

SUPPORTING INFORMATION FOR

Elucidating the mechanism and origin of stereoselectivity on the activation/transformation of an acetic ester catalyzed by an N-heterocyclic carbene

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Part 2: Test of methods and solvation models

Table S1. Test of different methods and solvation models for stereoselective transition states

13-ts	M06-2X		B3LYP		ω B97X-D	
	SMD	IEF-PCM	SMD	IEF-PCM	SMD	IEF-PCM
R	0	0	0	0	0	0
S	2.4	3.1	1.2	1.9	2.1	3.4

Table S2. Test of different methods and basis sets for stereoselective transition states using IEF-PCM solvation model (L1=6-311+G(d, p), L2=6-311++G(2df, 2pd))

13-ts	M06-2X-D3		B3LYP		B3LYP-D3		ω B97X-D	
	L1	L2	L1	L2	L1	L2	L1	L2
R	0	0	0	0	0	0	0	0
S	4.0	4.2	1.7	1.7	2.5	2.6	3.2	3.2

Part 3: Energy profiles for the unfavorable S-configured pathway involved in the reaction between **10** and **R2a**

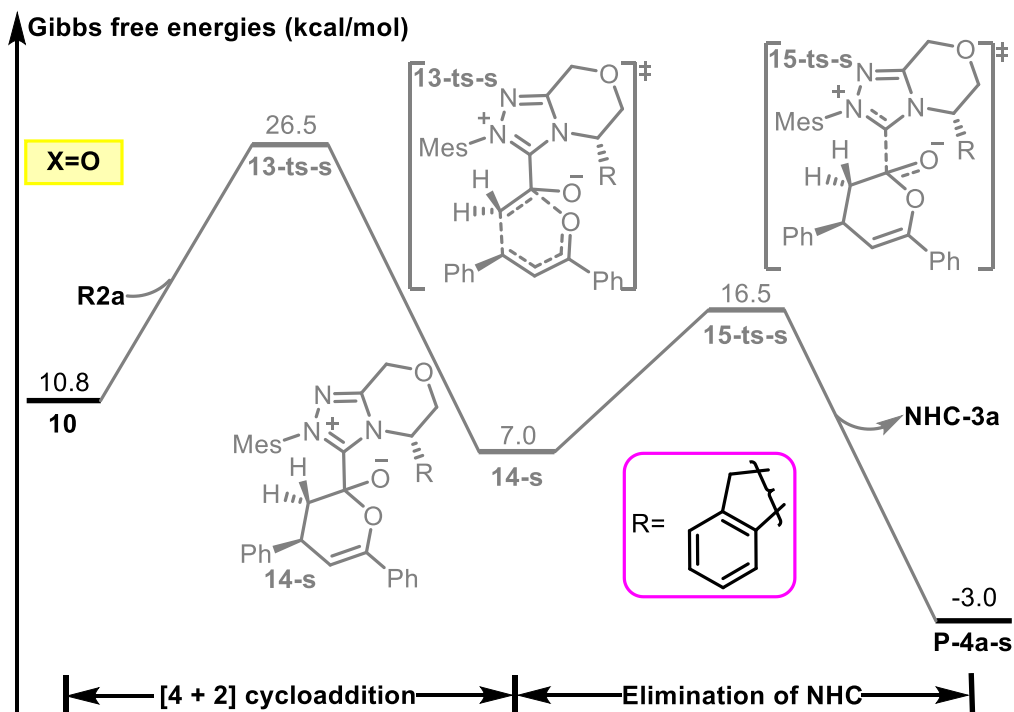


Fig. S3 Energy profiles for the unfavorable S-configured pathway involved in the reaction between **10** and **R2a**

Part 4: Energy profiles for the unfavorable *S*-configured pathway involved in the reaction between 10 and R2b

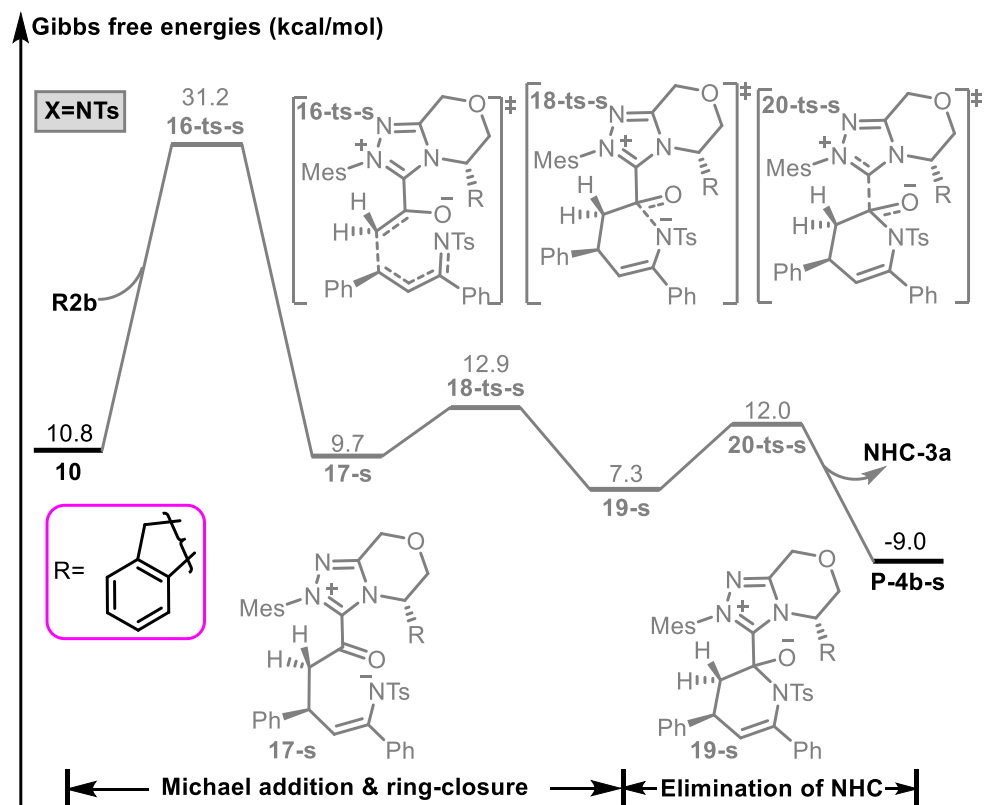


Fig. S4 Energy profiles for the unfavorable *S*-configured pathway involved in the reaction between 10 and R2b

Part 5: Possible configurations of the transition states involved in reaction between 10 and R2a

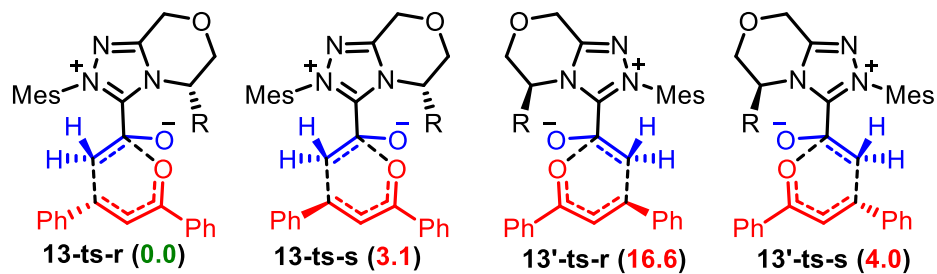


Fig. S5 The four possible configurations of the transition states involved in [4 + 2] cycloaddition step (The relative Gibbs free energies are given in parentheses and the unit of energy is given in kcal/mol)

Part 6: Energy profile for the formation of enolate intermediate 26

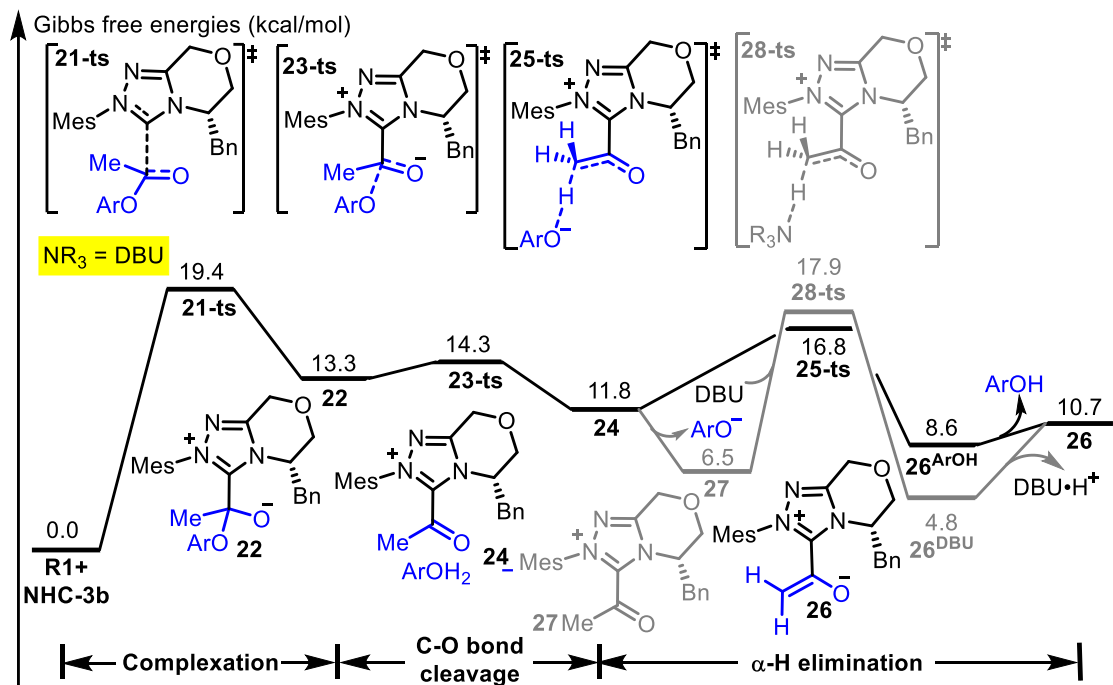


Fig. S6 Energy profile for the formation of the enolate 26 catalyzed by NHC-3b.

Part 7: Energy profiles for the unfavorable S-configured pathway involved in the reaction between 26 and R2b

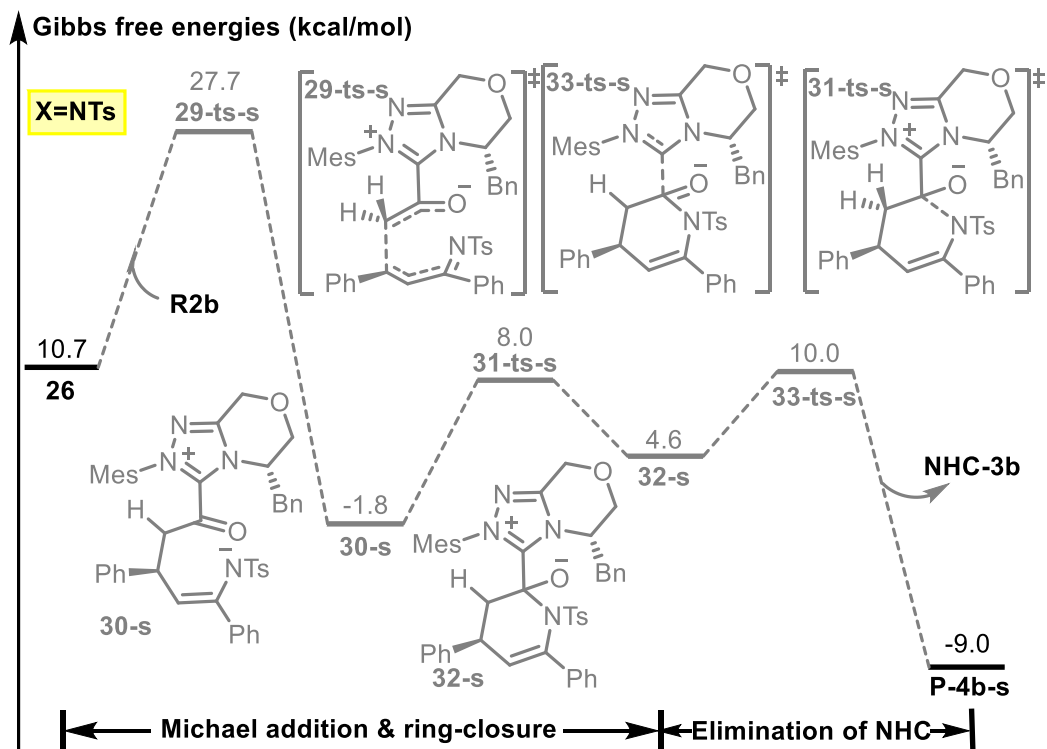


Fig. S7 Energy profiles for the unfavorable *S*-configured pathway involved in the reaction between 26 and R2b

Part 8: Energy profiles for reaction of the enolate intermediate 26 with R2a catalyzed by NHC-3b

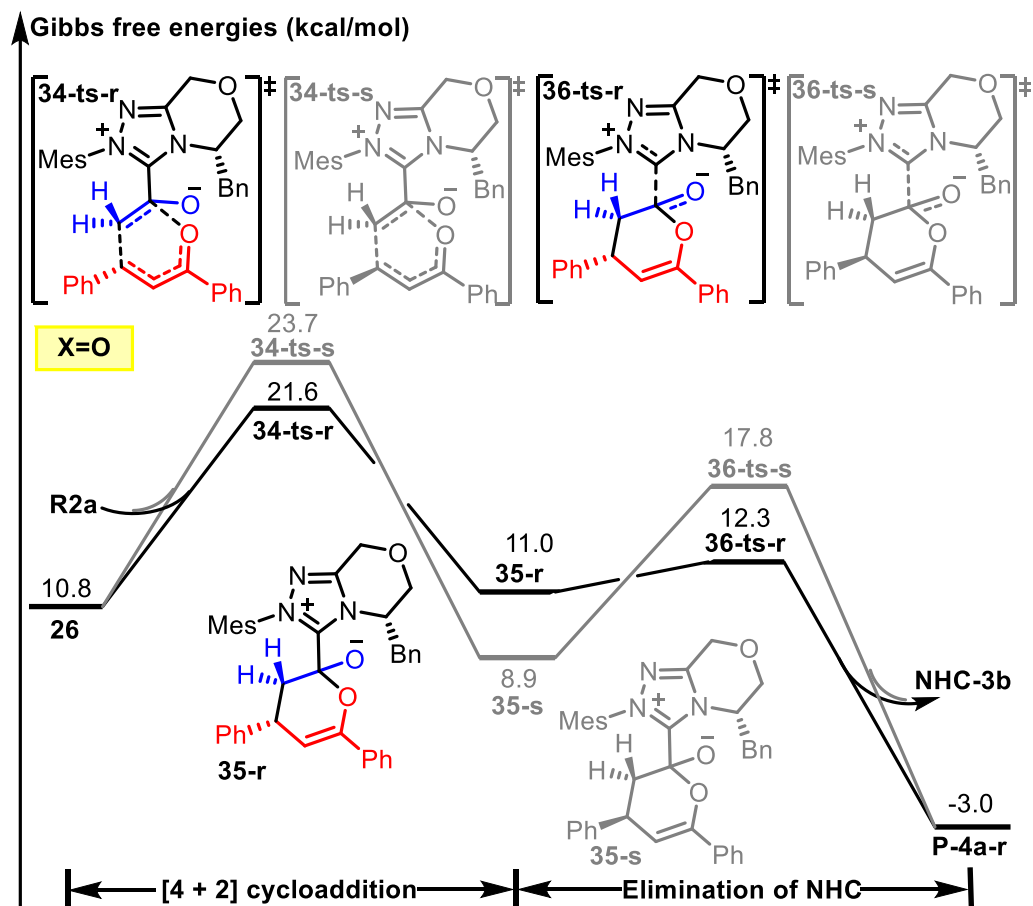


Fig. S8 Energy profiles for reaction of the enolate intermediate **26** with **R2a** catalyzed by NHC-

3b

Part 9: derivation of the calculated ee value

The predicted ee value is calculated by using Boltzmann distribution along with the stereoselective transition states through the following equations:

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

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

In the equation (1), the ΔG^\ddagger is the difference in Gibbs free energies of the stereoselective transition states, R is the gas constant ($R=8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$), T is the temperature ($T=298.15 \text{ K}$ in the reaction).

For the present study, the computational results show that the reaction between enolate intermediate **10** and chalcone **R2a** determines the stereoselectivity associated with transition state **13-ts**. The calculated results also indicate that the *R*-configured pathway has the lowest energy barrier and the energy difference between **13-ts-r** and **13-ts-s** is 3.2 kcal/mol. That is, the value of ΔG^\ddagger in equation (1) is 3.2 kcal/mol. Thus, we can obtain the value of $[R]/[S]$, which is calculated to be 226.9. Then, the value of $[R]/[S]$ is substituted into equation, the calculated ee value can be obtained by 99.1 %, which is very closed to the experimental observed ee value (98%).

Part 10: Energies of all the stationary points (SP)

SP	E^a	G^b	$G_{\text{correction}}$	IF (cm ⁻¹)
R1a	-664.56176	-664.268127	0.107155	–
R2a	-653.931953	-653.590269	0.184709	–
R2b	-1452.927381	-1452.343428	0.302559	–
NHC-3a	-1052.168533	-1051.587702	0.330955	–
NHC-3b	-1053.369168	-1052.765927	0.350957	–
Pre-NHC-3a	-1514.669061	-1513.740975	0.581795	–
Pre-NHC-3b	-1053.596428	-1053.232128	0.364300	–
DBU	-462.00664	-461.68408	0.21325	–
DBU•H⁺	-462.479238	-462.148871	0.227556	–
ArO[•]	-511.465437	-511.241213	0.062763	–
ArOH	-511.927322	-511.70527	0.076086	–
TS0	-1514.666124	-1513.736442	0.577810	-1216.18
TS1	-1515.510647	-1514.913475	0.597171	-1196.17
P-4a-r	-806.578598	-806.156727	0.22311	–
P-4a-s	-806.577378	-806.154633	0.224062	–
P-4b-r	-1605.585425	-1604.917158	0.342798	–
P-4b-s	-1605.585676	-1604.917291	0.342822	–
5-ts	-1716.725589	-1715.829219	0.465906	-141.30
6	-1716.734686	-1715.83665	0.467013	–
7-ts	-1716.734892	-1715.834073	0.468004	-96.17
8	-1716.741688	-1715.844606	0.461303	–
9-ts	-1716.720716	-1715.824269	0.46287	-1263.74
10^{ArOH}	-1716.727606	-1715.826766	0.465990	–
10^{DBU}	-1204.792513	-1666.279614	0.619203	–
10	-1204.792513	-1204.129992	0.368704	–
11	-1205.254832	-1204.591945	0.38034	–
12-ts	-1667.266437	-1666.265597	0.61238	-1343.33
13-ts-r	-1858.730703	-1857.704904	0.579701	-332.44
13'-ts-r	-1858.704762	-1857.675085	0.580342	-465.63
13-ts-s	-1858.724773	-1857.699357	0.578815	-374.63
13'-ts-s	-1858.726700	-1857.698868	0.582198	-332.36
14-r	-1858.761273	-1857.731792	0.586188	–
14-s	-1858.758406	-1857.733148	0.581358	–
15-ts-r	-1858.741902	-1857.718707	0.581084	-155.88
15-ts-s	-1858.742922	-1857.71924	0.580954	-161.18
16-ts-r	-2657.719571	-2656.446679	0.699872	-292.00
16-ts-s	-2657.71825	-2656.442217	0.70226	-459.84
17-r	-2657.755248	-2656.474991	0.70685	–
17-s	-2657.752691	-2656.475965	0.702402	–

18-ts-r	-2657.756438	-2656.478327	0.708248	-81.28
18-ts-s	-2657.753939	-2656.473708	0.708714	-49.86
19-r	-2657.76414	-2656.483846	0.711573	–
19-s	-2657.760477	-2656.485732	0.706311	–
20-ts-r	-2657.751617	-2656.475841	0.70686	-120.98
20-ts-s	-2657.753088	-2656.477473	0.706509	-128.62
Energies for 3b-catalyzed reactions				
21-ts	-1717.931305	-1717.009705	0.489461	-199.20
22	-1717.942551	-1717.019320	0.490955	–
23-ts	-1717.938712	-1717.014440	0.488744	-84.82
24	-1717.941296	-1717.016701	0.487206	–
25-ts	-1717.931423	-1717.008845	0.485374	-1153.01
26^{ArOH}	-1717.947200	-1717.020828	0.488167	–
26	-1205.996041	-1205.308262	0.391434	–
27	-1206.462091	-1205.776079	0.402311	–
28-ts	-1668.467112	-1667.444204	0.632153	-1293.06
26^{DBU}	-1668.481921	-1667.468302	0.636334	–
29-ts-r	-2658.927126	-2657.648228	0.719893	-243.07
29-ts-s	-2658.914007	-2657.62709	0.720332	-301.06
30-r	-2658.982706	-2657.681197	0.727462	–
30-s	-2658.975605	-2657.673372	0.726536	–
31-ts-r	-2658.96611	-2657.660533	0.732362	-118.30
31-ts-s	-2658.964089	-2657.659522	0.730341	-68.34
32-r	-2658.966895	-2657.662580	0.731936	–
32-s	-2658.968034	-2657.667788	0.728928	–
33-ts-r	-2658.953668	-2657.651146	0.729825	-168.07
33-ts-s	-2658.957993	-2657.658898	0.727497	-142.99
34-ts-r	-1859.93438	-1858.884699	0.599969	-330.74
34-ts-s	-1859.931815	-1858.874944	0.600776	-391.45
35-r	0.606525	-1858.906536	-1859.95775	–
35-s	0.605186	-1858.909192	-1859.959808	–
36-ts-r	-1859.953872	-1858.905754	0.604656	-187.29
36-ts-s	-1859.946554	-1858.895447	0.606121	-191.07

^a The E value is obtained at M06-2X/6-311+g(d, p)//IEF-PCM_{acetonitrile} level

^b The G value is obtained at M06-2X/6-31g(d, p)//IEF-PCM_{acetonitrile} level

Part 11: Cartesian coordinates of all the stationary points involved in the calculations

R1a

C	-3.16593200	-0.21425400	0.21895000
O	-2.84946100	-1.08610900	0.98199900
C	-4.55823700	0.20073300	-0.14767000
H	-4.69499700	1.26121300	0.07262000
H	-4.70625800	0.06012700	-1.22065200
H	-5.27251400	-0.39815300	0.41266600
O	-2.25572200	0.56263700	-0.44705100
C	-0.90596400	0.33368200	-0.27561200
C	-0.34816700	-0.93243000	-0.45121500
C	-0.11986600	1.44781700	0.00559900
C	1.02546400	-1.08400700	-0.33318500
H	-0.98053600	-1.78152200	-0.67648100
C	1.25481100	1.30133000	0.12036300
H	-0.59399700	2.41421500	0.12935600
C	1.80035000	0.03462800	-0.04821200
H	1.49663200	-2.04988500	-0.46280800
H	1.89668900	2.14463200	0.34005600
N	3.24963400	-0.12885200	0.07791400
O	3.91781000	0.86123400	0.32364100
O	3.71397200	-1.24697000	-0.06787200

R2a

C	-1.18086700	-0.96589700	-0.03791800
O	-1.17640300	-2.18841600	-0.09720800
C	0.08211900	-0.19151800	0.03771900
C	1.25779100	-0.82596300	-0.09124000
H	0.02814600	0.87491000	0.22275500
H	1.21761200	-1.90113300	-0.26298500
C	2.59714800	-0.23434700	-0.02417700
C	3.70830400	-1.07533700	-0.17150000
C	2.81303200	1.13682300	0.18444200
C	5.00166100	-0.56580900	-0.11128400
H	3.54975100	-2.13795700	-0.33330100
C	4.10335500	1.64534700	0.24405800
H	1.97018900	1.81101000	0.29886900
C	5.20167500	0.79623000	0.09717400
H	5.85070700	-1.23154700	-0.22597100
H	4.25671100	2.70731600	0.40538400

H	6.20859300	1.19793400	0.14500100
C	-2.48273300	-0.22448700	-0.01933200
C	-2.58401600	1.13848000	-0.31584900
C	-3.64066800	-0.94950700	0.28429300
C	-3.82722000	1.76536300	-0.30453300
H	-1.70465000	1.71500200	-0.58192600
C	-4.87839800	-0.32059500	0.30875500
H	-3.54593600	-2.00790800	0.50283000
C	-4.97286200	1.03995700	0.01372400
H	-3.90016400	2.82069300	-0.54526500
H	-5.77018200	-0.88671800	0.55653900
H	-5.93948100	1.53329500	0.02975600

R2b

C	-0.45269200	1.14665900	-0.03789900
C	-1.75871900	0.57329900	0.32008200
C	-2.31442700	-0.45103200	-0.34765600
H	-2.29815900	1.09293300	1.10634700
H	-1.76619100	-0.88865000	-1.18110100
C	-3.62974800	-1.04503200	-0.08845200
C	-4.10455300	-2.02276500	-0.97275400
C	-4.42389800	-0.68547500	1.01126900
C	-5.34267200	-2.62434600	-0.77092000
H	-3.49344100	-2.31011100	-1.82379000
C	-5.65888000	-1.28656600	1.21279000
H	-4.07313300	0.05889200	1.71902300
C	-6.12279100	-2.25655800	0.32232900
H	-5.69689200	-3.37913900	-1.46503200
H	-6.26209900	-1.00243300	2.06860900
H	-7.08846400	-2.72436200	0.48385100
C	-0.34300400	2.63076400	-0.00956300
C	-1.48444600	3.43318400	-0.11896900
C	0.91474000	3.23474500	0.11563200
C	-1.36888400	4.81963300	-0.10434200
H	-2.46147700	2.97597700	-0.23862300
C	1.02563400	4.61853900	0.13863500
H	1.79347600	2.60472000	0.20271900
C	-0.11587100	5.41327400	0.02807900
H	-2.25733200	5.43502500	-0.19729000
H	2.00137400	5.08015700	0.24712600
H	-0.02735400	6.49468100	0.04629700
N	0.62260600	0.51486700	-0.38846800
S	0.81148200	-1.14301000	-0.29102700
O	0.48721600	-1.70834700	-1.60452400

O	0.19171400	-1.73863900	0.89251800
C	2.56863200	-1.20645800	-0.06633800
C	3.40355700	-0.72150500	-1.07315300
C	3.08026000	-1.76991000	1.09433000
C	4.77642100	-0.80065400	-0.89718000
H	2.98093200	-0.28882700	-1.97440900
C	4.46292700	-1.84241200	1.25171100
H	2.40459700	-2.14281500	1.85589900
C	5.32511200	-1.35946200	0.26645800
H	5.43937600	-0.42567300	-1.67154300
H	4.87519300	-2.28076700	2.15544700
C	6.81912500	-1.42200500	0.44139300
H	7.09102500	-1.99595400	1.32897600
H	7.29387200	-1.88331500	-0.42869700
H	7.23637500	-0.41586100	0.54507100

NHC-3a

C	-2.93368600	0.62513700	0.73925700
C	-3.78070500	0.57715900	-0.37086100
C	-4.47167300	1.71600600	-0.77164600
C	-4.29668100	2.89752100	-0.05186200
C	-3.44336500	2.94228000	1.05300300
C	-2.75292500	1.80083100	1.45801900
C	-2.30452200	-0.72549400	0.98151300
C	-3.22800600	-1.66708400	0.16614200
C	-3.78277700	-0.80013300	-0.98541100
H	-5.13741900	1.68656000	-1.62896300
H	-4.83272900	3.79263700	-0.35125300
H	-3.32179700	3.87075300	1.60135200
H	-2.08608200	1.82563900	2.31387800
H	-4.05813700	-1.94837200	0.81862400
H	-3.12167900	-0.82197900	-1.85976500
H	-2.26322900	-1.00172500	2.03766700
H	-4.76927200	-1.13622800	-1.31171700
C	-0.53678700	-1.74055400	-0.47115700
C	0.10196800	0.01006000	0.80486500
N	0.72204000	-1.59129600	-0.75156000
N	-0.94263100	-0.80207900	0.44147900
N	1.07862800	-0.51643200	0.03932500
C	-1.48528800	-2.75261400	-1.03602500
H	-1.77311800	-2.46923600	-2.05645200
H	-1.00259700	-3.73024400	-1.08208600
O	-2.61655100	-2.88758200	-0.19805600
C	2.43146600	-0.05192200	-0.00968100

C	2.70760500	1.14789500	-0.67052200
C	3.42983100	-0.82249500	0.59354900
C	4.03435900	1.57805800	-0.70906600
C	4.74203000	-0.35677400	0.52448100
C	5.06154400	0.84100200	-0.11838700
H	4.27078800	2.50774200	-1.22115300
H	5.53314100	-0.94183800	0.98795200
C	1.60503800	1.93993500	-1.32210200
H	1.04618400	1.31847800	-2.02891300
H	0.88850300	2.29633300	-0.57681500
H	2.01264600	2.79817700	-1.85891600
C	6.48430500	1.33768800	-0.14943100
H	6.64847200	2.01533000	-0.99019100
H	6.72332700	1.88416200	0.76869000
H	7.19044000	0.50778000	-0.22981400
C	3.08611000	-2.10801600	1.29772400
H	2.27163800	-1.95217500	2.01194700
H	2.74731900	-2.86646900	0.58624300
H	3.95270400	-2.49694400	1.83501100

Pre-NHC-3a

C	-2.93534100	0.62732800	0.77026500
C	-3.69926600	0.64599200	-0.40086800
C	-4.32652700	1.82060600	-0.79896700
C	-4.17175700	2.96441100	-0.01523000
C	-3.41145100	2.93714900	1.15546400
C	-2.78684600	1.75926900	1.56337900
C	-2.36507000	-0.74940200	0.98658600
C	-3.27044100	-1.63321700	0.09402800
C	-3.71056000	-0.71003100	-1.06310200
H	-4.93024200	1.84733900	-1.70044900
H	-4.65783700	3.88715800	-0.31458800
H	-3.31525300	3.83451100	1.75682600
H	-2.21358300	1.72723500	2.48531600
H	-4.14527300	-1.89037800	0.69410000
H	-2.99718800	-0.73162100	-1.89543900
H	-2.32637200	-1.08105300	2.02492400
H	-4.68617100	-0.99498300	-1.46050000
C	-0.56650400	-1.78149100	-0.47085200
C	0.08197700	-0.10178300	0.73501100
N	0.69855400	-1.62381600	-0.75224100
N	-0.98392900	-0.85238800	0.44440000
N	1.08499600	-0.56888400	0.01201200
C	-1.52240700	-2.78014600	-1.04917900

H	-1.75661800	-2.49975900	-2.08303100
H	-1.05665300	-3.76619400	-1.05863800
O	-2.67874900	-2.86763500	-0.24789000
C	2.43886800	-0.07593900	-0.02653000
C	2.70299600	1.06752600	-0.78214100
C	3.41345700	-0.78935300	0.67585100
C	4.02415400	1.51285300	-0.80737500
C	4.71612000	-0.30121900	0.61485600
C	5.03671000	0.84700300	-0.11462300
H	4.26664600	2.39773300	-1.38944400
H	5.49966500	-0.83203500	1.14887000
C	1.61466800	1.78203000	-1.53954900
H	1.01068300	1.08149300	-2.12323200
H	0.94139700	2.31679200	-0.86217900
H	2.04819300	2.51271600	-2.22298600
C	6.45010600	1.36651100	-0.13489300
H	6.63733500	1.96807400	-1.02640500
H	6.63587400	1.99845400	0.73932900
H	7.17110600	0.54668300	-0.10793200
C	3.06426600	-2.03070700	1.45210600
H	2.27972600	-1.83072300	2.18832200
H	2.69670200	-2.81750600	0.78714800
H	3.94045600	-2.40733900	1.98052600
H	0.12714200	0.72575000	1.42797200

Pre-NHC-3b

C	0.01130200	1.71379300	-0.32277700
C	0.92556800	2.85466700	-0.66750800
C	2.57278200	1.76032100	0.58934600
C	1.93468300	0.37039900	0.58904600
C	-0.54512600	-0.21164100	0.50420800
H	0.71130300	3.20911900	-1.67612500
H	3.65718600	1.66179000	0.64441400
H	2.00724100	-0.08035900	1.58180900
N	-1.27855800	1.62407500	-0.49901700
N	-1.60707400	0.41313000	0.02497700
N	0.49908000	0.59632400	0.30344700
H	2.22149700	2.34567700	1.44875600
H	0.75184000	3.67339000	0.04345000
O	2.26650400	2.42103400	-0.62801300
C	2.51546600	-0.56031300	-0.48697200
H	1.91542200	-1.47541900	-0.51799300
H	2.41588000	-0.06108300	-1.45562700
C	3.96019800	-0.89329900	-0.20540900

C	4.28775000	-1.87800700	0.73081500
C	4.98863800	-0.20145400	-0.85016600
C	5.61923300	-2.16748900	1.01589800
H	3.49367300	-2.42575000	1.23239600
C	6.32190700	-0.48955200	-0.56673800
H	4.73984400	0.56591200	-1.57924800
C	6.63918300	-1.47327900	0.36705600
H	5.86094500	-2.93754000	1.74120100
H	7.11114300	0.05255100	-1.07725900
H	7.67711100	-1.70048700	0.58702700
C	-2.96912600	-0.05895700	0.01750200
C	-3.74984000	0.16910400	1.15207400
C	-3.43562300	-0.69165500	-1.13656500
C	-5.06630900	-0.28637500	1.11134300
C	-4.75941600	-1.12583000	-1.12389500
C	-5.58299200	-0.93707800	-0.01130100
H	-5.70421800	-0.12228900	1.97559600
H	-5.15693100	-1.61980000	-2.00630800
C	-3.19164200	0.88042900	2.35593600
H	-2.43421300	0.27281000	2.86083300
H	-2.72110200	1.82640600	2.07276600
H	-3.98508800	1.09199800	3.07316000
C	-7.00070500	-1.44519100	-0.01489900
H	-7.03873600	-2.46916000	0.37007900
H	-7.64197900	-0.82920300	0.61879200
H	-7.41341600	-1.45585800	-1.02568800
C	-2.54553100	-0.88447900	-2.33514900
H	-2.15770800	0.07301200	-2.69467900
H	-1.68600100	-1.51738300	-2.09291900
H	-3.09803400	-1.35915300	-3.14640700
H	-0.53423100	-1.18682400	0.96914500

TS0

C	3.32375500	1.13401800	-0.37891300
C	4.47707700	0.89968100	0.37679000
C	4.91734200	1.85774400	1.28249900
C	4.18867200	3.04055700	1.41837500
C	3.04111900	3.26957500	0.65689200
C	2.59747400	2.31183000	-0.25611700
C	3.05865700	-0.03760500	-1.28624200
C	4.43955400	-0.73176800	-1.34010700
C	5.07654700	-0.44441000	0.03792000
H	5.81468800	1.69345600	1.87068400
H	4.52379800	3.79750900	2.11992400

H	2.49517500	4.20074500	0.77192000
H	1.70492000	2.48076400	-0.85422400
H	5.02294900	-0.22023100	-2.10876700
H	4.77815500	-1.19134400	0.78345700
H	2.67826500	0.22888300	-2.27393800
H	6.16701500	-0.44059100	-0.00737100
C	2.32032000	-2.33389000	-0.56106300
C	0.85793000	-0.71586500	-0.23553500
N	1.27513900	-2.93097200	-0.06231300
N	2.10066300	-0.98618200	-0.68248000
N	0.38864600	-1.90896500	0.12643200
C	3.64422500	-2.93995900	-0.91432600
H	4.19560000	-3.16548800	0.00696800
H	3.49162200	-3.87358400	-1.45713400
O	4.37375800	-2.07732900	-1.76084700
C	-0.93323100	-2.14118400	0.63913000
C	-1.21902900	-1.73965900	1.94558900
C	-1.88066800	-2.72052800	-0.21006700
C	-2.52755700	-1.91529800	2.39551400
C	-3.17116900	-2.88278200	0.29028100
C	-3.51374200	-2.47627500	1.58232400
H	-2.77890800	-1.61158000	3.40825800
H	-3.92978400	-3.32784900	-0.34900300
C	-0.14862700	-1.16526000	2.83551700
H	0.69919000	-1.85219100	2.91698300
H	0.23777100	-0.22059300	2.44164400
H	-0.54224900	-0.98031900	3.83584100
C	-4.92995400	-2.62160900	2.07485700
H	-4.97497400	-2.59512400	3.16527600
H	-5.55203000	-1.80526200	1.69373100
H	-5.37225000	-3.55911600	1.73012400
C	-1.51510500	-3.15091600	-1.60606500
H	-1.03790400	-2.33777800	-2.16419900
H	-0.80566500	-3.98299000	-1.58523100
H	-2.40401400	-3.46737200	-2.15367900
H	0.12701700	0.36836700	-0.06918100
C	-4.44272600	0.99121400	-2.46954600
C	-4.18255800	2.48312200	-2.24839400
C	-3.97749600	2.85410800	-0.78163300
C	-3.51544300	0.11231000	-1.62770300
C	-2.08003100	0.65367700	-1.59176300
C	-1.80262700	1.63059500	-0.46579400
H	-4.30611700	0.75917300	-3.53103600
H	-5.03384800	3.05939600	-2.62168500

H	-4.20768800	3.91386500	-0.65572400
H	-3.89100800	0.02247100	-0.60093400
H	-1.82550400	1.12375400	-2.54819900
C	-2.27336900	3.68743900	0.77804800
H	-2.88185500	3.50049200	1.67198200
C	-0.79503600	3.65201800	1.12349500
H	-0.60563600	4.28971200	1.98952400
C	-0.41442600	2.20796200	1.39857900
H	-0.96039000	1.84045100	2.27820700
N	-0.73667000	1.37985800	0.24444800
N	-2.61012100	2.69582800	-0.25493400
H	-1.37940700	-0.17064200	-1.45138100
H	-3.50169700	-0.90535900	-2.02975600
H	-5.48424300	0.75828000	-2.22491700
H	-3.31088700	2.82184200	-2.81782500
H	-4.68121000	2.30158900	-0.14379800
H	-2.55146200	4.67044600	0.38816500
H	-0.20511900	4.03315800	0.28257300
H	0.65474600	2.10168400	1.60618300

TS1

C	1.23679500	2.89493800	-0.85894200
C	0.70239600	4.24665700	-1.23213800
C	-1.41811500	3.26437200	-1.37345200
C	-1.09118100	1.96828900	-0.62895500
C	1.09506300	0.76721800	-0.28955700
H	1.25543000	5.02667900	-0.70814200
H	-2.47138500	3.51286600	-1.23529700
H	-1.47754400	1.11544000	-1.19480400
N	2.47139600	2.50389200	-0.73128800
N	2.35706400	1.18526700	-0.37694100
N	0.37482100	1.85959700	-0.61188400
H	-1.21890900	3.14762700	-2.44683700
H	0.81031200	4.39908800	-2.31446000
O	-0.65320900	4.33454300	-0.84297900
C	-1.62583700	1.93040500	0.81174700
H	-1.13085500	1.10359000	1.33474100
H	-1.33806100	2.86183500	1.31003700
C	-3.12054500	1.72839500	0.84368500
C	-3.65357400	0.43754000	0.75757400
C	-3.99611700	2.81351100	0.92562600
C	-5.03074000	0.23539800	0.74735000
H	-2.98384800	-0.42018900	0.71736500
C	-5.37572600	2.61498200	0.91236900

H	-3.59385400	3.82018600	1.00871000
C	-5.89574900	1.32633200	0.82088200
H	-5.42823000	-0.77334400	0.69126700
H	-6.04313600	3.46795300	0.97869000
H	-6.96951100	1.17121500	0.81463400
C	3.52731300	0.39251900	-0.12872300
C	3.72917400	-0.76630800	-0.88515100
C	4.40885100	0.80574300	0.87844300
C	4.87530900	-1.51601100	-0.61486800
C	5.53819200	0.02219200	1.10271400
C	5.79152200	-1.13603800	0.36436300
H	5.05413600	-2.41982900	-1.19143900
H	6.23338400	0.31988500	1.88367900
C	2.75594600	-1.22519700	-1.94100300
H	1.90150700	-1.73762900	-1.48383800
H	2.36861300	-0.38976900	-2.53045300
H	3.24209900	-1.92902900	-2.61824300
C	7.03836700	-1.94399500	0.61292500
H	7.89203000	-1.50362500	0.08802500
H	7.28504400	-1.96864000	1.67691500
H	6.92232800	-2.97008400	0.25850200
C	4.14422600	2.03303900	1.71089000
H	4.33863700	2.94608600	1.14285800
H	3.10082900	2.07167700	2.03773500
H	4.78425000	2.03154300	2.59437800
H	0.56211900	-0.40419200	0.06503200
C	-2.87771400	-3.37937500	-2.52748200
C	-3.62756800	-3.29910500	-1.19566300
C	-2.83686600	-3.85624700	-0.01449000
C	-1.41313300	-2.95699500	-2.39088900
C	-1.25415400	-1.73870800	-1.47042500
C	-1.05363500	-2.08100800	-0.00693100
H	-3.37989300	-2.73704000	-3.25834900
H	-4.55828400	-3.86865400	-1.26843900
H	-3.53933600	-4.13607000	0.77270500
H	-0.81054400	-3.78401600	-1.99813200
H	-2.12894400	-1.08324000	-1.56746100
C	-1.67844500	-3.20956700	2.06084200
H	-1.07541200	-4.12025200	2.16686100
C	-1.00888800	-2.03730900	2.75716500
H	-0.77718300	-2.30740400	3.78929100
C	0.24899000	-1.67765000	1.98599600
H	0.99802900	-2.47245400	2.08283000
N	-0.05852300	-1.46972000	0.57709200

N	-1.89120200	-2.92761900	0.63260700
H	-0.38156900	-1.15191800	-1.76689300
H	-1.00022000	-2.71824700	-3.37393500
H	-2.92576300	-4.40176400	-2.91583400
H	-3.92063400	-2.26798300	-0.96673100
H	-2.30566400	-4.77287800	-0.30538200
H	-2.65799700	-3.40559400	2.50295300
H	-1.69200100	-1.18079500	2.77718700
H	0.70587300	-0.75538100	2.36357400

DBU

C	2.94577200	-0.00104100	0.07589700
C	2.11418500	-1.14090800	-0.51846100
C	0.84785300	-1.45629900	0.27580200
C	2.07465400	1.16332200	0.55189900
C	0.92406600	1.46861700	-0.41732800
C	-0.36901700	0.71992800	-0.14078800
H	3.65548000	0.35437300	-0.67957500
H	2.72400000	-2.04853800	-0.56059500
H	0.56669600	-2.49325200	0.07132100
H	1.65847300	0.94370300	1.54263000
H	1.24509500	1.27583100	-1.44873800
C	-1.58325200	-1.35090400	0.28303400
H	-1.68173700	-1.43755600	1.37664000
C	-2.77566300	-0.60903200	-0.29195900
H	-3.70548400	-1.09542500	0.01491900
C	-2.71530200	0.83342900	0.18776800
H	-2.94087500	0.87585000	1.26296200
N	-1.42093200	1.45774800	-0.05319900
N	-0.33971800	-0.66512300	-0.06587800
H	0.64622200	2.52133900	-0.36291800
H	2.69297400	2.05728600	0.67509000
H	3.54147900	-0.37791800	0.91471200
H	1.82346400	-0.91740900	-1.55035100
H	1.05571900	-1.40089100	1.35696500
H	-1.52915300	-2.36754300	-0.11934000
H	-2.72466800	-0.63744700	-1.38594100
H	-3.48291500	1.43655200	-0.30942900

DBU•H⁺

C	2.96667500	-0.00437000	-0.02832200
C	2.09023600	-1.09584000	-0.64376800
C	0.91035200	-1.49786700	0.23429700
C	2.12881900	1.10841600	0.60098400

C	0.93438900	1.49842700	-0.27663800
C	-0.30841400	0.66410600	-0.06635900
H	3.61492900	0.41392400	-0.80500300
H	2.68825200	-1.99489300	-0.81510300
H	0.57609900	-2.49270700	-0.06151000
H	1.76444000	0.80423800	1.58842700
H	1.19912300	1.45443200	-1.33907200
C	-1.56620100	-1.34652300	0.41185700
H	-1.73319800	-1.33825800	1.49447300
C	-2.72302700	-0.69843900	-0.32946400
H	-3.65439100	-1.19909000	-0.06152800
C	-2.79097700	0.76922400	0.04475200
H	-3.14178500	0.90074600	1.07270100
N	-1.45055700	1.33976600	-0.08071300
N	-0.29767900	-0.64636900	0.12455800
H	0.64959800	2.53241000	-0.07381000
H	2.74361300	1.99667000	0.76287200
H	3.62032300	-0.43950500	0.73409900
H	1.70977900	-0.79450600	-1.62560400
H	1.20164600	-1.55462500	1.28986800
H	-1.44400500	-2.38226300	0.09541800
H	-2.57324400	-0.80575400	-1.40733100
H	-3.45327200	1.32473100	-0.62021900
H	-1.38136500	2.33786300	-0.21961600

ArO⁻

O	-3.44847800	0.00006200	-0.00008600
C	-2.19684800	0.00006000	-0.00016200
C	-1.41539500	-1.22567300	0.00014600
C	-1.41510300	1.22577100	-0.00000200
C	-0.04747700	-1.22191300	0.00014200
H	-1.96446900	-2.16280500	0.00041200
C	-0.04714400	1.22198200	0.00004200
H	-1.96427900	2.16300600	-0.00014400
C	0.65821100	0.00000600	0.00000000
H	0.51601500	-2.14827500	0.00039100
H	0.51662000	2.14821300	0.00009800
N	2.06796900	-0.00002100	0.00002700
O	2.67457900	1.07936400	0.00013300
O	2.67425700	-1.07959900	-0.00029000

ArOH

H	-3.80031100	-0.79778700	-0.00051100
O	-3.41310300	0.08780500	-0.00002600

C	-2.06838900	0.01495300	0.00011500
C	-1.36625000	1.22775900	0.00039600
C	-1.38000600	-1.20438400	-0.00033200
C	0.01644300	1.22272000	0.00031500
H	-1.92442000	2.15662500	0.00069200
C	0.00514600	-1.21250800	-0.00033000
H	-1.93106900	-2.13922800	-0.00073100
C	0.68523000	0.00061800	0.00001300
H	0.58134600	2.14624700	0.00055100
H	0.55947700	-2.14243500	-0.00060600
N	2.14072500	-0.00747200	0.00002700
O	2.71193000	-1.08731600	0.00090000
O	2.72328000	1.06625300	-0.00095400

P-4a-r

C	-0.17114600	2.50254300	0.36296400
O	-0.33740000	3.68283100	0.52033000
C	1.14944800	1.78591600	0.46327700
H	1.94463400	2.52747800	0.38271000
H	1.19326700	1.34393200	1.46739100
C	-1.13865900	0.37499800	-0.17948700
O	-1.26460100	1.72689700	0.12861600
C	0.02847700	-0.15555200	-0.55106900
C	1.29045400	0.66222600	-0.57523300
H	0.06194100	-1.19294300	-0.86340300
H	1.40291200	1.11609000	-1.56969300
C	2.53835100	-0.15087100	-0.29166300
C	3.72053800	0.10786500	-0.98688700
C	2.53951200	-1.13029000	0.70525800
C	4.88464700	-0.59979600	-0.69468800
H	3.72803100	0.86857800	-1.76357500
C	3.70087000	-1.83981900	0.99830400
H	1.62299400	-1.33872100	1.25242500
C	4.87717500	-1.57600000	0.29855900
H	5.79595600	-0.38887300	-1.24516700
H	3.68694900	-2.60013900	1.77296300
H	5.78212300	-2.12989800	0.52623900
C	-2.43986400	-0.32007100	-0.11037400
C	-2.49608000	-1.71205500	0.03420400
C	-3.63351800	0.40554300	-0.19321800
C	-3.72191600	-2.36544700	0.06974700
H	-1.57859000	-2.28221300	0.14048700
C	-4.85907800	-0.25270200	-0.15284500
H	-3.59684500	1.48411200	-0.29477600

C	-4.90808100	-1.63842800	-0.02518400
H	-3.75175300	-3.44388700	0.18562100
H	-5.77799900	0.32036700	-0.22173300
H	-5.86439000	-2.15006900	0.00895700

P-4a-s

C	0.39979400	2.25132900	0.17612800
O	0.65765100	3.23915500	-0.46194400
C	1.17043800	1.76523700	1.37550800
H	2.13493700	2.27422900	1.38293900
H	0.60500200	2.09298900	2.25578600
C	-0.96986500	0.29636500	0.41682700
O	-0.69396900	1.52747100	-0.17435300
C	-0.05889400	-0.35400500	1.14302200
C	1.29893700	0.24092600	1.42383600
H	-0.28659100	-1.34835800	1.50818500
H	1.59186700	-0.03517100	2.44214000
C	2.33714600	-0.34435300	0.47339700
C	2.78572800	-1.65111600	0.69493300
C	2.83011100	0.35536000	-0.62930000
C	3.69894300	-2.24821800	-0.16677400
H	2.41558700	-2.20142600	1.55688500
C	3.74637100	-0.24232500	-1.49523400
H	2.51798300	1.37724000	-0.82440300
C	4.18157600	-1.54388400	-1.26952300
H	4.03798700	-3.26150200	0.02419400
H	4.12026600	0.31710900	-2.34695000
H	4.89553900	-2.00555400	-1.94375700
C	-2.32671400	-0.17350800	0.06983700
C	-2.96774200	-1.14626300	0.84696400
C	-2.98712200	0.34886800	-1.04786100
C	-4.23386400	-1.60162800	0.49844600
H	-2.48504600	-1.53228200	1.73912700
C	-4.25651400	-0.10697600	-1.39059800
H	-2.50069300	1.10873300	-1.64837400
C	-4.88273700	-1.08457800	-0.62216500
H	-4.72067300	-2.35314500	1.11139100
H	-4.75563000	0.30392600	-2.26217000
H	-5.87353800	-1.43718700	-0.88927400

P-4b-r

C	0.53891000	-1.74506900	-0.23130100
O	-0.11875600	-2.75911200	-0.29507500
C	1.97821000	-1.64616200	-0.68857300

H	1.98114000	-1.27993500	-1.72274000
H	2.37609100	-2.66306700	-0.68443500
C	0.71686000	0.68809000	0.17496600
C	2.05140500	0.64448200	0.14174500
C	2.76578700	-0.68652400	0.20995700
H	2.60919700	1.55145800	-0.06725900
H	2.69875300	-1.06324400	1.24223000
C	4.23755400	-0.55814100	-0.13417200
C	5.05104800	0.20294800	0.71353900
C	4.81114200	-1.14935300	-1.25934400
C	6.40395000	0.37113000	0.44313700
H	4.61301500	0.66573300	1.59509700
C	6.16963900	-0.98309500	-1.53266700
H	4.20851400	-1.74802400	-1.93473400
C	6.96887200	-0.22361800	-0.68523100
H	7.01881300	0.96472200	1.11214100
H	6.59976200	-1.45014000	-2.41289600
H	8.02488500	-0.09474500	-0.89912400
C	-0.07511200	1.91225400	-0.08481100
C	-1.14345700	1.87993700	-0.98596400
C	0.27623500	3.12093100	0.52162900
C	-1.85240500	3.04284300	-1.27352300
H	-1.41311500	0.94336500	-1.46642200
C	-0.43036800	4.28284900	0.22812500
H	1.09326300	3.13941800	1.23675900
C	-1.49817300	4.24642500	-0.66748700
H	-2.68170900	3.00649700	-1.97291000
H	-0.15446100	5.21592100	0.70862100
H	-2.05316800	5.15178700	-0.89030100
N	0.00562100	-0.55574900	0.30395500
S	-1.26428800	-0.68501600	1.46197200
O	-1.24539000	0.58538000	2.16769100
O	-1.05306600	-1.91924800	2.19708900
C	-2.76542600	-0.80463300	0.53564200
C	-3.57400800	0.32494900	0.44400700
C	-3.12947400	-2.02154200	-0.03777300
C	-4.77188400	0.23013400	-0.25484500
H	-3.26546800	1.25381800	0.91117400
C	-4.33061700	-2.09031000	-0.73186500
H	-2.47859300	-2.88311100	0.05633300
C	-5.16335100	-0.97128400	-0.85352800
H	-5.41533900	1.10153800	-0.32996200
H	-4.63247500	-3.03095100	-1.18293800
C	-6.44801200	-1.05830400	-1.63286900

H	-6.90183100	-2.04680000	-1.53472300
H	-7.16594600	-0.30783700	-1.29642600
H	-6.25831800	-0.88569900	-2.69711500

P-4b-s

C	-0.24860000	-0.36258800	1.61158800
O	-1.19953800	-0.67281600	2.29531700
C	1.07876800	-1.08732200	1.62371800
H	0.89221200	-2.07327700	2.05368400
H	1.76442500	-0.54442900	2.28602700
C	0.82706400	1.16893800	-0.00888000
C	1.80015200	0.28594900	-0.25741400
C	1.65651400	-1.14702400	0.20442800
H	2.74547300	0.63047500	-0.66323600
H	0.91343700	-1.64532600	-0.43806600
C	2.95735500	-1.91708700	0.07834800
C	3.64312800	-2.43757100	1.17517500
C	3.49488500	-2.10220400	-1.20085100
C	4.84208600	-3.12932200	0.99744200
H	3.25168100	-2.31230400	2.17955500
C	4.68948000	-2.78934800	-1.38048400
H	2.96555400	-1.70169900	-2.06270600
C	5.36872300	-3.30669300	-0.27738600
H	5.36273800	-3.52836300	1.86215600
H	5.09071300	-2.92330500	-2.37998400
H	6.30200900	-3.84330500	-0.41351100
C	0.95054700	2.62798900	-0.22901100
C	1.65314300	3.11534600	-1.33448400
C	0.41729400	3.53242000	0.69674600
C	1.83504900	4.48448800	-1.50250600
H	2.04082100	2.41910000	-2.07192900
C	0.59750600	4.90044300	0.52317300
H	-0.13702200	3.16116200	1.55422400
C	1.30892100	5.38119500	-0.57442100
H	2.37890100	4.85133500	-2.36700000
H	0.18339100	5.59264800	1.24904900
H	1.44654600	6.44894500	-0.70985300
N	-0.33592300	0.69129800	0.68588400
S	-1.91084900	1.18880700	0.19896300
O	-1.70205300	1.90637900	-1.04908700
O	-2.56233200	1.84825400	1.31742600
C	-2.74067600	-0.33052500	-0.16478700
C	-2.40245100	-1.00698300	-1.33434900
C	-3.73128300	-0.79215000	0.69422200

C	-3.07637500	-2.18354000	-1.63719500
H	-1.63614800	-0.61536400	-1.99643200
C	-4.40026600	-1.96440900	0.36583100
H	-3.96234100	-0.24052300	1.59807200
C	-4.07973400	-2.67693800	-0.79502000
H	-2.82658500	-2.72373000	-2.54511000
H	-5.18118200	-2.33537000	1.02272500
C	-4.78615700	-3.96605200	-1.11819700
H	-4.28898900	-4.80493700	-0.62065900
H	-5.82194500	-3.94443600	-0.77316700
H	-4.77769100	-4.16389400	-2.19179300

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C	-1.40394500	2.09875600	0.31414500
C	-2.11546500	3.29178700	0.40052300
C	-3.02779800	3.48502900	1.43180100
C	-3.20697800	2.46991100	2.37261500
C	-2.47621100	1.28344300	2.28803100
C	-1.55990500	1.08615500	1.25741000
C	-0.48576100	2.10448900	-0.88711300
C	-0.48809300	3.59613600	-1.37386200
C	-1.73151000	4.23678400	-0.71105500
H	-3.58494600	4.41578700	1.51260900
H	-3.91656800	2.61001700	3.18337500
H	-2.61901500	0.51096700	3.03655800
H	-0.97604000	0.16716500	1.19407800
H	-0.55131000	3.63755300	-2.46183400
H	-1.49102000	5.24231000	-0.35739000
H	-0.83427400	1.43822400	-1.67665100
H	-2.54237000	4.33277500	-1.44112300
C	1.72246700	2.53595100	0.08358200
C	1.41168600	0.43449200	-0.60416200
N	2.82748000	1.93377400	0.40524400
N	0.85772700	1.67210200	-0.53196500
N	2.60329700	0.63966000	-0.02156200
C	1.30743400	3.96708400	0.17740300
H	0.60813200	4.11839100	1.01027500
H	2.17097900	4.61428500	0.31428100
O	0.71339700	4.29421500	-1.06921800
C	3.61945800	-0.35181200	0.17497400
C	3.70618200	-0.97778300	1.42263700
C	4.48021800	-0.64272800	-0.88413300
C	4.69267200	-1.94909900	1.58376500
C	5.44916300	-1.62513800	-0.67677600

C	5.56491400	-2.28826800	0.54668800
H	4.78274400	-2.45262300	2.54314900
H	6.13051500	-1.86915800	-1.48659900
C	2.76537800	-0.60262300	2.53499100
H	2.86900500	0.45557600	2.79183100
H	1.72859300	-0.77207700	2.22164800
H	2.96688300	-1.19863200	3.42618500
C	6.60048300	-3.36573400	0.74282200
H	7.39881600	-3.28709400	0.00209200
H	7.04168000	-3.31084500	1.73839000
H	6.14700800	-4.35964000	0.63834600
C	4.35090600	0.07589800	-2.20034000
H	3.41602200	-0.19444400	-2.70145300
H	4.33603500	1.15987800	-2.05454900
H	5.18095800	-0.17795500	-2.85996000
C	0.43016000	-1.46932300	-0.61364300
O	0.40295500	-1.78559700	0.56515200
C	1.26705600	-2.16058400	-1.65785300
H	0.81029700	-3.13781400	-1.84867200
H	1.28595600	-1.58723000	-2.58411600
H	2.27872200	-2.31002200	-1.27459900
O	-0.76594500	-0.94254500	-1.21921200
C	-1.97607600	-1.44058200	-0.86314200
C	-2.17322400	-2.68200400	-0.24260500
C	-3.07972400	-0.64534300	-1.21100100
C	-3.46134400	-3.11399200	0.03009000
H	-1.32841400	-3.29745200	0.03063600
C	-4.36454700	-1.07531500	-0.94259200
H	-2.90693800	0.31285000	-1.68940200
C	-4.53968800	-2.30781100	-0.31868800
H	-3.63762700	-4.07325600	0.50479900
H	-5.22526200	-0.47261000	-1.20141400
N	-5.88889100	-2.76933400	-0.02651400
O	-6.82512500	-2.04771300	-0.34180500
O	-6.02569500	-3.85023400	0.52333700

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C	-1.05399500	2.65013800	0.49449500
C	-0.83841600	4.00288200	0.77574000
C	-1.38722500	4.58882300	1.91165400
C	-2.16269100	3.80594000	2.76345800
C	-2.39385300	2.46036800	2.47253500
C	-1.84685200	1.87232800	1.33411800
C	-0.41660900	2.27197600	-0.82917200

C	-0.14999500	3.67304300	-1.46303800
C	-0.00773400	4.66129000	-0.28988600
H	-1.22097400	5.64090700	2.12203300
H	-2.60069600	4.24814100	3.65278500
H	-3.01337200	1.86456900	3.13501000
H	-2.01800700	0.82642400	1.12409800
H	-1.05445900	3.92420700	-2.02119700
H	1.03010700	4.76192800	0.04477200
H	-1.05432500	1.65178900	-1.45556600
H	-0.35999300	5.65839200	-0.56231700
C	2.07088100	2.07359300	-1.14716100
C	1.15459600	0.29097800	-0.26870900
N	3.06042100	1.25759500	-0.94396400
N	0.88075500	1.54090700	-0.71460400
N	2.47538300	0.16112200	-0.38559100
C	2.15134800	3.38473800	-1.86407400
H	2.51813800	4.17147500	-1.19591100
H	2.85646100	3.28483000	-2.69011900
O	0.89117400	3.69084600	-2.41411100
C	3.31768800	-0.94456300	-0.01093600
C	3.63961300	-1.10363800	1.33845700
C	3.78905200	-1.78088700	-1.02385000
C	4.44955500	-2.18888400	1.66965200
C	4.59733000	-2.84930000	-0.63920400
C	4.92807500	-3.07251300	0.69901300
H	4.71602900	-2.34519500	2.71190600
H	4.97522700	-3.52385700	-1.40297100
C	3.11963600	-0.14822700	2.37868500
H	3.39080800	0.88255400	2.12774400
H	2.02641100	-0.20065100	2.43484800
H	3.54013300	-0.38563000	3.35698600
C	5.77209400	-4.25603800	1.09446600
H	6.40422000	-4.01894000	1.95311900
H	5.13700200	-5.10206100	1.37597600
H	6.41008200	-4.57981000	0.26958500
C	3.43863400	-1.53286300	-2.46652800
H	2.35969400	-1.40303700	-2.60111800
H	3.91959200	-0.62030800	-2.83106600
H	3.76388400	-2.36787000	-3.08828400
C	0.18026500	-0.76086000	0.36921800
O	-0.08318000	-0.47733800	1.58114200
C	0.59059200	-2.20765800	0.05162400
H	-0.28259400	-2.83821500	0.23481500
H	0.90907200	-2.34500700	-0.98541700

H	1.38549000	-2.52689700	0.72675800
O	-0.98895300	-0.51350900	-0.66643500
C	-2.17478300	-1.10109600	-0.50793800
C	-2.61591200	-1.70799200	0.68747100
C	-3.03455100	-1.07449000	-1.62558900
C	-3.87611700	-2.28004600	0.74445800
H	-1.96586500	-1.70250500	1.55240500
C	-4.29189700	-1.64123200	-1.56505500
H	-2.67924900	-0.60524700	-2.53643300
C	-4.70099700	-2.24412500	-0.37604300
H	-4.22987000	-2.74886900	1.65464200
H	-4.95570800	-1.63004800	-2.42041800
N	-6.01858200	-2.84656500	-0.30699800
O	-6.72390300	-2.81435000	-1.30599800
O	-6.36757300	-3.36222200	0.74593600

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C	-0.82329800	2.83792300	0.43936200
C	-0.42233400	4.15281100	0.69665000
C	-0.90585000	4.83215400	1.80963900
C	-1.80298500	4.18176600	2.65468400
C	-2.21963300	2.87699500	2.38285200
C	-1.73598300	2.19547500	1.26867800
C	-0.23452000	2.35305600	-0.86702400
C	0.15788400	3.69862800	-1.53957500
C	0.49535800	4.66076500	-0.38344900
H	-0.60190800	5.85563400	2.00686200
H	-2.19383200	4.69984200	3.52493600
H	-2.93222700	2.39144000	3.04175500
H	-2.04354900	1.18042900	1.05553300
H	-0.74896400	4.05766600	-2.03182100
H	1.54154300	4.57932200	-0.06707100
H	-0.92389400	1.76187700	-1.46522400
H	0.31385200	5.70205300	-0.65715300
C	2.19046700	1.86196200	-1.32243500
C	1.18260000	0.28846500	-0.19505000
N	3.09796600	0.94891000	-1.14208900
N	0.99838900	1.51442900	-0.73373400
N	2.45681100	-0.01587200	-0.43003600
C	2.36751400	3.12257400	-2.11019200
H	2.88827200	3.87483600	-1.50617900
H	2.97986700	2.90372800	-2.98581300
O	1.11677300	3.57906500	-2.56529500
C	3.18808200	-1.18922300	-0.02873100

C	3.63770000	-1.27063600	1.29149600
C	3.41507500	-2.17542300	-0.98885500
C	4.32475300	-2.42753500	1.65199600
C	4.10700100	-3.31312500	-0.57520800
C	4.56068400	-3.45753400	0.73673700
H	4.68837100	-2.52599200	2.67162400
H	4.29302000	-4.10419100	-1.29662000
C	3.37843200	-0.15826800	2.27298100
H	3.73641800	0.79857600	1.88032500
H	2.30738400	-0.05225800	2.47517400
H	3.89001400	-0.35672200	3.21553200
C	5.28671000	-4.70385500	1.17093200
H	6.18191300	-4.45369900	1.74591000
H	4.64669100	-5.31694200	1.81272800
H	5.58330500	-5.30909900	0.31247000
C	2.93082900	-2.01081900	-2.40447500
H	1.86932400	-1.74316400	-2.43690100
H	3.47893700	-1.21103300	-2.91121600
H	3.06932300	-2.93555600	-2.96572900
C	0.22729100	-0.57428800	0.66104600
O	-0.04887900	-0.09113300	1.76330300
C	0.34458600	-2.07801400	0.47718500
H	-0.59764300	-2.52404700	0.80062700
H	0.54199000	-2.36184300	-0.55769000
H	1.14037400	-2.45965200	1.12154700
O	-1.11107800	-0.32300800	-0.64217800
C	-2.27289000	-0.90053000	-0.50914500
C	-2.83954000	-1.23199800	0.75369700
C	-3.02926700	-1.20132100	-1.67468900
C	-4.08142400	-1.83079600	0.83561300
H	-2.27655400	-1.00648000	1.65288800
C	-4.27265600	-1.78883500	-1.59098300
H	-2.59687900	-0.95179100	-2.63769400
C	-4.79436700	-2.10456000	-0.33256200
H	-4.51520400	-2.08540200	1.79528900
H	-4.84814800	-2.01622100	-2.48023200
N	-6.09208800	-2.72493500	-0.23955600
O	-6.70619100	-2.95723800	-1.27515900
O	-6.53320800	-2.99817600	0.87145400

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C	3.29745200	-1.22044200	-0.49802600
C	4.52672400	-0.95222200	0.11184500
C	5.67829100	-0.84219800	-0.66016100

C	5.57765300	-1.01797500	-2.03986400
C	4.35134200	-1.31843900	-2.63809500
C	3.19557100	-1.43060500	-1.86833700
C	2.22502400	-1.37321800	0.55035700
C	3.07540200	-1.69927100	1.80145400
C	4.37908900	-0.89434500	1.61277100
H	6.63945800	-0.64323500	-0.19618000
H	6.46853100	-0.94140900	-2.65536400
H	4.30236800	-1.47447400	-3.71083900
H	2.23125200	-1.66668100	-2.30646000
H	3.31482500	-2.76282500	1.73047700
H	4.27423200	0.14294500	1.95363000
H	1.47692800	-2.12407000	0.30265800
H	5.21733100	-1.33937700	2.15210600
C	1.27882700	0.35313000	2.11942800
C	0.66316400	0.63853000	0.05331900
N	0.45845600	1.36467500	2.15145800
N	1.45278100	-0.12010100	0.84098500
N	0.09061200	1.53092900	0.85675400
C	1.98394200	-0.23872200	3.30070200
H	2.83219900	0.40179100	3.57229400
H	1.29547600	-0.27085700	4.14599100
O	2.38671500	-1.55626100	3.02276300
C	-0.75038300	2.63474100	0.46770900
C	-0.14398900	3.74628500	-0.12125700
C	-2.12435200	2.53201200	0.70500000
C	-0.98612600	4.78101700	-0.52971900
C	-2.91636400	3.59517800	0.28135600
C	-2.36774500	4.71749900	-0.34666700
H	-0.54766800	5.66073400	-0.99270500
H	-3.98973900	3.54601200	0.44477900
C	1.35090900	3.83592200	-0.29265500
H	1.86871600	3.58246400	0.63712900
H	1.71395200	3.15698700	-1.07036800
H	1.63519600	4.85002300	-0.57579100
C	-3.26238700	5.83417000	-0.81582000
H	-2.68453900	6.72183800	-1.07853100
H	-3.82838600	5.52416100	-1.69947300
H	-3.98590300	6.10525900	-0.04297800
C	-2.71121700	1.32657200	1.38697500
H	-2.46275400	0.40125700	0.85540100
H	-2.32059800	1.22568000	2.40401000
H	-3.79731300	1.40993700	1.43894400
C	0.51383400	0.71050600	-1.46529800

O	1.52569000	0.83714700	-2.11089700
C	-0.87147700	0.83645400	-2.03494100
H	-0.89958900	0.25079100	-2.95469300
H	-1.63877400	0.47294500	-1.34984200
H	-1.06243900	1.88798200	-2.27101600
O	0.08822100	-1.68165400	-1.33149100
C	-1.06648500	-2.08736000	-0.97980300
C	-2.02935300	-2.55715300	-1.93867200
C	-1.49470300	-2.07886900	0.39394000
C	-3.28241500	-2.97613400	-1.56407300
H	-1.72943500	-2.57126400	-2.98190800
C	-2.75084200	-2.49886300	0.76740200
H	-0.79187700	-1.73587900	1.15044400
C	-3.65036800	-2.94834000	-0.20894100
H	-3.99989300	-3.32789200	-2.29635900
H	-3.06112900	-2.48674200	1.80607700
N	-4.95380300	-3.38307700	0.17886100
O	-5.26161900	-3.34677000	1.37061600
O	-5.73161500	-3.77624100	-0.68941600

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C	-3.69232300	-0.61221700	0.43619000
C	-4.57712700	-0.77062000	-0.63535500
C	-5.88103600	-0.29738000	-0.54445400
C	-6.28935600	0.31924200	0.63741400
C	-5.41572400	0.44011100	1.71963400
C	-4.10885600	-0.03445400	1.63029200
C	-2.37014500	-1.27359100	0.12350400
C	-2.78235800	-2.24887800	-1.01154300
C	-3.92936900	-1.53665500	-1.75919100
H	-6.57397200	-0.42246800	-1.37057900
H	-7.30545300	0.69042300	0.72567600
H	-5.76035800	0.89610400	2.64176200
H	-3.43219300	0.04894000	2.47298800
H	-3.18358900	-3.13793800	-0.52022700
H	-3.55684000	-0.85045500	-2.52847000
H	-1.89490500	-1.76501600	0.97497300
H	-4.59980200	-2.24701400	-2.24659500
C	-0.71233700	-0.55317000	-1.64779600
C	-0.70826100	0.68965500	0.13923500
N	0.20763300	0.34204900	-1.86330100
N	-1.33005800	-0.35711100	-0.43512500
N	0.19152900	1.10972300	-0.74208600
C	-1.06129400	-1.70231700	-2.54181300

H	-1.67784500	-1.35938700	-3.38051500
H	-0.13963000	-2.12685300	-2.94310800
O	-1.70140700	-2.71054000	-1.79237800
C	1.05824100	2.25179800	-0.61594200
C	0.48654400	3.52452500	-0.69510100
C	2.42698700	2.02429100	-0.44967000
C	1.34888800	4.61140100	-0.55688600
C	3.24148100	3.14632800	-0.31619900
C	2.71992700	4.44173800	-0.35739000
H	0.93753500	5.61547900	-0.61656600
H	4.31013400	3.00379600	-0.17749300
C	-0.98536400	3.71635400	-0.95512100
H	-1.30207300	3.14471000	-1.83328700
H	-1.59200500	3.38445400	-0.10732100
H	-1.19959800	4.76994800	-1.13824600
C	3.62372600	5.63247500	-0.17511700
H	3.79272100	5.82336900	0.88947600
H	4.59868900	5.46134200	-0.63700800
H	3.18465300	6.53288300	-0.60927900
C	2.99240200	0.62971100	-0.44036300
H	2.35086000	-0.06263700	0.11303100
H	3.07951400	0.24112900	-1.46011900
H	3.98368200	0.61824200	0.01669100
C	-0.91894300	1.29135600	1.53921200
O	-1.97763700	1.88442400	1.72416100
C	0.11585200	0.94476500	2.45133800
H	0.04988600	1.44103900	3.41672100
H	-0.05556700	-0.45223400	2.50387700
H	1.11947500	0.92777600	2.01948100
O	-0.11529400	-1.63990200	2.23662100
C	1.01416300	-2.00453800	1.67003900
C	1.01718300	-2.65346900	0.40994300
C	2.26082400	-1.73319900	2.28808700
C	2.20558100	-2.99231900	-0.21000700
H	0.06871300	-2.88772200	-0.06672100
C	3.44963200	-2.07104200	1.67129200
H	2.26188300	-1.25458100	3.26190200
C	3.41316200	-2.69052500	0.42149500
H	2.21507300	-3.47950600	-1.17790500
H	4.40506700	-1.85964000	2.13615500
N	4.65747300	-3.02033500	-0.23949800
O	5.70760000	-2.70765100	0.30685300
O	4.60890300	-3.59516800	-1.31945600

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C	-3.80697000	-0.54345200	0.39039200
C	-4.65077700	-0.83067500	-0.68733900
C	-5.97334100	-0.40098000	-0.68603200
C	-6.44770200	0.30461000	0.41766500
C	-5.61637800	0.55523400	1.51115900
C	-4.29103500	0.12528200	1.51100400
C	-2.45280800	-1.19585800	0.19171200
C	-2.79118600	-2.26406900	-0.89118400
C	-3.94816300	-1.66961800	-1.71882700
H	-6.62746200	-0.62835700	-1.52197300
H	-7.47857700	0.64371100	0.43705300
H	-6.00868100	1.08159900	2.37500600
H	-3.64196000	0.32927200	2.35225200
H	-3.16048100	-3.13802700	-0.35090400
H	-3.58962600	-1.04401100	-2.54323400
H	-2.03578200	-1.63691400	1.09841900
H	-4.57841200	-2.45039300	-2.14889300
C	-0.75520600	-0.53919400	-1.56298000
C	-0.71917700	0.71434400	0.22517700
N	0.18612700	0.32959100	-1.78414500
N	-1.37631000	-0.31508800	-0.35635300
N	0.18545500	1.10904000	-0.66890800
C	-1.07696200	-1.72307400	-2.42043500
H	-1.70925200	-1.43639400	-3.26735100
H	-0.14364100	-2.13099000	-2.81164200
O	-1.67499400	-2.72176000	-1.62395700
C	1.07278100	2.23882300	-0.58553900
C	0.51597600	3.52156700	-0.61530600
C	2.44582200	1.99540300	-0.52287200
C	1.40085600	4.59519100	-0.54114900
C	3.28589100	3.10629200	-0.45152400
C	2.78243000	4.40762200	-0.45077500
H	1.00004400	5.60520200	-0.56399700
H	4.35959400	2.94726800	-0.39453300
C	-0.96930600	3.73590000	-0.75431300
H	-1.35647900	3.20117700	-1.62793000
H	-1.51645300	3.37419800	0.12176200
H	-1.18403400	4.79765100	-0.88274100
C	3.70831700	5.59036600	-0.33642300
H	3.81837500	5.89001300	0.71068700
H	4.70264300	5.35261300	-0.71983100
H	3.31870900	6.45023700	-0.88573400
C	2.99782500	0.59571500	-0.54987100

H	2.35753200	-0.09844600	0.00141800
H	3.06309700	0.22404800	-1.57739100
H	3.99730100	0.56682400	-0.11121600
C	-0.90098400	1.31319000	1.62265600
O	-2.02992900	1.81027700	1.85797100
C	0.21680500	1.17573500	2.41762800
H	0.21359800	1.61300400	3.40969400
H	-0.05119300	-0.78667200	2.57388600
H	1.17108600	0.89552000	1.98176500
O	-0.09742000	-1.70703100	2.19570000
C	1.08666900	-2.01826600	1.63098100
C	1.08102100	-2.70234300	0.40670900
C	2.30104200	-1.68435700	2.25068400
C	2.28010900	-3.03613100	-0.20342500
H	0.13127000	-2.95635400	-0.05601300
C	3.50093100	-2.01531100	1.64318100
H	2.28834600	-1.16988600	3.20550100
C	3.47259600	-2.68185800	0.42164300
H	2.30257800	-3.55241800	-1.15510900
H	4.45042100	-1.76222800	2.09775600
N	4.73452900	-3.00473000	-0.23257400
O	5.76904700	-2.62796400	0.29567800
O	4.69634300	-3.63270600	-1.27894700

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C	-1.45778100	1.55973200	0.55675600
C	-2.29991900	2.58549300	0.97877100
C	-3.17947400	2.36637500	2.03793500
C	-3.18182700	1.12125100	2.66428200
C	-2.31479000	0.10514000	2.24689600
C	-1.44029900	0.31441700	1.18218100
C	-0.58363400	2.01520400	-0.58895500
C	-0.83442100	3.56389600	-0.70002400
C	-2.07972500	3.84351400	0.17724800
H	-3.84036600	3.15653100	2.37980400
H	-3.85415300	0.94073300	3.49656200
H	-2.31366800	-0.84462600	2.77331600
H	-0.74264100	-0.46185300	0.86134800
H	-1.01157100	3.83133800	-1.74120600
H	-1.90513600	4.72170900	0.80640300
H	-0.81109700	1.50545900	-1.52787100
H	-2.94474900	4.06855200	-0.45424700
C	1.58115500	2.57122400	0.47710200
C	1.53559000	0.62795200	-0.52656400

N	2.74231100	2.04126400	0.72811600
N	0.82190500	1.74158100	-0.30212200
N	2.68952800	0.82526900	0.10255600
C	0.98329200	3.89680000	0.82399400
H	0.31466600	3.79987100	1.69036500
H	1.76193200	4.62254000	1.05492200
O	0.29434700	4.34134500	-0.33006500
C	3.80748900	-0.07799900	0.14446800
C	3.92879100	-0.91793500	1.25393700
C	4.70996700	-0.06063900	-0.91783800
C	5.03071900	-1.76809300	1.28428200
C	5.79573100	-0.93385700	-0.84066800
C	5.97035600	-1.78830100	0.24849200
H	5.15790500	-2.43401500	2.13403400
H	6.52037400	-0.94319400	-1.65041600
C	2.88572400	-0.90486600	2.33705000
H	2.80570200	0.08429300	2.79798900
H	1.91348800	-1.15643700	1.89955400
H	3.12764900	-1.63085100	3.11437900
C	7.13828500	-2.73845600	0.30451500
H	7.58636500	-2.75007700	1.30111100
H	6.81348900	-3.75920600	0.08003400
H	7.90771200	-2.46370100	-0.41934700
C	4.50379500	0.85325900	-2.09643100
H	3.60978100	0.55988700	-2.65768900
H	4.36719700	1.89001200	-1.77477000
H	5.36035900	0.80994900	-2.77005200
C	1.08162500	-0.66342500	-1.18627300
O	1.04235400	-1.64203200	-0.37925400
C	0.75076400	-0.55553500	-2.51020900
H	0.48761300	-1.44242100	-3.07813100
H	-1.56418500	-0.68740200	-2.21708000
H	0.88555800	0.38062000	-3.04040600
C	-2.81858300	-4.40637400	0.79677200
C	-4.19261600	-3.96616800	0.29030600
C	-4.53354900	-2.51765100	0.62487700
C	-1.75906000	-3.33574200	0.54545800
C	-1.86683100	-2.71160800	-0.84627200
C	-2.85566700	-1.57928700	-0.97549300
H	-2.53400100	-5.33692700	0.29499900
H	-4.96960200	-4.59427600	0.73412900
H	-5.61602800	-2.39273900	0.57985700
H	-1.83695600	-2.54238800	1.29735600
H	-2.12285000	-3.46704900	-1.59897400

C	-4.78262800	-0.25845100	-0.41405300
H	-4.34468400	0.48946800	0.25888800
C	-4.77783200	0.23378400	-1.85217600
H	-5.36559600	1.14867500	-1.93781000
C	-3.34005100	0.50409300	-2.25054000
H	-2.99014100	1.42417700	-1.76843100
N	-2.50271300	-0.61623800	-1.82234100
N	-3.99684900	-1.50167700	-0.30815900
H	-0.88703600	-2.30547800	-1.11286200
H	-0.75431500	-3.75125100	0.65096800
H	-2.87004800	-4.62379300	1.86834400
H	-4.27572700	-4.09993100	-0.79367300
H	-4.22041300	-2.25578300	1.64341000
H	-5.79446300	-0.47491400	-0.07408000
H	-5.22334000	-0.52490200	-2.50130300
H	-3.22748500	0.61703200	-3.33018200

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C	-2.94534100	0.53502600	0.42926600
C	-4.19702600	0.30558400	-0.13366600
C	-4.96850200	1.38231400	-0.56562800
C	-4.45952000	2.67189000	-0.42734800
C	-3.19677900	2.88972900	0.13262100
C	-2.42178100	1.81787600	0.56975300
C	-2.27762300	-0.76461200	0.81499100
C	-3.20906800	-1.88706700	0.22581800
C	-4.51739900	-1.16680900	-0.18073400
H	-5.94556900	1.21984600	-1.01042800
H	-5.04835600	3.51943900	-0.76343900
H	-2.81758600	3.90213700	0.22514100
H	-1.43021400	1.97250200	0.99606500
H	-3.38837100	-2.65029500	0.98212800
H	-4.83949400	-1.50551800	-1.17052800
H	-2.14427700	-0.86707300	1.89425700
H	-5.31941300	-1.41705200	0.52040400
C	-0.75792100	-1.21327200	-1.08963300
C	0.22693200	-0.38136700	0.67877800
N	0.47630700	-1.02979100	-1.45611500
N	-0.94519500	-0.84336300	0.21441800
N	1.07062100	-0.49930400	-0.34243200

C	-1.93774000	-1.79611500	-1.79806100
H	-2.57981300	-0.99671000	-2.19326100
H	-1.61791900	-2.43458900	-2.62097400
O	-2.61608300	-2.60022700	-0.85133900
C	2.46386800	-0.14793900	-0.34752900
C	2.81800000	1.10908200	-0.84145900
C	3.38484400	-1.08007800	0.12949100
C	4.17531100	1.41991300	-0.86592000
C	4.73193400	-0.72059100	0.08490100
C	5.14167100	0.51898100	-0.40913400
H	4.48685300	2.38940000	-1.24661100
H	5.47614700	-1.42610600	0.44523400
C	1.75699100	2.07513600	-1.29034500
H	1.15822600	1.65540900	-2.10466800
H	1.08948200	2.28134100	-0.44627700
H	2.20396200	3.00889700	-1.63463400
C	6.60032500	0.89622600	-0.42347600
H	6.84559500	1.48680800	-1.30923600
H	6.84876100	1.50155400	0.45414000
H	7.23827600	0.01025900	-0.40817300
C	2.92825500	-2.40447300	0.68062000
H	2.32853800	-2.25225300	1.58502300
H	2.30662000	-2.94154000	-0.04225500
H	3.78388800	-3.03092200	0.93569000
C	0.49890100	0.31200400	2.00286700
O	0.78644800	1.54331100	1.86555400
C	0.35716300	-0.49236600	3.09360100
H	0.51490300	-0.09781300	4.09069600
H	0.10174600	-1.53961100	2.97825000

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C	-3.02672200	-0.56165500	-0.49208800
C	-3.78440700	-0.35256500	0.66557100
C	-4.51265300	-1.39830200	1.21897700
C	-4.47706500	-2.64478100	0.59444700
C	-3.74459400	-2.84024000	-0.57776400
C	-3.01669100	-1.79235500	-1.13791000
C	-2.36974400	0.73025300	-0.90773900
C	-3.26790700	1.77765000	-0.20309700
C	-3.70789800	1.08786300	1.10590900
H	-5.10933600	-1.24412800	2.11249600
H	-5.04279700	-3.47004400	1.01474300
H	-3.75101300	-3.81037900	-1.06267900
H	-2.46597500	-1.93877000	-2.06225700

H	-4.14306600	1.91189800	-0.84239800
H	-2.96190100	1.20745200	1.90077900
H	-2.28761300	0.88624400	-1.98492600
H	-4.65476900	1.48290300	1.47773000
C	-0.58724300	2.00196200	0.36826200
C	0.09066200	0.12008900	-0.47291200
N	0.67490400	1.92168300	0.68449500
N	-0.99387000	0.89783100	-0.34306200
N	1.08005000	0.74230600	0.15026600
C	-1.53548800	3.10720200	0.72072400
H	-1.79138500	3.03991200	1.78494500
H	-1.04833900	4.06697100	0.54450000
O	-2.67569000	3.05129400	-0.10352800
C	2.43939300	0.27722200	0.26765700
C	2.72253500	-0.69920800	1.22494500
C	3.39672800	0.84537500	-0.57895100
C	4.04269800	-1.14320400	1.29359400
C	4.69820600	0.36434500	-0.46560100
C	5.03466500	-0.63249400	0.45498900
H	4.30117000	-1.90136800	2.02785100
H	5.46825500	0.77958500	-1.11013000
C	1.66097300	-1.22112100	2.15718100
H	1.14569700	-0.39771400	2.66080000
H	0.90702300	-1.80702600	1.62260000
H	2.10967600	-1.86093700	2.91764200
C	6.44449100	-1.15582400	0.52790600
H	6.64749700	-1.60938300	1.49989400
H	6.60491800	-1.92062200	-0.23852600
H	7.17008500	-0.35824500	0.35437000
C	3.03467700	1.94102500	-1.54627900
H	2.18545700	1.66349700	-2.17937400
H	2.75299400	2.85206900	-1.01018000
H	3.88050500	2.17023200	-2.19481300
C	0.25143700	-1.23616600	-1.16308800
O	-0.09560100	-2.21568900	-0.55557600
C	0.85979600	-1.20722900	-2.52673700
H	0.88160700	-2.21674700	-2.93457400
H	0.28923600	-0.53855400	-3.17879500
H	1.87970900	-0.81147300	-2.45673900

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C	1.52931800	1.59843700	-0.59034300
C	2.37623000	2.65061800	-0.92707000
C	3.32467500	2.48064200	-1.93385000

C	3.39135700	1.25641300	-2.59594200
C	2.51991800	0.21284600	-2.26696400
C	1.57762400	0.37645200	-1.25466800
C	0.61175400	1.99250100	0.54231400
C	0.80628700	3.54528200	0.70064400
C	2.09497800	3.87279500	-0.09077000
H	3.99175300	3.29242600	-2.20602000
H	4.12080200	1.11333500	-3.38628400
H	2.57292400	-0.72271700	-2.81537300
H	0.88981300	-0.42891000	-0.99783500
H	0.90904300	3.79448800	1.75660700
H	1.94597400	4.77560700	-0.69098100
H	0.85603500	1.47831400	1.47148900
H	2.91962600	4.07649600	0.59948300
C	-1.53986300	2.49807000	-0.55449900
C	-1.50229400	0.56703800	0.45900100
N	-2.70241100	1.96614200	-0.80254900
N	-0.78299100	1.67545700	0.23277200
N	-2.65615300	0.75684700	-0.17548400
C	-0.95191800	3.82772800	-0.90160100
H	-0.25087100	3.73032100	-1.74163900
H	-1.73710600	4.53321400	-1.17096200
O	-0.31752900	4.29868300	0.27222200
C	-3.81346500	-0.10338800	-0.17680800
C	-3.96105700	-1.01024800	-1.22422100
C	-4.73452800	0.04621400	0.86234100
C	-5.10534900	-1.80779100	-1.20962900
C	-5.85884400	-0.77436900	0.82969000
C	-6.05857500	-1.70344200	-0.19553800
H	-5.25191600	-2.52845700	-2.00949300
H	-6.59814800	-0.68388100	1.62137600
C	-2.91298600	-1.12590500	-2.29612600
H	-2.72943600	-0.16005500	-2.77634000
H	-1.97088300	-1.46667800	-1.85443200
H	-3.22117100	-1.83946800	-3.06115800
C	-7.28759900	-2.57477400	-0.19503800
H	-7.31464700	-3.22241900	-1.07305500
H	-7.31313200	-3.20594400	0.69786000
H	-8.19512100	-1.96467100	-0.18893000
C	-4.50913900	1.04637400	1.96536100
H	-3.64218400	0.77311200	2.57678200
H	-4.32658700	2.04677200	1.56162000
H	-5.37947700	1.09318300	2.62070300
C	-1.10400700	-0.71167900	1.19363300

O	-1.40519600	-1.74637200	0.60689200
C	-0.34829500	-0.56806100	2.40496800
H	-0.44353200	-1.44500900	3.04581300
H	0.95740400	-0.62329200	2.07383800
H	-0.51026500	0.37053700	2.93693400
C	2.89346600	-4.35996600	-0.95432100
C	4.22325500	-3.96324900	-0.31057600
C	4.59239500	-2.49925000	-0.53172900
C	1.82565200	-3.28764500	-0.74005000
C	1.82986300	-2.74165100	0.69080000
C	2.77227800	-1.58375200	0.96386500
H	2.55523000	-5.31047400	-0.52797800
H	5.02875900	-4.57601800	-0.72511800
H	5.67255800	-2.39459600	-0.41204600
H	1.98326200	-2.46203600	-1.44345200
H	2.07051000	-3.54348200	1.39995200
C	4.80035600	-0.32218900	0.64160500
H	4.48183300	0.45967000	-0.06284600
C	4.61759600	0.14514000	2.07597400
H	5.20665200	1.04549200	2.26341900
C	3.13876100	0.42453100	2.27445700
H	2.89042000	1.35664200	1.74852000
N	2.30870600	-0.66433400	1.77157600
N	4.00678800	-1.53636700	0.41753800
H	0.83024100	-2.39965500	0.95830900
H	0.83390200	-3.69168800	-0.96154900
H	3.03572100	-4.52451300	-2.02756400
H	4.21376500	-4.15838700	0.76709400
H	4.35818500	-2.19080200	-1.56059900
H	5.84475700	-0.55893900	0.43418800
H	4.95941900	-0.63796900	2.75964000
H	2.89302600	0.57540400	3.33068900

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C	3.42202300	-0.98876400	1.04454200
C	4.74326300	-1.19092600	0.65630500
C	5.66551100	-1.70485900	1.56521500
C	5.23978800	-2.01252500	2.85562000
C	3.91173000	-1.80446300	3.23887100
C	2.98906700	-1.28629100	2.33338500
C	2.60192000	-0.42321500	-0.09088800
C	3.55334000	-0.48149200	-1.34283000
C	4.96354900	-0.77447300	-0.77531400
H	6.69801900	-1.86905500	1.27146700

H	5.94686200	-2.41915300	3.57164700
H	3.59941500	-2.04757300	4.24924800
H	1.95706100	-1.10452400	2.61893100
H	3.51601500	0.47907800	-1.85687700
H	5.45624600	-1.54477100	-1.37715100
H	2.27505300	0.59710400	0.10187100
H	5.58627400	0.12422600	-0.82848900
C	1.40918400	-2.32132000	-1.11661200
C	0.11298800	-1.02696600	0.07908400
N	0.22424600	-2.83936700	-1.24925000
N	1.38807800	-1.21652400	-0.31699400
N	-0.57019600	-2.03262100	-0.48368600
C	2.69102700	-2.65068600	-1.80432800
H	3.40825100	-3.10339300	-1.10636000
H	2.51216100	-3.33617300	-2.63200400
O	3.16634000	-1.42598400	-2.33118700
C	-1.98556300	-2.27065000	-0.45833200
C	-2.52741600	-2.96368600	0.62481200
C	-2.74705000	-1.77040300	-1.51708100
C	-3.91112000	-3.13024000	0.64533200
C	-4.12645000	-1.96225100	-1.44811200
C	-4.72339200	-2.62462800	-0.37233200
H	-4.36553500	-3.65664200	1.48058800
H	-4.75036500	-1.58060200	-2.25288100
C	-1.64792400	-3.44724100	1.74546600
H	-1.25348800	-2.59467100	2.31097000
H	-2.21148100	-4.08010200	2.43204500
H	-0.79417700	-4.01532500	1.36525900
C	-6.22161200	-2.76218800	-0.30096900
H	-6.51328800	-3.60689100	0.32625200
H	-6.66464600	-1.85764200	0.12891400
H	-6.65326500	-2.89934100	-1.29492000
C	-2.09803000	-1.07055300	-2.68215800
H	-2.85011100	-0.54592200	-3.27475800
H	-1.34023300	-0.34928600	-2.35479400
H	-1.59898000	-1.79765400	-3.33136700
C	-0.33080400	0.03659000	1.04705900
O	0.58150100	0.76312900	1.50678000
C	-1.69325800	0.28115600	1.25973300
H	-1.90506900	0.90508800	2.12053000
H	-2.47309200	-0.40257500	0.95498800
C	0.28995200	2.21484300	-0.81606700
O	0.28127100	1.17412000	-1.51446400
C	-0.85787800	2.67603500	-0.10916400

C	-1.99842700	1.87920900	-0.13091700
H	-0.79915400	3.57477400	0.49303800
H	-2.04869800	1.16873300	-0.95246000
C	-3.32390900	2.31623300	0.37116500
C	-4.47406700	1.69398000	-0.12843900
C	-3.47033700	3.31789700	1.33869700
C	-5.73950600	2.07020600	0.31195100
H	-4.36626200	0.90258100	-0.86738600
C	-4.73449200	3.69563600	1.77987000
H	-2.59001100	3.79731900	1.75666400
C	-5.87371500	3.07592700	1.26694700
H	-6.61993000	1.57885600	-0.09056400
H	-4.83247600	4.47453500	2.52948900
H	-6.85828200	3.37272200	1.61354800
C	1.56819400	3.00193800	-0.73656900
C	1.92543000	3.73667500	0.39829400
C	2.44384400	2.96380700	-1.82597700
C	3.13231700	4.42985200	0.43595800
H	1.27206200	3.73210300	1.26485700
C	3.64776400	3.66175600	-1.79257000
H	2.16003400	2.38180100	-2.69774400
C	3.99381500	4.39768200	-0.65970400
H	3.40624400	4.98877800	1.32518700
H	4.31506000	3.63340700	-2.64836700
H	4.93347600	4.94002200	-0.62858300

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C	3.80239500	-0.82862100	1.24357900
C	5.05661400	-0.22471700	1.28581200
C	6.18891300	-0.99141200	1.54736400
C	6.03890200	-2.36069600	1.76108400
C	4.77574300	-2.95756300	1.72216000
C	3.64034500	-2.19209300	1.46457500
C	2.72838300	0.18863100	0.93367000
C	3.51775200	1.47352100	0.50079300
C	4.94956300	1.26024400	1.04022600
H	7.17281400	-0.53291000	1.57833600
H	6.91395000	-2.97130100	1.96015200
H	4.67994300	-4.02474200	1.89399900
H	2.64617800	-2.62980000	1.44333800
H	3.03439300	2.35564700	0.92198800
H	5.68405200	1.64307500	0.32606100
H	2.07501800	0.39408700	1.77873000
H	5.08351000	1.81371700	1.97565800

C	2.25712400	-0.15890600	-1.45706900
C	0.61569600	-0.76321300	-0.14864200
N	1.33038400	-0.57621200	-2.27072700
N	1.86518500	-0.26873700	-0.15673000
N	0.31890700	-0.96795600	-1.43574100
C	3.54514500	0.54853100	-1.71790400
H	4.40355600	-0.09371800	-1.48394800
H	3.60168800	0.86563100	-2.75856100
O	3.51312300	1.70955700	-0.90521900
C	-0.83821500	-1.60591100	-2.00501300
C	-1.84251000	-0.80082000	-2.54826200
C	-0.88221900	-2.99991700	-2.00378300
C	-2.93615600	-1.45044200	-3.11557100
C	-1.99998100	-3.60135400	-2.58238100
C	-3.02847400	-2.84513200	-3.14393500
H	-3.73761300	-0.85298500	-3.54337000
H	-2.06369000	-4.68613600	-2.59553300
C	-1.76827100	0.69742200	-2.44706800
H	-1.93043100	1.00994600	-1.40651000
H	-0.78816900	1.07791800	-2.74867700
H	-2.53404700	1.16638300	-3.06638400
C	-4.21731100	-3.50978600	-3.78992700
H	-5.15244800	-3.12654100	-3.36680900
H	-4.23290300	-3.30108400	-4.86598100
H	-4.18737600	-4.59416400	-3.65047800
C	0.21714000	-3.80929200	-1.36910400
H	1.20303600	-3.48857500	-1.71920500
H	0.19842700	-3.69613500	-0.27898500
H	0.09699800	-4.86827500	-1.60101300
C	-0.15859700	-1.12883200	1.09679900
O	0.55243200	-1.37078300	2.09852200
C	-1.55937100	-1.12549500	1.04048000
H	-2.05617900	-1.69464100	1.81664600
H	-2.08561000	-1.01411900	0.10159700
C	-0.77284500	2.21953900	0.72020200
O	0.25465400	1.59811500	1.06933700
C	-2.05879800	1.81359100	1.17242100
C	-2.13061100	0.72577100	2.04011600
H	-2.95443200	2.24258700	0.73846000
H	-1.25779000	0.54204700	2.66646400
C	-3.42783800	0.27586600	2.59870000
C	-3.47266700	-0.28226000	3.88155500
C	-4.61954400	0.38408700	1.87125300
C	-4.67973500	-0.69760600	4.43573300

H	-2.54941100	-0.38698200	4.44579900
C	-5.82604600	-0.03482200	2.42201500
H	-4.59709800	0.78174200	0.86059300
C	-5.86145900	-0.57267300	3.70789300
H	-4.69802300	-1.11882100	5.43574600
H	-6.74122300	0.05221500	1.84486400
H	-6.80331000	-0.90005800	4.13626800
C	-0.64126500	3.32889400	-0.28216000
C	-1.61163000	4.32262000	-0.44432000
C	0.50095000	3.35093000	-1.08921600
C	-1.44318400	5.31832700	-1.40341100
H	-2.49106500	4.33209900	0.19248400
C	0.66389500	4.33889700	-2.05453400
H	1.25624100	2.58321200	-0.94748200
C	-0.30899600	5.32548100	-2.21407300
H	-2.19704300	6.09075500	-1.51739600
H	1.55040600	4.34123000	-2.68130300
H	-0.18237300	6.09919700	-2.96462700

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C	-3.59449200	-1.00767600	-0.97526600
C	-4.92837300	-0.88686700	-0.59342500
C	-5.88527900	-1.73667600	-1.14189600
C	-5.47871900	-2.69940600	-2.06493800
C	-4.13774000	-2.80916200	-2.44295400
C	-3.17631800	-1.95670800	-1.90226300
C	-2.74006400	0.01536900	-0.26050300
C	-3.67276100	0.57907000	0.86869100
C	-5.10448000	0.22951500	0.40653500
H	-6.92816100	-1.65789200	-0.84966300
H	-6.21295800	-3.37443300	-2.49330600
H	-3.84423900	-3.56442000	-3.16515300
H	-2.12780800	-1.99699300	-2.19040700
H	-3.52225900	1.65452200	0.98401500
H	-5.72224600	-0.04377800	1.26676600
H	-2.39708900	0.80565900	-0.92566400
H	-5.56739600	1.10265700	-0.06593300
C	-1.70133800	-1.40289900	1.44016800
C	-0.26903900	-0.69684500	-0.06601300
N	-0.59150200	-2.00171500	1.74442100
N	-1.55251400	-0.60756600	0.33751000
N	0.28884100	-1.56249100	0.78661000
C	-3.01142600	-1.33081900	2.15726500
H	-3.76519500	-1.96439900	1.67258300

H	-2.89098100	-1.64521600	3.19381000
O	-3.37869900	0.03761000	2.15238300
C	1.63756300	-2.05974700	0.83598200
C	2.04844900	-2.98519200	-0.12549600
C	2.45443200	-1.62455000	1.88513100
C	3.36858500	-3.43187900	-0.05066300
C	3.76056200	-2.10715300	1.91833900
C	4.23740800	-2.99662300	0.95118400
H	3.72270400	-4.14405800	-0.79134100
H	4.42338700	-1.77405600	2.71299700
C	1.10368000	-3.48055400	-1.18811400
H	0.20067500	-3.89987300	-0.73103300
H	0.78149300	-2.66937000	-1.85173600
H	1.58093300	-4.26096500	-1.78269000
C	5.67054900	-3.45907800	0.98289400
H	5.79499200	-4.40106800	0.44517800
H	6.32099100	-2.71576600	0.51004000
H	6.01881700	-3.59422900	2.00949200
C	1.94538200	-0.66084000	2.92485500
H	1.37573600	0.15645600	2.46769500
H	1.27744700	-1.16605800	3.62848100
H	2.77762700	-0.23115200	3.48448200
C	0.24878000	-0.05688000	-1.41492800
O	-0.25867000	-0.71280500	-2.39501200
C	1.76362200	0.19849000	-1.46013100
H	1.89642900	0.73603200	-2.40511100
H	2.30376200	-0.74877700	-1.54726100
C	0.06657000	2.09770800	-0.28485900
O	-0.36041400	1.32589500	-1.32705400
C	1.30868800	2.01410200	0.21440300
C	2.33031200	1.03576000	-0.29715400
H	1.59112500	2.66571900	1.03589500
H	2.57577800	0.35505100	0.52511200
C	3.64543800	1.67743900	-0.70217400
C	4.84268200	0.98975200	-0.48766000
C	3.68577100	2.91915200	-1.34014700
C	6.05778100	1.53053000	-0.90096300
H	4.81475500	0.02140400	0.01032900
C	4.89928700	3.46398900	-1.75297400
H	2.75654400	3.45809000	-1.50837800
C	6.08889800	2.77105600	-1.53508400
H	6.98027200	0.98585800	-0.72448000
H	4.91715200	4.43154600	-2.24534600
H	7.03442800	3.19639800	-1.85617500

C	-1.00241200	2.97454500	0.25468600
C	-1.08068200	3.25779000	1.62269300
C	-1.99127800	3.47636700	-0.60104400
C	-2.11567000	4.04355800	2.12227700
H	-0.34361300	2.83668700	2.29979400
C	-3.02606200	4.26042600	-0.10014700
H	-1.94212400	3.24291000	-1.66015700
C	-3.09115900	4.54704300	1.26331600
H	-2.16962400	4.24839100	3.18662700
H	-3.78375400	4.64658000	-0.77440800
H	-3.90199600	5.15267800	1.65488500

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C	3.61371300	-0.79019200	1.07840000
C	4.98914900	-0.81724200	0.85989400
C	5.82934000	-1.41702200	1.79435200
C	5.26711100	-1.98660500	2.93553800
C	3.88593100	-1.95231900	3.14646400
C	3.04101100	-1.34736100	2.21771200
C	2.90122500	-0.10389900	-0.06861500
C	4.00288200	0.02588200	-1.18221400
C	5.34607300	-0.13947700	-0.43895500
H	6.90263800	-1.44844700	1.63284400
H	5.91015400	-2.46374500	3.66849100
H	3.46922100	-2.39862400	4.04371700
H	1.96511300	-1.28030200	2.35976400
H	3.92594600	0.99262700	-1.68101200
H	6.04656200	-0.71218400	-1.05370000
H	2.48371900	0.86517900	0.20736700
H	5.79811300	0.84066200	-0.25488600
C	2.04310900	-2.04693400	-1.30716800
C	0.47156700	-0.88307000	-0.32534900
N	0.95336100	-2.71718300	-1.53379900
N	1.79305800	-0.92578700	-0.56641300
N	-0.01736000	-1.97887900	-0.90333700
C	3.43593800	-2.21607200	-1.82132500
H	4.09354500	-2.63869400	-1.05079500
H	3.44172600	-2.86632700	-2.69543100
O	3.85374000	-0.92517600	-2.23110500
C	-1.35837400	-2.49341600	-0.84484300
C	-2.18830700	-2.32437100	-1.95237000
C	-1.75349600	-3.13723600	0.32970100
C	-3.48489600	-2.82649800	-1.85462500
C	-3.05972800	-3.61996400	0.37821300

C	-3.93419500	-3.47453100	-0.70177100
H	-4.16155900	-2.70319000	-2.69631700
H	-3.40335700	-4.11674600	1.28190300
C	-1.69680100	-1.61015600	-3.18242300
H	-1.35960000	-0.59676600	-2.93913900
H	-0.84671300	-2.13597800	-3.62689900
H	-2.48934300	-1.53821600	-3.92813400
C	-5.33285500	-4.02988800	-0.63389800
H	-6.02084700	-3.43977500	-1.24310300
H	-5.35499200	-5.05772700	-1.01008600
H	-5.70180000	-4.04549000	0.39380000
C	-0.81192300	-3.24875000	1.49983300
H	0.13150300	-3.71751000	1.20017000
H	-0.56945000	-2.25585700	1.90085100
H	-1.25803100	-3.84806400	2.29466200
C	-0.18390200	0.19154400	0.58765300
O	0.29127300	0.09191700	1.78021600
C	-1.71498300	0.27176200	0.46562600
H	-2.17588800	-0.62221100	0.89293600
H	-2.02833900	0.35753100	-0.58296400
C	-0.22873400	2.59815300	0.14554100
O	0.33090700	1.40293000	-0.18038400
C	-1.39552200	2.70990900	0.79885000
C	-2.17574600	1.50742400	1.25370700
H	-1.79578900	3.69599600	1.00753700
H	-1.94381400	1.30704400	2.30884400
C	-3.67493300	1.68528900	1.12506100
C	-4.53258600	1.17083000	2.10033500
C	-4.23246900	2.31810900	0.00999800
C	-5.91468700	1.28619700	1.96902400
H	-4.10929600	0.67774400	2.97224700
C	-5.61322900	2.43690900	-0.12519700
H	-3.57168900	2.72177500	-0.75340200
C	-6.45943100	1.92134100	0.85521300
H	-6.56642100	0.88428500	2.73867000
H	-6.03004800	2.93314900	-0.99633100
H	-7.53579800	2.01616500	0.75223000
C	0.58451600	3.74556800	-0.33168600
C	0.44656500	5.02569600	0.21982000
C	1.52116500	3.55218300	-1.35454500
C	1.21221300	6.08576900	-0.25237400
H	-0.24684700	5.19015000	1.03822800
C	2.28855600	4.61429700	-1.82488700
H	1.63441400	2.56195400	-1.78309800

C	2.13607600	5.88587300	-1.27763900
H	1.09568800	7.06986300	0.19049600
H	3.00771200	4.44704400	-2.62069200
H	2.73673600	6.71386300	-1.64005900

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C	2.97652900	-0.99986400	0.96541300
C	4.28503400	-1.46014700	1.08579100
C	4.94745900	-1.36080500	2.30697800
C	4.27645300	-0.80071500	3.39250700
C	2.96109500	-0.34580200	3.26337600
C	2.29345700	-0.44267200	2.04357900
C	2.45849400	-1.19734400	-0.44235600
C	3.53991400	-2.10457100	-1.13330900
C	4.78730700	-2.01817200	-0.22196000
H	5.96613600	-1.72141400	2.41451600
H	4.77910400	-0.72073400	4.35129700
H	2.45557900	0.08432100	4.12206800
H	1.26970100	-0.08945400	1.92931800
H	3.75060700	-1.73572900	-2.13757500
H	5.24872200	-3.00544300	-0.12337300
H	2.35281500	-0.24466600	-0.96475800
H	5.53437500	-1.35252000	-0.66676300
C	1.04852400	-3.19994900	-0.27933200
C	-0.08906400	-1.29600400	-0.50199200
N	-0.19479900	-3.57075200	-0.23737200
N	1.15157100	-1.84384000	-0.44776600
N	-0.87100600	-2.37627700	-0.36518400
C	2.31729100	-3.98740600	-0.29413400
H	2.82720700	-3.92764500	0.67716200
H	2.12120000	-5.03319300	-0.52944900
O	3.11129100	-3.44575100	-1.33719700
C	-2.30469700	-2.36224000	-0.36004000
C	-2.96677800	-2.32733200	0.86972900
C	-2.97459600	-2.36285000	-1.58527000
C	-4.35956700	-2.26727300	0.84635800
C	-4.36763500	-2.29842800	-1.55807300
C	-5.07303300	-2.24753000	-0.35443200
H	-4.90055700	-2.23105800	1.78895200
H	-4.91343100	-2.28895700	-2.49834800
C	-2.18931700	-2.34117500	2.15810100
H	-1.54520500	-3.22380500	2.21395000
H	-1.55175400	-1.45349100	2.21578300
H	-2.86530400	-2.34973700	3.01480800

C	-6.57949400	-2.20507400	-0.34698000
H	-6.95208300	-1.60135000	0.48392600
H	-6.96825100	-1.79090900	-1.27968300
H	-6.99297000	-3.21231700	-0.23272500
C	-2.21069800	-2.43040000	-2.88094900
H	-1.55915800	-1.55945900	-3.00348800
H	-1.56912000	-3.31643300	-2.90705300
H	-2.89451500	-2.47136100	-3.72997500
C	-0.64974700	0.64399200	0.06011000
O	-0.88032600	0.54152500	1.25875200
C	-1.71729400	0.95335800	-0.96747700
H	-2.64890900	0.47427300	-0.65705500
H	-1.41104800	0.56377600	-1.94076900
C	0.61705500	2.42121900	-0.92906500
O	0.61583000	1.20154600	-0.29936200
C	-0.50051500	3.07928600	-1.26692300
C	-1.86911100	2.48721800	-1.06999200
H	-0.41189100	4.07389600	-1.68853500
H	-2.46434800	2.68613800	-1.96964100
C	-2.63778800	3.07459200	0.10590500
C	-4.03502600	3.09278000	0.06515800
C	-1.99455000	3.56732900	1.24276500
C	-4.77535800	3.58932300	1.13417600
H	-4.54581700	2.71315300	-0.81719200
C	-2.73165000	4.06696000	2.31423000
H	-0.90938100	3.55677000	1.28580000
C	-4.12364100	4.08030600	2.26401200
H	-5.85970100	3.59829300	1.08298000
H	-2.21645000	4.44790000	3.19077900
H	-4.69680900	4.47247600	3.09818800
C	1.99770400	2.91046800	-1.15138900
C	2.28450200	3.81337300	-2.18206000
C	3.04015400	2.46191700	-0.33115200
C	3.58281700	4.27191600	-2.37542300
H	1.49213800	4.13919300	-2.84852200
C	4.34025600	2.91725200	-0.53240700
H	2.82403700	1.76118700	0.46944500
C	4.61577100	3.82528900	-1.55213900
H	3.79127400	4.96914200	-3.18052400
H	5.13809200	2.56240600	0.11266300
H	5.62944100	4.17932500	-1.70949700

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C	-3.38855800	-0.78250700	-0.35536000
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C	-4.72391600	-0.93783900	0.00623400
C	-5.69283800	-1.13127700	-0.97552100
C	-5.29729700	-1.17380600	-2.31121800
C	-3.95285100	-1.02709800	-2.66441300
C	-2.97952200	-0.83062500	-1.68562800
C	-2.52038600	-0.56886400	0.86469800
C	-3.45747300	-0.91647600	2.07541300
C	-4.89297900	-0.86036900	1.50328400
H	-6.73721000	-1.25662600	-0.70546700
H	-6.04127700	-1.32824300	-3.08626000
H	-3.66520800	-1.06789200	-3.71009900
H	-1.92957300	-0.70740500	-1.94797500
H	-3.31756700	-0.19200000	2.87823600
H	-5.49415000	-1.67680000	1.91457100
H	-2.16781400	0.46288800	0.92515900
H	-5.37710800	0.07854800	1.79224500
C	-1.45335500	-2.75078400	1.19984400
C	-0.08822800	-1.17168500	0.41253500
N	-0.32240200	-3.36743300	1.03642300
N	-1.34742300	-1.43142900	0.84683500
N	0.49444700	-2.37299200	0.54093800
C	-2.75277100	-3.19440600	1.78795000
H	-3.49991700	-3.36914200	1.00179500
H	-2.62451700	-4.10968500	2.36562900
O	-3.16179300	-2.17013700	2.68057200
C	1.85927700	-2.66168500	0.21271500
C	2.14334600	-3.20758900	-1.03970600
C	2.84849800	-2.36697100	1.15586000
C	3.48434300	-3.43824900	-1.35114300
C	4.17265700	-2.61025500	0.79849400
C	4.50770000	-3.13764300	-0.45179700
H	3.73262600	-3.86116600	-2.32151100
H	4.96143200	-2.38819100	1.51341400
C	1.03446200	-3.52364900	-2.00630800
H	0.32747800	-4.23537800	-1.56969900
H	0.48498300	-2.60975800	-2.25232500
H	1.43661500	-3.95345700	-2.92539900
C	5.95180800	-3.36697400	-0.81718100
H	6.03950700	-3.96771800	-1.72465600
H	6.46170500	-2.41450400	-0.99253700
H	6.48426400	-3.87798500	-0.01075600
C	2.48157000	-1.80938200	2.50529700
H	2.04652100	-0.80910900	2.41467600
H	1.73527600	-2.44049500	2.99719200

H	3.36136600	-1.74467400	3.14723300
C	0.51354200	0.30016500	-1.00219900
O	0.44603500	-0.28926500	-2.07088400
C	1.81575600	0.76050200	-0.38416000
H	2.59832500	0.03944700	-0.63227800
H	1.71031400	0.82883100	0.70147500
C	-0.30282300	2.50510000	-0.54825200
O	-0.57218200	1.16379200	-0.67770900
C	0.92096500	3.02824800	-0.70397100
C	2.13219000	2.16413800	-0.93886500
H	1.03882900	4.10525400	-0.66217300
H	2.31755600	2.07186500	-2.01845500
C	3.39312500	2.70681000	-0.29736300
C	4.62677300	2.54488300	-0.93197400
C	3.35668300	3.32351100	0.95618700
C	5.80030800	2.99322000	-0.33103600
H	4.66541700	2.06485900	-1.90682900
C	4.52808500	3.77461000	1.55933300
H	2.40040200	3.45203000	1.45777000
C	5.75396600	3.61141500	0.91661600
H	6.75090400	2.86345900	-0.83886500
H	4.48281800	4.25548900	2.53158800
H	6.66704600	3.96548600	1.38437800
C	-1.53466400	3.27537800	-0.26125000
C	-1.47859700	4.50877000	0.39890800
C	-2.78143800	2.76317400	-0.63947800
C	-2.64426300	5.22194000	0.65634200
H	-0.52188800	4.89835100	0.73312200
C	-3.94716300	3.47536200	-0.37188200
H	-2.83032800	1.80661200	-1.14979100
C	-3.88281900	4.70797200	0.27347100
H	-2.58683700	6.17491500	1.17245900
H	-4.90625800	3.06499600	-0.67265500
H	-4.79124300	5.26266700	0.48473600

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C	-0.73191000	0.38324500	0.88426900
O	-0.16891800	1.49774900	0.90739400
C	-0.23704500	-0.76914600	1.49245000
H	0.50837000	-0.60959300	2.26243500
H	-0.78751000	-1.69847600	1.53658300
C	2.59025200	1.09355200	0.38081800
C	1.91981100	0.09597000	-0.36580900
C	1.44899900	-1.14786700	0.04397300

H	1.59611500	0.44157100	-1.34161600
H	1.88156900	-1.64469200	0.90251200
C	0.81864200	-2.05334900	-0.94378900
C	0.96068700	-3.43786700	-0.78876000
C	0.08938200	-1.57248600	-2.04186000
C	0.42027200	-4.31832800	-1.72322400
H	1.51388300	-3.82179400	0.06473600
C	-0.45478100	-2.45043800	-2.97289300
H	-0.06524900	-0.50303100	-2.16548600
C	-0.27945500	-3.82709800	-2.82337900
H	0.55114500	-5.38784600	-1.59401800
H	-1.02710200	-2.06221100	-3.80900700
H	-0.70034000	-4.51214900	-3.55241700
C	2.61791200	2.44430600	-0.26867700
C	3.10976000	2.59130200	-1.56825600
C	2.15740200	3.56508800	0.42496000
C	3.14152200	3.84843900	-2.16813200
H	3.47790800	1.72085100	-2.10498800
C	2.17053100	4.81520700	-0.18355500
H	1.76386400	3.43551700	1.42728000
C	2.66473700	4.96171700	-1.48018500
H	3.53782000	3.95621500	-3.17282600
H	1.78910800	5.67918400	0.35271300
H	2.67948600	5.94034900	-1.94982800
N	3.23610300	1.08470000	1.54263700
S	3.71546800	-0.24262600	2.35213300
O	2.62224200	-1.04184300	2.93548800
O	4.72496700	0.22249500	3.30859400
C	4.53725800	-1.27851700	1.15086200
C	4.35511100	-2.65640200	1.20817800
C	5.37445000	-0.70436800	0.19776700
C	5.01600300	-3.46677900	0.29069000
H	3.68706900	-3.08017700	1.95184300
C	6.02649700	-1.52771400	-0.71262400
H	5.49696100	0.37406100	0.15528800
C	5.85949100	-2.91649800	-0.67912300
H	4.86914900	-4.54268200	0.32355700
H	6.67235500	-1.08614900	-1.46605600
C	6.58864800	-3.80275400	-1.65396300
H	7.52079000	-4.17092200	-1.21325500
H	5.98587300	-4.67303700	-1.92307400
H	6.84464300	-3.25997300	-2.56616900
C	-3.62947400	-2.33596900	1.05446200
C	-4.63362900	-3.25985400	0.77482100

C	-5.60413400	-3.54594000	1.73257700
C	-5.55808400	-2.88867100	2.95903500
C	-4.55622900	-1.95262600	3.22948900
C	-3.58312000	-1.66755300	2.27661300
C	-2.70352400	-2.15826300	-0.13103300
C	-3.34256000	-3.04126600	-1.27359000
C	-4.50133200	-3.82594800	-0.61304400
H	-6.39053500	-4.26394800	1.52092900
H	-6.31235900	-3.09817100	3.71057200
H	-4.53710200	-1.44240500	4.18658000
H	-2.80813000	-0.93547300	2.48581200
H	-2.57767600	-3.71474200	-1.65511200
H	-5.41796700	-3.71887300	-1.20246200
H	-1.67927400	-2.48694500	0.04427900
H	-4.26537800	-4.89353200	-0.58575000
C	-3.60206600	-0.21574100	-1.35538200
C	-1.92742100	0.30464300	-0.04387700
N	-3.50926400	1.07827300	-1.43186200
N	-2.65434200	-0.73511600	-0.51800100
N	-2.47443100	1.39054900	-0.60448700
C	-4.51550400	-1.15303400	-2.07245800
H	-5.37868000	-1.40577200	-1.44128400
H	-4.87324900	-0.69567100	-2.99460100
O	-3.75036900	-2.29292700	-2.40372400
C	-2.23894700	2.79495500	-0.34815900
C	-3.01868000	3.40089300	0.63365600
C	-1.30818200	3.47987500	-1.12806100
C	-2.84593000	4.77358200	0.82450000
C	-1.17513200	4.84580600	-0.90175900
C	-1.93621600	5.50863000	0.06590700
H	-3.43705500	5.27450700	1.58678500
H	-0.44359200	5.40213500	-1.48296600
C	-3.97720000	2.60039800	1.47544600
H	-4.64812100	1.99558900	0.85794200
H	-3.43334500	1.91838500	2.13884100
H	-4.58422000	3.25953300	2.09734300
C	-1.76529200	6.99054400	0.27822400
H	-2.34464100	7.33747000	1.13602600
H	-0.71410800	7.24024200	0.44932000
H	-2.09275300	7.55001100	-0.60322300
C	-0.44911600	2.74328000	-2.11299200
H	0.12516800	1.98630600	-1.56863000
H	-1.04962600	2.24201500	-2.87959200
H	0.25500400	3.42198500	-2.59782600

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C	-3.75948800	-1.38411300	1.86060300
C	-5.08715100	-1.10171700	2.20298400
C	-5.45452200	-0.93689200	3.53332100
C	-4.48005800	-1.05761600	4.52199000
C	-3.16009900	-1.35551700	4.18302500
C	-2.78896500	-1.52623000	2.85042000
C	-3.63273000	-1.51145200	0.35399400
C	-5.10805700	-1.74803400	-0.07518800
C	-5.96771900	-1.03235800	0.98475400
H	-6.48606800	-0.72337700	3.79550800
H	-4.75191500	-0.93106800	5.56491100
H	-2.41393600	-1.46594600	4.96249400
H	-1.76268700	-1.77354800	2.60754200
H	-5.27441000	-2.82521600	-0.00373200
H	-6.16613500	0.01182600	0.71673200
H	-2.97706000	-2.30496300	-0.01072800
H	-6.93395500	-1.52247500	1.11854300
C	-3.94054000	0.47849700	-1.15955400
C	-2.08729900	0.51118900	-0.01132000
N	-3.39162600	1.62865300	-1.43160000
N	-3.18222100	-0.23398900	-0.26904500
N	-2.24416900	1.63935700	-0.70360700
C	-5.22338100	-0.05097900	-1.72410400
H	-6.06430000	0.54920000	-1.35717300
H	-5.19167400	0.03868400	-2.81192700
O	-5.36884800	-1.41741500	-1.41911500
C	-1.49433400	2.87443700	-0.61976000
C	-1.81879600	3.72308100	0.44755700
C	-0.56960600	3.19619200	-1.60606400
C	-1.17427000	4.95131200	0.49962200
C	0.05241100	4.44507700	-1.50368400
C	-0.23744600	5.32939900	-0.47055500
H	-1.40412700	5.63266100	1.31506500
H	0.78669300	4.72098300	-2.25598600
C	-2.80151500	3.29412800	1.50282800
H	-3.75597900	2.98393200	1.06439200
H	-2.39644800	2.44607400	2.06583800
H	-2.99543900	4.10929500	2.20102000
C	0.43142300	6.67659500	-0.38774200
H	-0.30016500	7.47979400	-0.51769400
H	0.90017600	6.81844200	0.58991300
H	1.19844900	6.78675400	-1.15633200

C	-0.19570300	2.24652400	-2.70829900
H	0.64613400	1.62195400	-2.38198100
H	-1.03176500	1.60257900	-2.99309800
H	0.12108900	2.79959100	-3.59481300
C	-0.81262000	0.18873100	0.75437500
O	-0.26337300	1.14794900	1.30034300
C	-0.30770700	-1.12952600	0.58493100
H	0.63415900	-1.31725200	1.09285400
H	-1.00265900	-1.95812300	0.57202500
C	2.63691000	-1.09036000	-1.27444200
C	1.54204100	-1.93751700	-1.41866100
C	0.22529900	-1.41842000	-1.47198300
H	1.70942900	-3.00868300	-1.41796800
H	0.16048600	-0.37276800	-1.75975400
C	-0.91713700	-2.25353900	-1.91729500
C	-1.91150600	-1.69243400	-2.72585100
C	-1.04879700	-3.59083600	-1.51755100
C	-3.01857600	-2.44200300	-3.11765500
H	-1.81374200	-0.65903700	-3.05328200
C	-2.15817200	-4.33719900	-1.89988000
H	-0.29186300	-4.03615700	-0.87723000
C	-3.15025400	-3.76278400	-2.69602100
H	-3.78110400	-1.99467800	-3.74701500
H	-2.25408600	-5.36652200	-1.56994600
H	-4.02034000	-4.34234800	-2.98601500
C	3.97249200	-1.73381500	-1.08310800
C	5.05135900	-1.43249500	-1.92033500
C	4.14328400	-2.66304300	-0.05130500
C	6.28378600	-2.04713700	-1.71922300
H	4.92124900	-0.70832300	-2.71605200
C	5.38136500	-3.26199400	0.15955000
H	3.30502600	-2.88904900	0.60201100
C	6.45444900	-2.95433700	-0.67486600
H	7.11460000	-1.81501700	-2.37804400
H	5.50910100	-3.96670600	0.97522800
H	7.42051000	-3.42258500	-0.51447600
N	2.43059600	0.24144200	-1.29562600
S	3.50343600	1.32538200	-0.75931400
O	2.73755600	2.54992700	-0.48698500
O	4.67849900	1.50445400	-1.63102300
C	4.09246600	0.69088800	0.80020500
C	3.16397800	0.44106700	1.80880600
C	5.43972900	0.39470500	0.96947400
C	3.60312900	-0.13050000	2.99838200

H	2.11348400	0.68556500	1.66199100
C	5.86124800	-0.17305800	2.16722500
H	6.13447500	0.58446400	0.15810900
C	4.95139600	-0.45200700	3.19136900
H	2.88830600	-0.33125400	3.79180800
H	6.91150100	-0.41579800	2.30572100
C	5.41449000	-1.11142500	4.46433800
H	6.36458800	-0.69136100	4.80383600
H	4.67831500	-0.99429300	5.26217400
H	5.56951900	-2.18382100	4.30611800

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C	0.49610200	0.40078100	-1.09849300
O	0.01817500	1.12037000	-1.94103500
C	0.30444000	-1.09251000	-1.07627100
H	-0.36764700	-1.27932500	-1.91413800
H	1.25762700	-1.59647300	-1.28039700
C	-2.47606900	-0.26803500	0.12606800
C	-1.41108700	-0.75872200	0.80045500
C	-0.34378800	-1.65839500	0.22189800
H	-1.35882800	-0.55964200	1.86580300
H	-0.82156100	-2.58172800	-0.12393300
C	0.68345200	-2.10381400	1.25057800
C	1.29791600	-3.34898300	1.06269500
C	1.06064900	-1.33873600	2.35811500
C	2.25833400	-3.81923200	1.95317700
H	1.00614300	-3.95512300	0.20651200
C	2.01906500	-1.80816800	3.25707000
H	0.60700600	-0.36646400	2.53609500
C	2.61696900	-3.05017600	3.06079400
H	2.71610300	-4.78999700	1.79113200
H	2.30214000	-1.19593200	4.10656600
H	3.35862800	-3.41625800	3.76335200
C	-3.48632000	0.54306500	0.87132500
C	-3.85436800	0.22611500	2.18455700
C	-4.05170100	1.67166300	0.26956800
C	-4.74217900	1.03358100	2.88953200
H	-3.45402800	-0.67134400	2.64767900
C	-4.93559000	2.48318000	0.97465000
H	-3.77548700	1.90908900	-0.75305800
C	-5.27921800	2.17208300	2.29004700
H	-5.02166400	0.76964000	3.90488300
H	-5.35451100	3.36525300	0.49851000
H	-5.97096900	2.80343700	2.83873600

N	-2.62221200	-0.40877800	-1.26115500
S	-3.70995500	-1.44064600	-1.74847400
O	-3.77617900	-1.39541300	-3.22068700
O	-5.01239200	-1.37562400	-1.05015000
C	-3.03694900	-3.04774800	-1.32416000
C	-2.13018600	-3.65510100	-2.18835200
C	-3.25310100	-3.56863200	-0.04812600
C	-1.41763800	-4.77405800	-1.76360000
H	-1.98006200	-3.23980500	-3.18038200
C	-2.53141200	-4.68279100	0.36708100
H	-3.96912900	-3.08912100	0.61225900
C	-1.59374500	-5.29175500	-0.47614500
H	-0.70726300	-5.24695300	-2.43644900
H	-2.68733300	-5.08491800	1.36490800
C	-0.79501500	-6.47438400	0.00827800
H	-1.45187600	-7.29711800	0.30542400
H	-0.11746600	-6.83999900	-0.76592000
H	-0.19768900	-6.20343100	0.88517000
C	4.19915800	-0.12594100	-1.06885100
C	5.56826800	-0.10927400	-0.81160300
C	6.46846600	0.13459200	-1.84634700
C	5.97909300	0.36763700	-3.12824300
C	4.60479000	0.35288900	-3.38112700
C	3.70354500	0.10249100	-2.35078300
C	3.41138600	-0.41000700	0.18914600
C	4.50282600	-0.59787800	1.31295300
C	5.87657000	-0.38000900	0.63547400
H	7.53655900	0.14611300	-1.65286100
H	6.67145800	0.56220900	-3.94071500
H	4.23664900	0.53284400	-4.38525400
H	2.63832900	0.08851400	-2.56504300
H	4.41028800	-1.61709300	1.68606700
H	6.41765500	0.44773700	1.10514300
H	2.79165000	-1.30438400	0.13011300
H	6.50206500	-1.26848400	0.75428400
C	2.88862300	1.72970100	1.35712000
C	1.34684100	1.10218900	-0.04407700
N	2.02450500	2.70641900	1.34137800
N	2.51148300	0.72229400	0.51664000
N	1.08341100	2.31435300	0.44818400
C	4.13957500	1.58279100	2.15865700
H	4.99296400	1.99147600	1.60176100
H	4.04199700	2.12593800	3.09858300
O	4.29451600	0.21270000	2.45271300

C	0.04573300	3.25317500	0.07926000
C	0.27218600	4.03663400	-1.05558400
C	-1.05916700	3.40079800	0.91820900
C	-0.70816300	4.97199900	-1.38040200
C	-2.00460600	4.35488700	0.54716500
C	-1.85254600	5.13706600	-0.59841700
H	-0.56882500	5.58952100	-2.26379200
H	-2.88610800	4.48111000	1.17047400
C	1.52129500	3.88809100	-1.88145400
H	2.41697300	3.88752200	-1.25218600
H	1.50374300	2.95072000	-2.44487700
H	1.60618700	4.71185800	-2.59120100
C	-2.90181400	6.15444500	-0.96222800
H	-2.72235000	6.57449400	-1.95349800
H	-3.89791300	5.70312700	-0.95238200
H	-2.90922800	6.97684800	-0.24036300
C	-1.21032700	2.60063600	2.18158200
H	-1.01062400	1.54228600	1.99763100
H	-0.50996500	2.95154200	2.94650800
H	-2.22938100	2.68953300	2.56522500

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C	-3.67081800	-1.39791300	1.70805800
C	-5.01649700	-1.16880200	2.01401000
C	-5.41450300	-0.98515800	3.33299900
C	-4.45218000	-1.03000300	4.34025900
C	-3.11241300	-1.27225200	4.03534700
C	-2.71171100	-1.46522500	2.71452400
C	-3.50072800	-1.55648300	0.21309700
C	-4.95030000	-1.86292700	-0.25470000
C	-5.86901900	-1.17010000	0.77279800
H	-6.45902000	-0.81403700	3.57350200
H	-4.74918000	-0.88737500	5.37411500
H	-2.37723300	-1.32461700	4.83098200
H	-1.67189200	-1.68648800	2.50045300
H	-5.07263500	-2.94525000	-0.17565300
H	-6.11250500	-0.14254100	0.47882500
H	-2.78932300	-2.31972600	-0.10954800
H	-6.81265600	-1.70521100	0.89430900
C	-3.84234600	0.39877800	-1.35117000
C	-2.03596700	0.51339400	-0.15174600
N	-3.31707900	1.56064100	-1.63085200
N	-3.09176100	-0.27082300	-0.42262300
N	-2.19648900	1.62120700	-0.86791500

C	-5.08828800	-0.19255500	-1.93609300
H	-5.96114900	0.37874100	-1.59928900
H	-5.03267800	-0.12048100	-3.02413500
O	-5.18184100	-1.55869200	-1.61084500
C	-1.47159000	2.86754800	-0.74847500
C	-1.85904500	3.70082800	0.31102200
C	-0.50381000	3.20531200	-1.68913700
C	-1.21479000	4.92651600	0.41539500
C	0.10958500	4.45228900	-1.53518300
C	-0.22832000	5.31674900	-0.49810800
H	-1.49035100	5.59760600	1.22473200
H	0.87379500	4.74649000	-2.24970200
C	-2.92607700	3.27963000	1.28591400
H	-3.84279500	2.97713500	0.76920000
H	-2.58373100	2.43305000	1.89046900
H	-3.17096000	4.10191600	1.95900600
C	0.44045500	6.65857700	-0.35611000
H	-0.29144700	7.46606300	-0.45103800
H	0.90740600	6.75603900	0.62785700
H	1.20916000	6.80119100	-1.11741600
C	-0.08303100	2.27454300	-2.79207600
H	0.76111000	1.66256800	-2.44742500
H	-0.89650300	1.61352500	-3.10240400
H	0.24179600	2.84441200	-3.66469900
C	-0.80540800	0.22257700	0.70283200
O	-0.52287900	1.03015800	1.55338500
C	0.00877800	-0.99471700	0.35762900
H	0.96592500	-0.85268500	0.86305800
H	-0.47191000	-1.88301100	0.78536200
C	2.68503400	-0.82508000	-1.25014400
C	1.64846200	-1.67946700	-1.41258900
C	0.23111200	-1.21964000	-1.17533000
H	1.82024100	-2.69517600	-1.75304900
H	0.11079600	-0.24818700	-1.66984400
C	-0.79170300	-2.17470600	-1.75539000
C	-1.70174400	-1.74966900	-2.72496300
C	-0.86614100	-3.49696600	-1.30073800
C	-2.69558800	-2.60525900	-3.19784400
H	-1.64144500	-0.73013400	-3.10351700
C	-1.85241100	-4.35822400	-1.77534300
H	-0.15285900	-3.84966100	-0.55874800
C	-2.77898500	-3.90943300	-2.71619300
H	-3.40628800	-2.25123600	-3.93768600
H	-1.90277800	-5.37715700	-1.40518700

H	-3.55673100	-4.57480500	-3.07607000
C	4.07182400	-1.34046700	-1.46433200
C	4.98147400	-0.65919300	-2.28038100
C	4.47276000	-2.53855000	-0.86286300
C	6.26067900	-1.16596100	-2.48801900
H	4.68045900	0.27804400	-2.73478900
C	5.75417600	-3.04428200	-1.06540500
H	3.77551000	-3.05699800	-0.21101600
C	6.65308900	-2.35746900	-1.87822400
H	6.95508900	-0.62932300	-3.12730600
H	6.05293100	-3.96895800	-0.58111500
H	7.65442000	-2.74659200	-2.03428400
N	2.39598100	0.50534100	-0.95146300
S	3.35820000	1.40769700	-0.06733600
O	2.57131500	2.56903900	0.38905300
O	4.65770300	1.76297200	-0.67800600
C	3.77181000	0.47102800	1.40386800
C	2.83097300	0.36372500	2.42610800
C	5.00170700	-0.17296400	1.50198600
C	3.12883900	-0.39844200	3.55150100
H	1.87855800	0.87966700	2.33609300
C	5.28651800	-0.93137800	2.63385800
H	5.72137800	-0.07411700	0.69492500
C	4.35687500	-1.05824600	3.67042900
H	2.40061300	-0.47887900	4.35411600
H	6.24805900	-1.43150100	2.71647700
C	4.66520100	-1.90515800	4.87802700
H	5.72479100	-1.84947700	5.13889700
H	4.07778000	-1.59056600	5.74337600
H	4.43050300	-2.95661600	4.68220300

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C	0.36612900	0.87976300	0.37946300
O	0.74018500	1.33566900	1.47115800
C	0.38326300	1.80679600	-0.83628700
H	-0.21386200	2.67049400	-0.54204300
H	1.40568100	2.18094000	-0.95429100
C	-2.11974500	0.27622100	-0.92849900
C	-1.40470700	0.50209700	-2.05103400
C	-0.11021400	1.24935800	-2.17396400
H	-1.82428700	0.14769300	-2.98896900
H	-0.32949200	2.13411800	-2.79054200
C	0.97550700	0.49858600	-2.94006900
C	2.03000400	1.22468900	-3.50387600

C	0.95403500	-0.88543900	-3.11800400
C	3.03413300	0.58410500	-4.22547600
H	2.05529000	2.30645800	-3.38798800
C	1.96302100	-1.53351800	-3.82853900
H	0.13638700	-1.45863000	-2.69559800
C	3.00580200	-0.80035700	-4.38639500
H	3.83840400	1.16696100	-4.66445700
H	1.92960900	-2.61310500	-3.94474900
H	3.79279600	-1.30190100	-4.93992700
C	-3.47749500	-0.33886600	-1.05871800
C	-4.27819100	-0.05045700	-2.17044700
C	-3.96641300	-1.22774400	-0.09681800
C	-5.51431000	-0.66934200	-2.34001700
H	-3.93946900	0.68089000	-2.89794100
C	-5.19551500	-1.85374500	-0.26855900
H	-3.37100200	-1.42222900	0.78839400
C	-5.97408300	-1.58118800	-1.39332800
H	-6.12118800	-0.42843900	-3.20714000
H	-5.54701900	-2.55747100	0.48115900
H	-6.93704900	-2.06507900	-1.52317000
N	-1.56541800	0.47643600	0.36035900
S	-2.37916500	1.39562000	1.44310400
O	-1.81828900	1.12445600	2.76678900
O	-3.83142700	1.26079000	1.28604000
C	-2.02847700	3.09609200	1.04328300
C	-1.07035200	3.80238600	1.76123400
C	-2.66684400	3.66281700	-0.06014500
C	-0.74900900	5.09749800	1.36392000
H	-0.57233200	3.32448000	2.59646800
C	-2.32566200	4.95222500	-0.44943100
H	-3.41742100	3.09631500	-0.60379600
C	-1.36374700	5.68665500	0.25555300
H	-0.00146700	5.65781200	1.91851300
H	-2.81256900	5.40019400	-1.31114900
C	-1.02367100	7.09381500	-0.16022500
H	-1.74420200	7.80296800	0.25989200
H	-0.03074000	7.38171800	0.19107200
H	-1.05387100	7.20142600	-1.24703300
C	4.03830900	0.15817700	1.31568400
C	5.41776400	0.05900800	1.15067900
C	6.24272400	-0.07287800	2.26443900
C	5.66271100	-0.10570900	3.53117700
C	4.27833900	0.00045700	3.68716200
C	3.44897600	0.13863700	2.57614100

C	3.34913700	0.28707800	-0.02880100
C	4.47179900	-0.05570500	-1.07333300
C	5.79729300	0.13476100	-0.30588000
H	7.31898100	-0.15561700	2.14706700
H	6.29393400	-0.21477800	4.40740000
H	3.84584300	-0.02302500	4.68204600
H	2.37257200	0.24502900	2.67856900
H	4.39045700	0.60108700	-1.93917700
H	6.51932300	-0.62751300	-0.61195000
H	2.96177500	1.29172400	-0.19026200
H	6.23220800	1.11195600	-0.54047900
C	2.51289900	-1.98970200	-0.33073300
C	0.91518900	-0.55203500	0.10796900
N	1.44623500	-2.71151800	-0.18349900
N	2.23751200	-0.66768200	-0.14103100
N	0.45148500	-1.80877000	0.10548100
C	3.90626800	-2.36062300	-0.72258900
H	4.54750700	-2.44511200	0.16501500
H	3.90319500	-3.31238000	-1.25393200
O	4.35538100	-1.36255600	-1.61574100
C	-0.75243900	-2.41379200	0.64497100
C	-0.94160200	-2.32148800	2.03079200
C	-1.52338700	-3.24136800	-0.17167000
C	-1.99775300	-3.04286100	2.58068400
C	-2.54196800	-3.97582300	0.44126600
C	-2.80380100	-3.88154200	1.80451400
H	-2.17174500	-2.97664700	3.65191300
H	-3.16058100	-4.61894300	-0.17915400
C	-0.00909000	-1.52619600	2.90133500
H	1.02780700	-1.85117600	2.74996300
H	-0.07498100	-0.45567400	2.68419300
H	-0.25705100	-1.68043700	3.95293700
C	-3.92083800	-4.66562000	2.44204700
H	-4.60501300	-4.00032900	2.97688100
H	-4.49310200	-5.21827700	1.69427900
H	-3.52850400	-5.38163800	3.17045200
C	-1.32644200	-3.33542400	-1.65957400
H	-1.69636200	-2.42326500	-2.14170100
H	-0.27400000	-3.46548100	-1.92370400
H	-1.88861000	-4.17997400	-2.06129600

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C	-4.68602500	-1.26797000	-0.97072800
C	-6.05795300	-1.29647500	-0.73236300

C	-6.83864200	-2.30257900	-1.29450400
C	-6.22106700	-3.26914600	-2.08609800
C	-4.84371100	-3.23154000	-2.31947000
C	-4.05866400	-2.22333600	-1.76415800
C	-4.04859600	-0.09341900	-0.25839900
C	-5.16671300	0.42776300	0.71377200
C	-6.48263400	-0.14929200	0.14914500
H	-7.90829400	-2.33846300	-1.11234300
H	-6.81658400	-4.06332000	-2.52499100
H	-4.38262600	-3.99328600	-2.93947200
H	-2.98876800	-2.16603100	-1.94621900
H	-5.16974900	1.51768600	0.73894100
H	-7.14243300	-0.44841800	0.96859800
H	-3.74301100	0.68379300	-0.95594000
H	-7.00869500	0.61414400	-0.43295200
C	-3.06084100	-1.25091400	1.65392100
C	-1.55414700	-0.51629500	0.23496700
N	-1.93548400	-1.72364300	2.08691000
N	-2.87531100	-0.52138300	0.51507300
N	-0.99981700	-1.27030100	1.18863300
C	-4.43618900	-1.26751800	2.23986900
H	-5.06370400	-2.02706600	1.75669100
H	-4.38634100	-1.47064300	3.30916800
O	-4.94427000	0.04269500	2.06401600
C	0.32047600	-1.82665500	1.38097500
C	0.79873400	-2.75197600	0.44486900
C	0.95268100	-1.56957400	2.59748700
C	1.97752600	-3.42138000	0.76562100
C	2.11659500	-2.28953000	2.87828800
C	2.64222200	-3.21415900	1.97929400
H	2.37796200	-4.14127200	0.05505500
H	2.63383700	-2.09818900	3.81488800
C	0.06951100	-3.02694900	-0.84066500
H	-0.98506900	-3.25955700	-0.65207700
H	0.10429700	-2.16045400	-1.51073700
H	0.51664800	-3.88345300	-1.34937000
C	3.91384800	-3.96372800	2.28078100
H	4.33799900	-3.65522900	3.23828700
H	3.73327900	-5.04214600	2.31633000
H	4.66049400	-3.78501700	1.50047400
C	0.41996000	-0.55143300	3.57055200
H	0.03682400	0.32716800	3.04266700
H	-0.39716200	-0.96651500	4.16736200
H	1.21384600	-0.22954500	4.24689300

C	-1.12316500	0.23019700	-1.06391600
O	-1.45834400	-0.38203400	-2.08159600
C	-1.30718800	1.74645200	-0.99780400
H	-0.63452000	2.17424800	-1.74673900
H	-2.32842300	1.98072500	-1.31624800
C	1.22289000	1.19622700	0.26842900
C	0.35017700	2.04614500	0.84308100
C	-1.03936900	2.36599000	0.37148000
H	0.69250800	2.59584200	1.71629400
H	-1.77457200	1.97311400	1.09222600
C	-1.25454800	3.86966600	0.30841100
C	-2.37913900	4.45612300	0.88906200
C	-0.33771600	4.68319300	-0.36512700
C	-2.58785200	5.83181700	0.80206100
H	-3.09570700	3.83055100	1.41615900
C	-0.54387700	6.05638400	-0.45436400
H	0.54004700	4.22805600	-0.81923800
C	-1.67013700	6.63506500	0.13074900
H	-3.46614000	6.27466600	1.26119800
H	0.17501100	6.67724700	-0.97986500
H	-1.82952800	7.70648500	0.06369500
C	2.62194600	1.17763000	0.79464400
C	3.27959900	2.37913300	1.08094200
C	3.29524200	-0.02570000	1.01404800
C	4.57472000	2.37289000	1.59398800
H	2.77640400	3.32095800	0.87980200
C	4.58261900	-0.03603400	1.53535500
H	2.80406200	-0.95078900	0.74428900
C	5.22829700	1.16500800	1.82866700
H	5.07567800	3.31303700	1.80300500
H	5.08548300	-0.98532700	1.70182600
H	6.23876300	1.15983500	2.22591200
N	0.84689200	0.26854000	-0.74607900
S	1.63526000	0.41058900	-2.17778600
O	1.68974200	1.81676100	-2.62052700
O	1.05594900	-0.56899300	-3.10102100
C	3.32820600	-0.10696500	-1.95744000
C	4.35376700	0.83016300	-1.90424800
C	3.58387900	-1.46743100	-1.81866100
C	5.65193400	0.39293300	-1.67170200
H	4.12533200	1.88419700	-2.02091000
C	4.88643800	-1.88896100	-1.57695800
H	2.76628800	-2.18027700	-1.88178700
C	5.93279200	-0.96497000	-1.48574000

H	6.46004500	1.11704200	-1.61262600
H	5.09492000	-2.94831600	-1.45280200
C	7.33180400	-1.41094500	-1.15313200
H	7.46653000	-2.47816500	-1.34052200
H	8.07320800	-0.85782900	-1.73498100
H	7.54300100	-1.22625100	-0.09398500

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C	-0.17585000	0.80947100	0.08709700
O	-0.67958000	1.51516300	-0.88444000
C	-0.52586700	1.34680200	1.50243000
H	-0.06722300	2.33905500	1.53291600
H	-1.60093500	1.50439100	1.59120300
C	2.03421700	0.19312900	1.20756500
C	1.35373100	-0.02810000	2.34907400
C	-0.01522700	0.49229200	2.66529700
H	1.84676500	-0.60911100	3.12323100
H	0.09610300	1.16052900	3.53187900
C	-1.01138100	-0.57750200	3.09961600
C	-2.20767900	-0.18211900	3.70958600
C	-0.78002200	-1.94097500	2.92018900
C	-3.14417300	-1.12450800	4.12362200
H	-2.40067200	0.87679600	3.87064600
C	-1.72119400	-2.88911900	3.32048200
H	0.14732500	-2.26487800	2.46323800
C	-2.90605700	-2.48422400	3.92545700
H	-4.06252000	-0.79673600	4.60189200
H	-1.52050000	-3.94454300	3.15987300
H	-3.64077700	-3.21829600	4.23989500
C	3.44573500	-0.27110200	1.07407300
C	4.27291000	-0.32372100	2.20322300
C	3.97512300	-0.66709700	-0.15726800
C	5.57802700	-0.79839500	2.11058400
H	3.90323600	0.03583900	3.15826500
C	5.27981800	-1.13628800	-0.25193500
H	3.35436000	-0.61102200	-1.04614800
C	6.08691000	-1.21153400	0.88167600
H	6.20147100	-0.82833100	2.99851900
H	5.66417400	-1.45030000	-1.21831700
H	7.10589900	-1.57733700	0.80567400
N	1.37379100	0.73743900	0.05937300
S	2.09463100	2.04482800	-0.75514100
O	1.93619600	1.83685600	-2.18954400
O	3.45133100	2.16422200	-0.22144500

C	1.29767400	3.57666900	-0.30849800
C	0.33830400	4.13786600	-1.14534600
C	1.71496900	4.21917500	0.85302800
C	-0.21040000	5.36571000	-0.80359100
H	0.02763200	3.59725100	-2.03016500
C	1.13682900	5.43994500	1.19078700
H	2.48060100	3.77174200	1.47865300
C	0.17335100	6.02997200	0.36864600
H	-0.95746600	5.81692200	-1.45053600
H	1.44653200	5.94547600	2.10074200
C	-0.42355400	7.36808800	0.71561900
H	0.08556200	8.16799400	0.16835400
H	-1.48145100	7.40804200	0.44540900
H	-0.32734400	7.58075100	1.78226900
C	-3.78749700	0.10843500	-1.34482400
C	-5.15781300	-0.14263100	-1.34396000
C	-5.88239700	-0.05593000	-2.52988000
C	-5.21298400	0.28380900	-3.70414500
C	-3.84118900	0.55017200	-3.69242800
C	-3.11329600	0.47301500	-2.50656200
C	-3.21334800	-0.04818600	0.05019200
C	-4.37227500	-0.72171600	0.86927000
C	-5.65054100	-0.46182300	0.04380200
H	-6.94976900	-0.25509600	-2.53998200
H	-5.76410300	0.34602500	-4.63724300
H	-3.33922600	0.82499500	-4.61464100
H	-2.05433700	0.70932000	-2.45765100
H	-4.42586400	-0.29180200	1.86906800
H	-6.30819700	-1.33476600	0.08742100
H	-2.93601200	0.91636300	0.46659900
H	-6.20390800	0.38615900	0.46089000
C	-2.20546700	-2.25943600	-0.16121100
C	-0.70280100	-0.66338300	-0.06437600
N	-1.08515900	-2.85104500	-0.43160300
N	-2.02617400	-0.92010900	0.04054800
N	-0.15058900	-1.84144700	-0.38803500
C	-3.58125300	-2.81324100	0.01996500
H	-4.16375400	-2.71674600	-0.90621500
H	-3.52459000	-3.86561700	0.29868000
O	-4.16324100	-2.10718400	1.09559800
C	1.10493400	-2.16151800	-1.03595300
C	1.26957600	-1.69670500	-2.34767600
C	1.97440100	-3.08083100	-0.44569100
C	2.39483800	-2.13116400	-3.04637200

C	3.06520600	-3.50851900	-1.20259800
C	3.29835200	-3.04145700	-2.49441700
H	2.54949900	-1.77069100	-4.06022500
H	3.76255500	-4.21339600	-0.75692800
C	0.25004200	-0.80611500	-3.00034300
H	-0.74065400	-1.27714500	-2.97393400
H	0.18059900	0.16372000	-2.49526900
H	0.51386100	-0.63714500	-4.04595500
C	4.48057600	-3.53024900	-3.28987100
H	4.85426300	-2.75130400	-3.95855100
H	5.29461700	-3.84516800	-2.63286300
H	4.20107400	-4.38991300	-3.90751600
C	1.79057700	-3.57977300	0.96005900
H	2.06444200	-2.79352500	1.67329300
H	0.75557500	-3.87481200	1.15119500
H	2.43529400	-4.44039800	1.14489200

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C	3.79633700	-1.80335200	0.44000800
C	4.99824700	-2.37779900	0.03363600
C	5.95369100	-2.72837600	0.98299000
C	5.67765900	-2.49882200	2.33020000
C	4.46673300	-1.92469000	2.72567800
C	3.50683400	-1.56672600	1.78041000
C	2.92264400	-1.49762900	-0.75595200
C	3.61610400	-2.24582100	-1.95639300
C	5.05624800	-2.51992200	-1.46609900
H	6.89321500	-3.18088500	0.68031200
H	6.41112300	-2.77404800	3.08163500
H	4.27167300	-1.75778200	3.78011300
H	2.55564700	-1.11553200	2.06135900
H	3.60249900	-1.61456500	-2.84554600
H	5.38003800	-3.51067600	-1.79812200
H	2.90318900	-0.43678500	-0.98479700
H	5.74633900	-1.78897200	-1.89961200
C	1.30160000	-3.30837900	-0.72136300
C	0.38520800	-1.39120100	-0.13491600
N	0.07283600	-3.60257700	-0.44702100
N	1.54059500	-1.96910000	-0.56124700
N	-0.48670100	-2.40655000	-0.07952400
C	2.38751000	-4.16560900	-1.28089300
H	3.13408500	-4.41045200	-0.51423000
H	1.96623200	-5.08750500	-1.68032600
O	2.94675800	-3.43107900	-2.35306100

C	-1.89570400	-2.48743300	0.23045100
C	-2.28776800	-2.59211400	1.56774000
C	-2.76730300	-2.67080600	-0.84359900
C	-3.64159800	-2.82076100	1.80985800
C	-4.10177500	-2.94787400	-0.54487800
C	-4.55810600	-3.00925800	0.77054300
H	-3.98267100	-2.88916100	2.84022400
H	-4.80433300	-3.08471700	-1.36298800
C	-1.28002600	-2.53874900	2.68083300
H	-0.64818600	-3.43456200	2.64827400
H	-0.63742500	-1.65760600	2.58732000
H	-1.78714300	-2.51393400	3.64713900
C	-6.01267100	-3.25620100	1.07699000
H	-6.56339600	-3.54476100	0.17945700
H	-6.12897600	-4.04604800	1.82399400
H	-6.47889000	-2.35347600	1.48513500
C	-2.29095700	-2.55746200	-2.26706800
H	-1.69386500	-1.64985000	-2.40599900
H	-1.66535900	-3.41200400	-2.54325200
H	-3.14171400	-2.51619700	-2.94924500
C	0.29702700	0.03844800	0.56248800
O	0.63535400	-0.13432100	1.80272400
C	1.14429400	1.07574200	-0.20238500
H	0.89573500	2.04373400	0.23973200
H	2.20157400	0.92128800	0.02182300
C	-1.57073000	0.88573700	-0.93382800
C	-0.64736800	1.05458400	-1.90092700
C	0.84064100	1.11682100	-1.69867700
H	-0.99852300	1.15127300	-2.92354400
H	1.28407600	0.24309300	-2.20145800
C	1.44765300	2.35171000	-2.34353900
C	2.60598100	2.25822400	-3.11552300
C	0.87765100	3.61092600	-2.13001600
C	3.18975900	3.40039700	-3.66152100
H	3.05467700	1.28358500	-3.29382900
C	1.45747500	4.75288500	-2.67355200
H	-0.02905100	3.68836200	-1.53395000
C	2.61702000	4.65034800	-3.44145900
H	4.09069400	3.31260700	-4.26060800
H	1.00326500	5.72366100	-2.50069700
H	3.06895500	5.54019300	-3.86762400
C	-3.02193900	0.92361800	-1.27255500
C	-3.46889600	1.72178000	-2.33276600
C	-3.96067900	0.17024200	-0.56247700

C	-4.80971400	1.72685900	-2.70553400
H	-2.76692000	2.36498700	-2.85457800
C	-5.29947300	0.17180700	-0.93659700
H	-3.63729100	-0.41911800	0.28938400
C	-5.73083900	0.94419200	-2.01353500
H	-5.13471400	2.35384000	-3.52968300
H	-6.00799100	-0.43656100	-0.38149500
H	-6.77739700	0.94724200	-2.30120000
N	-1.17627100	0.50070400	0.38730100
S	-1.76667900	1.40198600	1.70677100
O	-1.95293900	0.50950100	2.84121100
O	-2.92564300	2.14309700	1.21283300
C	-0.56612700	2.64982100	2.12326100
C	0.39921000	2.42391600	3.09841200
C	-0.62836600	3.85488200	1.42534500
C	1.32359400	3.42776600	3.36505800
H	0.42759800	1.46955700	3.60837100
C	0.31642500	4.83837700	1.69292000
H	-1.41102400	4.01472000	0.69092100
C	1.30679600	4.63677900	2.66081900
H	2.07868900	3.26883900	4.12941200
H	0.28061000	5.77783400	1.14866300
C	2.34412900	5.69619500	2.92296300
H	1.91691000	6.69721400	2.82986200
H	2.77484600	5.59043500	3.92063000
H	3.16002700	5.61759900	2.19717600

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C	0.03204200	1.06368100	-0.05780900
O	-0.28503300	1.60777900	-1.11918600
C	-0.62071600	1.50767200	1.24334200
H	-0.20403200	2.51472700	1.37872100
H	-1.68838200	1.64983800	1.07572200
C	1.88930600	0.15086300	1.34978500
C	1.03629000	0.02493000	2.37930500
C	-0.30673000	0.67733500	2.49964800
H	1.34769400	-0.59405800	3.21562400
H	-0.21991200	1.39874000	3.32460100
C	-1.39454700	-0.28912500	2.95794900
C	-2.47919000	0.21353200	3.68588300
C	-1.32263300	-1.66717600	2.74023300
C	-3.45397700	-0.63772100	4.20025400
H	-2.54513500	1.28340200	3.87134700
C	-2.30009400	-2.52338900	3.24583900

H	-0.48630100	-2.07356700	2.17887200
C	-3.36131500	-2.01357300	3.98924400
H	-4.27839800	-0.22836600	4.77569800
H	-2.22307500	-3.59112100	3.06571700
H	-4.11473500	-2.68102900	4.39500800
C	3.24010800	-0.47295400	1.40207500
C	3.91007300	-0.57552300	2.62784900
C	3.86396900	-0.96869100	0.25453600
C	5.15683000	-1.18728500	2.70814100
H	3.46452500	-0.14832500	3.52063500
C	5.11415200	-1.57229900	0.33413800
H	3.36447700	-0.88404000	-0.70654500
C	5.76504800	-1.69022700	1.55994700
H	5.66017600	-1.25552000	3.66735000
H	5.57520400	-1.95981600	-0.56994300
H	6.74148500	-2.16028900	1.61967500
N	1.46662100	0.77151900	0.13131500
S	2.48117100	1.93774200	-0.61421300
O	2.50943000	1.67701100	-2.04543800
O	3.73475500	1.93396300	0.13092000
C	1.74266600	3.52777600	-0.32030900
C	1.02308200	4.16543500	-1.32425600
C	1.94004900	4.11931000	0.92635700
C	0.48911100	5.42236400	-1.06732100
H	0.88497000	3.67467400	-2.28030500
C	1.38552100	5.37051000	1.16832800
H	2.52228200	3.60923600	1.68739500
C	0.65261300	6.03637500	0.17927600
H	-0.06766100	5.93509700	-1.84599600
H	1.53094600	5.84176000	2.13581800
C	0.03356900	7.37917000	0.46208700
H	-0.14215100	7.93547200	-0.46073500
H	-0.93084100	7.25491200	0.96510800
H	0.67117400	7.97808000	1.11612500
C	-3.92682500	0.27774900	-1.08075900
C	-5.30192400	0.05408700	-1.08977000
C	-6.09126100	0.59824500	-2.09906600
C	-5.48111000	1.36074100	-3.09337000
C	-4.10112800	1.57869000	-3.07859100
C	-3.30726500	1.03827000	-2.06809900
C	-3.27464900	-0.41172900	0.10081700
C	-4.40737400	-1.33713400	0.68348300
C	-5.72354000	-0.79778300	0.07904700
H	-7.16298400	0.42383000	-2.11625900

H	-6.08345000	1.78587800	-3.89011200
H	-3.64324000	2.17347800	-3.86254100
H	-2.23369100	1.20839800	-2.03790200
H	-4.40466300	-1.27799100	1.77109900
H	-6.37526000	-1.63001600	-0.20388100
H	-2.96928900	0.28934300	0.87505500
H	-6.26296000	-0.20073600	0.82186300
C	-2.30549800	-2.40561900	-0.89123900
C	-0.76603500	-0.90628100	-0.26939900
N	-1.18403900	-2.93244900	-1.26406600
N	-2.10369300	-1.18921200	-0.29730700
N	-0.25278200	-1.98653300	-0.88197300
C	-3.68563400	-2.97312900	-0.88924400
H	-4.30228100	-2.52595900	-1.68053700
H	-3.65062500	-4.05301300	-1.03163900
O	-4.21366100	-2.71504100	0.39996300
C	1.09113800	-2.27893600	-1.29900700
C	1.53360100	-1.73353900	-2.50950500
C	1.81928900	-3.23232600	-0.58764100
C	2.76772600	-2.16436100	-2.99405900
C	3.03127700	-3.65861800	-1.13160400
C	3.51946500	-3.13782700	-2.32889600
H	3.13872300	-1.75003500	-3.92872400
H	3.61808600	-4.39661300	-0.59016000
C	0.68416000	-0.74694800	-3.26251100
H	-0.29254700	-1.18479500	-3.49900500
H	0.51506600	0.15587700	-2.66715600
H	1.17053800	-0.46257200	-4.19745500
C	4.82980900	-3.61033500	-2.90487700
H	4.66493100	-4.20901200	-3.80628700
H	5.46037600	-2.76303500	-3.18926700
H	5.37917900	-4.22434700	-2.18785300
C	1.34802300	-3.73597900	0.74912900
H	1.52304400	-2.96538900	1.51080300
H	0.27939700	-3.96830200	0.74262400
H	1.89909500	-4.63100600	1.04281900

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C	-3.76619800	-1.76269000	-0.47760100
C	-5.00240000	-2.30742400	-0.13535600
C	-6.00629900	-2.41110800	-1.09314900
C	-5.74750000	-1.96685400	-2.38927500
C	-4.50458300	-1.42543500	-2.72404900
C	-3.49522600	-1.31681300	-1.76729500

C	-2.84459300	-1.74429700	0.72441600
C	-3.55748500	-2.67841900	1.76824200
C	-5.03343400	-2.71051300	1.31733600
H	-6.97120600	-2.83964300	-0.83889800
H	-6.51893300	-2.04972400	-3.14832800
H	-4.32125300	-1.08951800	-3.73959100
H	-2.52184500	-0.89835200	-2.01669200
H	-3.44641300	-2.27134400	2.77456300
H	-5.45746900	-3.70401800	1.48703300
H	-2.76608800	-0.74476900	1.15111300
H	-5.62133900	-1.99689000	1.90477200
C	-1.31110200	-3.57581300	0.28792300
C	-0.31436000	-1.57652100	0.20148800
N	-0.07736000	-3.84772500	0.00794400
N	-1.49856300	-2.22432600	0.42020000
N	0.51311100	-2.60221700	-0.05125900
C	-2.45060200	-4.47684900	0.62932800
H	-3.19752000	-4.49979300	-0.17463200
H	-2.09108100	-5.48880200	0.81406000
O	-2.99303000	-3.98051400	1.84276000
C	1.93761400	-2.60919500	-0.24587300
C	2.44346400	-2.59538900	-1.54823400
C	2.74074700	-2.78492400	0.88162600
C	3.82151400	-2.74843000	-1.69865900
C	4.10859900	-2.96743900	0.67784300
C	4.66394700	-2.95163500	-0.60125500
H	4.24452900	-2.73099200	-2.70044800
H	4.75597000	-3.10137500	1.54109000
C	1.52062100	-2.44691600	-2.72611200
H	0.79668400	-3.26873200	-2.74722400
H	0.96477500	-1.50634600	-2.66274500
H	2.08737100	-2.46160700	-3.65896200
C	6.14358000	-3.15335000	-0.80702000
H	6.68683600	-3.09094800	0.13848600
H	6.34415800	-4.13553100	-1.24667400
H	6.55006700	-2.40249100	-1.49034400
C	2.14418800	-2.74520600	2.26265300
H	1.68703900	-1.76627300	2.44790300
H	1.36145100	-3.50117800	2.38025600
H	2.91073800	-2.91769000	3.01961400
C	-0.20797300	0.28941100	-0.70393200
O	-0.50844400	0.03421800	-1.87446200
C	-1.16547600	1.07722200	0.17614300
H	-1.08189600	2.11172100	-0.18460000

H	-2.18796600	0.76045700	-0.04450100
C	1.57815500	0.98327800	0.90157200
C	0.64946400	1.09442800	1.86611500
C	-0.83692900	1.03748300	1.66684800
H	0.99839000	1.17142400	2.89144000
H	-1.17202500	0.08029000	2.08988500
C	-1.56206800	2.14003800	2.41877000
C	-2.64375800	1.84518800	3.24888900
C	-1.17155400	3.47395100	2.26558600
C	-3.32936100	2.86301100	3.91104500
H	-2.95066600	0.81013500	3.38342400
C	-1.85298600	4.49218900	2.92458900
H	-0.32386600	3.70997300	1.62585900
C	-2.93573300	4.18847900	3.74990500
H	-4.16908700	2.61770200	4.55347500
H	-1.53789400	5.52317600	2.79700400
H	-3.46664500	4.98201900	4.26571300
C	3.02454200	1.01232900	1.24899000
C	3.47565500	1.84604800	2.27818800
C	3.94599300	0.19902100	0.58562800
C	4.81451100	1.84156300	2.65800900
H	2.77704500	2.51932200	2.76618900
C	5.28294900	0.19331300	0.96696800
H	3.60907400	-0.43169400	-0.23146100
C	5.72347100	1.01118300	2.00620100
H	5.14899700	2.49754700	3.45537700
H	5.98164600	-0.45746200	0.44851800
H	6.76863500	1.00878000	2.29881800
N	1.20686200	0.66918800	-0.44608200
S	1.85761900	1.63081500	-1.71207800
O	2.03570900	0.79170300	-2.88526200
O	3.01247600	2.32867700	-1.16199200
C	0.63138700	2.87206000	-2.03290300
C	-0.30271900	2.70715900	-3.04899100
C	0.60753000	3.98394000	-1.18999100
C	-1.28399600	3.67957900	-3.21619800
H	-0.26293000	1.82562700	-3.67756800
C	-0.38906900	4.93527300	-1.36455600
H	1.36168800	4.09764800	-0.41726000
C	-1.34937100	4.79418900	-2.37456100
H	-2.01656400	3.56648500	-4.00958500
H	-0.42025500	5.80347800	-0.71238100
C	-2.43810000	5.82165400	-2.53362700
H	-2.03972600	6.83344500	-2.42709400

H	-2.92337400	5.73770500	-3.50764900
H	-3.20333700	5.68747500	-1.76266200

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C	2.73675600	1.47100400	-0.78279500
C	4.10437900	1.78888100	-1.31092600
C	4.88107200	1.50295200	0.88023700
C	3.65102000	0.76813000	1.42133800
C	1.20032200	0.91236500	0.73159900
H	4.22143900	1.37088300	-2.31217000
H	5.76902200	1.16840300	1.42008300
H	3.40744100	1.20167200	2.39485800
N	1.60659600	1.59563200	-1.40850000
N	0.67770000	1.24435800	-0.45441800
N	2.53603200	1.06931400	0.51283500
H	4.76165200	2.58532800	1.03335100
H	4.21725400	2.88119300	-1.36853600
O	5.10055200	1.22535100	-0.48997400
C	3.83004600	-0.75464100	1.57922500
H	4.67474200	-0.91172500	2.25818100
H	2.92991300	-1.14679300	2.06399200
C	4.03780000	-1.50118200	0.28316800
C	5.31546100	-1.80063300	-0.19486100
C	2.92649100	-1.90036100	-0.46523400
C	5.48111700	-2.46858100	-1.40446600
H	6.18639300	-1.50082800	0.38281800
C	3.08856100	-2.56213800	-1.68099200
H	1.93229900	-1.70656100	-0.06706500
C	4.36741200	-2.84542000	-2.15492100
H	6.48010000	-2.69566300	-1.76357000
H	2.21531700	-2.86682100	-2.25067300
H	4.49757800	-3.36396300	-3.09948000
C	-0.70510400	1.30125500	-0.84095100
C	-1.41310700	2.47990000	-0.61155200
C	-1.25713900	0.19699600	-1.49486700
C	-2.72805300	2.54214300	-1.07555100
C	-2.57759500	0.29878300	-1.92579300
C	-3.32281600	1.46431800	-1.73201400
H	-3.30251100	3.44979200	-0.90654000
H	-3.03801000	-0.55358800	-2.42077800
C	-0.77890300	3.61992400	0.13797000
H	-0.56796200	3.32183100	1.17084700
H	0.17155100	3.91456200	-0.31734400
H	-1.44003500	4.48768700	0.15603700

C	-4.75758800	1.52401300	-2.18729700
H	-5.36875700	0.81014500	-1.62295400
H	-5.18041300	2.52027500	-2.04301700
H	-4.84572700	1.26169500	-3.24547600
C	-0.44476800	-1.05378200	-1.69153000
H	0.46786000	-0.84452600	-2.25973600
H	-0.14138300	-1.46020700	-0.72029300
H	-1.02345700	-1.81294400	-2.22085900
C	0.28089700	-0.20409900	2.18774500
O	0.49744900	-1.37213900	1.86531900
C	0.87495200	0.42089900	3.43334300
H	0.78790300	1.50743500	3.41653900
H	0.31762700	0.02955300	4.29042800
H	1.91762200	0.12322000	3.54050400
O	-1.01656200	0.37373400	2.05121200
C	-2.11229000	-0.25493100	1.56400300
C	-3.25019500	0.56804300	1.53193000
C	-2.20326600	-1.59127400	1.13975500
C	-4.45014200	0.09757500	1.03894400
H	-3.15479500	1.58851400	1.88488700
C	-3.40798300	-2.06102500	0.63685100
H	-1.34122800	-2.23659800	1.18705700
C	-4.50855400	-1.21426800	0.57540100
H	-5.32806400	0.73042800	0.99649800
H	-3.49604600	-3.08096300	0.28319700
N	-5.75338500	-1.70909700	0.01208600
O	-5.81739900	-2.88465400	-0.31322200
O	-6.68262000	-0.92253800	-0.11600400

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C	-2.70238600	-1.55966200	-0.45140700
C	-4.07826000	-2.03191200	-0.81698600
C	-4.75622200	-1.35438100	1.31241000
C	-3.53380100	-0.49318600	1.64808100
C	-1.11986800	-0.67753000	0.78621900
H	-4.26186900	-1.83935600	-1.87508700
H	-5.62659800	-0.94712200	1.83012300
H	-3.22435800	-0.74770700	2.66303400
N	-1.60925400	-1.74131300	-1.12742700
N	-0.63327200	-1.18804600	-0.34573500
N	-2.44972600	-0.91690600	0.73382600
H	-4.59041900	-2.38498600	1.65703700
H	-4.13736600	-3.11488200	-0.63695100
O	-5.05052500	-1.34234100	-0.07049200

C	-3.76838800	1.02631900	1.54765500
H	-4.55406900	1.26860700	2.27072900
H	-2.84813900	1.52912900	1.86115900
C	-4.14300800	1.51198000	0.16778200
C	-5.47639800	1.70620000	-0.19923200
C	-3.13721600	1.76706600	-0.76996600
C	-5.80253100	2.12849300	-1.48450900
H	-6.26407100	1.51923300	0.52666600
C	-3.46236600	2.18171300	-2.06027800
H	-2.09742000	1.66516400	-0.46242400
C	-4.79588400	2.35983000	-2.42148700
H	-6.84288500	2.27755700	-1.75620000
H	-2.67261400	2.37820600	-2.77960400
H	-5.05075200	2.68725900	-3.42440700
C	0.72181600	-1.25719200	-0.83748400
C	1.44889000	-2.41839400	-0.57720800
C	1.21346800	-0.19403900	-1.59441700
C	2.73996700	-2.49257100	-1.09675200
C	2.51560400	-0.31102100	-2.08028100
C	3.29327700	-1.44280100	-1.83299700
H	3.33657000	-3.37876400	-0.89438900
H	2.93520200	0.51004700	-2.65708800
C	0.87177700	-3.50678600	0.28517600
H	0.67627300	-3.11875300	1.29119000
H	-0.07574400	-3.87816200	-0.11684400
H	1.56597000	-4.34447400	0.36621400
C	4.72397400	-1.49590200	-2.30043700
H	5.35888300	-0.89994200	-1.63345000
H	5.10597000	-2.51888600	-2.30204400
H	4.82908400	-1.08253700	-3.30668200
C	0.37437900	1.02879300	-1.84305300
H	-0.55709700	0.76337600	-2.35620200
H	0.10892800	1.49593900	-0.88743100
H	0.91683500	1.74816900	-2.45869400
C	-0.38588200	0.28374400	1.79047200
O	-0.50164400	1.48291200	1.34741700
C	-0.79183800	0.04211000	3.25108300
H	-0.79837900	-1.01811500	3.51895100
H	-0.04888400	0.55545400	3.86532300
H	-1.76350500	0.49055100	3.46133800
O	1.00468400	-0.35945000	1.78875300
C	2.14302900	0.25039500	1.44453800
C	3.28084000	-0.58269000	1.49413800
C	2.29569000	1.59715600	1.05197100

C	4.51449700	-0.12978600	1.07786300
H	3.15126200	-1.60390000	1.83488000
C	3.53797300	2.05230600	0.64100200
H	1.43697100	2.24970400	1.05315300
C	4.62767500	1.18606100	0.63041300
H	5.38329400	-0.77678600	1.08455900
H	3.66726500	3.07610000	0.31104500
N	5.90622400	1.65610600	0.14076800
O	6.02498000	2.84055000	-0.14085900
O	6.81638000	0.84396900	0.02120800

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C	2.81398400	0.19849200	1.48931600
C	4.16214800	0.12405800	2.14549300
C	4.13749500	-2.16295500	1.65892200
C	3.02428100	-2.12427700	0.60910800
C	1.03014400	-0.50703800	0.43945300
H	4.72401300	1.03384700	1.92927800
H	4.81875800	-2.98139100	1.42151700
H	2.36626200	-2.97462800	0.79352800
N	2.00018900	1.21215500	1.48211500
N	0.89735300	0.76171000	0.82252700
N	2.25203900	-0.88637000	0.86512400
H	3.70377700	-2.33891000	2.65299800
H	4.01641200	0.04413600	3.23190500
O	4.89676100	-0.97091300	1.65426600
C	3.50978800	-2.16210800	-0.85425000
H	4.20163400	-3.00631000	-0.93434200
H	2.65073100	-2.39965200	-1.48906400
C	4.14647100	-0.89252100	-1.36879300
C	5.51688800	-0.65278900	-1.23515300
C	3.35325100	0.06304000	-2.00907500
C	6.07992100	0.52314400	-1.72047700
H	6.14223400	-1.39067000	-0.74101500
C	3.91525100	1.24151900	-2.49859500
H	2.28828400	-0.12723200	-2.13952100
C	5.27973800	1.47453700	-2.35241800
H	7.14574700	0.69569400	-1.61037400
H	3.28792400	1.97004800	-3.00331900
H	5.71998000	2.38916000	-2.73609000
C	-0.22883600	1.65372400	0.68327300
C	-1.08052100	1.80162100	1.78312000
C	-0.35548900	2.39482000	-0.49099600
C	-2.15965900	2.66828400	1.63463200

C	-1.45301500	3.25320200	-0.58573600
C	-2.37300600	3.38463400	0.45365700
H	-2.84978000	2.79236900	2.46545300
H	-1.58227900	3.83669100	-1.49381300
C	-0.82366500	1.07514200	3.07480400
H	-0.77421400	-0.00140700	2.89569600
H	0.12421400	1.39794100	3.51705000
H	-1.62143400	1.27946800	3.79078800
C	-3.58009000	4.27338400	0.30936600
H	-4.45328700	3.68211000	0.01422200
H	-3.82210600	4.76723500	1.25343700
H	-3.42170700	5.03776100	-0.45410500
C	0.64822500	2.28673400	-1.60377500
H	1.66908900	2.31159800	-1.21106100
H	0.51476400	1.34006700	-2.13496500
H	0.52910200	3.11214100	-2.30783000
C	0.04521100	-1.29368100	-0.43352800
O	-0.30002700	-0.72793400	-1.46896800
C	0.02960700	-2.80178600	-0.30904800
H	0.17149300	-3.13525200	0.71870600
H	-0.95232200	-3.13379800	-0.65289900
H	0.78103400	-3.24828100	-0.96695800
O	-1.31855900	-1.11507200	0.98836800
C	-2.52145600	-1.14964500	0.50487400
C	-3.40526000	-2.21176600	0.85197400
C	-3.00815800	-0.15160100	-0.38762100
C	-4.69296600	-2.26670000	0.36282400
H	-3.03544800	-2.97659300	1.52742200
C	-4.29470400	-0.20901000	-0.88324600
H	-2.34859700	0.66443000	-0.65677400
C	-5.13263300	-1.26352900	-0.50686700
H	-5.36597800	-3.07159800	0.63284500
H	-4.67113800	0.55268800	-1.55614000
N	-6.47587300	-1.31628500	-1.02287900
O	-6.85016900	-0.42797400	-1.78229800
O	-7.19935600	-2.24832100	-0.68539300

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C	2.73980300	0.02286900	1.48644700
C	4.02552300	-0.19464200	2.22979900
C	3.89526800	-2.43172400	1.55008700
C	2.87234400	-2.23021400	0.42844600
C	1.00718100	-0.46920700	0.25408400
H	4.66004500	0.68676100	2.12637300

H	4.54110000	-3.27211100	1.29187800
H	2.15233000	-3.04716200	0.49032100
N	1.99640100	1.09090600	1.49790200
N	0.92535900	0.77546500	0.72307000
N	2.16045900	-0.96917100	0.73929800
H	3.37200000	-2.66183900	2.48837600
H	3.79020400	-0.34264000	3.29312600
O	4.72516400	-1.29918200	1.70895700
C	3.46019800	-2.17261700	-0.99682000
H	4.10510700	-3.04986000	-1.10738100
H	2.63737400	-2.29898700	-1.70832700
C	4.20796500	-0.90534500	-1.34087000
C	5.57465100	-0.76972400	-1.08254200
C	3.52642800	0.15929500	-1.93674100
C	6.24044500	0.41068000	-1.39710200
H	6.11443100	-1.59153500	-0.62124200
C	4.19014600	1.34376300	-2.25295400
H	2.46835500	0.05299700	-2.17332200
C	5.54911400	1.47203200	-1.98013100
H	7.30203400	0.50169100	-1.19104700
H	3.64896300	2.15819600	-2.72478500
H	6.07051400	2.39061300	-2.22843800
C	-0.15652500	1.72569600	0.61267100
C	-0.98201500	1.89570900	1.73134300
C	-0.27425300	2.48666400	-0.55075500
C	-2.03533900	2.79701300	1.60520400
C	-1.35211000	3.37152600	-0.62384800
C	-2.25316300	3.51991600	0.42932600
H	-2.70482000	2.93933900	2.44980400
H	-1.47471900	3.96958400	-1.52338500
C	-0.72628700	1.17125100	3.02479100
H	-0.64710900	0.09669200	2.84785200
H	0.20141100	1.52391200	3.48566400
H	-1.54462400	1.35212400	3.72394800
C	-3.44061000	4.43782000	0.30745800
H	-4.32985100	3.86880500	0.01647800
H	-3.66082400	4.92739600	1.25897100
H	-3.27369300	5.20561300	-0.45075800
C	0.73208000	2.40582500	-1.66546200
H	1.74172500	2.27537800	-1.26627400
H	0.51528500	1.56173300	-2.32481600
H	0.71399900	3.32414300	-2.25516800
C	0.04698200	-1.13688800	-0.71722000
O	-0.41473600	-0.44303400	-1.59754800

C	-0.11933500	-2.63162500	-0.67399800
H	-0.01320500	-3.02570100	0.33505900
H	-1.12813700	-2.84502500	-1.03327700
H	0.59174500	-3.10939200	-1.35582500
O	-1.40220900	-1.06616900	1.09735800
C	-2.58224500	-1.12710400	0.61826400
C	-3.44292700	-2.24362500	0.89836500
C	-3.11508200	-0.10820500	-0.24560500
C	-4.71654500	-2.32501900	0.38920600
H	-3.05257600	-3.02618200	1.54180400
C	-4.38876200	-0.19591600	-0.75721500
H	-2.48263300	0.74156600	-0.48182100
C	-5.19564600	-1.30014300	-0.44116400
H	-5.35905900	-3.16883900	0.61239200
H	-4.78700600	0.57707200	-1.40479200
N	-6.51779500	-1.38389000	-0.97276300
O	-6.92458600	-0.48035200	-1.70362000
O	-7.21401500	-2.35824500	-0.68543700

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C	2.74435200	-0.54381600	1.57780900
C	4.02548300	-0.76747600	2.32473800
C	4.65792200	-2.24166400	0.62246400
C	3.58015800	-1.85631500	-0.39779800
C	1.31392500	-0.74003000	-0.05087100
H	4.32975500	0.15695900	2.81694200
H	5.54760600	-2.57723400	0.08714800
H	3.12774800	-2.77578500	-0.77544500
N	1.70050400	0.13941900	1.95553800
N	0.82079300	0.01013300	0.92538000
N	2.53721400	-1.12121000	0.35184100
H	4.29358900	-3.06445400	1.25264100
H	3.86273400	-1.54217400	3.08671700
O	5.04099000	-1.14203600	1.42521300
C	4.06540600	-1.01183100	-1.59172800
H	4.88617900	-1.56739400	-2.05582600
H	3.25519900	-0.97620300	-2.32902200
C	4.49332500	0.39368000	-1.24309800
C	5.80730000	0.67987100	-0.86342900
C	3.56207700	1.43472300	-1.28982300
C	6.17894700	1.97674600	-0.52365000
H	6.54178000	-0.12065100	-0.82915800
C	3.93118500	2.73484900	-0.94755100
H	2.54489800	1.22974200	-1.62099100

C	5.24038700	3.00739800	-0.56094300
H	7.20365900	2.18506600	-0.23301300
H	3.19764100	3.53419100	-0.99677700
H	5.53185600	4.01923900	-0.29872400
C	-0.50179200	0.58063300	1.02068200
C	-1.48466200	-0.17404600	1.66495800
C	-0.71408700	1.86803900	0.52160600
C	-2.74539400	0.40732900	1.79215500
C	-1.99637100	2.39291500	0.66273500
C	-3.01831500	1.68074100	1.29624400
H	-3.53456200	-0.15851200	2.27963400
H	-2.19812600	3.39001900	0.27872100
C	-1.20055200	-1.55710800	2.18658900
H	-1.06140800	-2.25996700	1.35725100
H	-0.30287300	-1.57270400	2.81164300
H	-2.04258300	-1.91150200	2.78359700
C	-4.38608400	2.29228800	1.44773500
H	-4.72048200	2.73212800	0.50379400
H	-5.12137000	1.54581400	1.75898200
H	-4.37311900	3.09005700	2.19716400
C	0.38540700	2.65024600	-0.14293800
H	1.33514800	2.53357300	0.38756600
H	0.53007300	2.29510000	-1.16807300
H	0.13465200	3.71192200	-0.17079300
C	0.65355500	-0.98429000	-1.40646900
O	0.35701000	0.03218800	-2.02446800
C	0.36937000	-2.34639400	-1.74521200
H	1.00482200	-3.08903500	-1.26349300
H	-0.80362100	-2.58522900	-1.23780000
H	0.25034600	-2.49917400	-2.81739900
O	-1.95980600	-2.97508200	-0.69499700
C	-2.90538800	-2.09230000	-0.71172200
C	-4.08222400	-2.30777000	0.06580300
C	-2.83525800	-0.88743400	-1.47597700
C	-5.11803000	-1.40228000	0.07092400
H	-4.13717000	-3.21899400	0.65218100
C	-3.87400800	0.01611600	-1.47133500
H	-1.94790400	-0.68310700	-2.06742000
C	-5.01483600	-0.23788800	-0.70040000
H	-6.01156300	-1.57443400	0.65971200
H	-3.82104900	0.93109100	-2.04997600
N	-6.09169100	0.70552500	-0.70093000
O	-6.02066600	1.68742700	-1.43824000
O	-7.05007400	0.50937500	0.04354500

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C	2.83862600	-0.61337200	1.51250100
C	4.15884100	-0.78514400	2.20456300
C	4.81284700	-2.13631200	0.40707400
C	3.68959800	-1.74909400	-0.55992700
C	1.36249200	-0.83804100	-0.08132000
H	4.42566100	0.13639900	2.72308700
H	5.70370900	-2.39830900	-0.16576000
H	3.27712800	-2.66112000	-0.99628100
N	1.76258600	-0.03664700	1.96516700
N	0.85463000	-0.18273400	0.95632100
N	2.62780300	-1.13614800	0.26358000
H	4.50532400	-3.00817200	1.00082300
H	4.07176000	-1.59656900	2.94066100
O	5.16575100	-1.06359200	1.26059500
C	4.09011800	-0.79412300	-1.70067600
H	4.95027500	-1.24569000	-2.20484100
H	3.26447400	-0.78331400	-2.42005600
C	4.39661700	0.61989700	-1.26806600
C	5.68338800	1.00040700	-0.87802500
C	3.37237900	1.57138900	-1.24717500
C	5.94019300	2.30324000	-0.46232500
H	6.48601700	0.26795000	-0.89467300
C	3.62769200	2.87668800	-0.82815000
H	2.37489500	1.28434800	-1.57988000
C	4.91127400	3.24434600	-0.43276000
H	6.94445200	2.58625300	-0.16351900
H	2.82495200	3.60812400	-0.82290500
H	5.11277300	4.26090700	-0.11080000
C	-0.50218300	0.26449100	1.14631400
C	-1.40146600	-0.62869800	1.73323400
C	-0.82886700	1.57945100	0.81069400
C	-2.68996100	-0.16032500	1.98796400
C	-2.13009700	1.99696000	1.08290500
C	-3.06663100	1.14708100	1.67699000
H	-3.41531700	-0.83562500	2.43453900
H	-2.41827400	3.01357700	0.82704200
C	-0.98645700	-2.03482300	2.07671000
H	-0.67468100	-2.58073100	1.18065900
H	-0.14802900	-2.03674800	2.78033300
H	-1.81851300	-2.57800600	2.52710300
C	-4.45329200	1.64432200	1.99355600
H	-4.75404600	2.43287900	1.29862300

H	-5.18576900	0.83423500	1.94138000
H	-4.49138700	2.06169100	3.00489000
C	0.18235000	2.48579100	0.16760900
H	1.12000500	2.49545900	0.73229900
H	0.40306000	2.11524200	-0.83865700
H	-0.19711300	3.50682400	0.10465400
C	0.70258900	-1.04778100	-1.43517100
O	0.36154100	0.02770500	-2.00457300
C	0.57777200	-2.35772400	-1.82528100
H	0.97589600	-3.16088200	-1.21464400
H	-1.27162200	-2.65493900	-1.21003100
H	0.22783300	-2.58781500	-2.82632300
O	-2.15990300	-2.95628300	-0.89337700
C	-3.04071800	-1.94714600	-0.91939100
C	-4.31344500	-2.19441900	-0.37825100
C	-2.72825200	-0.68592500	-1.45418800
C	-5.26129900	-1.18966200	-0.34999700
H	-4.52717000	-3.17797000	0.02426000
C	-3.67771300	0.31988700	-1.42211700
H	-1.73920700	-0.48527400	-1.86195500
C	-4.93074700	0.06086500	-0.87051100
H	-6.24424100	-1.35451800	0.07350100
H	-3.45495100	1.30761300	-1.80634400
N	-5.90421000	1.13149900	-0.79896000
O	-5.59179200	2.23186000	-1.23551700
O	-6.99153000	0.89644000	-0.28970800

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C	-0.97828400	-0.92391900	-1.37830500
C	-2.12113400	-1.18442500	-2.31440900
C	-3.21071900	-2.25251600	-0.54053200
C	-2.29950300	-1.75960300	0.58801600
C	0.10257100	-0.92783300	0.52266500
H	-2.22718200	-0.35079400	-3.00963100
H	-4.21470900	-2.41313200	-0.14430300
H	-2.02587000	-2.61287900	1.21206900
N	0.18705600	-0.41393000	-1.65484300
N	0.84350600	-0.42210600	-0.45710900
N	-1.06338000	-1.27262200	-0.05498100
H	-2.82962400	-3.20492600	-0.93468400
H	-1.91404400	-2.10089400	-2.88494500
O	-3.32051900	-1.30383500	-1.58572300
C	-2.89199500	-0.66107600	1.49162400
H	-3.85783900	-1.03133300	1.85018400

H	-2.23447600	-0.57379300	2.36272200
C	-3.03980300	0.69010300	0.83323100
C	-4.19468300	1.03337800	0.12501300
C	-1.99588900	1.61635000	0.92040600
C	-4.30061100	2.27351800	-0.49707600
H	-5.01116200	0.31950200	0.05361400
C	-2.10003200	2.85808500	0.29411800
H	-1.10585700	1.36012300	1.49683400
C	-3.25098700	3.18812100	-0.41700400
H	-5.20294700	2.52832600	-1.04386200
H	-1.28531500	3.57203800	0.37294000
H	-3.33549400	4.15629200	-0.90034400
C	2.22073800	-0.01493200	-0.37699200
C	3.19884900	-1.00630200	-0.48136600
C	2.51081400	1.34106300	-0.23086500
C	4.52940900	-0.59361100	-0.44371000
C	3.85655700	1.70347800	-0.20266500
C	4.87421500	0.75297700	-0.30664200
H	5.31411900	-1.34117400	-0.52829700
H	4.11427800	2.75367500	-0.09159900
C	2.81915900	-2.45718000	-0.61522100
H	2.33070000	-2.80974200	0.30017000
H	2.12014600	-2.60895000	-1.44346500
H	3.70331600	-3.07100800	-0.79222000
C	6.32128700	1.16730000	-0.24157900
H	6.70241000	1.06966800	0.78004700
H	6.94096800	0.53826400	-0.88470900
H	6.44843200	2.20850900	-0.54524100
C	1.40468600	2.34261700	-0.05866400
H	0.65960200	2.26146100	-0.85615400
H	0.90066500	2.13334300	0.89145700
H	1.79745100	3.36060200	-0.04736300
C	0.47342100	-0.93090000	1.99546500
O	0.74741300	0.22735400	2.44249900
C	0.43280000	-2.16236600	2.57977000
H	0.67639600	-2.28002700	3.62930900
H	0.18539900	-3.04464900	2.00013500

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C	-1.06195600	-0.79277500	-1.22738500
C	-2.21884600	-1.01994700	-2.15931400
C	-3.08728600	-2.38296500	-0.44310800
C	-2.32776900	-1.71601800	0.70372700
C	0.11932500	-0.89937300	0.59466000

H	-2.46454500	-0.08220700	-2.66298700
H	-4.04674100	-2.74454500	-0.07188300
H	-2.01413700	-2.47773500	1.41882100
N	0.11579800	-0.32009300	-1.54952900
N	0.83624700	-0.39765000	-0.40994200
N	-1.09827900	-1.16258000	0.08447600
H	-2.51194400	-3.23451800	-0.83128300
H	-1.90318500	-1.75656500	-2.91050800
O	-3.36626800	-1.45097300	-1.46987400
C	-3.10987900	-0.60555300	1.44090600
H	-4.11417900	-1.00048100	1.62243200
H	-2.63272700	-0.46522600	2.41323700
C	-3.18184900	0.72255000	0.72213200
C	-4.22240800	1.02314800	-0.16109500
C	-2.18859600	1.68268500	0.93856100
C	-4.25590800	2.24330100	-0.82962600
H	-5.00184000	0.28746200	-0.33302600
C	-2.21671400	2.90530700	0.26945700
H	-1.39835800	1.48046100	1.65964600
C	-3.24927000	3.18523500	-0.62175400
H	-5.07142100	2.46100900	-1.51172100
H	-1.44140300	3.64245700	0.45506300
H	-3.27671900	4.13657800	-1.14284900
C	2.21486800	0.03000500	-0.40203000
C	3.17087500	-0.86156900	-0.90071700
C	2.51418500	1.29788400	0.09349100
C	4.49750600	-0.44601300	-0.85480100
C	3.86101400	1.66324300	0.11376200
C	4.85994800	0.80597800	-0.34690100
H	5.26888200	-1.11595200	-1.22530600
H	4.13037900	2.64362000	0.49673400
C	2.77688700	-2.20680400	-1.44978100
H	2.25354900	-2.81047100	-0.70045100
H	2.10726700	-2.09907600	-2.30778600
H	3.66081300	-2.75920800	-1.76897900
C	6.30806500	1.21662700	-0.31970700
H	6.91515100	0.45928400	0.18303900
H	6.69564300	1.32289400	-1.33702300
H	6.44165000	2.16793200	0.19743900
C	1.44133700	2.22053600	0.60675800
H	0.55486300	2.19954000	-0.03311200
H	1.13132600	1.94617300	1.62239100
H	1.81209500	3.24539900	0.64750900
C	0.52619500	-1.17619000	2.02643600

O	-0.37835100	-1.36098900	2.80673200
C	1.97722000	-1.23281500	2.38975200
H	2.42448200	-0.23492900	2.34675400
H	2.04813100	-1.62026300	3.40497400
H	2.53188700	-1.87253000	1.69844100

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C	2.46982900	-0.85255800	1.64974300
C	3.42467900	-1.58792900	2.54579400
C	3.59057200	-3.16047700	0.83209800
C	3.08491500	-2.27660100	-0.30548900
C	1.35966800	-0.37673200	-0.16805700
H	4.01865100	-0.87054500	3.11468000
H	4.28443300	-3.89938100	0.43060900
H	2.39389100	-2.84373700	-0.92714900
N	1.68386700	0.13458500	1.98030900
N	0.99840400	0.41511200	0.84399600
N	2.29243700	-1.20562000	0.34298400
H	2.75611300	-3.68322300	1.31834800
H	2.84589800	-2.20463200	3.24667100
O	4.30181600	-2.37950300	1.77896600
C	4.22788000	-1.69772500	-1.18677200
H	5.14041800	-2.24775700	-0.93573700
H	3.98186600	-1.91738300	-2.22581500
C	4.50023200	-0.21667900	-1.05057700
C	5.12771900	0.29663900	0.09082200
C	4.16266000	0.66065800	-2.08418100
C	5.42060200	1.65437500	0.18989800
H	5.40781500	-0.38397800	0.89148300
C	4.46985200	2.01784200	-1.99353600
H	3.66680900	0.27064500	-2.96854800
C	5.09903500	2.51823400	-0.85684000
H	5.91263700	2.03592800	1.07902400
H	4.21294200	2.68346500	-2.81185400
H	5.33615800	3.57489300	-0.78453600
C	0.01394700	1.46647700	0.88532500
C	-1.21431500	1.18614700	1.48765400
C	0.35165100	2.70941600	0.34888600
C	-2.14426900	2.22279300	1.52778600
C	-0.62102100	3.70686600	0.40318800
C	-1.87007100	3.48043700	0.98424600
H	-3.11174500	2.04227400	1.99174800
H	-0.39560000	4.68217800	-0.01947000
C	-1.51406100	-0.16138900	2.08619600

H	-1.07266600	-0.97074500	1.49789500
H	-1.10871200	-0.23296200	3.10034200
H	-2.59342700	-0.32534000	2.13741400
C	-2.91091500	4.56712900	1.03926400
H	-3.87201300	4.20035600	0.66809400
H	-3.06434600	4.90157400	2.06968800
H	-2.61545100	5.43104800	0.44169600
C	1.68645700	2.92935200	-0.30599100
H	2.50803400	2.54096100	0.30407700
H	1.73384500	2.41506400	-1.27334200
H	1.86067800	3.99150900	-0.48419500
C	0.87991700	-0.44108400	-1.62032600
O	1.55460400	-1.17919500	-2.33513400
C	-0.33894300	0.22126000	-1.97051200
H	-0.55251200	1.16073600	-1.46727800
H	-0.47098600	0.26392500	-3.05087800
H	-1.31936900	-0.58175400	-1.51050600
C	-6.25115400	0.90500100	-0.71591600
C	-6.09955400	-0.00710400	0.50245500
C	-5.81420200	-1.46153400	0.13943500
C	-5.19018600	0.61314400	-1.77636500
C	-3.80316000	0.40681600	-1.15936900
C	-3.48727700	-1.01663900	-0.73622500
H	-6.17471600	1.94954000	-0.39402200
H	-7.01900600	0.01456900	1.09418600
H	-6.11056600	-2.09191600	0.98057800
H	-5.46436800	-0.27604800	-2.35571200
H	-3.66650200	1.07298700	-0.29871100
C	-4.06873600	-3.20982100	0.10612700
H	-4.31546300	-3.78713400	-0.79440900
C	-2.59768600	-3.36393000	0.45582900
H	-2.34878200	-4.42134900	0.56817300
C	-1.77124800	-2.72967100	-0.65123600
H	-1.76304400	-3.37262900	-1.53945600
N	-2.27951200	-1.41708000	-1.01756900
N	-4.40097000	-1.79584200	-0.10941700
H	-3.02855800	0.67642300	-1.87881400
H	-5.14177400	1.43908200	-2.49074400
H	-7.24784100	0.77784400	-1.15129100
H	-5.30191900	0.34742200	1.16530200
H	-6.42582300	-1.77061700	-0.71974100
H	-4.69549100	-3.57917700	0.91988600
H	-2.40424500	-2.86688300	1.41131900
H	-0.72307700	-2.61001600	-0.34189700

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C	-2.29540000	-0.48912000	-1.54167100
C	-3.25826000	-1.27570500	-2.38180700
C	-2.86662600	-3.08532100	-0.95593000
C	-2.17623700	-2.31418500	0.17048400
C	-0.92273600	-0.08933400	0.11427300
H	-4.05332300	-0.61996700	-2.73850300
H	-3.37944500	-3.95108500	-0.53387400
H	-1.27114600	-2.84174100	0.47032600
N	-1.83287000	0.70523400	-1.77270100
N	-0.97692700	0.93997400	-0.73613800
N	-1.74463100	-1.02278300	-0.40818400
H	-2.11502200	-3.43843100	-1.67636700
H	-2.71892800	-1.68583500	-3.24739700
O	-3.84338000	-2.30229300	-1.61804300
C	-3.02432000	-2.06008300	1.43088700
H	-3.42157500	-3.02957100	1.74791500
H	-2.33272100	-1.72339100	2.20967100
C	-4.13724900	-1.05332300	1.26098500
C	-5.39949100	-1.43514500	0.79705800
C	-3.91124800	0.29339600	1.56082500
C	-6.40749800	-0.49200900	0.62382500
H	-5.58917400	-2.47932800	0.56454100
C	-4.91807800	1.24212600	1.38577500
H	-2.94131600	0.59248000	1.95691700
C	-6.16797600	0.85094800	0.91379400
H	-7.38270600	-0.80489500	0.26481900
H	-4.72964500	2.28327800	1.62959200
H	-6.95503500	1.58600400	0.78089300
C	-0.20950100	2.15823500	-0.72711200
C	1.10893900	2.10652100	-1.18421800
C	-0.82717100	3.33058200	-0.28988500
C	1.83532200	3.29517400	-1.16888300
C	-0.06097400	4.49520100	-0.30262000
C	1.26701100	4.49522800	-0.73425300
H	2.86693000	3.28424300	-1.51118000
H	-0.51276100	5.42304600	0.03810700
C	1.70757300	0.81392200	-1.66799900
H	1.72543300	0.06837400	-0.86592400
H	1.12076700	0.39146600	-2.49056500
H	2.73062800	0.96733700	-2.01575600
C	2.06441300	5.77282500	-0.76084400
H	3.12474600	5.57952200	-0.58509400

H	1.97391900	6.25932700	-1.73721900
H	1.70771100	6.47608600	-0.00565300
C	-2.24440000	3.31894100	0.21613500
H	-2.91473900	2.79959900	-0.47403100
H	-2.30308200	2.79950900	1.17984100
H	-2.60912100	4.33668800	0.36058200
C	-0.13725200	-0.26787000	1.38134900
O	0.18252100	-1.49986200	1.63819300
C	0.10954300	0.84052600	2.11982800
H	-0.22099400	1.82525500	1.81840800
H	0.64422600	0.73898600	3.05734400
H	1.40333300	-1.96503300	0.77623600
C	5.59041400	0.38283000	2.02243600
C	5.74712600	0.30372700	0.50330100
C	5.79319800	-1.12587700	-0.02821600
C	4.55267400	-0.61476500	2.53593200
C	3.30053100	-0.65508600	1.65689300
C	3.37712200	-1.57376400	0.45597100
H	5.29494600	1.40014400	2.29913000
H	6.67453800	0.79826300	0.20221800
H	6.28812500	-1.12343700	-1.00021800
H	4.98411000	-1.62036500	2.59435500
H	3.03990300	0.35054900	1.29926800
C	4.45363900	-2.76497200	-1.34535100
H	4.67681000	-3.74817500	-0.91579400
C	3.10058200	-2.76941900	-2.03885000
H	3.08290800	-3.53891400	-2.81216100
C	2.02357600	-3.03533800	-1.00344900
H	2.02901600	-4.08565800	-0.69490500
N	2.24668300	-2.19057800	0.16567000
N	4.47789400	-1.75479200	-0.27267000
H	2.43510300	-0.99811700	2.22810400
H	4.25373500	-0.35260200	3.55373400
H	6.55337900	0.18717000	2.50478700
H	4.93719800	0.83831400	-0.00573500
H	6.38433500	-1.77312000	0.63120000
H	5.24646800	-2.51668300	-2.05073100
H	2.93708400	-1.79957700	-2.51886500
H	1.02774900	-2.80505000	-1.39303600

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C	-1.51507200	-2.21421400	-1.45884400
C	-1.26745500	-3.56319800	-2.06449700
C	-0.07341900	-4.07600200	-0.13655100

C	-0.60321000	-2.94382300	0.74229500
C	-1.41092300	-0.60808200	0.02141900
H	-2.13209000	-3.87040900	-2.65476100
H	0.18494400	-4.92602900	0.49772300
H	0.23759100	-2.48356400	1.25979400
N	-1.99173900	-1.17104100	-2.07011100
N	-1.92223800	-0.17573300	-1.14037500
N	-1.15084600	-1.91860700	-0.17687400
H	0.82515800	-3.73269600	-0.66421600
H	-0.39110300	-3.47388800	-2.72258600
O	-1.04928800	-4.52634000	-1.06357700
C	-1.66290600	-3.36142900	1.78195800
H	-1.30280900	-4.28192300	2.25317000
H	-1.67326800	-2.58057100	2.54635100
C	-3.06167200	-3.55180000	1.24545600
C	-3.48601600	-4.76749400	0.70101800
C	-3.96595900	-2.48723900	1.28966300
C	-4.77863500	-4.91073600	0.20494800
H	-2.79298600	-5.60236700	0.66049400
C	-5.26207700	-2.62605700	0.79545500
H	-3.65119800	-1.54442900	1.73521700
C	-5.67020500	-3.83946000	0.24827300
H	-5.09379500	-5.86204400	-0.21231400
H	-5.95267400	-1.78938200	0.84658400
H	-6.67871700	-3.95363300	-0.13583400
C	-2.38216200	1.13090400	-1.53660000
C	-1.52706500	1.93332200	-2.29458900
C	-3.69807700	1.49504400	-1.22915100
C	-2.01182300	3.18170500	-2.69330600
C	-4.12727200	2.75456200	-1.63734300
C	-3.29475000	3.61454100	-2.35975400
H	-1.36548900	3.82810600	-3.28164600
H	-5.14031300	3.06720400	-1.39688700
C	-0.15506500	1.46103200	-2.68899800
H	0.37200300	2.24749400	-3.23295300
H	0.43354400	1.16616200	-1.81429200
H	-0.22141700	0.57468700	-3.32752300
C	-3.78286200	4.98060600	-2.76487900
H	-3.84635300	5.63847500	-1.89242800
H	-3.10997300	5.44327600	-3.48913400
H	-4.78237000	4.92499800	-3.20390700
C	-4.60060300	0.56039400	-0.47230300
H	-4.58980300	-0.44084800	-0.91281600
H	-4.27265100	0.46307200	0.56939600

H	-5.62676800	0.93102400	-0.47335900
C	-1.20262200	0.08939400	1.34428800
O	-0.47870500	-0.52099400	2.17696300
C	-1.73971000	1.35123300	1.53631300
H	-1.71073600	1.73742800	2.54752900
H	-2.37723200	1.85345400	0.82393700
C	1.84670200	0.65600600	1.30533700
C	1.20605700	1.80252700	1.85319100
C	0.27559400	2.53239700	1.14981500
H	1.44335600	2.04048500	2.88403500
H	0.16928800	2.31323800	0.09037800
C	-0.28195500	3.82942500	1.57742100
C	-0.98748400	4.59378600	0.63868400
C	-0.14010900	4.32783900	2.87966500
C	-1.52689400	5.82825200	0.98352500
H	-1.11561000	4.20436700	-0.36899200
C	-0.68274700	5.56035600	3.22541300
H	0.39118300	3.75121200	3.63028000
C	-1.37557600	6.31627800	2.27995900
H	-2.06483300	6.40923400	0.24112500
H	-0.56471100	5.93438300	4.23733000
H	-1.79628300	7.27821400	2.55450200
C	2.82914000	-0.02147500	2.20972500
C	4.19083300	0.02248500	1.90189100
C	2.40418300	-0.60485200	3.40502000
C	5.12092700	-0.54023300	2.77110400
H	4.52291700	0.50848100	0.98907800
C	3.33768400	-1.17537500	4.26647400
H	1.34149600	-0.62002700	3.62453500
C	4.69521200	-1.14685900	3.95141600
H	6.17801400	-0.50099700	2.52745100
H	3.00442500	-1.64234800	5.18806500
H	5.42002700	-1.58909400	4.62742200
N	1.62633600	0.34349100	0.03615400
S	2.17411000	-1.02991700	-0.66484800
O	1.20938300	-1.33034600	-1.73271700
O	2.47205800	-2.12374200	0.27056500
C	3.69694800	-0.57534200	-1.46571200
C	3.68007900	0.43312500	-2.42784200
C	4.87334100	-1.23537900	-1.13130700
C	4.86801000	0.78440300	-3.05426300
H	2.75000200	0.93650700	-2.67549800
C	6.05492100	-0.87225000	-1.77221700
H	4.85617000	-2.00956000	-0.37119400

C	6.06955700	0.13675500	-2.73821900
H	4.86786900	1.57350800	-3.80096200
H	6.98005400	-1.38008100	-1.51561000
C	7.34440200	0.51001500	-3.44746400
H	8.22107200	0.19896700	-2.87597400
H	7.39376100	0.02422300	-4.42730900
H	7.40079000	1.58841900	-3.61339300

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C	0.37205300	-2.33319700	1.09805300
C	-0.65819000	-3.31453300	1.58617400
C	-1.64367100	-3.01761300	-0.52666400
C	-0.37307100	-2.60111200	-1.25585300
C	1.43215500	-1.03644100	-0.31003500
H	-0.16768800	-4.10023500	2.16524500
H	-2.31349000	-3.52730800	-1.22054600
H	-0.60723000	-1.82174000	-1.97912200
N	1.20493200	-1.65344700	1.83405300
N	1.85683800	-0.84970600	0.94807000
N	0.47658600	-1.98233000	-0.21644400
H	-2.16147900	-2.13091100	-0.13365200
H	-1.35768500	-2.77702800	2.24267400
O	-1.33852800	-3.92764600	0.51722800
C	0.34617600	-3.78743300	-1.94498300
H	-0.42811600	-4.48578600	-2.27807200
H	0.84836000	-3.38354300	-2.82351700
C	1.36270300	-4.50883600	-1.09016200
C	1.01921200	-5.61269300	-0.30389800
C	2.68795800	-4.06032000	-1.07661200
C	1.97583900	-6.25042900	0.48269400
H	-0.00800700	-5.96405900	-0.30317000
C	3.64834300	-4.70260100	-0.29681000
H	2.95657800	-3.20442100	-1.69387500
C	3.29335300	-5.79674900	0.48928600
H	1.69290900	-7.10735500	1.08602200
H	4.67628700	-4.35224500	-0.30817900
H	4.04048700	-6.29697800	1.09701000
C	2.82809900	0.08300200	1.45919200
C	2.36494300	1.13106100	2.26095600
C	4.18064700	-0.10867000	1.15848000
C	3.30974100	2.05655300	2.70737500
C	5.08056200	0.84333900	1.63223000
C	4.66272100	1.94066000	2.38831700
H	2.97455100	2.88765100	3.32306700

H	6.13655900	0.72141100	1.40525700
C	0.92329400	1.24954300	2.67733500
H	0.67737600	2.28760000	2.91432400
H	0.24039600	0.90445900	1.89924100
H	0.73407800	0.64236400	3.56807700
C	5.65285000	2.98130400	2.84046500
H	6.63218600	2.53689600	3.03134800
H	5.78227600	3.74474500	2.06635900
H	5.31333500	3.48309800	3.74888600
C	4.64673900	-1.28017200	0.34003100
H	4.13102000	-2.19832500	0.63361300
H	4.44527700	-1.11007300	-0.72370700
H	5.72058800	-1.42848200	0.46517300
C	1.88969100	-0.45379900	-1.63756500
O	1.59929000	-1.16327800	-2.63358100
C	2.52593400	0.77452800	-1.61102400
H	2.92656000	1.14704700	-2.54664400
H	2.87202700	1.22657700	-0.69460100
C	-1.21589300	1.50281400	-0.40294600
C	-0.02947600	2.28662600	-0.42373600
C	0.75054400	2.42214700	-1.55176000
H	0.20297500	2.85727400	0.46884300
H	0.38216800	1.97471900	-2.47159900
C	1.76003500	3.48699100	-1.67768800
C	2.02432800	4.03413300	-2.93871600
C	2.45783400	3.97812100	-0.56480900
C	2.94463600	5.06832400	-3.08236700
H	1.49786300	3.64802800	-3.80737600
C	3.38374200	5.00323000	-0.71068700
H	2.29685200	3.53105100	0.41344400
C	3.62553400	5.55608100	-1.96936900
H	3.13231900	5.49038800	-4.06428500
H	3.92339400	5.36853300	0.15743000
H	4.34951300	6.35640100	-2.08186300
C	-2.09878000	1.69659000	0.78410300
C	-2.43148200	2.98361000	1.21650500
C	-2.55169500	0.58926800	1.50833700
C	-3.24530700	3.15705100	2.33236600
H	-2.07718200	3.84452400	0.65719300
C	-3.35584000	0.76282500	2.62750700
H	-2.26393900	-0.40788700	1.18684200
C	-3.71159100	2.04852300	3.03542300
H	-3.51868100	4.15793200	2.64965200
H	-3.70717400	-0.10324500	3.17936400

H	-4.34659300	2.18457700	3.90527900
N	-1.43792700	0.62542400	-1.37091300
S	-2.86687700	0.26617900	-2.08333400
O	-2.74774700	-1.11440900	-2.56629600
O	-3.11753800	1.31303300	-3.08135900
C	-4.26023700	0.29480000	-0.97690800
C	-4.74041600	-0.90002400	-0.45331900
C	-4.82420400	1.51815100	-0.61792500
C	-5.76737900	-0.86200000	0.48586600
H	-4.31924600	-1.84279500	-0.78470300
C	-5.83718900	1.53935600	0.32859400
H	-4.45619500	2.43821500	-1.06049100
C	-6.30883200	0.35371400	0.90760300
H	-6.14722700	-1.79061900	0.90172200
H	-6.26446400	2.49001400	0.63554400
C	-7.35825500	0.40588600	1.98438600
H	-6.90986300	0.74148900	2.92607700
H	-8.15156900	1.11339400	1.73049100
H	-7.80583600	-0.57506700	2.15462300

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C	-2.04812700	-1.71948200	-1.78779700
C	-2.08673000	-2.92103000	-2.68363100
C	-1.11516700	-4.10496900	-0.93238000
C	-1.44980800	-3.12366200	0.19119000
C	-1.66893000	-0.58478200	0.02446900
H	-2.96837300	-2.88359300	-3.32533900
H	-1.06318600	-5.11364800	-0.52012400
H	-0.56018200	-2.96373700	0.80574600
N	-2.23418000	-0.47339700	-2.12605200
N	-1.99121900	0.22294400	-0.98644000
N	-1.71991600	-1.83101100	-0.47041900
H	-0.15371800	-3.84693000	-1.38871900
H	-1.17925000	-2.90231400	-3.30159500
O	-2.14976300	-4.09727600	-1.90937700
C	-2.64843100	-3.59158300	1.06815100
H	-2.84535400	-4.63757500	0.81114100
H	-2.32883300	-3.56596800	2.11031200
C	-3.94127500	-2.81687600	0.93564600
C	-4.70300600	-2.88117200	-0.23830200
C	-4.42796900	-2.06574200	2.00808400
C	-5.92164300	-2.21442900	-0.33240800
H	-4.34293500	-3.48272700	-1.06970500
C	-5.65421500	-1.40709300	1.92068400

H	-3.84312500	-2.00704600	2.92177200
C	-6.40403600	-1.47884100	0.74996700
H	-6.50139800	-2.27850000	-1.24792900
H	-6.02007500	-0.83647300	2.76882300
H	-7.35756900	-0.96526900	0.67897900
C	-2.18582900	1.65079400	-0.98368200
C	-3.32006600	2.15557000	-0.33692700
C	-1.25116400	2.45340400	-1.63840800
C	-3.46554300	3.53930400	-0.30159400
C	-1.44620300	3.83388200	-1.57214000
C	-2.53242700	4.39137100	-0.90141400
H	-4.32635500	3.96337000	0.20924100
H	-0.71037900	4.48666600	-2.03556100
C	-4.31379200	1.23675300	0.32185800
H	-4.50921300	0.34527400	-0.28295200
H	-3.96106100	0.88652900	1.30016700
H	-5.26139900	1.75212900	0.48731900
C	-2.71146800	5.88496800	-0.83780700
H	-3.39080900	6.22651800	-1.62558600
H	-3.13811900	6.18696100	0.12186200
H	-1.75512600	6.39596400	-0.96653400
C	-0.07983700	1.87669300	-2.38716400
H	0.17043000	0.86117200	-2.06391600
H	-0.30414600	1.83140700	-3.45784900
H	0.79257700	2.52411700	-2.25857800
C	-1.33117000	-0.26450000	1.46929700
O	-1.42622000	-1.17644800	2.25873500
C	-0.96134500	1.14046000	1.85534700
H	-0.87519300	1.14681800	2.94469100
H	-1.79145400	1.79386400	1.57050000
C	1.93382900	-0.27670700	1.31570700
C	1.54809000	0.93561300	1.77419400
C	0.34555900	1.62596500	1.18828900
H	2.06943500	1.40312300	2.60410700
H	0.30617000	1.30372700	0.14091600
C	0.48010300	3.13774400	1.15999200
C	1.52675600	3.67660900	0.40024900
C	-0.40595000	4.01525900	1.78395400
C	1.66119400	5.04968700	0.23434600
H	2.23710300	2.99696400	-0.06800900
C	-0.27043300	5.39551800	1.62679400
H	-1.22109500	3.63774800	2.39376500
C	0.75374500	5.91744800	0.84423700
H	2.47133800	5.44462900	-0.37099900

H	-0.97578200	6.06195400	2.11419800
H	0.85097800	6.99073300	0.71430400
C	3.15566200	-0.93213700	1.86531800
C	4.31959300	-0.18718000	2.08662700
C	3.15902200	-2.29879700	2.16670500
C	5.46039600	-0.79183900	2.60609600
H	4.32854500	0.86577100	1.81906500
C	4.29894000	-2.90274400	2.68913900
H	2.26504000	-2.88212000	1.97352000
C	5.45312900	-2.15257100	2.90898600
H	6.35987500	-0.20444500	2.76329100
H	4.28771800	-3.96254400	2.92465100
H	6.34403100	-2.62658700	3.30879900
N	1.12086600	-0.90475000	0.36921300
S	1.71585100	-1.74048600	-0.83944700
O	0.80180800	-1.55583700	-1.99543900
O	1.98899700	-3.16727800	-0.55141600
C	3.29046800	-1.00781200	-1.26648300
C	3.34809100	0.36304700	-1.51135600
C	4.43878800	-1.78768400	-1.30613600
C	4.57156900	0.95236500	-1.80218800
H	2.44007000	0.95848300	-1.46477700
C	5.65919100	-1.18500700	-1.60224500
H	4.36859600	-2.84896200	-1.09306600
C	5.74465200	0.18747200	-1.84786100
H	4.62199400	2.02073400	-1.99543900
H	6.56133900	-1.78947300	-1.63604400
C	7.07205400	0.84213900	-2.12914600
H	7.80045900	0.11687200	-2.49763500
H	6.96975700	1.63890200	-2.86973100
H	7.48001000	1.29092800	-1.21761400

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C	-0.53325900	2.44305300	1.03823100
C	0.37015600	3.54571900	1.51760900
C	1.45573200	3.29886200	-0.56851700
C	0.26216900	2.70308000	-1.30442600
C	-1.31501600	0.93882900	-0.31763800
H	-0.21715200	4.29744300	2.04967500
H	2.05831300	3.88369700	-1.26498900
H	0.62440900	1.92853600	-1.98253800
N	-1.31222100	1.69253700	1.77460200
N	-1.79402400	0.76025800	0.91605000
N	-0.52878700	2.02386000	-0.25668200

H	2.07397200	2.48911500	-0.15653800
H	1.09335900	3.10165100	2.21655900
O	1.02479000	4.18844600	0.44985800
C	-0.59346800	3.75050500	-2.05761200
H	0.10182600	4.48304700	-2.47888500
H	-1.07816100	3.23810200	-2.89020700
C	-1.65088700	4.44386800	-1.22964800
C	-1.39069600	5.62401200	-0.52737500
C	-2.93203200	3.88856800	-1.15420100
C	-2.38190200	6.22247500	0.24696100
H	-0.40116700	6.06676900	-0.58102600
C	-3.92618600	4.48371100	-0.37992200
H	-3.15111700	2.98782600	-1.72538900
C	-3.65071900	5.65178100	0.32730600
H	-2.16321500	7.13915100	0.78544200
H	-4.91753700	4.04218600	-0.33767700
H	-4.42279600	6.11932900	0.92963500
C	-2.71967100	-0.24091600	1.38688300
C	-2.27979800	-1.14834100	2.35634800
C	-4.01691000	-0.25749900	0.85802000
C	-3.17011400	-2.15565600	2.73164800
C	-4.86208900	-1.28487700	1.26994500
C	-4.45018300	-2.25417800	2.18720000
H	-2.84572000	-2.88267900	3.47175700
H	-5.86958900	-1.32580000	0.86466400
C	-0.93413100	-1.04764500	3.01827300
H	-0.57856800	-2.03872200	3.30918000
H	-0.18683400	-0.59417900	2.36938000
H	-1.00832800	-0.43330700	3.92118300
C	-5.36369500	-3.38960400	2.56424200
H	-6.40982000	-3.07648100	2.54958600
H	-5.25450100	-4.21291400	1.85039600
H	-5.12644300	-3.77632600	3.55720700
C	-4.49283700	0.77277200	-0.13122600
H	-4.12225300	1.76901700	0.12301300
H	-4.17037500	0.54020800	-1.15379800
H	-5.58322300	0.80426300	-0.14103000
C	-1.57990600	0.18022100	-1.60160800
O	-1.52634900	0.83920400	-2.61714900
C	-1.94556700	-1.27763300	-1.58416000
H	-2.43331200	-1.46540600	-2.54437400
H	-2.66154100	-1.48486200	-0.78620800
C	1.05740000	-1.21893900	-0.02258500
C	0.04206400	-2.09713100	-0.15585000

C	-0.73570000	-2.24393200	-1.44113900
H	-0.20208900	-2.76723800	0.66596000
H	-0.05262700	-2.02294700	-2.26691300
C	-1.25495000	-3.66134400	-1.59857500
C	-0.84662700	-4.45168000	-2.67303500
C	-2.15918800	-4.19514800	-0.67317400
C	-1.33271500	-5.74953100	-2.82621800
H	-0.13980300	-4.04628200	-3.39228400
C	-2.64682100	-5.48959900	-0.82362400
H	-2.48144900	-3.59405200	0.17684000
C	-2.23539400	-6.27088400	-1.90318000
H	-1.00612900	-6.35181500	-3.66816400
H	-3.34839900	-5.88982100	-0.09821900
H	-2.61692600	-7.27980200	-2.02218200
C	1.91677200	-1.23012000	1.19892000
C	2.22373900	-2.42598600	1.85769800
C	2.43336500	-0.03442800	1.70997000
C	3.01404600	-2.42303100	3.00402200
H	1.86164000	-3.36550800	1.45037700
C	3.22433600	-0.02762200	2.85319400
H	2.21120800	0.88922500	1.18575800
C	3.51781500	-1.22447900	3.50629800
H	3.24932200	-3.36082400	3.49785300
H	3.61760800	0.91124500	3.23181200
H	4.14007800	-1.22338800	4.39565000
N	1.23831300	-0.19179000	-0.96986300
S	2.43113000	-0.31415000	-2.00431200
O	2.39528400	0.88877700	-2.86304900
O	2.46598700	-1.61181700	-2.71442300
C	3.97679600	-0.23209300	-1.10604200
C	4.55083300	1.00617400	-0.83848300
C	4.50873700	-1.39327200	-0.54928600
C	5.64723700	1.08271700	0.01608300
H	4.14200800	1.89762500	-1.30382500
C	5.59982200	-1.30376400	0.30581200
H	4.05639300	-2.35366000	-0.77604200
C	6.17298000	-0.06522400	0.61463100
H	6.09855400	2.04875200	0.22571500
H	6.00876400	-2.20686000	0.75145200
C	7.31149900	0.02260300	1.59667100
H	6.93713300	-0.09112500	2.61986100
H	8.04455500	-0.77030900	1.42777700
H	7.82093300	0.98622800	1.53122500

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C	-1.39212500	-3.04629300	-1.61423500
C	-1.41028100	-4.47663700	-2.07352100
C	0.52360700	-4.72654000	-0.80269600
C	0.31326400	-3.53453000	0.12446900
C	-0.77646100	-1.28750300	-0.47161000
H	-2.44234100	-4.82612400	-2.14091200
H	1.09836000	-5.49365300	-0.28229900
H	1.25618900	-3.00757400	0.24486500
N	-2.08158700	-2.06435900	-2.11831800
N	-1.68995000	-0.97931200	-1.39557800
N	-0.58613000	-2.61578400	-0.60198900
H	1.07206500	-4.41540900	-1.70270300
H	-0.95153500	-4.53261700	-3.07013200
O	-0.72582300	-5.29927800	-1.15729400
C	-0.26681100	-3.93995700	1.50897300
H	-0.18637600	-5.02873900	1.59342200
H	0.37109000	-3.49623000	2.27339400
C	-1.70131500	-3.54024100	1.77713400
C	-2.76251500	-4.24362700	1.19530500
C	-1.99216400	-2.47582500	2.63576100
C	-4.08299100	-3.90552800	1.48365800
H	-2.54052200	-5.07310300	0.52759900
C	-3.31317100	-2.14005200	2.93044200
H	-1.17121200	-1.91254300	3.07006000
C	-4.36205800	-2.85774300	2.36026700
H	-4.89422200	-4.46600600	1.02953200
H	-3.52115800	-1.31567200	3.60665300
H	-5.39069900	-2.59750200	2.58959100
C	-2.35045100	0.27009800	-1.66148300
C	-3.51869100	0.55600000	-0.94466400
C	-1.82110200	1.12126600	-2.63331400
C	-4.10442800	1.80195200	-1.15312600
C	-2.45898900	2.35022300	-2.81349400
C	-3.58088600	2.71596700	-2.06972600
H	-4.98481700	2.07056300	-0.57334000
H	-2.05462800	3.04340500	-3.54743600
C	-4.14365500	-0.42420700	0.01314700
H	-3.49547300	-1.27230500	0.24548100
H	-4.39999100	0.07170600	0.95471300
H	-5.06995600	-0.82564400	-0.40998600
C	-4.23404400	4.05852600	-2.26515900
H	-5.06607400	3.98429000	-2.97282700
H	-4.62988100	4.43615800	-1.31941700

H	-3.52321500	4.78801500	-2.65964900
C	-0.59648400	0.78163300	-3.43690500
H	-0.30332400	-0.26439800	-3.33150000
H	-0.77776300	0.98966500	-4.49468600
H	0.25326800	1.38751900	-3.11217100
C	-0.10927000	-0.45058500	0.65500700
O	0.56831800	-1.14924800	1.43646000
C	-1.02638000	0.61614800	1.27694100
H	-0.69210800	0.66544400	2.31825100
H	-2.03676200	0.19104600	1.28763600
C	1.37392400	1.87684700	0.21508700
C	0.37206800	2.57499000	0.77039400
C	-1.02714000	2.02964100	0.68665600
H	0.58250400	3.48147400	1.32801600
H	-1.27465600	1.95852700	-0.37686300
C	-2.06753500	2.94468900	1.30196000
C	-2.25795700	4.20535700	0.72098800
C	-2.86979800	2.58709700	2.38657700
C	-3.22405700	5.08048700	1.20260500
H	-1.64738700	4.48706300	-0.13483500
C	-3.84454500	3.46214300	2.87135000
H	-2.74912200	1.61922800	2.86430100
C	-4.02727700	4.70824000	2.28216600
H	-3.35844300	6.04973100	0.73160900
H	-4.46050700	3.16363700	3.71400900
H	-4.78623100	5.38640800	2.65868900
C	2.78706700	2.35285200	0.36012100
C	3.52002600	2.00974800	1.50059500
C	3.37885400	3.15698200	-0.61529400
C	4.83392900	2.44040800	1.65033300
H	3.05661300	1.38031600	2.25546000
C	4.69064300	3.60064300	-0.45985400
H	2.81046500	3.41984600	-1.50157800
C	5.42142900	3.23803200	0.66885000
H	5.39991700	2.15433700	2.53172800
H	5.14247800	4.22731800	-1.22253100
H	6.44646600	3.57635200	0.78463600
N	1.04529700	0.65348600	-0.41839900
S	2.14568000	-0.06472000	-1.38183400
O	2.54200800	0.83327500	-2.47468500
O	1.56854300	-1.36479200	-1.76328100
C	3.64712000	-0.42357500	-0.47754700
C	4.85651200	0.05461800	-0.96715000
C	3.58672200	-1.17605200	0.69247100

C	6.02558700	-0.22490700	-0.26680000
H	4.86844900	0.65620900	-1.86886300
C	4.76537500	-1.44551300	1.37793300
H	2.62351700	-1.49650200	1.08151100
C	5.99782200	-0.97147900	0.91367100
H	6.97437600	0.15337000	-0.63768900
H	4.73046100	-2.02600400	2.29592500
C	7.26064700	-1.22474300	1.69437200
H	7.21116700	-2.17521500	2.23060100
H	8.13541600	-1.23848700	1.04060500
H	7.41484000	-0.43454800	2.43694900

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C	1.30678000	-2.25763400	1.71341000
C	1.10618600	-3.53958400	2.47088000
C	-0.12282600	-4.27724500	0.61790400
C	0.43651000	-3.27913300	-0.39449900
C	1.12282600	-0.85756900	0.04700400
H	2.00040800	-3.77468600	3.05075800
H	-0.39176100	-5.20062000	0.10376200
H	-0.37119800	-2.89072200	-1.02139400
N	1.74085800	-1.12307200	2.18283200
N	1.62277300	-0.25948900	1.13101300
N	0.93224800	-2.14106300	0.40556700
H	-1.02083600	-3.88158300	1.11326200
H	0.26243500	-3.40363500	3.16281200
O	0.86272600	-4.60853100	1.58529300
C	1.54563600	-3.90321500	-1.29124000
H	1.46576500	-4.99113400	-1.18921200
H	1.30423600	-3.64563600	-2.32201100
C	2.97979100	-3.50233700	-1.01957300
C	3.64663100	-3.91620700	0.14027700
C	3.69052000	-2.76363000	-1.96926300
C	4.98723900	-3.59723200	0.34426100
H	3.11391100	-4.51996000	0.87032400
C	5.03742800	-2.46073700	-1.77728700
H	3.17571300	-2.42491200	-2.86258500
C	5.68938800	-2.87252200	-0.61774100
H	5.48805700	-3.92948700	1.24841800
H	5.57471700	-1.89546400	-2.53288000
H	6.73687300	-2.63316700	-0.46391600
C	2.17019300	1.06680700	1.27184400
C	3.38733600	1.32795200	0.63133600
C	1.51923200	1.99556900	2.08700800

C	3.90630300	2.61528900	0.74625500
C	2.07834800	3.27207700	2.15982500
C	3.25546500	3.60305100	1.48891800
H	4.83942600	2.85159900	0.24140100
H	1.57885500	4.02533300	2.76478900
C	4.09189200	0.25718000	-0.15876200
H	5.11292800	0.56281500	-0.39337900
H	4.13625400	-0.68748600	0.39467000
H	3.58594400	0.03972700	-1.10749900
C	3.82577300	4.99260700	1.59586400
H	4.60347500	5.15848100	0.84757900
H	3.04333700	5.74180900	1.45096400
H	4.26556200	5.15465500	2.58505100
C	0.31768000	1.63776200	2.91957300
H	-0.25152900	0.80969700	2.49660500
H	0.64215700	1.34272700	3.92273600
H	-0.34757400	2.49847800	3.02324100
C	0.78404300	-0.36324700	-1.37808200
O	1.06654300	-1.19381200	-2.25311700
C	0.94534700	1.12617600	-1.68603100
H	1.12973100	1.14915000	-2.76282600
H	1.87033200	1.43383800	-1.19881900
C	-1.50536200	0.53277400	0.01340700
C	-0.96749500	1.75391500	-0.11905100
C	-0.15907900	2.14370900	-1.33212500
H	-1.12969700	2.49396500	0.65909400
H	-0.85765100	2.12475300	-2.17924400
C	0.36450300	3.57253000	-1.21759500
C	1.66774200	3.94739200	-1.55352700
C	-0.51000600	4.57569500	-0.77596700
C	2.09364600	5.26885400	-1.41599200
H	2.37640300	3.21560400	-1.92574500
C	-0.09054800	5.89369400	-0.63707900
H	-1.53914600	4.31986100	-0.53678500
C	1.22180800	6.24669400	-0.94957300
H	3.11683800	5.52791500	-1.67198600
H	-0.78954400	6.64607800	-0.28520600
H	1.55697800	7.27289800	-0.83720600
C	-2.36501900	0.15771300	1.16809200
C	-3.29906600	1.05324200	1.69801400
C	-2.25200100	-1.11439200	1.73911300
C	-4.09884800	0.68151800	2.77612400
H	-3.42212700	2.02994200	1.23874200
C	-3.03977400	-1.48345100	2.82320000

H	-1.54537200	-1.81251900	1.30233500
C	-3.97175300	-0.58538800	3.34286000
H	-4.83113000	1.38064700	3.16824800
H	-2.93236200	-2.47290400	3.25768300
H	-4.59761900	-0.87267800	4.18159800
N	-1.13281500	-0.50662000	-0.87712100
S	-2.07064900	-0.78779200	-2.16830800
O	-1.87222500	-2.19014000	-2.56828100
O	-1.90456100	0.21624800	-3.23567400
C	-3.72630600	-0.60023300	-1.54243200
C	-4.27754400	-1.62061100	-0.77146900
C	-4.38294600	0.61354900	-1.70799500
C	-5.50117100	-1.41027300	-0.14982700
H	-3.74145200	-2.55689100	-0.64853900
C	-5.61100800	0.80755000	-1.08206000
H	-3.92852900	1.39174100	-2.31261500
C	-6.17646000	-0.19128200	-0.28507900
H	-5.93546200	-2.19585500	0.46245900
H	-6.13103700	1.75353200	-1.20334700
C	-7.46560700	0.04691800	0.45508300
H	-8.02394800	0.88114400	0.02573000
H	-8.10051000	-0.84228900	0.44267600
H	-7.25537100	0.28574600	1.50335600

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C	-1.42565900	3.05537000	1.54240100
C	-1.47559100	4.50123900	1.94986400
C	0.58438500	4.67342600	0.86847600
C	0.40825800	3.48214300	-0.06621500
C	-0.71309600	1.24354000	0.53698000
H	-2.50218700	4.86619000	1.87638300
H	1.22721800	5.41625900	0.39412200
H	1.34595400	2.93953500	-0.14221700
N	-2.14507700	2.09627200	2.04563700
N	-1.69312200	0.97880400	1.40745500
N	-0.54346000	2.58044100	0.61520200
H	1.04434700	4.35266000	1.81408000
H	-1.14724800	4.57708700	2.99548100
O	-0.66918900	5.29417100	1.11089800
C	-0.09329300	3.89955300	-1.47575000
H	0.07492800	4.97643900	-1.58111700
H	0.52816400	3.38185900	-2.20567200
C	-1.54496900	3.59721100	-1.77349200
C	-2.56981300	4.43250400	-1.31616700

C	-1.88282200	2.46785700	-2.52672700
C	-3.90210400	4.15130000	-1.61488800
H	-2.31278500	5.31257600	-0.73173900
C	-3.21384000	2.19247900	-2.83578300
H	-1.08639400	1.80460600	-2.85231300
C	-4.22786400	3.03342100	-2.38151100
H	-4.68516400	4.81230200	-1.25632900
H	-3.45992200	1.31579300	-3.42866000
H	-5.26494000	2.81724000	-2.61870000
C	-2.36969400	-0.25769100	1.68706500
C	-3.54539500	-0.53237700	0.97513900
C	-1.85290100	-1.10967200	2.66322400
C	-4.15044200	-1.76551700	1.19643100
C	-2.51045800	-2.32749500	2.85769900
C	-3.63997000	-2.68061800	2.12153500
H	-5.03865700	-2.02425200	0.62370900
H	-2.11744600	-3.01845200	3.59954200
C	-4.15620700	0.44855700	0.00838100
H	-3.50616700	1.29891300	-0.20718400
H	-4.39129600	-0.04603300	-0.93941300
H	-5.09230300	0.84348300	0.41539200
C	-4.31706000	-4.01074100	2.31998900
H	-5.30559800	-3.88008000	2.77052900
H	-4.45689200	-4.51268000	1.35800700
H	-3.72918600	-4.66248000	2.96920600
C	-0.62160000	-0.78255800	3.46172600
H	-0.33122700	0.26595700	3.37142000
H	-0.79323100	-1.00770700	4.51742800
H	0.22579800	-1.38401400	3.12223300
C	0.04169300	0.33806300	-0.52004800
O	0.68857400	1.08174500	-1.34685300
C	-0.99661600	-0.61415000	-1.20016300
H	-0.64433400	-0.66328800	-2.23569400
H	-1.96561000	-0.10444600	-1.21800800
C	1.29693900	-1.91474700	-0.22803200
C	0.27561400	-2.62728500	-0.71249700
C	-1.10693900	-2.03790100	-0.65117000
H	0.46421400	-3.56727400	-1.22056100
H	-1.38436800	-1.99274100	0.40695900
C	-2.15743900	-2.89608700	-1.32638400
C	-2.40133200	-4.17054500	-0.79859100
C	-2.91502500	-2.47418200	-2.41949900
C	-3.37344400	-5.00039900	-1.34380800
H	-1.82603300	-4.50120000	0.06438000

C	-3.89736200	-3.30279300	-2.96675100
H	-2.74950600	-1.49243400	-2.85349200
C	-4.13070200	-4.56554000	-2.43303100
H	-3.54629300	-5.98349200	-0.91600100
H	-4.47940700	-2.95583100	-3.81504000
H	-4.89438800	-5.20813000	-2.85915600
C	2.70516200	-2.38824100	-0.39969000
C	3.43580500	-1.97789300	-1.51969300
C	3.28945200	-3.26196800	0.51733800
C	4.74254300	-2.41521800	-1.70480000
H	2.97560400	-1.29479300	-2.22851100
C	4.59552900	-3.70924000	0.32689700
H	2.72091600	-3.57241400	1.38803600
C	5.32471700	-3.28191800	-0.77953300
H	5.30731300	-2.08168300	-2.57008800
H	5.04298800	-4.38881800	1.04533600
H	6.34497200	-3.62400800	-0.92301400
N	0.99840500	-0.63847200	0.35559700
S	2.13870000	0.02560300	1.36323600
O	2.46398800	-0.96879800	2.38580400
O	1.59318900	1.31475300	1.80073100
C	3.66087500	0.36279700	0.49239000
C	4.83946500	-0.17031300	1.00254700
C	3.65223100	1.15671600	-0.65144800
C	6.03533600	0.10044400	0.34662900
H	4.81072900	-0.80167300	1.88320200
C	4.85910300	1.41220200	-1.29158100
H	2.70195300	1.49787800	-1.05655100
C	6.06297900	0.88730400	-0.80779400
H	6.96174400	-0.31705000	0.73140400
H	4.86755900	2.02117300	-2.19139500
C	7.35596300	1.12808600	-1.54115000
H	7.33662300	2.07949100	-2.07722700
H	8.20613700	1.13061600	-0.85554500
H	7.52800800	0.33623900	-2.27799400

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C	3.19289000	0.88318500	0.73034300
C	4.60406700	0.70678100	1.22148400
C	4.16595700	-1.60074700	1.03212700
C	3.09172100	-1.46091100	-0.04608000
C	1.21635300	0.31072800	-0.03214000
H	5.24947700	1.45429600	0.75453300
H	4.69877700	-2.54272600	0.89649200

H	2.31939500	-2.22381800	0.06684000
N	2.47433500	1.96273400	0.82975600
N	1.24704100	1.59215100	0.35126700
N	2.46426300	-0.14821000	0.21112800
H	3.71888800	-1.58642500	2.03700500
H	4.60235500	0.86749000	2.30837400
O	5.12271300	-0.56360100	0.90283400
C	3.67552400	-1.55361100	-1.47787800
H	4.47562700	-2.30045200	-1.44509100
H	2.87051300	-1.92578200	-2.10952400
C	4.20217200	-0.26038900	-2.05846200
C	5.55506400	0.08357800	-1.98321900
C	3.32039000	0.61200100	-2.70710200
C	6.01828000	1.27534000	-2.53545400
H	6.24462200	-0.58572900	-1.47741200
C	3.78432300	1.80190700	-3.26587700
H	2.27068100	0.32828700	-2.76927500
C	5.13339200	2.13919400	-3.17827300
H	7.07243000	1.52649100	-2.46946300
H	3.09199400	2.46354600	-3.77888700
H	5.49475000	3.06569300	-3.61322900
C	0.20500500	2.58992600	0.40012800
C	-0.02747900	3.36325200	-0.74360500
C	-0.43521700	2.82293200	1.61831500
C	-1.01789200	4.33669000	-0.66777200
C	-1.43319100	3.80042300	1.63528900
C	-1.74451100	4.55530000	0.50656800
H	-1.23554600	4.93515000	-1.54903100
H	-1.96717500	3.98273600	2.56503900
C	0.78333000	3.15292500	-1.99392500
H	0.53782400	3.90830700	-2.74198100
H	1.85335200	3.21507700	-1.77274100
H	0.60855700	2.16535700	-2.43776700
C	-2.80128900	5.62624900	0.56458900
H	-3.58518300	5.36349500	1.27851600
H	-2.36424400	6.58064300	0.87698500
H	-3.26508500	5.77031300	-0.41376100
C	-0.02353600	2.13283700	2.89116100
H	0.44772800	1.16483200	2.71559100
H	0.69336500	2.76012900	3.43133800
H	-0.88594500	1.97724300	3.54462900
C	0.15906100	-0.61364400	-0.76398200
O	0.75084600	-1.16480100	-1.76923200
C	-1.14927400	0.13328400	-1.13353700

H	-1.45409900	-0.31928400	-2.07997900
H	-0.89635800	1.17002200	-1.34762700
C	-0.84611900	-1.03066400	1.54159800
C	-1.80467400	-0.13074000	1.27805100
C	-2.31374000	0.08297700	-0.12583600
H	-2.21659400	0.45893200	2.09012600
H	-2.89612900	-0.81881200	-0.37223300
C	-3.28556600	1.25058900	-0.24927100
C	-3.32835900	2.05718000	-1.38898900
C	-4.21669400	1.50354700	0.76648300
C	-4.24508100	3.10183800	-1.49791000
H	-2.63908100	1.88371300	-2.20913500
C	-5.13175200	2.54641400	0.66375800
H	-4.23960100	0.87263900	1.65057100
C	-5.14641700	3.35651900	-0.47025000
H	-4.24727500	3.71989900	-2.39087200
H	-5.83803600	2.72272300	1.46920100
H	-5.85492200	4.17493100	-0.55107400
C	-0.33006600	-1.31121600	2.90321300
C	-1.11164600	-1.06127200	4.03804400
C	0.97241000	-1.78911000	3.08036000
C	-0.58615600	-1.24265900	5.31298100
H	-2.14079600	-0.73438800	3.92363600
C	1.49862400	-1.97240200	4.35528000
H	1.56344500	-2.02421200	2.20212300
C	0.72380600	-1.69103000	5.47810300
H	-1.20542700	-1.04167100	6.18138200
H	2.51340600	-2.34076900	4.47152800
H	1.13154100	-1.83337900	6.47348100
N	-0.15147000	-1.61372300	0.43456200
S	-0.44022900	-3.21529600	0.09662000
O	-0.88942600	-3.82249500	1.34935800
O	0.73490400	-3.78033200	-0.55839700
C	-1.81194400	-3.29482600	-1.03402000
C	-3.06905700	-3.61142200	-0.52481400
C	-1.62055800	-3.02525600	-2.38799900
C	-4.15642800	-3.64412500	-1.39173100
H	-3.18399100	-3.83384100	0.53041100
C	-2.72096800	-3.06551800	-3.23608400
H	-0.63341300	-2.74586900	-2.74166500
C	-3.99985600	-3.36839400	-2.75354000
H	-5.14056200	-3.89407800	-1.00603900
H	-2.58675300	-2.85866200	-4.29414500
C	-5.18615400	-3.37608100	-3.68082700

H	-5.60663600	-2.36934100	-3.77161300
H	-4.90126700	-3.70551700	-4.68246000
H	-5.97489700	-4.03274100	-3.30801500

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C	-1.88656400	2.98135400	1.63263000
C	-2.04779800	4.41434600	2.05197400
C	0.02017700	4.77241900	1.03002400
C	-0.00914000	3.54873400	0.12046700
C	-0.93421600	1.22129100	0.65177600
H	-3.09681000	4.70989300	1.98528400
H	0.60070400	5.56905000	0.56236700
H	0.97845200	3.09427000	0.08583600
N	-2.57367600	1.96856100	2.06433600
N	-1.96776100	0.90003900	1.44701600
N	-0.89456300	2.57707700	0.77920100
H	0.47301100	4.52082700	1.99987000
H	-1.72162900	4.51435400	3.09691100
O	-1.29860300	5.26913600	1.21597000
C	-0.47708900	3.91875100	-1.31767500
H	-0.51763400	5.01141700	-1.38311100
H	0.28939300	3.57069000	-2.01015900
C	-1.81371900	3.37264300	-1.76502700
C	-3.01077700	3.92728100	-1.29687700
C	-1.87801200	2.33968300	-2.70409200
C	-4.24008300	3.47061500	-1.76636300
H	-2.96660000	4.74342600	-0.57897700
C	-3.10731000	1.88556900	-3.18241100
H	-0.95061600	1.89548100	-3.05477600
C	-4.29180700	2.45244500	-2.71750800
H	-5.15834600	3.91692600	-1.39708200
H	-3.13795300	1.09116800	-3.92303900
H	-5.24893800	2.10037000	-3.08936600
C	-2.55972800	-0.39018600	1.64107500
C	-3.64768600	-0.74116600	0.83915300
C	-2.02769400	-1.24107900	2.61493500
C	-4.19124500	-2.01545300	1.01154000
C	-2.60568800	-2.50123700	2.75059700
C	-3.68058400	-2.90641600	1.95273200
H	-5.00871000	-2.32929800	0.36624400
H	-2.20054300	-3.18898500	3.48955500
C	-4.21285700	0.21677300	-0.17457300
H	-3.44395000	0.86254800	-0.60936800
H	-4.70166500	-0.32859500	-0.98568500

H	-4.95469100	0.87812300	0.28688700
C	-4.25514900	-4.29074100	2.10236500
H	-5.03311700	-4.47559600	1.35874200
H	-3.47545200	-5.04722000	1.97061900
H	-4.68608800	-4.43152400	3.09832400
C	-0.83078700	-0.83224600	3.42933900
H	-0.89278600	0.21638100	3.73251400
H	-0.74722300	-1.45174000	4.32444700
H	0.09076700	-0.95181700	2.84846400
C	0.36078100	0.31465200	-0.74934400
O	0.84587200	1.27538100	-1.34846800
C	-0.67542400	-0.59655500	-1.41709500
H	-0.31459800	-0.75974700	-2.44110100
H	-1.60896000	-0.03489900	-1.48013600
C	1.55105600	-1.84060400	-0.26632500
C	0.52225500	-2.58361800	-0.67884600
C	-0.84011400	-1.94361900	-0.71310600
H	0.69649900	-3.57207700	-1.09133900
H	-1.11550500	-1.73532000	0.32875400
C	-1.93056300	-2.82946200	-1.27814500
C	-2.09194000	-4.11601600	-0.75055000
C	-2.83540700	-2.38992800	-2.24542600
C	-3.13869400	-4.93321300	-1.16095400
H	-1.40270600	-4.46559900	0.01565900
C	-3.88927500	-3.20622900	-2.65866700
H	-2.73838400	-1.39872100	-2.67850200
C	-4.04819900	-4.47728300	-2.11595100
H	-3.25215300	-5.92304100	-0.72908400
H	-4.58666500	-2.84214300	-3.40693400
H	-4.87029500	-5.11010700	-2.43457900
C	2.96902300	-2.28726300	-0.38243100
C	3.74289500	-1.82562900	-1.45296000
C	3.52608800	-3.17403300	0.53800400
C	5.06274400	-2.23742600	-1.59243700
H	3.30392900	-1.12921500	-2.16286700
C	4.84903600	-3.59009500	0.39566700
H	2.92358900	-3.51867100	1.37243300
C	5.61817500	-3.12045600	-0.66531200
H	5.65944500	-1.87041400	-2.42183000
H	5.27805200	-4.27859600	1.11669300
H	6.64991200	-3.44064700	-0.77140900
N	1.26553700	-0.49111800	0.14007900
S	2.26558100	0.23277000	1.26488200
O	2.50020000	-0.76710000	2.30287700

O	1.64955300	1.50322300	1.63192100
C	3.83601100	0.58500600	0.50939800
C	4.97927900	0.00368200	1.04560200
C	3.89176200	1.43866900	-0.58982500
C	6.20667900	0.27693900	0.45265600
H	4.89916700	-0.66930800	1.89196500
C	5.12854400	1.69193100	-1.16969500
H	2.97534600	1.85556600	-0.99794900
C	6.29833500	1.11251200	-0.66372200
H	7.10728000	-0.17817100	0.85516700
H	5.18890800	2.34722400	-2.03403900
C	7.62508500	1.35225600	-1.33391300
H	7.65228000	2.32818900	-1.82339900
H	8.44646300	1.29726800	-0.61626200
H	7.80432500	0.59134200	-2.10090200

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C	3.36358900	0.86718500	0.60526400
C	4.77591300	0.60498700	1.05041100
C	4.09665900	-1.64625100	1.22307800
C	2.96344100	-1.54215300	0.20526100
C	1.27634700	0.36957500	0.00999600
H	5.46961300	1.20894300	0.46116100
H	4.52438900	-2.64974200	1.20586300
H	2.12841600	-2.18678300	0.49152700
N	2.75820100	2.01654800	0.56918200
N	1.47588000	1.68350900	0.19637900
N	2.50253900	-0.14865700	0.28024900
H	3.72902400	-1.43215900	2.23810200
H	4.86447600	0.89343900	2.10704000
O	5.13729800	-0.74847300	0.87331900
C	3.42434300	-1.93446400	-1.22507100
H	4.23026800	-2.66797100	-1.12027700
H	2.57839200	-2.42532800	-1.70695700
C	3.88141600	-0.79045100	-2.09952000
C	5.21646400	-0.37611300	-2.13864200
C	2.94738600	-0.12735200	-2.90206500
C	5.60994900	0.67739800	-2.96078800
H	5.94609200	-0.88039700	-1.51218300
C	3.34232700	0.91843700	-3.73436600
H	1.90811800	-0.45157200	-2.86747600
C	4.67384100	1.32712000	-3.76319400
H	6.65073200	0.98594800	-2.98039800
H	2.60817000	1.41551300	-4.36198100

H	4.98093100	2.14315900	-4.40956100
C	0.50032200	2.73687100	0.11754200
C	0.24866800	3.33171200	-1.12331000
C	-0.10940700	3.17500000	1.29628400
C	-0.68909500	4.36077200	-1.17143400
C	-1.05274500	4.19851300	1.19410800
C	-1.35576100	4.80091700	-0.02672600
H	-0.90694200	4.82794200	-2.12902400
H	-1.55213800	4.54175100	2.09769300
C	0.98578000	2.88252000	-2.35547700
H	0.74329000	3.52312100	-3.20533700
H	2.06785900	2.90649800	-2.19424900
H	0.73677200	1.84981100	-2.62453400
C	-2.34487600	5.93436100	-0.09814200
H	-3.16947000	5.77660300	0.60123200
H	-1.86275200	6.88372900	0.15854700
H	-2.76351500	6.02642300	-1.10260900
C	0.28288700	2.62113100	2.63910600
H	0.59925000	1.57852600	2.57724200
H	1.11734000	3.19753600	3.05293100
H	-0.54971700	2.68510300	3.34437400
C	-0.19484800	-0.97697200	-0.65085000
O	0.37029500	-1.73416800	-1.44280900
C	-1.24840100	0.01417500	-1.15747400
H	-1.65576800	-0.44353400	-2.06524400
H	-0.74666900	0.93663000	-1.44551800
C	-1.01844600	-0.62826000	1.68093600
C	-1.84557100	0.33417200	1.25283400
C	-2.37779000	0.31625000	-0.16118200
H	-2.11871200	1.14368700	1.92209900
H	-3.07575900	-0.53535000	-0.20827200
C	-3.18616500	1.55434100	-0.51944000
C	-3.10601600	2.15158300	-1.77862400
C	-4.08875800	2.09028500	0.40818900
C	-3.88863100	3.26077000	-2.09818100
H	-2.42479900	1.76156500	-2.52809000
C	-4.86855900	3.19853800	0.09521400
H	-4.19344200	1.62948800	1.38693400
C	-4.77039100	3.79107900	-1.16296900
H	-3.79975600	3.71197700	-3.08190000
H	-5.55769900	3.59745700	0.83322500
H	-5.37420000	4.65895600	-1.40894400
C	-0.46961400	-0.70799900	3.05257500
C	-1.18894300	-0.19262500	4.13674000

C	0.80016100	-1.24919600	3.28199900
C	-0.63185000	-0.17908300	5.41084800
H	-2.19260200	0.19182700	3.98093700
C	1.35543700	-1.23932000	4.55759600
H	1.34732000	-1.68194800	2.45018000
C	0.64529000	-0.69532300	5.62576500
H	-1.20092500	0.22613500	6.24148000
H	2.34369300	-1.65963100	4.71724500
H	1.07696400	-0.68678500	6.62120900
N	-0.48123900	-1.51432400	0.69871000
S	-0.73334000	-3.17057200	0.83291300
O	-1.38881700	-3.36294000	2.12274700
O	0.51532500	-3.87544100	0.56908200
C	-1.90458700	-3.58189500	-0.43606500
C	-3.25695500	-3.38834900	-0.16401700
C	-1.46956000	-4.07486200	-1.66269600
C	-4.18821800	-3.68702500	-1.15173900
H	-3.57181200	-3.02309000	0.80862100
C	-2.41751600	-4.37452700	-2.63361400
H	-0.40944000	-4.20870100	-1.84271100
C	-3.78313100	-4.17924800	-2.39703700
H	-5.24563200	-3.54459100	-0.95022300
H	-2.09294500	-4.76566200	-3.59347200
C	-4.79373500	-4.47659900	-3.47246000
H	-4.86322800	-3.63739600	-4.17200300
H	-4.50798100	-5.36036800	-4.04734200
H	-5.78615700	-4.64072700	-3.04829000

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C	-1.97680600	-1.53563900	1.40471400
C	-3.28126400	-1.66961300	2.14021000
C	-3.71590600	0.49403400	1.33947900
C	-2.80343100	0.42121200	0.12191400
C	-0.47925400	-0.66430200	0.07103600
H	-3.66455100	-2.68587400	2.02394400
H	-4.55647800	1.15711000	1.12904000
H	-2.30083800	1.37778800	-0.00367200
N	-0.90238600	-2.24277300	1.60847500
N	0.01805900	-1.69492700	0.76406700
N	-1.76195800	-0.56023100	0.47558200
H	-3.15152800	0.88961300	2.19656600
H	-3.09223000	-1.48137800	3.20585100
O	-4.25456300	-0.78421900	1.63703200
C	-3.52444000	0.02336100	-1.19040000

H	-4.55735900	0.37939700	-1.12389200
H	-3.03029600	0.56233000	-2.00041800
C	-3.49813500	-1.45617300	-1.49800600
C	-4.46103200	-2.33249100	-0.98863100
C	-2.46407500	-1.97687000	-2.28268600
C	-4.38769300	-3.69843900	-1.25281900
H	-5.26210100	-1.93910400	-0.37009200
C	-2.39189600	-3.34200100	-2.55326800
H	-1.71593600	-1.29666400	-2.68559900
C	-3.35255900	-4.20776900	-2.03453300
H	-5.14328500	-4.36626300	-0.85087600
H	-1.58627900	-3.72829800	-3.17086100
H	-3.29810100	-5.27142000	-2.24290900
C	1.37190100	-2.17154100	0.81032700
C	2.19086900	-1.69684600	1.83758800
C	1.80322100	-3.06399900	-0.17198500
C	3.51681200	-2.12947800	1.83892800
C	3.13674500	-3.46615900	-0.12572300
C	4.00782600	-2.99787700	0.86132200
H	4.18344400	-1.77353400	2.62096400
H	3.50577900	-4.15318600	-0.88274600
C	1.65638100	-0.77357100	2.90063100
H	1.02397800	0.01448900	2.47612900
H	1.04774400	-1.33381200	3.61813200
H	2.47998600	-0.30728200	3.44507600
C	5.46032200	-3.39615100	0.85689400
H	6.05690100	-2.64389000	0.33007300
H	5.85179500	-3.47415100	1.87359600
H	5.60833500	-4.35245900	0.35126900
C	0.86832700	-3.51132600	-1.26139800
H	-0.07641600	-3.88053600	-0.85162400
H	0.62807500	-2.66901700	-1.92212800
H	1.32275300	-4.29950200	-1.86340100
C	0.14174100	0.19153300	-0.99981000
O	-0.62983900	1.01570400	-1.54357200
C	1.52565500	0.16656200	-1.21601300
H	1.84231700	0.65860800	-2.12867600
H	2.17072600	-0.61417400	-0.83769700
C	-0.06368700	2.63980100	0.61976100
O	-0.25573100	1.70220000	1.42973900
C	1.15741500	2.79867900	-0.09630900
C	2.12309500	1.80503100	0.02967300
H	1.27774100	3.62373000	-0.78752000
H	2.03306700	1.18144900	0.91591200

C	3.51043200	1.93315900	-0.47948400
C	4.52135200	1.16723500	0.11307900
C	3.84830500	2.78314500	-1.53959700
C	5.83852900	1.25798600	-0.32682700
H	4.26308500	0.49129700	0.92569400
C	5.16434300	2.87502700	-1.98101100
H	3.07539600	3.36885900	-2.02869900
C	6.16500300	2.11548700	-1.37520100
H	6.60943800	0.65981000	0.14916000
H	5.41053600	3.53911400	-2.80359700
H	7.19054700	2.18889100	-1.72233800
C	-1.17610800	3.62895600	0.40723200
C	-1.34725400	4.31116600	-0.80129500
C	-2.09721600	3.83339900	1.43982600
C	-2.40845700	5.19665100	-0.96596900
H	-0.66906800	4.11667300	-1.62584000
C	-3.15586400	4.72227000	1.27838800
H	-1.96321800	3.28681700	2.36850900
C	-3.31191100	5.40830300	0.07462000
H	-2.53807400	5.71345300	-1.91166500
H	-3.86021100	4.88074900	2.08909400
H	-4.13833500	6.09989400	-0.05516700

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C	-2.32049400	1.09812400	0.58807200
C	-3.29168100	2.24523900	0.55793300
C	-2.36310900	2.67001100	-1.57238400
C	-1.96834700	1.22784800	-1.87065400
C	-0.83225900	-0.30033300	-0.16920200
H	-4.25202700	1.92539600	0.97026800
H	-2.61931100	3.18414400	-2.49974600
H	-1.00909900	1.20781000	-2.38548500
N	-1.86399600	0.49167500	1.64943500
N	-0.94309900	-0.38797400	1.15643300
N	-1.73093300	0.62469000	-0.54574200
H	-1.52033600	3.18373000	-1.08948000
H	-2.88594800	3.04858700	1.18779200
O	-3.52384800	2.69771700	-0.75608400
C	-3.02814600	0.44031100	-2.67361900
H	-3.45562100	1.12903200	-3.40914000
H	-2.49516600	-0.34532100	-3.21082900
C	-4.12428400	-0.19245800	-1.84822300
C	-5.34160800	0.45146000	-1.61218800
C	-3.91836600	-1.46240200	-1.29925600

C	-6.32771000	-0.15547000	-0.83788400
H	-5.50955500	1.43914400	-2.03087600
C	-4.90350100	-2.07360000	-0.52618000
H	-2.97343200	-1.96778200	-1.49360600
C	-6.11090100	-1.41897000	-0.29103500
H	-7.26894600	0.35684300	-0.66482100
H	-4.73108800	-3.06316000	-0.11275300
H	-6.88072700	-1.89314900	0.30925200
C	-0.30513600	-1.31083400	2.05938400
C	0.73971300	-0.84570800	2.85983200
C	-0.78401900	-2.62265100	2.10801000
C	1.31651500	-1.75603800	3.74558000
C	-0.17126800	-3.49300700	3.00571800
C	0.87432200	-3.07658800	3.83345000
H	2.13609000	-1.42341600	4.37730900
H	-0.52180900	-4.52039500	3.06258400
C	1.26756600	0.55396500	2.71340700
H	1.91309700	0.81372900	3.55397400
H	1.85965000	0.63948700	1.79294500
H	0.46224200	1.29017200	2.64973700
C	1.49375500	-4.03307500	4.81861000
H	1.55229900	-5.04194700	4.40365900
H	2.49888700	-3.71368200	5.10121100
H	0.89130000	-4.08647100	5.73103900
C	-1.89861600	-3.07500100	1.20568200
H	-2.71796600	-2.35009400	1.19216000
H	-1.53939100	-3.18756200	0.17544700
H	-2.29206900	-4.03860700	1.53279100
C	0.01900000	-1.10037500	-1.12028300
O	-0.46077700	-1.22857000	-2.26873800
C	1.28322200	-1.52898200	-0.68931800
H	1.70619900	-2.36528600	-1.23175700
H	1.58220300	-1.41621200	0.34500500
C	1.88893300	1.90313700	-0.50501000
O	0.70990300	1.79996200	-0.91478900
C	2.88697100	0.94722600	-0.83017300
C	2.55151900	-0.10240200	-1.68771200
H	3.84986000	0.97627400	-0.33451100
H	1.72548500	0.07964200	-2.37531600
C	3.58456300	-1.03388100	-2.20512700
C	3.41303400	-1.60467300	-3.47214800
C	4.72445000	-1.37142600	-1.46542700
C	4.36518500	-2.47242600	-3.99829200
H	2.51981200	-1.36309100	-4.04243500

C	5.67534200	-2.24168200	-1.98865200
H	4.86150600	-0.96097800	-0.46927000
C	5.50174200	-2.79218600	-3.25825000
H	4.21924600	-2.90092300	-4.98480400
H	6.55323400	-2.49518000	-1.40287800
H	6.24436500	-3.47118200	-3.66452200
C	2.22921200	3.05114100	0.40484700
C	3.53548900	3.52198200	0.56860000
C	1.18974600	3.67640500	1.10136600
C	3.79659500	4.59215800	1.42051600
H	4.34930700	3.06722700	0.01224900
C	1.44979000	4.73818700	1.96080600
H	0.17917300	3.30354800	0.95951600
C	2.75630300	5.19889300	2.12189000
H	4.81269300	4.95649100	1.53353100
H	0.63630100	5.20950500	2.50343000
H	2.96239400	6.03055700	2.78821300

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C	-2.52243800	-0.31371400	1.30275800
C	-3.81444900	0.08546500	1.96263700
C	-3.58241200	2.10553700	0.74624400
C	-2.73725000	1.49305500	-0.36794000
C	-0.76157200	-0.12026100	0.00583200
H	-4.49632800	-0.76824700	1.97528700
H	-4.20680400	2.90204200	0.33850100
H	-2.01391800	2.21192100	-0.74763500
N	-1.73895100	-1.28623500	1.66331700
N	-0.64905300	-1.15620600	0.84090700
N	-1.96966700	0.41591800	0.28816900
H	-2.93588300	2.52565400	1.53125700
H	-3.58517400	0.37174100	2.99810300
O	-4.46348300	1.13580900	1.28352900
C	-3.57103200	0.96471300	-1.55838100
H	-4.31513500	1.73619500	-1.78252100
H	-2.87836100	0.88651900	-2.39717200
C	-4.24293900	-0.37363000	-1.35631300
C	-5.56911000	-0.48543300	-0.92922100
C	-3.51997000	-1.54050100	-1.62392000
C	-6.15653700	-1.73625200	-0.75754800
H	-6.13668200	0.41574600	-0.71632500
C	-4.10671600	-2.79366200	-1.45408100
H	-2.49484700	-1.43697500	-1.97628900
C	-5.42538500	-2.89493700	-1.01653500

H	-7.18750200	-1.80681300	-0.42492700
H	-3.54032800	-3.69299700	-1.67822500
H	-5.88430400	-3.86986800	-0.88632400
C	0.40866100	-2.12066500	0.99006100
C	1.22996900	-2.02078400	2.11773000
C	0.52397500	-3.14173400	0.04592200
C	2.23082600	-2.97837200	2.26516800
C	1.55138000	-4.06781900	0.23112300
C	2.41189100	-3.99997200	1.32790900
H	2.89117600	-2.91978500	3.12650900
H	1.67172700	-4.86718400	-0.49508900
C	1.05919300	-0.89289000	3.10003500
H	1.10734600	0.07642900	2.58909800
H	0.08797700	-0.95052100	3.59922600
H	1.84415000	-0.92281900	3.85665100
C	3.53928300	-4.98626600	1.48559100
H	4.46775000	-4.57186800	1.07756700
H	3.71790200	-5.21556000	2.53850000
H	3.32913300	-5.91689700	0.95496500
C	-0.43934200	-3.24887700	-1.10515700
H	-1.46002500	-3.36284700	-0.72593800
H	-0.42650900	-2.35179000	-1.73511600
H	-0.20098200	-4.11541200	-1.72359200
C	0.05828000	0.35196400	-1.24896500
O	-0.68681900	0.12946200	-2.27642100
C	1.49641600	-0.17583100	-1.36672400
H	1.84797700	0.28839200	-2.29521400
H	1.47753500	-1.25470100	-1.53941900
C	1.17706500	2.31310200	-0.19413700
O	0.17445400	1.84623700	-0.98968300
C	2.22358200	1.58074200	0.21925700
C	2.46814300	0.17375000	-0.23268800
H	2.93860100	2.03697200	0.89600800
H	2.30496600	-0.51046300	0.60619300
C	3.89592600	-0.06875100	-0.69265800
C	4.46738700	-1.33386800	-0.52863400
C	4.63845000	0.92650900	-1.33244100
C	5.75425700	-1.59960600	-0.98937700
H	3.89012500	-2.11360000	-0.03424400
C	5.92690300	0.66495800	-1.79267700
H	4.19955100	1.91206000	-1.46725800
C	6.48963400	-0.59862800	-1.62189700
H	6.18471200	-2.58690200	-0.85096000
H	6.49285500	1.44982700	-2.28509100

H	7.49477800	-0.80126000	-1.97775400
C	1.01616500	3.74412300	0.17503200
C	2.14011900	4.56217900	0.34535600
C	-0.25215000	4.30647200	0.34860000
C	1.99785500	5.89856300	0.70354100
H	3.13017400	4.15085700	0.17393300
C	-0.39633400	5.64427000	0.70387100
H	-1.13081300	3.68731700	0.21681200
C	0.72849300	6.44530900	0.88452800
H	2.88032700	6.51850000	0.82612000
H	-1.38939100	6.06049200	0.84015100
H	0.61741300	7.48989800	1.15665500

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C	-2.92943400	-0.03929700	1.27562200
C	-4.26018500	0.50003900	1.72497400
C	-3.61542400	2.48280300	0.61183500
C	-2.65546700	1.80713600	-0.36378000
C	-0.99814200	-0.04335900	0.24920300
H	-5.02241100	-0.27675300	1.63305100
H	-4.07089000	3.35337700	0.13800900
H	-1.78685400	2.43937300	-0.55352900
N	-2.30405000	-1.07865300	1.74970500
N	-1.10085700	-1.06479400	1.09505200
N	-2.16190400	0.62074800	0.35805300
H	-3.08123900	2.80690700	1.51644700
H	-4.16939100	0.78593000	2.78188800
O	-4.67258600	1.59611100	0.94063100
C	-3.32818800	1.40960800	-1.70262600
H	-4.06089700	2.18740100	-1.94056300
H	-2.54069200	1.41963600	-2.45547200
C	-3.99048300	0.05004500	-1.70497100
C	-5.34865500	-0.10857400	-1.41556600
C	-3.22579200	-1.08593700	-1.99804300
C	-5.93051700	-1.37416300	-1.40537000
H	-5.94665800	0.76667600	-1.18024400
C	-3.80838700	-2.35201600	-1.99052000
H	-2.16968000	-0.94920200	-2.22936500
C	-5.16098300	-2.50055000	-1.69024400
H	-6.98685900	-1.48031700	-1.17839700
H	-3.20738200	-3.22512300	-2.22798800
H	-5.61405400	-3.48688200	-1.68463100
C	-0.08913500	-2.01221200	1.48036200
C	0.82108400	-1.62010900	2.46276900

C	-0.06884700	-3.26128100	0.86116300
C	1.80339300	-2.54142800	2.82169600
C	0.93103900	-4.14804800	1.25557400
C	1.87032600	-3.80548400	2.23153900
H	2.53490500	-2.26310400	3.57599200
H	0.98160500	-5.12734400	0.78630300
C	0.75715600	-0.24110800	3.06363300
H	1.52148800	-0.12083100	3.83222500
H	0.91236600	0.52709200	2.29575900
H	-0.22228600	-0.05653900	3.51641700
C	2.92469700	-4.79528300	2.65286800
H	3.27876100	-5.37866200	1.79973900
H	3.77896400	-4.29257400	3.11053600
H	2.51823400	-5.49876900	3.38645900
C	-1.07435700	-3.60337200	-0.20356800
H	-2.09712000	-3.50198100	0.17212100
H	-0.98095000	-2.92410100	-1.05891000
H	-0.93084200	-4.62463800	-0.55903100
C	0.10192100	0.40194800	-0.76027300
O	-0.42127700	0.62077500	-1.91412700
C	1.36179400	-0.47883100	-0.75592100
H	1.11776700	-1.47524700	-1.13978500
H	1.78972600	-0.58608500	0.24646500
C	1.65880300	2.25610800	-0.43085000
O	0.50023800	1.67393200	-0.01968200
C	2.57016600	1.62832600	-1.19227700
C	2.38780400	0.21081600	-1.66663900
H	3.47891500	2.15100200	-1.46919000
H	1.96232600	0.21689100	-2.67924700
C	3.68012100	-0.57892200	-1.69812900
C	3.91979000	-1.49673500	-2.72360800
C	4.63006700	-0.45011700	-0.68016300
C	5.08007600	-2.26780300	-2.73608700
H	3.18726400	-1.60594800	-3.51975400
C	5.79216400	-1.21745500	-0.68912900
H	4.45250900	0.26234400	0.12196300
C	6.02103600	-2.12955300	-1.71796300
H	5.25057500	-2.97444000	-3.54245700
H	6.52146300	-1.10230500	0.10684000
H	6.92728600	-2.72663700	-1.72707400
C	1.80541000	3.63808300	0.09648800
C	2.74162700	4.53839000	-0.42951900
C	0.98952100	4.06152800	1.15289600
C	2.87162600	5.81646000	0.10183700

H	3.36055300	4.24886400	-1.27240500
C	1.12103200	5.34214300	1.68353600
H	0.25316400	3.37503700	1.55616000
C	2.06436900	6.22409000	1.16355700
H	3.59989600	6.50124900	-0.32100600
H	0.48406200	5.65004900	2.50685300
H	2.16690300	7.22270500	1.57574100

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C	-2.01901600	-1.25380700	1.56668800
C	-3.29300900	-1.28831100	2.36150000
C	-3.67472900	0.88216700	1.55195500
C	-2.71765600	0.79664800	0.36343300
C	-0.47432400	-0.43089800	0.18923100
H	-3.73214200	-2.28678900	2.31082400
H	-4.50172500	1.55045600	1.30450700
H	-2.19535000	1.75070100	0.27982100
N	-1.03142700	-2.09124700	1.65540700
N	-0.09603900	-1.56557000	0.79527600
N	-1.72221900	-0.23407000	0.69927100
H	-3.14329500	1.28610300	2.42668400
H	-3.05242000	-1.06202200	3.41024300
O	-4.24268000	-0.37746400	1.85992000
C	-3.38887100	0.48731500	-0.98979100
H	-4.18709900	1.22475300	-1.12764700
H	-2.63182900	0.65553600	-1.76128400
C	-3.93028900	-0.91763800	-1.12860300
C	-5.26328600	-1.22435400	-0.84196700
C	-3.07970300	-1.94601800	-1.54912800
C	-5.73323100	-2.52983800	-0.95337300
H	-5.93289600	-0.43261600	-0.51572300
C	-3.54588800	-3.25542100	-1.65513200
H	-2.05230900	-1.69989600	-1.81095300
C	-4.87335200	-3.55175700	-1.35475100
H	-6.77171700	-2.75104500	-0.72680900
H	-2.87451300	-4.04278000	-1.98612900
H	-5.24001500	-4.56974700	-1.44110700
C	1.17163900	-2.23336100	0.70841900
C	2.06512600	-2.08043000	1.77416600
C	1.43921000	-3.04736500	-0.39452500
C	3.28557200	-2.74847900	1.69368900
C	2.68086100	-3.68360700	-0.43658600
C	3.61485700	-3.54099900	0.59083400
H	4.00101300	-2.63802400	2.50495100

H	2.91749000	-4.31554400	-1.28883400
C	1.71211700	-1.22641300	2.96364400
H	1.29973000	-0.26037400	2.65209300
H	0.95097100	-1.71546000	3.57892000
H	2.59314800	-1.04443900	3.58087200
C	4.96644500	-4.20046400	0.50333600
H	5.70382300	-3.50321200	0.09114500
H	5.32043000	-4.50792600	1.48999400
H	4.93950100	-5.07750700	-0.14652700
C	0.41516800	-3.23945000	-1.48112200
H	-0.54237400	-3.55046500	-1.04922600
H	0.23340800	-2.30901000	-2.03125300
H	0.74453300	-4.00679100	-2.18380500
C	0.12331500	0.44303000	-1.54174400
O	-0.49773500	-0.14223200	-2.43496000
C	1.63682400	0.36420800	-1.46556900
H	1.98248100	0.93105900	-2.34061200
H	1.94709800	-0.67454500	-1.60208800
C	0.29113800	2.51718300	-0.32632500
O	-0.36127500	1.74409600	-1.25554500
C	1.48699700	2.20149800	0.18773400
C	2.25150500	0.96831900	-0.19997300
H	1.93908100	2.87741100	0.90523800
H	2.16542900	0.23288100	0.60922500
C	3.73481400	1.21322200	-0.41190400
C	4.63925500	0.17075600	-0.19140100
C	4.21761300	2.43645700	-0.88259800
C	5.99979000	0.34784800	-0.42815500
H	4.26667100	-0.78573500	0.17043400
C	5.57932200	2.61744100	-1.11761100
H	3.52035100	3.25025400	-1.06475900
C	6.47438700	1.57454300	-0.89018900
H	6.69077900	-0.47013900	-0.24792900
H	5.94124700	3.57500000	-1.47905200
H	7.53506100	1.71674600	-1.07094500
C	-0.48815200	3.73225500	0.01560700
C	-0.22814900	4.45699300	1.18620200
C	-1.51211300	4.16945100	-0.83457700
C	-0.95479800	5.60367100	1.48346700
H	0.53131400	4.11372300	1.88089100
C	-2.24131700	5.31641100	-0.53112500
H	-1.73122200	3.60600800	-1.73510000
C	-1.96320600	6.04025500	0.62515100
H	-0.74121300	6.15116400	2.39571600

H	-3.02841300	5.64422600	-1.20260000
H	-2.53291600	6.93267500	0.86238700

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C	-2.61522600	0.12498200	1.20703000
C	-3.98956500	0.50673200	1.68294200
C	-4.13580500	1.70891300	-0.33859200
C	-3.13523500	0.84437500	-1.10191500
C	-0.89764800	-0.01748400	-0.19785200
H	-4.46852200	-0.35092200	2.16077000
H	-4.88826800	2.10096300	-1.02418900
H	-2.55026400	1.44792700	-1.79849400
N	-1.64377700	-0.33977200	1.93354300
N	-0.59587700	-0.41918600	1.04507200
N	-2.20340600	0.33708800	-0.08246500
H	-3.63071600	2.55270000	0.15486200
H	-3.88627800	1.31232700	2.42294500
O	-4.81935700	0.91380600	0.61549500
C	-3.83538300	-0.29967700	-1.88394900
H	-4.84277100	0.04481000	-2.13844300
H	-3.27564100	-0.43898800	-2.80860300
C	-3.91542100	-1.62470500	-1.16267100
C	-5.01454400	-1.96724000	-0.36935300
C	-2.86695700	-2.54163900	-1.29368400
C	-5.06506100	-3.19776500	0.28173600
H	-5.82950400	-1.25829100	-0.25942700
C	-2.92197300	-3.77761000	-0.65238000
H	-2.01220800	-2.26885900	-1.91075400
C	-4.01888900	-4.10756600	0.14132600
H	-5.92660800	-3.45000800	0.89223200
H	-2.10786400	-4.48626900	-0.77435800
H	-4.06169600	-5.06989000	0.64155700
C	0.67085300	-0.85958300	1.56502200
C	1.41948900	0.03810100	2.33278400
C	1.05818900	-2.18795000	1.36587800
C	2.60611400	-0.43084200	2.89854200
C	2.25794800	-2.60620400	1.94089700
C	3.03636600	-1.74690800	2.71880300
H	3.20528700	0.24898300	3.49953900
H	2.58202100	-3.63299500	1.79064100
C	0.93841800	1.44291300	2.57275400
H	1.75424200	2.07390500	2.93066300
H	0.53402700	1.88468700	1.65893300
H	0.14108500	1.45148200	3.32305500

C	4.29906100	-2.23749100	3.37945400
H	4.72537400	-3.08591100	2.83899100
H	5.04996500	-1.44525800	3.43495500
H	4.09295200	-2.56667900	4.40312200
C	0.18780400	-3.13255900	0.58352300
H	-0.80824300	-3.19815700	1.03203900
H	0.04560500	-2.79109900	-0.44784100
H	0.62619700	-4.13160100	0.55856600
C	-0.10499000	0.18983200	-2.01552500
O	-0.96379400	-0.20548000	-2.80836300
C	1.24787500	-0.52844700	-1.91000100
H	1.25155600	-1.29196000	-2.69279500
H	1.34377400	-1.02645200	-0.94455800
C	0.98970800	2.16988900	-1.17157000
O	-0.01057700	1.62482100	-1.94179200
C	2.20719100	1.61387800	-1.17587100
C	2.44516100	0.42490700	-2.06999100
H	3.00602100	2.00444400	-0.55594800
H	2.46762600	0.77503200	-3.11189300
C	3.73809800	-0.30301500	-1.78119100
C	4.61884500	-0.65079400	-2.80555300
C	4.04439100	-0.68011200	-0.47021200
C	5.78765400	-1.35829300	-2.52694100
H	4.38855100	-0.36495300	-3.82877100
C	5.20939500	-1.38605400	-0.18837900
H	3.35992200	-0.41832400	0.33436600
C	6.08649500	-1.72718400	-1.21778300
H	6.46470500	-1.61933700	-3.33431300
H	5.43233100	-1.66938000	0.83633400
H	6.99662000	-2.27669200	-0.99966600
C	0.57831000	3.36667000	-0.40775900
C	1.52519800	4.23756700	0.14848900
C	-0.77970500	3.62414200	-0.19397300
C	1.11996600	5.31255300	0.93000300
H	2.58266100	4.07823900	-0.03632400
C	-1.18482100	4.70459200	0.58490900
H	-1.51220500	2.96403800	-0.64274200
C	-0.23651900	5.54830200	1.15672600
H	1.86487100	5.97668200	1.35639200
H	-2.24309200	4.88769600	0.74429500
H	-0.54899500	6.39064700	1.76504800