	-0.55301900	2.05928600
H	-4.96978400	-1.75851500	3.35098400
H	-7.30089200	-1.79675200	2.53348200
H	-7.91972100	-0.64233800	0.42658300
H	-6.52146100	0.24092200	-2.01973300
H	-4.50881800	2.24387800	-1.88460900
H	-6.63778900	1.72633900	-1.08294400
H	-3.33816800	1.77911600	0.07815800
N	-2.52005900	0.08656700	-0.78788500
O	-4.18706300	0.51986700	-2.82297900
C	-1.28925300	0.02261800	-0.24098500
C	-2.56919600	-0.81366200	-1.81699400
N	-0.65333300	-0.91125000	-0.95891700
N	-1.43659100	-1.42991200	-1.95456200
C	-3.81631800	-0.83404200	-2.63652800
H	-4.60555200	-1.40971100	-2.13357000
H	-3.62490700	-1.27357800	-3.61571900
C	0.68669700	-1.39008800	-0.79732800
C	1.16402700	-1.66166300	0.47887300
C	1.47917100	-1.55403800	-1.92476000
C	2.49047700	-2.05019600	0.61362400
C	2.79705200	-1.96938400	-1.76345600
C	3.33467000	-2.20759300	-0.49343900
H	2.87120300	-2.22145200	1.61628000
H	3.41010700	-2.08693200	-2.64951000
H	1.07285600	-1.34721800	-2.90924700
H	0.50753400	-1.51220300	1.33655500
C	4.80502400	-2.57358800	-0.27472100
C	5.48898300	-1.39892500	0.44602300
C	4.91330900	-3.83755900	0.59260100
C	5.54040100	-2.83086900	-1.59335300
H	5.45102000	-0.49495200	-0.17147900
H	5.00357600	-1.17722900	1.40216500
H	6.54036600	-1.63335500	0.64614400
H	6.57730100	-3.11175000	-1.38447200
H	5.07997300	-3.64791800	-2.15841800
H	5.56335700	-1.93992700	-2.22881300
C	0.97086300	1.95725800	-0.09122800
C	0.55347800	1.25310600	0.96216000
H	0.21406300	2.12100300	-0.86280800
C	2.28879200	2.55215200	-0.37982200
C	2.34698500	3.79687500	-1.01784600
C	3.48707400	1.88276900	-0.09844900

C	3.56961800	4.38193100	-1.32924200
H	1.42133200	4.31273600	-1.25966500
C	4.70858200	2.46747500	-0.41424200
H	3.45316800	0.89911700	0.36014800
C	4.75588500	3.71927100	-1.02478500
H	3.59628100	5.35336900	-1.81333300
H	5.63023300	1.93970400	-0.18653000
H	5.71191000	4.17289500	-1.26717700
Br	1.62963900	0.95167200	2.48559200
C	-0.88306600	0.66023300	1.10935000
H	-1.53411800	1.56938400	1.18313600
O	-1.07700100	-0.25979500	2.03342500
H	5.96615100	-4.09936800	0.74163900
H	4.46702500	-3.69698500	1.58074700
H	4.41510300	-4.68639900	0.11384300

Re-TS1 (L3)

C	5.50945100	0.96751600	-0.07262500
C	4.38754900	0.63657700	0.68630200
C	4.10700000	1.28877300	1.88180900
C	4.96682700	2.30048600	2.30198400
C	6.08827700	2.64096000	1.54342700
C	6.37010400	1.97317000	0.35386000
C	5.60340200	0.12122100	-1.31287200
C	4.58689000	-1.01391900	-1.04447900
C	3.60369800	-0.48289400	0.04380000
H	3.24428800	0.97422600	2.46298700
H	4.77145800	2.81951100	3.23505600
H	6.75414800	3.42596800	1.88856600
H	7.25031700	2.23184300	-0.22743800
H	5.33606400	0.70628600	-2.20026100
H	5.11322100	-1.86100900	-0.60122400
H	6.60480400	-0.27920100	-1.48908500
H	3.29718700	-1.24609300	0.76011600
N	2.36248900	-0.01008900	-0.59449700
O	3.95779800	-1.54847800	-2.19201900
C	1.25343700	0.46228400	0.02392800
C	2.12416700	-0.06679400	-1.93967900
N	0.43107700	0.72292000	-1.00198700
N	0.94048600	0.38499900	-2.22998700
C	3.13470300	-0.63522300	-2.87974100
H	3.71304300	0.17050800	-3.35126000
H	2.62528200	-1.18771000	-3.67014400
C	-0.90933600	1.18368100	-0.89386000

C	-1.21904300	2.19912300	0.00294300
C	-1.90505000	0.56586200	-1.63483400
C	-2.54679400	2.56361600	0.17626900
C	-3.22806900	0.94827700	-1.45119800
C	-3.58217900	1.94133300	-0.53483500
H	-2.77428900	3.35617900	0.88191000
H	-3.99048500	0.42655400	-2.01610400
H	-1.64662900	-0.23138600	-2.32185600
H	-0.42730900	2.68723000	0.56150400
C	-5.03490100	2.37901600	-0.31161600
C	-6.02703500	1.48591100	-1.06939100
C	-5.38146400	2.30898300	1.18696900
C	-5.19660700	3.82909500	-0.80661000
H	-5.88871900	1.55288100	-2.15313200
H	-5.93170000	0.43724900	-0.76887200
H	-7.04944500	1.80791300	-0.84962800
H	-6.22866100	4.16552700	-0.66132900
H	-4.54025200	4.51398200	-0.26131700
H	-4.95745100	3.90767100	-1.87162200
C	-1.59305700	-0.86906000	1.42444800
C	-0.29131700	-1.12598800	1.27886800
H	-1.78509800	0.05921700	1.96241300
C	-2.81795100	-1.54072200	0.96808500
C	-4.01388900	-1.21024000	1.61926700
C	-2.87958000	-2.39958000	-0.13705100
C	-5.23217700	-1.72436400	1.19257800
H	-3.98285600	-0.53511200	2.47016100
C	-4.09910500	-2.90759900	-0.56944800
H	-1.97317700	-2.65405000	-0.67112800
C	-5.27941700	-2.57405500	0.09021200
H	-6.14481800	-1.45488600	1.71491400
H	-4.12684100	-3.56544000	-1.43246400
H	-6.22848300	-2.97353400	-0.25269800
Br	0.43737500	-2.67214300	0.45498300
C	0.78101300	-0.17196200	1.79231800
H	-6.41893000	2.62125200	1.34492400
H	-5.27080500	1.28706800	1.55929000
H	-4.74537500	2.96268800	1.79033700
H	0.29393000	0.75334800	2.15889500
O	1.79017600	-0.63644200	2.36907200

***Si*-TS1 (L3)**

C	6.00608700	0.23068600	-0.18327700
C	4.68895100	0.04752500	-0.59395400

C	4.33163600	-0.94018000	-1.50509400
C	5.33968200	-1.76852400	-1.99217800
C	6.66398700	-1.59969700	-1.58201500
C	7.00855600	-0.59661000	-0.67866300
C	6.12007300	1.38026200	0.78303800
C	4.66750100	1.68709100	1.20611600
C	3.77208000	1.04613500	0.08197300
H	3.28886200	-1.02232400	-1.81249600
H	5.09320400	-2.55038900	-2.70333400
H	7.43460600	-2.25835300	-1.97070600
H	8.03973400	-0.46704300	-0.36386200
H	6.72747700	1.15887600	1.66508900
H	4.48158200	2.75914900	1.27854500
H	6.56320800	2.25581100	0.29573000
H	3.41497600	1.80927000	-0.61187400
N	2.60450800	0.41135200	0.68697900
O	4.37331100	1.19685800	2.50807100
C	1.33206600	0.28679300	0.25097700
C	2.72768000	-0.30130500	1.84608700
N	0.74955600	-0.49216600	1.16975000
N	1.60868400	-0.86731700	2.17752300
C	4.01888600	-0.17282400	2.58158900
H	4.78889700	-0.82639000	2.15195100
H	3.88385000	-0.42307700	3.63321500
C	-0.61906900	-0.91065300	1.21722300
C	-0.95704100	-2.20183500	0.83679600
C	-1.59030000	0.00141500	1.59158800
C	-2.29848400	-2.54713800	0.76913200
C	-2.92928800	-0.35008700	1.49068400
C	-3.31010500	-1.61788500	1.04643900
H	-2.55570400	-3.54527600	0.43075700
H	-3.67149100	0.40344200	1.72381500
H	-1.30627900	1.00051100	1.90204200
H	-0.18276300	-2.90275900	0.54723400
C	-4.77237400	-1.97081900	0.75985200
C	-5.73790800	-0.88612200	1.25839500
C	-4.92648200	-2.09374300	-0.76941600
C	-5.15129100	-3.30033100	1.43603500
H	-5.63273900	-0.71676000	2.33528800
H	-5.58264500	0.06569900	0.74124400
H	-6.76862400	-1.20118800	1.06943900
H	-6.20214300	-3.53403500	1.23674100
H	-4.55363800	-4.13844700	1.06741100
H	-5.01531500	-3.23791600	2.52026000

C	-1.20409000	2.07095600	-0.78497000
C	-0.62021100	0.97087700	-1.26769500
H	-0.50451300	2.78864600	-0.35083300
C	-2.62411000	2.39520700	-0.57381300
C	-2.95824000	3.13066700	0.57257600
C	-3.66134000	1.98280000	-1.42022900
C	-4.28378900	3.39465500	0.89782800
H	-2.16529600	3.48072400	1.22892600
C	-4.98680900	2.25627600	-1.10049500
H	-3.42975700	1.44312100	-2.32897800
C	-5.30685400	2.95026100	0.06389600
H	-4.51721900	3.94959900	1.80105700
H	-5.77428200	1.92500700	-1.77032600
H	-6.34378600	3.15243700	0.31213500
Br	-1.56849300	-0.45908100	-2.05497200
C	0.91169300	0.72366400	-1.19332000
H	1.32832600	1.76808400	-1.26112900
O	1.41519300	-0.17782400	-1.99495600
H	-5.97021300	-2.29820000	-1.03117200
H	-4.61503400	-1.16565900	-1.25916700
H	-4.30987100	-2.90516300	-1.16827800

Re-M1 (L3)

C	5.83630200	0.08253000	0.47467900
C	4.53487900	-0.19604200	0.87768900
C	4.14651200	-0.09035500	2.20969400
C	5.08458600	0.35303800	3.13623300
C	6.38648300	0.66471100	2.73511100
C	6.77454500	0.51932800	1.40611300
C	6.03515600	-0.19386700	-0.99031400
C	4.64309500	-0.62568600	-1.52180700
C	3.67228900	-0.63475300	-0.27960900
H	3.14209200	-0.40729600	2.48080500
H	4.80950200	0.44469000	4.18224300
H	7.10815700	1.00719000	3.47031500
H	7.79474800	0.73730900	1.10407400
H	6.40447600	0.67633900	-1.54346500
H	4.67990300	-1.63313000	-1.93518700
H	6.76760700	-0.99136200	-1.14736200
H	3.19895700	-1.59812800	-0.08925200
N	2.54508000	0.29494900	-0.50269300
O	4.20530100	0.17277800	-2.61045800
C	1.31893300	0.30552500	0.04607400
C	2.60410600	1.33602600	-1.38765500

N	0.70605000	1.35368200	-0.50827700
N	1.48740900	2.00093000	-1.42644000
C	3.82014100	1.47664300	-2.23484400
H	4.61653000	2.00441200	-1.69162500
H	3.58491800	2.03528300	-3.14041900
C	-0.67800500	1.68120800	-0.35717400
C	-1.14534200	2.20631200	0.83847900
C	-1.54328200	1.36435500	-1.39184200
C	-2.51268200	2.37665300	1.00264200
C	-2.90751600	1.55031400	-1.21112800
C	-3.42323700	2.03796400	-0.00750700
H	-2.87502200	2.77287000	1.94569700
H	-3.57391700	1.27602400	-2.01917400
H	-1.15247500	0.92960300	-2.30494400
H	-0.45053100	2.45254300	1.63423800
C	-4.92735300	2.19842400	0.23937300
C	-5.76309400	1.75414300	-0.96841300
C	-5.33459000	1.32968200	1.44432600
C	-5.23716600	3.67789300	0.53433800
H	-5.53735100	2.34400100	-1.86276900
H	-5.60376000	0.69457100	-1.19315500
H	-6.82530700	1.88969700	-0.74428700
H	-6.31020900	3.81044700	0.70683700
H	-4.71099800	4.03361800	1.42494900
H	-4.94495800	4.31405400	-0.30707100
C	-1.72253900	-1.25952200	1.09869300
C	-0.55234600	-1.26941100	0.46103400
H	-1.67172500	-0.79330300	2.08259500
C	-3.06150800	-1.75336800	0.73555800
C	-3.91171600	-2.16491400	1.77086600
C	-3.55994800	-1.75518500	-0.57329400
C	-5.21149900	-2.58237700	1.51022100
H	-3.54290000	-2.15477200	2.79276700
C	-4.86454300	-2.16114600	-0.83271300
H	-2.92733200	-1.42391500	-1.38706500
C	-5.69543900	-2.57695900	0.20464300
H	-5.85010200	-2.90177700	2.32759300
H	-5.23579900	-2.14792700	-1.85302400
H	-6.71344700	-2.89085800	-0.00245600
Br	-0.27587300	-2.08328600	-1.24040100
C	0.76235700	-0.73731000	1.07779200
H	-6.40563600	1.44517000	1.64115600
H	-5.13304100	0.27327000	1.24662600
H	-4.79661600	1.61479400	2.35331000

H	0.40291900	-0.08216600	1.91856300
O	1.64865500	-1.65356300	1.37318900

Si-M1 (L3)

C	-5.91173800	0.04276300	0.06038600
C	-4.60342600	0.02634000	0.53318300
C	-4.23040800	-0.70784100	1.65524600
C	-5.22013700	-1.44167500	2.30430900
C	-6.53794300	-1.43270600	1.84092500
C	-6.89467100	-0.69059400	0.71760700
C	-6.04830500	0.92037800	-1.15599600
C	-4.60203600	1.29722300	-1.55770000
C	-3.70803900	0.88892700	-0.32569200
H	-3.18972400	-0.70874300	1.99245800
H	-4.96312300	-2.02735300	3.18106500
H	-7.29352700	-2.01281000	2.36166800
H	-7.91962700	-0.68958100	0.35888900
H	-6.55020700	0.42710600	-1.99406000
H	-4.50433700	2.36680400	-1.74349600
H	-6.62368200	1.82343500	-0.92696900
H	-3.36205400	1.77849800	0.20447400
N	-2.52260900	0.16233400	-0.77653100
O	-4.19840900	0.70122700	-2.78077700
C	-1.29622400	0.06051100	-0.22558700
C	-2.56573300	-0.67305800	-1.85751200
N	-0.65290300	-0.82263800	-0.99951200
N	-1.43363400	-1.28154600	-2.03096300
C	-3.80622500	-0.65477900	-2.68285100
H	-4.58723000	-1.27918200	-2.22774400
H	-3.60349100	-1.01989100	-3.68892900
C	0.69042200	-1.29665600	-0.86568700
C	1.13944200	-1.73409200	0.37322600
C	1.52139800	-1.28501300	-1.97588500
C	2.46463400	-2.12504400	0.49320000
C	2.84091700	-1.69873200	-1.83308400
C	3.34450500	-2.11321600	-0.59635100
H	2.81712700	-2.43295500	1.47234600
H	3.48194100	-1.67446800	-2.70590800
H	1.14568300	-0.94302000	-2.93375400
H	0.46367300	-1.69116600	1.22599000
C	4.80985400	-2.51279500	-0.38867900
C	5.45843100	-1.51457800	0.58968700
C	4.88231900	-3.93457000	0.19898200
C	5.61165800	-2.49213400	-1.69689500

H	5.45273400	-0.50695400	0.16308700
H	4.93071000	-1.47921400	1.54710000
H	6.49879400	-1.79484100	0.78567700
H	6.64709900	-2.78252700	-1.49486900
H	5.20722700	-3.19553900	-2.43198900
H	5.63199300	-1.49402600	-2.14568800
C	0.98072700	1.91521400	0.01406000
C	0.54287900	1.19931600	1.05036800
H	0.23507100	2.09465700	-0.76394800
C	2.30773800	2.49190700	-0.26562600
C	2.38644700	3.73177700	-0.91073700
C	3.49635000	1.81220100	0.02814300
C	3.61744900	4.29943500	-1.21959900
H	1.46980000	4.25857900	-1.16235200
C	4.72613900	2.37927300	-0.28453100
H	3.45076200	0.83578600	0.49724700
C	4.79361900	3.62513800	-0.90343500
H	3.65843800	5.26729900	-1.70921500
H	5.64068000	1.84444200	-0.04574600
H	5.75649700	4.06562200	-1.14165300
Br	1.59277900	0.84425100	2.57904400
C	-0.89358100	0.60444500	1.15385200
H	-1.54528500	1.50349100	1.30559800
O	-1.09298700	-0.39187400	2.00109300
H	5.92742500	-4.22541500	0.34780500
H	4.37758400	-4.00387900	1.16629000
H	4.41820100	-4.65902000	-0.47735600

Re-TS1 (L4)

C	5.98172900	-0.02337200	0.60695200
C	4.63792900	-0.05660800	0.98558700
C	4.23598900	0.36848100	2.24892600
C	5.20299100	0.83786500	3.13764500
C	6.54904900	0.87333900	2.76355400
C	6.94705800	0.44106900	1.49815500
C	6.15705000	-0.55397100	-0.79125800
C	4.72807200	-0.63034200	-1.37589400
C	3.78215100	-0.62121700	-0.12674400
H	3.18798300	0.34219600	2.53628000
H	4.90847500	1.17806400	4.12628300
H	7.29230000	1.24302300	3.46444600
H	7.99508900	0.47350200	1.21188000
H	6.79418900	0.07004000	-1.42625700
H	4.57504100	-1.54387300	-1.95344700

H	6.60751500	-1.55440300	-0.77289400
H	3.41260200	-1.63191000	0.09154500
N	2.59414100	0.18355100	-0.38461600
O	4.46840500	0.41493800	-2.31348700
C	1.32039900	0.01380500	0.04859700
C	2.67794300	1.33271600	-1.11916400
N	0.70612000	1.10834500	-0.44142100
N	1.52525300	1.93299100	-1.18640300
C	3.98173800	1.63309700	-1.77225900
H	4.68619200	2.07821800	-1.05478200
H	3.84457900	2.32874500	-2.60169200
C	-0.65063900	1.49367400	-0.25863100
C	-1.25576200	1.34298100	0.98308600
C	-1.35355500	2.06205400	-1.31963600
C	-2.57733100	1.74883100	1.15724600
C	-2.66454100	2.47304300	-1.12273800
C	-3.31126000	2.32627500	0.11561900
H	-3.02733600	1.61710200	2.13443300
H	-3.19529600	2.91375600	-1.96160100
H	-0.86961500	2.17935300	-2.28276700
H	-0.69318300	0.92169500	1.80974600
C	-4.76104200	2.79758100	0.28136000
C	-5.66028900	2.03838700	-0.71405600
C	-5.29515400	2.54594900	1.69780800
C	-4.84098100	4.30990900	-0.00558400
H	-5.35982800	2.21371800	-1.75153100
H	-5.62218200	0.96025700	-0.53003900
H	-6.70031300	2.36726200	-0.60919000
H	-5.87327100	4.66085600	0.10321800
H	-4.21406800	4.87572300	0.69140500
H	-4.51334600	4.54959100	-1.02158400
C	-1.62171200	-2.06910900	0.96205600
C	-0.62360300	-1.86581900	0.08758100
H	-1.26211700	-2.11801800	1.99192000
C	-3.06717800	-2.26763700	0.84963100
C	-3.74758900	-2.66364700	2.01708300
C	-3.82487800	-2.08215300	-0.32090900
C	-5.12020500	-2.88364700	2.01792300
H	-3.18133400	-2.80717900	2.93443000
C	-5.19937600	-2.30056500	-0.31699100
H	-3.33563600	-1.76378300	-1.23235000
C	-5.85473100	-2.70422200	0.84645500
H	-5.61627000	-3.19518100	2.93293300
H	-5.76310100	-2.15430000	-1.23435100

H	-6.92741200	-2.87580200	0.83999800
Br	-0.80018300	-1.79967600	-1.79782400
C	0.82276000	-1.82707300	0.53635000
H	-6.33088200	2.89433300	1.76499000
H	-5.28782900	1.48100100	1.95195500
H	-4.71719200	3.08689700	2.45475800
H	0.85694200	-1.67942800	1.63722200
O	1.65496100	-2.56931900	-0.03908300

Si-TS1 (L4)

C	4.34136600	-2.89961500	-0.08631600
C	3.17036300	-2.35640400	-0.61710000
C	2.61072700	-2.85211400	-1.79283500
C	3.24875900	-3.90963900	-2.43989100
C	4.42442300	-4.45473500	-1.91607700
C	4.97818500	-3.95429900	-0.73798900
C	4.74260800	-2.19346600	1.18074000
C	3.53111400	-1.30973300	1.55872700
C	2.66951700	-1.21700900	0.24469700
H	1.69118700	-2.43611200	-2.19615600
H	2.82689900	-4.31306000	-3.35555700
H	4.90871400	-5.28052000	-2.42952100
H	5.88842500	-4.38730400	-0.33181600
H	4.98327800	-2.87261100	2.00516200
H	3.84550100	-0.31041900	1.86610700
H	5.62894100	-1.56782300	1.01793300
H	2.83488400	-0.24566000	-0.22686200
N	1.24619100	-1.31986700	0.54414600
O	2.81857900	-1.80440400	2.68603600
C	0.17381900	-0.76044500	-0.07590200
C	0.81348300	-2.15034000	1.54052100
N	-0.86531200	-1.30130900	0.59673700
N	-0.48254600	-2.15750400	1.60778500
C	1.83809200	-2.79280900	2.40760600
H	2.27076200	-3.67899500	1.92132100
H	1.39910600	-3.09695300	3.35886200
C	-2.26865400	-1.08753400	0.41923200
C	-2.76399200	-0.62787100	-0.79887400
C	-3.13208200	-1.37264100	1.47345900
C	-4.13569500	-0.45447900	-0.93906000
C	-4.50293600	-1.19336000	1.30376200
C	-5.04063600	-0.73202800	0.09717400
H	-4.50275600	-0.09145900	-1.89496600
H	-5.15258300	-1.42124100	2.14152100

H	-2.73670000	-1.73315700	2.41564800
H	-2.08030100	-0.38587500	-1.61364300
C	-6.54423000	-0.52352900	-0.11972400
C	-6.80827600	0.95453900	-0.46800500
C	-7.01996700	-1.41603500	-1.28296000
C	-7.36705700	-0.87827900	1.12609300
H	-6.48474500	1.61236000	0.34531600
H	-6.27894100	1.25950600	-1.37537700
H	-7.87882500	1.11988700	-0.63436800
H	-8.43011700	-0.71379600	0.92250200
H	-7.24463900	-1.92881400	1.41058100
H	-7.09602300	-0.25515000	1.98502100
C	1.80545000	2.32017900	-0.87301800
C	0.61653500	1.69414200	-0.89067700
H	2.57269300	1.77567500	-1.42899200
C	2.28436100	3.58775600	-0.31596000
C	3.51019000	4.08114300	-0.80089000
C	1.62877400	4.32363000	0.68696500
C	4.04931900	5.27151500	-0.32659800
H	4.03770300	3.52131700	-1.56977400
C	2.17458700	5.51064200	1.16601400
H	0.69309100	3.96159600	1.09455400
C	3.38135700	5.99426300	0.66130500
H	4.99248200	5.63363900	-0.72622600
H	1.65191400	6.06091600	1.94357100
H	3.79960600	6.92360200	1.03744700
Br	-0.99761700	2.39148300	-0.18620700
C	0.41137300	0.37653400	-1.62647100
H	1.41939500	-0.04756700	-1.85151400
O	-0.49558100	0.26798400	-2.48233600
H	-8.09199100	-1.27109900	-1.45807800
H	-6.49589500	-1.18397200	-2.21479900
H	-6.85205100	-2.47458800	-1.05861100

Re-M1 (L4)

C	-5.81762200	-0.07184600	0.07730900
C	-4.50285100	-0.04503600	0.54334200
C	-4.12297100	-0.68717700	1.72178600
C	-5.10665900	-1.37406900	2.43287000
C	-6.42831300	-1.40787000	1.97656500
C	-6.79427800	-0.75684000	0.79872300
C	-5.96616700	0.71155300	-1.19879100
C	-4.52639800	1.07878800	-1.63158800
C	-3.62090100	0.76695400	-0.37881700

H	-3.08113300	-0.65742800	2.05555200
H	-4.84192200	-1.88817500	3.35245900
H	-7.17970700	-1.94875500	2.54549500
H	-7.82292100	-0.78798500	0.44921600
H	-6.46618400	0.15483500	-1.99900400
H	-4.44601600	2.13675500	-1.88796500
H	-6.55526900	1.62241400	-1.03800100
H	-3.29120600	1.69883500	0.08868600
N	-2.41886800	0.03844100	-0.78598100
O	-4.11692700	0.41288900	-2.81987500
C	-1.18164100	0.00032900	-0.23310700
C	-2.44951100	-0.86534700	-1.81114200
N	-0.52371600	-0.92744000	-0.95380900
N	-1.30459500	-1.46519700	-1.94879900
C	-3.68687500	-0.92709900	-2.63572400
H	-4.45584900	-1.54477000	-2.15007600
H	-3.47120200	-1.34631300	-3.61936300
C	0.80551000	-1.42441800	-0.78874100
C	1.29944800	-1.67657400	0.48893600
C	1.56713800	-1.69150900	-1.92162400
C	2.58916900	-2.17922800	0.61241500
C	2.85071000	-2.20768200	-1.76863700
C	3.39412900	-2.45976700	-0.50220600
H	2.96881600	-2.36238300	1.61332800
H	3.43071900	-2.40699100	-2.66260300
H	1.15998400	-1.50054500	-2.90872900
H	0.66554900	-1.46215600	1.35134900
C	4.80776800	-3.01935900	-0.30229100
C	5.63748800	-2.01965500	0.52739600
C	4.72219500	-4.36254400	0.44918200
C	5.53373900	-3.25848000	-1.63311100
H	5.71957500	-1.05662900	0.01308600
H	5.19220000	-1.83702500	1.50978600
H	6.64938400	-2.40905000	0.68636200
H	6.53576900	-3.65386300	-1.43794700
H	5.00911500	-3.98753300	-2.25983200
H	5.65185000	-2.33271900	-2.20624900
C	0.93398100	2.12128400	-0.03416300
C	0.57151900	1.35528200	1.00659500
H	0.16848900	2.14844700	-0.81497600
C	2.10411200	2.93530200	-0.37067400
C	2.01046900	3.73902000	-1.52359100
C	3.31277500	2.96514500	0.34922800
C	3.06358600	4.54770200	-1.93468300

H	1.08912500	3.72645700	-2.10166100
C	4.36764700	3.77114700	-0.06764400
H	3.42523300	2.35196200	1.23385400
C	4.25198400	4.56860200	-1.20568600
H	2.95734900	5.15964500	-2.82625200
H	5.29128900	3.77384200	0.50494800
H	5.07960800	5.19694800	-1.52250800
Br	1.58712500	1.11162700	2.58054000
C	-0.81312500	0.64428700	1.10693300
H	-1.52872900	1.50302500	1.20627900
O	-0.96154100	-0.31591400	2.00941700
H	5.72601700	-4.77380100	0.60349000
H	4.25356500	-4.25192700	1.43163900
H	4.13880300	-5.09382700	-0.11986000

Si-M1 (L4)

C	5.60273400	0.48707700	0.22032100
C	4.32070500	0.42764500	0.76599500
C	4.02465300	1.00393800	1.99931800
C	5.03558300	1.69573800	2.66395000
C	6.31658400	1.78911100	2.10908000
C	6.61271200	1.17537600	0.89222400
C	5.68825200	-0.30390600	-1.05655600
C	4.23075600	-0.70104500	-1.39767200
C	3.38503100	-0.37021500	-0.10974500
H	3.03282300	0.85101800	2.41966600
H	4.83240900	2.15514300	3.62740000
H	7.09433000	2.33206300	2.63949400
H	7.61655500	1.23062600	0.47886800
H	6.13210800	0.24905800	-1.89217200
H	4.14428600	-1.76503400	-1.62347900
H	6.30223500	-1.20168900	-0.91755400
H	3.01021500	-1.25339000	0.41268200
N	2.18382500	0.39892200	-0.48156400
O	3.76742100	-0.06638500	-2.58756400
C	0.95748100	0.43458500	0.07428600
C	2.18583300	1.26846400	-1.53696500
N	0.28408300	1.33872300	-0.65084200
N	1.03298800	1.86101700	-1.67634000
C	3.38850400	1.28768300	-2.41249200
H	4.19498500	1.89121300	-1.97154300
H	3.13921300	1.69817000	-3.39203500
C	-1.06990600	1.76675800	-0.48234900
C	-1.45434600	2.42264900	0.68509200

C	-1.98199900	1.54858200	-1.50688300
C	-2.77301000	2.83790400	0.82332000
C	-3.29697200	1.98125200	-1.35303600
C	-3.72514700	2.62772200	-0.18721500
H	-3.05810300	3.34648400	1.73938200
H	-3.99358600	1.79751600	-2.16284600
H	-1.66635100	1.04203500	-2.41284700
H	-0.72788300	2.61597000	1.46799800
C	-5.16849600	3.10474100	0.01423000
C	-6.06033800	2.78333000	-1.19232000
C	-5.76339700	2.40912300	1.25454900
C	-5.17433600	4.63123900	0.22842600
H	-5.70685100	3.27509400	-2.10469300
H	-6.11995500	1.70623500	-1.38057200
H	-7.07708200	3.13986100	-1.00000100
H	-6.19999200	4.98649400	0.37640600
H	-4.59234100	4.92408500	1.10752000
H	-4.75675300	5.15131600	-0.63980100
C	-1.69035100	-1.69318200	0.96267200
C	-0.38709900	-1.54776400	0.67786300
H	-2.05549700	-0.90693100	1.62575700
C	-2.71857500	-2.67837100	0.61498100
C	-3.89559200	-2.67024800	1.38731600
C	-2.63509400	-3.60199900	-0.44215600
C	-4.93424800	-3.55955400	1.13689600
H	-3.98494900	-1.95653100	2.20292600
C	-3.67897600	-4.48696100	-0.69578500
H	-1.75318300	-3.62272800	-1.07011400
C	-4.82981500	-4.47653600	0.09152200
H	-5.82644900	-3.53530300	1.75658700
H	-3.59169900	-5.18997300	-1.51985400
H	-5.63892100	-5.17276300	-0.11057100
Br	0.63266900	-2.78253000	-0.36461900
C	0.51044100	-0.43970500	1.28956300
H	-6.79405900	2.74357200	1.41557000
H	-5.77473700	1.32187800	1.12677800
H	-5.19554400	2.63552200	2.16196200
H	-0.23549500	0.20872000	1.82200100
O	1.54147000	-0.86116700	1.97873600

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