

Supporting Information

Enantioselective Synthesis of Chiral Tetrasubstituted Allenes: Harnessing Electrostatic and Noncovalent Interactions in Bifunctional Activation Model for N-Triflylphosphoramidate Catalysis

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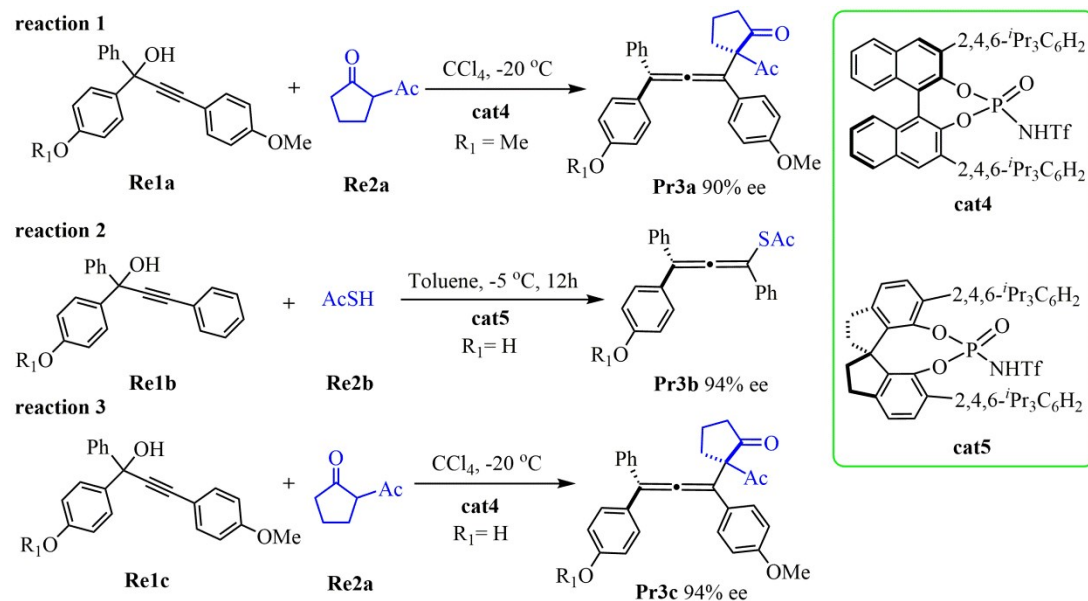
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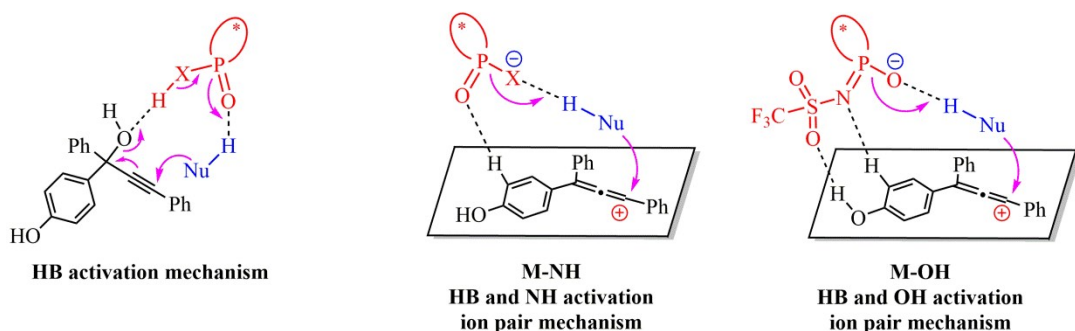
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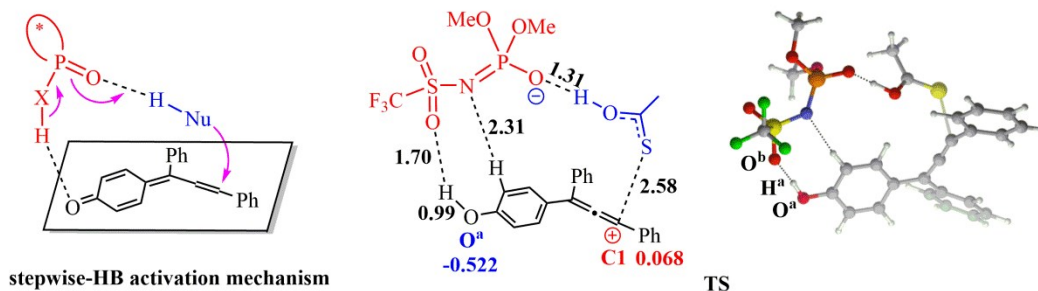
Scheme S1. Enantioselective reactions 1, 2, and 3 for catalytic asymmetric synthesis of chiral tetrasubstituted allenes from recemic propargylic alcohols, and possible activation mechanisms.



Activation Mechanism



The transition state structure of stepwise-HB activation mechanism proposed by Sun et al.



Sun group proposed the hydrogen bonding activation of quinone (denoted as stepwise-HB activation model in Scheme S1) for reactions 2 and 3 with –OH substituted substrate **Re1b/Re1c**. And the H^a shift from substrate **Re1b/Re1c** fragment to S=O group of catalyst and generate neutral complex to activate both of the reactants through the bifunctional model. Then we carefully check the Cartesian coordinate and geometry structure of the C-S bond formation **TS** located by Sun et al., and found that the H^a of the -OH group on the phenyl ring of substrate **Re1c** fragment is not transferred to the S=O group of the catalyst. Because the distance of O^a-H^a and O^b...H^a is 0.99 and 1.70 Å within van der Waals radius, indicating that H^a still connects with O^a and forms a hydrogen bonding with the S=O group of the catalyst. This is consistent with our calculation results that the realistic activation model is the cooperation HB and OH activation ion pair mechanism M-OH (M2-B model is revised to M-OH model) rather than the hydrogen bonding activation mechanism.

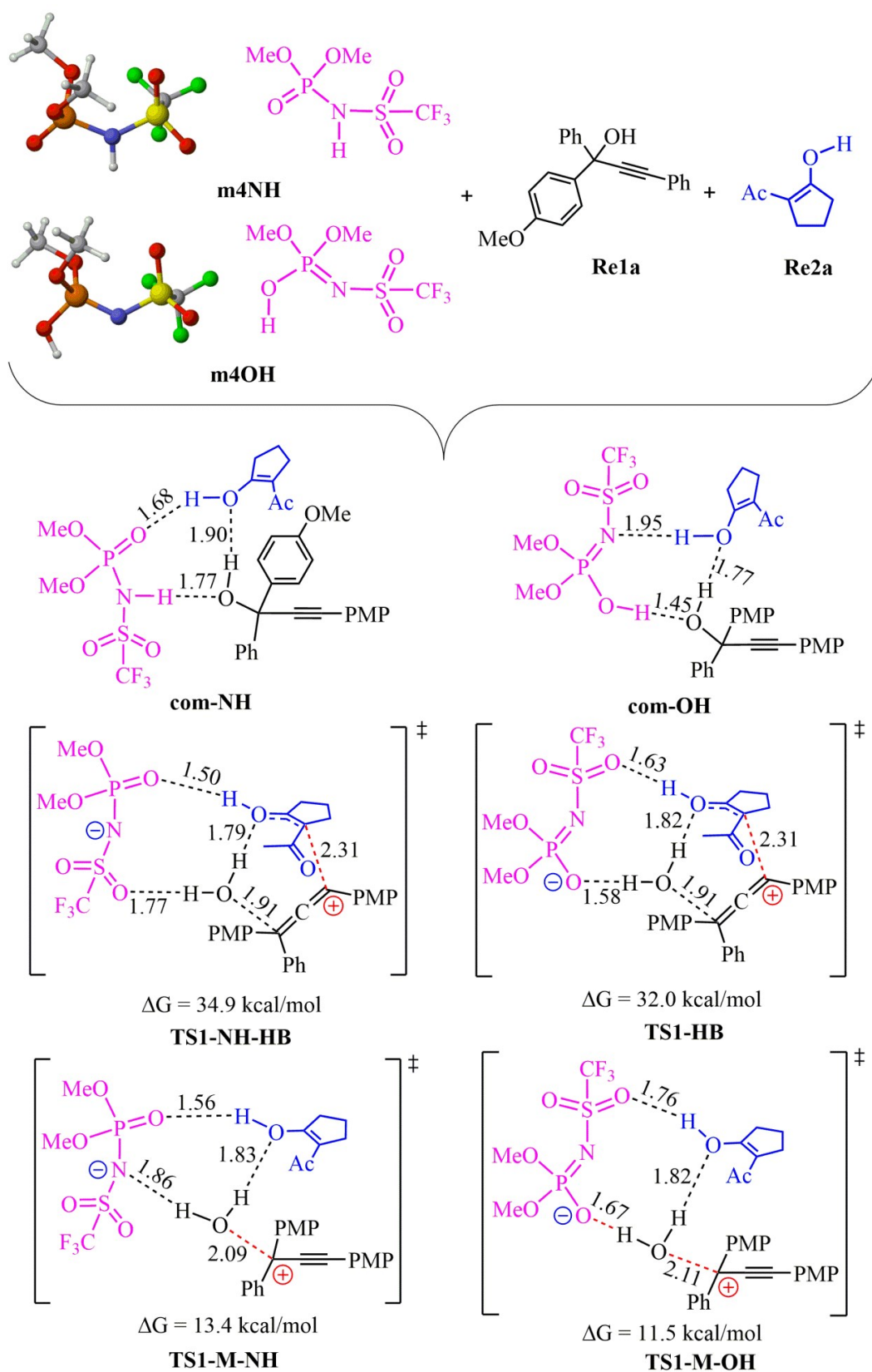


Figure S1. Optimized structures and Gibbs free energies of complexes and transition states for the reaction 1 of alcohol **Re1a**, 1,3-diketone **Re2a** catalyzed by **m4NH** or **m4OH**.

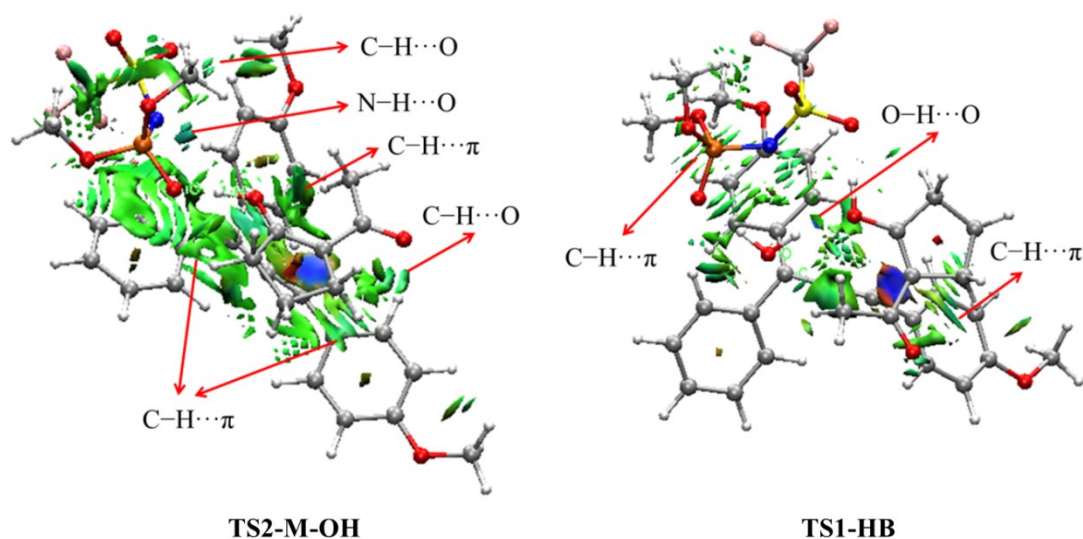


Figure S2. NCI analysis (blue, strong attraction; green, weak interaction; red, strong repulsion) of stereocontrolling TSs for **TS2-M-OH** and **TS1-HB**.

Conformational Analysis

For catalyst **4**, the orientation of the isopropyl group measured as H1-C2-C3-C4 dihedral angle as shown in Figure S1 can either be 0° or 180°, leading to a total of 4 possible conformations for each transition state. For the functional group of N-Triflylphosphoramides, additional conformational possibilities arising due to the dihedral angles differences along the P5-N6-S7-C8 (-180°, 90°, and 180°), which can result in more conformers **NH-I**, **NH-II**, and **NH-III** in NH tautomer and conformers **OH-I**, **OH-II**, and **OH-III** in OH tautomer. Thus, a total of 24 stereochemical possibilities for the catalyst are found for reactions 1 and 2. The energies of these conformations are provided in Table S1.

Scheme S2. Additional conformers for NH tautomer and OH tautomer.

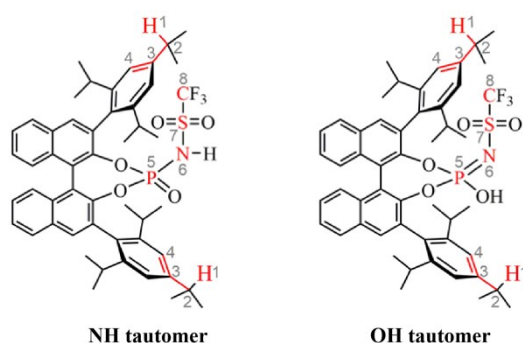


Table S1. Relative Energies (kcal/mol) of different conformation catalysts.

Conformation	G _{rel}
NH-I-1	0.0
NH-I-2	3.3
NH-I-3	4.0
NH-I-4	3.9
NH-II-1	2.9
NH-II-2	0.5
NH-II-3	1.5
NH-II-4	2.0
NH-III-1	2.9
NH-III-2	1.6
NH-III-3	2.1
NH-III-4	2.7
OH-I-1	2.1
OH-I-2	3.0
OH-I-3	3.5
OH-I-4	3.0
OH-II-1	2.9
OH-II-2	2.5
OH-II-3	3.5
OH-II-4	3.3
OH-III-1	2.2
OH-III-2	3.2
OH-III-3	2.9
OH-III-4	2.7

The definition of the activation energy:

The activation energy (ΔE) is the sum of the distortion energy ($\Delta E_{\text{dist}}^{\ddagger} = \Delta E_{\text{dist}}(\text{cat}) + \Delta E_{\text{dist}}(\text{sub})$) and the interaction energy (ΔE_{int}) between the distorted substrates and the catalyst ($\Delta E = \Delta E_{\text{dist}}^{\ddagger} + \Delta E_{\text{int}}$) in the TS structures.

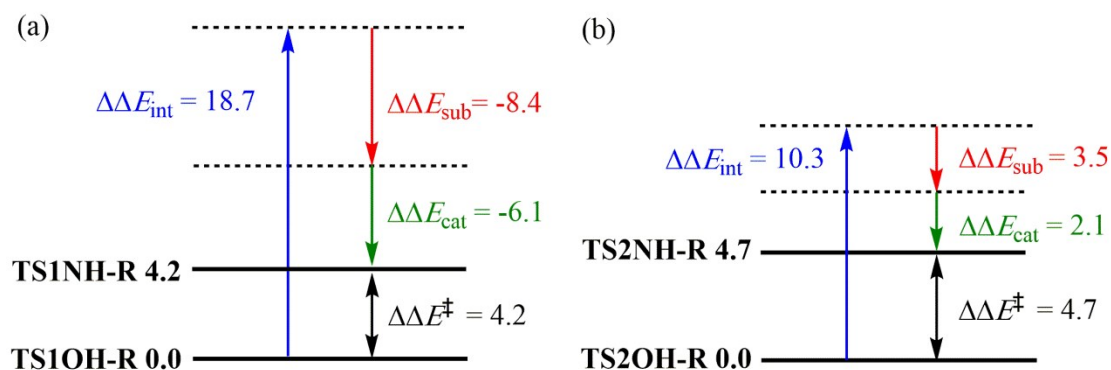


Figure S3. (a) Decomposition of the energy difference between **TS1OH-R** and **TS1NH-R**, (b) analogous decomposition of the energy difference between **TS2NH-R** and **TS2OH-R**. $\Delta E^\ddagger$, into contributions from the difference in energy of the substrate ($\Delta\Delta E_{\text{sub}}$), the difference in energy of the catalyst ($\Delta\Delta E_{\text{cat}}$), and the difference in interaction energies of the substrate with the catalyst ($\Delta\Delta E_{\text{int}}$) in kcal/mol.

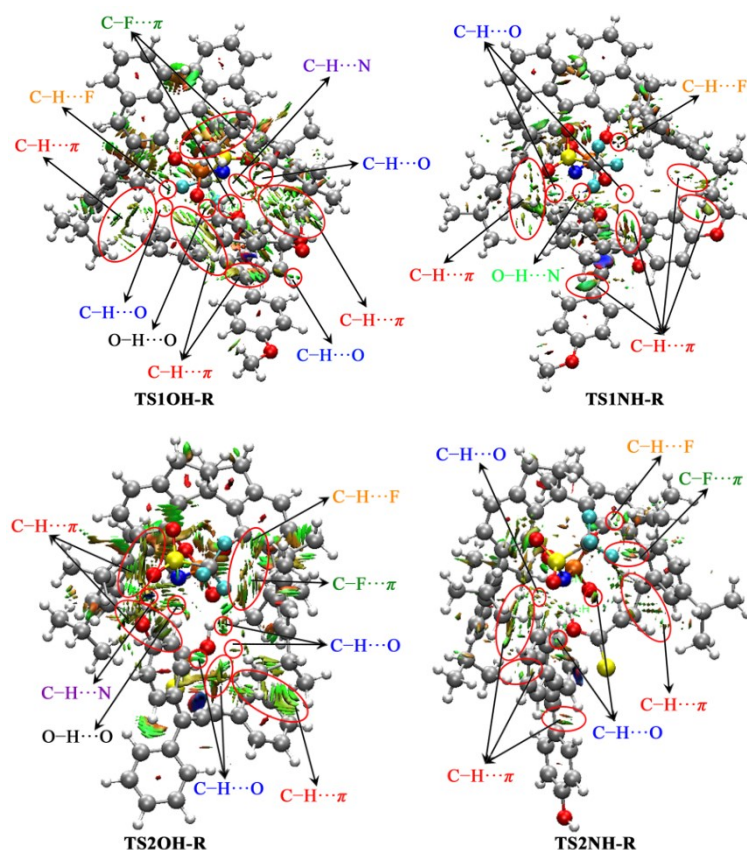


Figure S4. NCI analysis (blue, strong attraction; green, weak interaction; and red, strong repulsion) of stereocontrolling transition states **TS1OH-R**, **TS1NH-R**, **TS2OH-R**, and **TS2NH-R** for reactions 1 and 2.

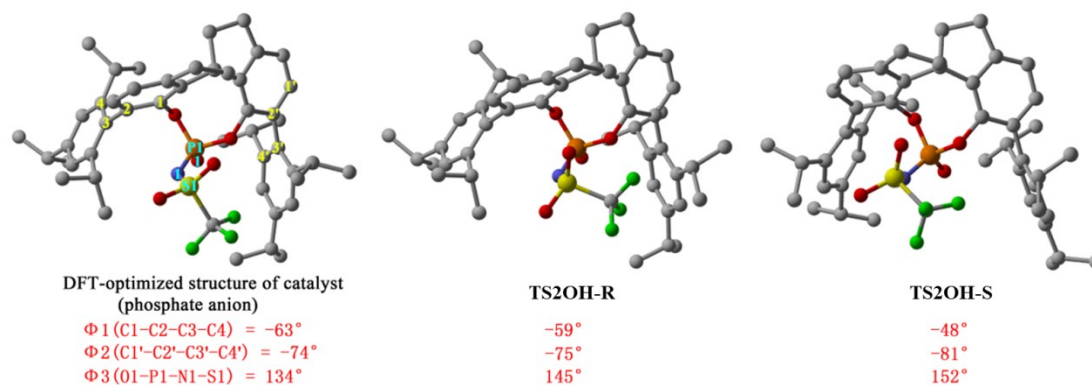


Figure S5. Key angles ($\Phi 1$, $\Phi 2$, and $\Phi 3$) for deprotonated catalyst in TS2OH-R and TS2NH-S. The optimized structure of the free phosphate anion of NTPAA is shown for comparison.

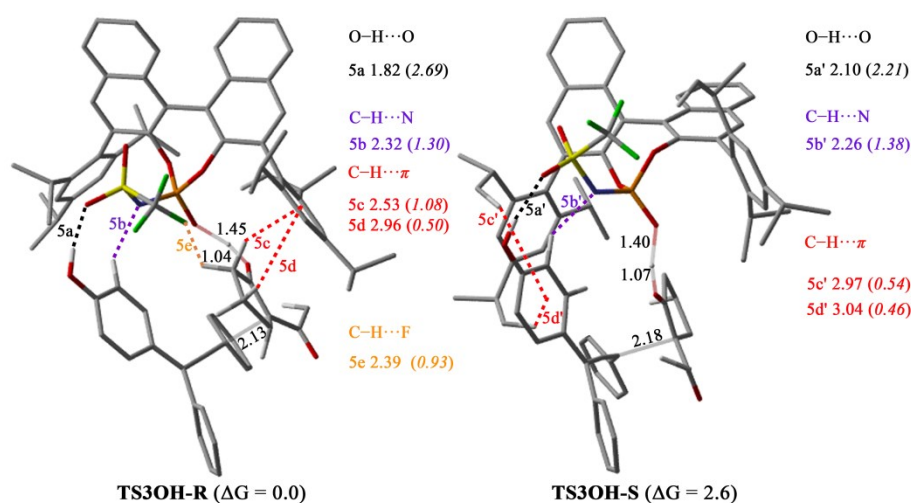


Figure S6. Competing lowest-lying TSs TS3OH-R and TS3OH-S for OH tautomer of reaction 3. All energies are in kcal/mol. Distances are given in Å.

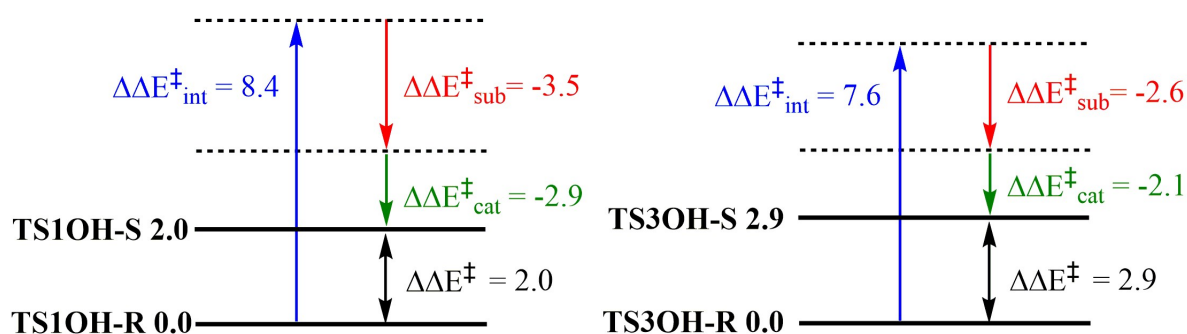


Figure S7. Distortion-interaction analysis for transition states TS1OH-R, TS1OH-S, TS3OH-R, and TS3OH-S.

Table S2. Estimation of Noncovalent Interaction Energies Using Espinosa Equation in the Lower Energy Enantiocontrolling **TS1OH-R** and **TS1OH-S** in model M2OH for reaction 1-1.

Noncovalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho$ -2G	E=1/2 V (kcal/mol)
TS1OH-R							
O-H $\cdots$ O	1a	1.40	0.048	-0.046	0.043	-0.097	-30.6
C-H $\cdots$ N	1b	2.40	0.012	-0.011	0.009	-0.020	-6.5
C-H $\cdots$ O	1c	2.57	0.009	-0.007	0.006	-0.013	-4.3
	1d	2.49	0.010	-0.009	0.008	-0.018	-5.7
	1e	2.55	0.009	-0.008	0.006	-0.014	-4.4
C-H $\cdots\pi$	1f	2.44	0.015	-0.014	0.012	-0.026	-8.1
	1g	2.83	0.006	-0.005	0.004	-0.009	-2.9
	1h	2.54	0.010	-0.009	0.008	-0.018	-5.7
	1i	2.61	0.009	-0.007	0.006	-0.013	-4.3
	1j	2.52	0.011	-0.009	0.008	-0.018	-5.7
C-H $\cdots$ F	1n	2.44	0.009	-0.007	0.006	-0.013	-4.3
total			0.148				-82.5
TS1OH-S							
O-H $\cdots$ O	1a'	1.76	0.029	-0.029	0.028	-0.063	-19.8
C-H $\cdots$ N	1b'	2.33	0.013	-0.011	0.01	-0.022	-7.1
C-H $\cdots$ O	1c'	2.34	0.012	-0.01	0.009	-0.020	-6.4
C-H $\cdots\pi$	1d'	2.42	0.013	-0.011	0.009	-0.020	-6.5
	1e'	2.51	0.012	-0.011	0.011	-0.024	-7.7
	1f'	2.61	0.009	-0.008	0.007	-0.016	-5.0
	1g'	2.52	0.011	-0.01	0.009	-0.020	-6.4
C-H $\cdots$ F	1m'	2.38	0.009	-0.007	0.007	-0.015	-4.9
total			0.108				-63.8

Table S3. Estimation of Noncovalent Interaction Energies Using Espinosa Equation in the Lower Energy Enantiocontrolling **TS1NH-R** and **TS1NH-S** in model A for reaction 1.

Noncovalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho$ -2G	E=1/2 V (kcal/mol)
TS1NH-R							
O–H $\cdots$ N	2a	1.71	0.037	-0.034	0.030	-0.061	-19.1
C–H $\cdots$ O	2b	2.16	0.020	-0.019	0.016	-0.036	-11.5
	2c	2.18	0.019	-0.017	0.015	-0.034	-10.7
C–H $\cdots\pi$	2d	2.59	0.010	-0.009	0.008	-0.018	-5.7
	2e	2.39	0.014	-0.013	0.01	-0.023	-7.3
	2f	2.53	0.011	-0.01	0.009	-0.020	-6.4
total			0.111				-60.7
TS1NH-S							
O–H $\cdots$ N	2a'	1.62	0.039	-0.038	0.036	-0.077	-24.1
C–H $\cdots$ O	2b'	2.33	0.013	-0.011	0.010	-0.022	-7.0
	2c'	2.06	0.022	-0.021	0.020	-0.041	-12.9
C–H $\cdots\pi$	2d'	2.63	0.008	-0.007	0.005	-0.011	-3.7
	2e'	2.61	0.010	-0.009	0.007	-0.016	-5.0
	2f'	2.54	0.011	-0.009	0.008	-0.018	-5.6
total			0.104				-58.3

Table S4. Estimation of Noncovalent Interaction Energies Using Espinosa Equation in the Lower Energy Enantiocontrolling **TS2OH-R** and **TS2OH-S** in oxygen activated model for reaction 2.

Noncovalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho$ -2G	E=1/2 V (kcal/mol)
TS2OH-R							
O–H···O	3a	1.70	0.020	-0.018	0.016	-0.037	-11.5
C–H···N	3b	2.45	0.011	-0.010	0.010	-0.022	-7.1
C–H···O	3c	2.30	0.015	-0.013	0.012	-0.027	-8.5
C–H··· π	3d	2.66	0.009	-0.008	0.007	-0.016	-5.0
	3e	2.78	0.006	-0.005	0.004	-0.009	-2.9
	3f	2.81	0.006	-0.005	0.004	-0.009	-2.9
total			0.067				-36.4
TS2OH-S							
O–H···O	3a'	2.01	0.018	-0.016	0.014	-0.032	-10.0
C–H···N	3b'	2.29	0.013	-0.012	0.011	-0.025	-7.8
C–H···O	3c'	2.37	0.012	-0.010	0.008	-0.019	-5.8
C–H··· π	3d'	2.94	0.005	-0.004	0.003	-0.007	-2.2
	3e'	2.68	0.008	-0.007	0.006	-0.014	-4.3
total			0.056				-31.6

Table S5. Estimation of Noncovalent Interaction Energies Using Espinosa Equation in the Lower Energy Enantiocontrolling **TS2NH-R** and **TS2NH-S** in nitrogen activated model for reaction 2.

Noncovalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	$V=1/4\nabla^2\rho$ -2G	E=1/2 V (kcal/mol)
TS2NH-R							
C–H···O	4a	2.30	0.015	-0.014	0.012	-0.028	-8.6
C–H··· π	4b	2.94	0.005	-0.004	0.004	-0.009	-2.8
	4c	2.90	0.006	-0.006	0.005	-0.012	-3.6
	4d	2.77	0.006	-0.005	0.004	-0.009	-2.9
	4e	2.73	0.008	-0.007	0.006	-0.014	-4.3
total			0.04				-22.2
TS2NH-S							
C–H··· π	4a'	2.99	0.005	-0.004	0.003	-0.007	-2.2
	4b'	3.05	0.005	-0.004	0.002	-0.005	-1.6
total			0.01				-3.8

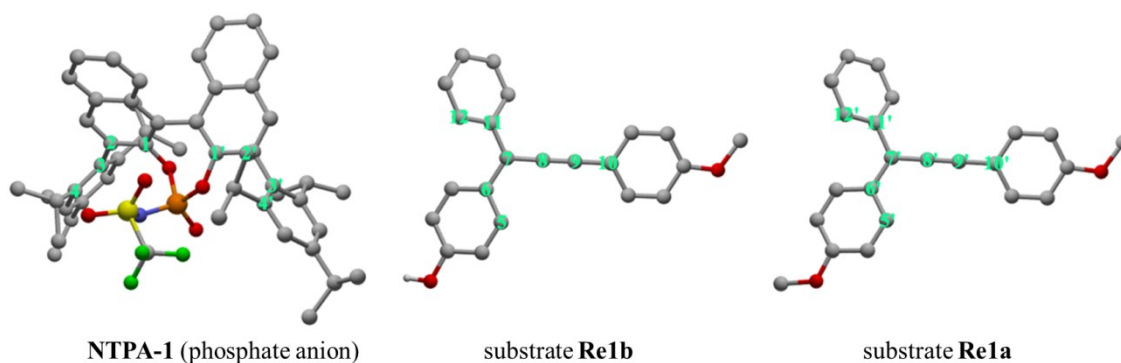


Figure S8. The deprotonated catalyst **NTPAA**, substrates **Re1a** and **Re1b** in transition states.

Table S6. The key changes of dihedral angles in transition states **TS3OH-R**, **TS3OH-S**, **TS1OH-R**, and **TS1OH-S**.

Dihedral angle	TS3OH-R	TS3OH-S	$\Delta\Phi$	TS1OH-R	TS1OH-S	$\Delta\Phi'$
Φ_4 (C1'-C2'-C3'-C4')	110.8	110.6	0.2	118.9	109.8	9.1
Φ_5 (C1-C2-C3-C4)	-59.9	-63.9	4.0	-61.2	-65.3	4.1
Φ_6 (C5-C6-C7-C8/C5'-C6'-C7'-C8')	-134.1	134.6	0.5	-126.5	130.9	4.4
Φ_7 (C7-C8-C9-C10/C7'-C8'-C9'-C10')	166.7	-170.0	3.3	165.5	-171.4	5.9
Φ_8 (C12-C11-C7-C8/C12'-C11'-C7'-C8')	-174.4	173.6	0.8	-177.8	175.1	2.7
$\angle C8-C7-C6/\angle C8'-C7'-C6'$	99.6	96.9	2.7	97.7	93.7	4.0
$\angle C8-C7-C11/\angle C8'-C7'-C11'$	79.6	82.0	2.4	78.6	82.8	4.2

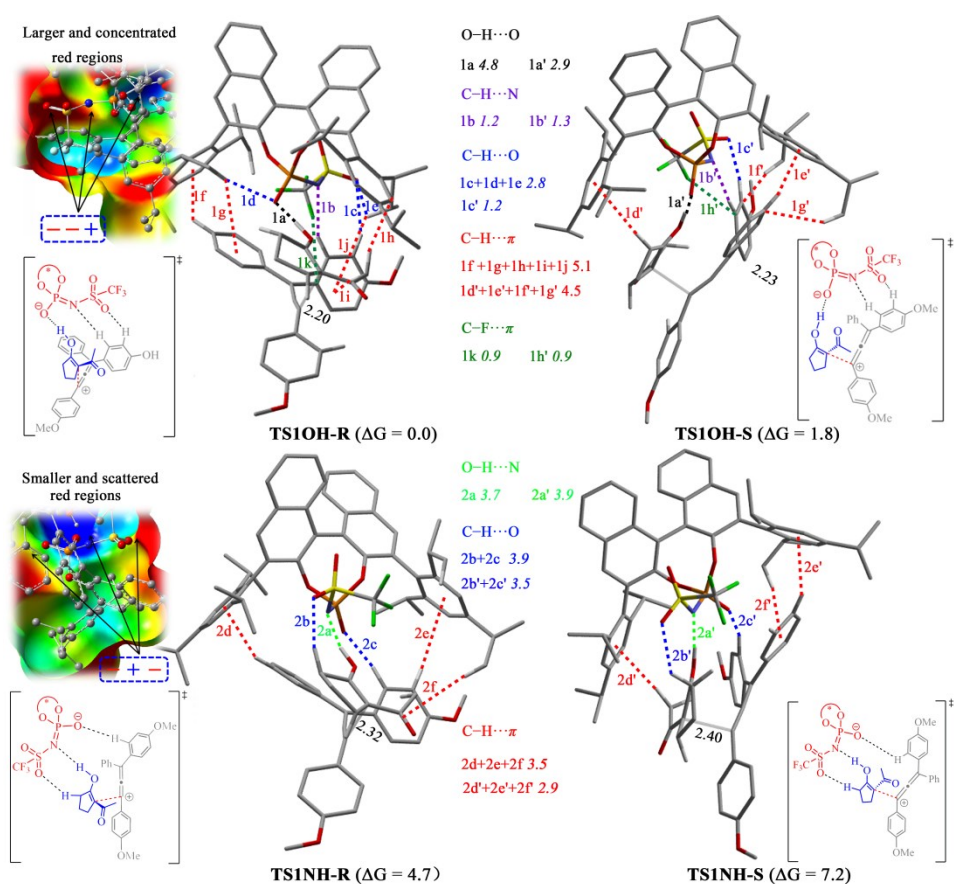


Figure S9. Enantiodetermining TS structures for nitrogen activated model and oxygen activated model of reaction 1. Electron densities ($\rho \times 10^{-2}$ au) at the bond critical points are given in parentheses. The hydrogen atoms that are not involved in any noticeable interaction are removed for improved clarity.

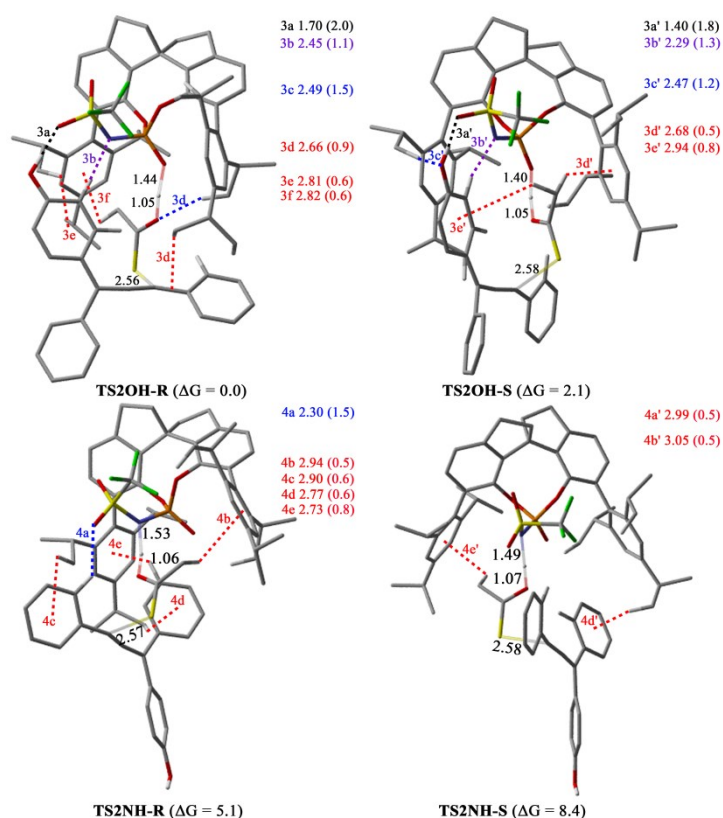


Figure S10. Enantiodetermining TS structures for OH and NH tautomers of reaction 2. The electron densities ($\rho \times 10^{-2}$ au) at the bond critical points are given in parentheses. The hydrogen atoms that are not involved in any noticeable interaction are removed for improved clarity.

S1. The optimized coordinates for key structures in the manuscript.

NH tautomer-I-1

C	1.59669400	6.01058900	1.88803700
C	0.34050300	5.82800900	1.26473300
C	-0.01553800	4.60592100	0.75193500
C	0.86633600	3.49650600	0.84186400
C	2.11934100	3.67612400	1.49066200
C	2.46388300	4.95516500	1.99824200
C	3.02006300	2.58346900	1.58217900
C	2.68267900	1.32777200	1.14643900
C	1.37244300	1.15314200	0.62148600
C	0.52062200	2.19617100	0.33944900
C	-0.70100000	1.97846600	-0.48030700

C	-1.63612800	1.04824800	-0.09971400
C	-2.88707300	0.85455600	-0.74193700
C	-3.13493300	1.62973800	-1.84711000
C	-2.16895000	2.52759900	-2.37067200
C	-0.92943100	2.70390700	-1.69671400
C	0.03823200	3.57091700	-2.27015700
C	-0.22919800	4.24451400	-3.43555200
C	-1.47535100	4.09435900	-4.08675500
C	-2.42124700	3.25171700	-3.56455300
H	3.42961300	5.07745000	2.48140400
H	1.86688700	6.98463100	2.28345800
H	-0.35099400	6.66187800	1.19577400
H	-0.98598300	4.47385600	0.28534000
H	4.02018200	2.75409400	1.97494700
O	0.99974500	-0.15394300	0.29219500
H	1.00312200	3.68453800	-1.78731100
H	0.52567700	4.89543300	-3.86539900
H	-1.67384100	4.63764800	-5.00514600
H	-3.37703500	3.11145700	-4.06244300
O	-1.39094200	0.28961300	1.04238200
H	-4.10055400	1.55743900	-2.33904400
P	-0.27316500	-0.85280100	0.98013900
N	-0.65566200	-1.89090800	-0.30876400
S	0.16417900	-2.04828500	-1.75390700
O	0.27539300	-0.76511500	-2.39986600
O	-0.40139400	-3.21326300	-2.39646300
C	1.88754200	-2.57591300	-1.22128400
F	2.73912500	-1.58971100	-1.39004200
F	1.86823100	-2.95235800	0.05113300
F	2.24003000	-3.60409000	-1.97598000
O	-0.15104500	-1.54533600	2.26288400
C	3.68036300	0.22365400	1.00726000
C	5.39853900	-1.93757600	0.52930400
C	-5.95725600	-1.74648000	0.80559800
C	-3.91010100	-0.08494600	-0.18881900
C	-4.50765500	0.19780000	1.05876800
C	-4.31958400	-1.21339200	-0.92727000
C	-5.34392300	-2.01335900	-0.41289000
H	-5.67530900	-2.88016600	-0.97994600
C	-5.51636800	-0.64010700	1.52913900
H	-5.97939300	-0.41434100	2.48815900
C	5.40681700	-0.82493500	-0.30739100
H	6.06881700	-0.81435700	-1.16781400
C	4.55842300	0.26331100	-0.09486900

C	3. 69503300	-0. 86103500	1. 90064700
C	4. 55536600	-1. 92536000	1. 63973600
H	4. 56143200	-2. 78405100	2. 30681100
C	-4. 13437800	1. 41000100	1. 90097300
C	-3. 66017600	1. 00114700	3. 30002900
C	-5. 30979100	2. 39258400	1. 98190200
H	-4. 46681100	0. 52368000	3. 86721500
H	-3. 33776200	1. 88385800	3. 86193500
H	-2. 82130400	0. 30229800	3. 24169400
H	-5. 02619500	3. 28184600	2. 55451300
H	-6. 17227600	1. 93413600	2. 47801600
H	-5. 62613400	2. 71046500	0. 98348000
C	-7. 06815800	-2. 63372300	1. 33249000
C	-6. 66918800	-3. 30377500	2. 65177800
C	-8. 37650100	-1. 85197800	1. 49395400
H	-6. 50514500	-2. 55454000	3. 43405300
H	-5. 74517600	-3. 87822600	2. 53942900
H	-7. 45881800	-3. 97985600	2. 99572800
H	-9. 18404100	-2. 51441200	1. 82260300
H	-8. 67502800	-1. 38232200	0. 55215400
H	-8. 26634000	-1. 06132800	2. 24439300
C	-3. 70084900	-1. 60458900	-2. 26338500
C	-4. 59590800	-1. 18324000	-3. 43785200
C	-3. 44657500	-3. 11478700	-2. 36116200
H	-4. 75809800	-0. 10327400	-3. 47066200
H	-5. 57670600	-1. 66501400	-3. 35341500
H	-4. 14628000	-1. 48971900	-4. 38801500
H	-2. 82209000	-3. 33793200	-3. 22915300
H	-4. 38558800	-3. 66699200	-2. 47240700
H	-2. 93464300	-3. 50257200	-1. 47536400
C	2. 84562500	-0. 83596700	3. 16002800
C	2. 48038600	-2. 22409300	3. 68559900
C	3. 56567400	-0. 02573800	4. 24787900
H	3. 34981500	-2. 72536300	4. 12678700
H	2. 07199800	-2. 85514400	2. 89235400
H	1. 71563900	-2. 13234800	4. 46156600
H	2. 96390300	0. 00781100	5. 16208700
H	3. 75324500	1. 00242700	3. 92256200
H	4. 53029200	-0. 48736200	4. 48730000
C	6. 19586200	-3. 18827500	0. 21212600
C	5. 33741100	-4. 11541800	-0. 66107300
C	7. 54363700	-2. 91335300	-0. 45614200
H	5. 09634600	-3. 62213200	-1. 61003300
H	4. 39361500	-4. 36080600	-0. 16361400

H	5.86537700	-5.04880600	-0.88368600
H	8.11476000	-3.84239000	-0.54845500
H	8.13794100	-2.19873900	0.12122000
H	7.41353000	-2.51029400	-1.46624900
C	4.54408500	1.41049100	-1.10022700
C	5.91991900	1.69472500	-1.71037300
C	3.51835500	1.15365700	-2.21458900
H	6.22922100	0.90370300	-2.40166600
H	6.69002300	1.79306500	-0.93920900
H	5.88455900	2.62634700	-2.28361800
H	3.47768100	2.00992300	-2.89680900
H	2.51098300	0.98107100	-1.82255600
H	3.80180000	0.26950400	-2.79606400
H	-3.30903500	1.93952200	1.41756300
H	-7.23502100	-3.42297400	0.58813300
H	-2.73784600	-1.08863700	-2.36286700
H	4.23463300	2.31849200	-0.57404900
H	1.90673900	-0.32117200	2.92925900
H	6.38833000	-3.70320700	1.16262300
H	-1.12444500	-2.75470300	-0.03947400

NH tautomer-I-2

C	1.54667800	5.92818200	2.16979900
C	0.27136500	5.76160500	1.58172400
C	-0.07789800	4.57279000	0.99187300
C	0.83029100	3.48130200	0.96561400
C	2.10410100	3.64387000	1.57703000
C	2.44081500	4.88969600	2.16613100
C	3.02812500	2.56739800	1.55864900
C	2.69668800	1.33524100	1.05566700
C	1.37101700	1.16896600	0.56766700
C	0.49067500	2.21121700	0.38702300
C	-0.75988800	2.02485100	-0.39709600
C	-1.66146100	1.05031100	-0.04682500
C	-2.93387300	0.87489500	-0.65111000
C	-3.24700100	1.72608600	-1.68112700
C	-2.32341800	2.68450200	-2.17321800
C	-1.05715600	2.83448000	-1.54358800
C	-0.13456800	3.76700400	-2.08801200
C	-0.47051300	4.52845600	-3.17894800
C	-1.74320400	4.40330100	-3.78267200
C	-2.64582000	3.49746700	-3.29065000
H	3.42135500	4.99911700	2.62175600

H	1. 80983900	6. 87563400	2. 62937400
H	-0. 44048300	6. 58080100	1. 60312400
H	-1. 06324900	4. 45243000	0. 55426600
H	4. 03831700	2. 73183200	1. 92755000
O	1. 00704500	-0. 12186600	0. 17046000
H	0. 84890700	3. 86462500	-1. 64069200
H	0. 25017000	5. 23015800	-3. 58688800
H	-1. 99604500	5. 01575900	-4. 64225000
H	-3. 62093900	3. 37572900	-3. 75478700
O	-1. 36160500	0. 22393100	1. 03252400
H	-4. 23257800	1. 67033600	-2. 13410800
P	-0. 22228900	-0. 88579300	0. 86904700
N	-0. 63205800	-1. 86812800	-0. 45523500
S	0. 16170100	-1. 96637700	-1. 92070300
O	0. 23488700	-0. 66341900	-2. 53160400
O	-0. 39495700	-3. 12330000	-2. 58537100
C	1. 90732300	-2. 47196300	-1. 43986600
F	2. 73420000	-1. 46652400	-1. 61651900
F	1. 93210000	-2. 86895700	-0. 17458000
F	2. 25807600	-3. 48034200	-2. 22255600
O	-0. 03899900	-1. 63860900	2. 10985400
C	3. 70799300	0. 25666800	0. 83445800
C	5. 47071600	-1. 83892500	0. 23849900
C	-5. 86787000	-1. 90860000	0. 84015500
C	-3. 90998700	-0. 12762500	-0. 12440600
C	-4. 47134100	0. 06451300	1. 15670300
C	-4. 30748100	-1. 22611700	-0. 91220200
C	-5. 28797400	-2. 08734900	-0. 41086400
H	-5. 61025600	-2. 93326300	-1. 01338800
C	-5. 43824100	-0. 82970400	1. 61055800
H	-5. 87464700	-0. 67345900	2. 59557700
C	5. 43459300	-0. 69247500	-0. 54954700
H	6. 08818400	-0. 63949400	-1. 41661700
C	4. 56275700	0. 36453600	-0. 28061800
C	3. 76434400	-0. 86641200	1. 67906900
C	4. 64213800	-1. 89998900	1. 35877300
H	4. 67057300	-2. 78285800	1. 99174700
C	-4. 10038000	1. 23458500	2. 05714100
C	-3. 56595100	0. 75511500	3. 41167000
C	-5. 29696900	2. 17717000	2. 23697000
H	-4. 33888900	0. 22051500	3. 97484200
H	-3. 24767700	1. 61072800	4. 01624600
H	-2. 71092200	0. 08573100	3. 28204300
H	-5. 01651700	3. 03919400	2. 85125800

H	-6.12878200	1.66633000	2.73404400
H	-5.65695000	2.54372400	1.27050100
C	-6.92845600	-2.86285700	1.35353800
C	-6.46241500	-3.58338200	2.62347300
C	-8.25891000	-2.14143900	1.59511800
H	-6.30373300	-2.86951100	3.43928500
H	-5.52032300	-4.11256200	2.45362700
H	-7.21335100	-4.30846400	2.95407400
H	-9.02850900	-2.85003700	1.91859600
H	-8.60752000	-1.64133800	0.68682200
H	-8.15292900	-1.38219100	2.37792300
C	-3.72042000	-1.51662800	-2.28793400
C	-4.65155800	-1.02593100	-3.40592400
C	-3.44996900	-3.01203400	-2.49899400
H	-4.82681500	0.05125700	-3.35707600
H	-5.62385100	-1.52610200	-3.33027200
H	-4.22386500	-1.25702900	-4.38705000
H	-2.84388400	-3.16292600	-3.39538100
H	-4.38418700	-3.56836900	-2.62881900
H	-2.91138000	-3.45507400	-1.65605800
C	2.94690600	-0.91459400	2.95880800
C	2.62030000	-2.33197900	3.42960700
C	3.68305200	-0.14402400	4.06472000
H	3.50727300	-2.83100000	3.83723500
H	2.21495100	-2.93868200	2.61617900
H	1.86517500	-2.29067100	4.21913800
H	3.10220800	-0.15787200	4.99285900
H	3.85199500	0.89956800	3.78137500
H	4.65793800	-0.60432900	4.26127000
C	6.33988200	-3.01736600	-0.15427000
C	7.22094000	-3.51360100	0.99510700
C	5.46017400	-4.15063500	-0.69819800
H	6.61440200	-3.91487200	1.81408700
H	7.83889300	-2.70557400	1.39747700
H	7.88180200	-4.31588500	0.65119100
H	6.07056600	-4.99799700	-1.02799000
H	4.85678600	-3.80900600	-1.54481100
H	4.77403200	-4.50771700	0.07865300
C	4.50138800	1.55483600	-1.23209700
C	5.85296900	1.88996300	-1.86922600
C	3.44658000	1.33142100	-2.32649700
H	6.15384800	1.13545000	-2.60368600
H	6.64441300	1.96877600	-1.11755600
H	5.78435100	2.84519400	-2.39900800

H	3.37668900	2.21483100	-2.97063400
H	2.45281600	1.13017000	-1.91388700
H	3.72380400	0.47592800	-2.95180400
H	-3.30652800	1.81487500	1.57892200
H	-7.09047800	-3.61988700	0.57533300
H	-2.76583200	-0.98259600	-2.37581900
H	4.19427900	2.43281300	-0.65575200
H	1.99354600	-0.40701100	2.77885200
H	6.99973100	-2.68224800	-0.96522700
H	-1.07906300	-2.74993000	-0.20739200

NH tautomer-I-3

C	-1.80095100	5.96453200	-1.99327600
C	-0.50535400	5.82338500	-1.44445500
C	-0.09961100	4.62828900	-0.90602700
C	-0.96908100	3.50533600	-0.89370000
C	-2.26398900	3.64335300	-1.46546800
C	-2.65861500	4.89576100	-2.00271000
C	-3.15187800	2.53653000	-1.45352100
C	-2.76666200	1.30267900	-0.99489300
C	-1.42211900	1.16540400	-0.55234700
C	-0.57109200	2.23037700	-0.36576300
C	0.70587800	2.06327100	0.37827200
C	1.62961400	1.13223900	-0.02715500
C	2.92282300	0.98109800	0.53895600
C	3.23317100	1.80915500	1.58871700
C	2.29071200	2.71793500	2.13629500
C	1.00431800	2.84443900	1.54366800
C	0.06351000	3.72343800	2.14291700
C	0.39976700	4.45717900	3.25250900
C	1.69097300	4.35671500	3.82044600
C	2.61266300	3.50272900	3.27393700
H	-3.65433500	4.98650400	-2.42847200
H	-2.10974400	6.91737300	-2.41145800
H	0.17654000	6.66780900	-1.45456500
H	0.90058000	4.52795500	-0.49809400
H	-4.17792100	2.67867900	-1.78617500
O	-1.00667300	-0.12424400	-0.20552500
H	-0.93375000	3.80098600	1.72273500
H	-0.33450000	5.11805000	3.70237800
H	1.94368700	4.94726500	4.69525200
H	3.60259900	3.39981000	3.71047800
O	1.32403800	0.33023700	-1.12354000

H	4. 23131300	1. 77331100	2. 01524900
P	0. 23128800	-0. 82476500	-0. 95495400
N	0. 71797400	-1. 81481300	0. 33627300
S	-0. 02430600	-1. 96353200	1. 82430800
O	-0. 12898200	-0. 67222100	2. 45481600
O	0. 59901400	-3. 10483600	2. 45555900
C	-1. 76360100	-2. 53304400	1. 39040600
F	-2. 62680500	-1. 57474900	1. 64094400
F	-1. 82362000	-2. 88208700	0. 11238300
F	-2. 03539400	-3. 58627100	2. 14459200
O	0. 03818700	-1. 55643800	-2. 20685200
C	-3. 73619700	0. 18864600	-0. 76357700
C	-5. 41198100	-1. 97194000	-0. 14991800
C	5. 88234000	-1. 68060700	-1. 11818100
C	3. 91583200	0. 02626500	-0. 04271300
C	4. 42845000	0. 26531900	-1. 33302600
C	4. 36975700	-1. 08277600	0. 70457500
C	5. 35100500	-1. 90509000	0. 15035200
H	5. 70829500	-2. 75618500	0. 72507500
C	5. 40255600	-0. 59545900	-1. 84213300
H	5. 80578700	-0. 40977200	-2. 83601800
C	-5. 37982600	-0. 84255100	0. 66241400
H	-6. 00063600	-0. 82846300	1. 55472100
C	-4. 55062600	0. 24634100	0. 38508400
C	-3. 78915500	-0. 91797000	-1. 62943900
C	-4. 62445300	-1. 98373200	-1. 30120200
H	-4. 64921100	-2. 85381700	-1. 95176600
C	4. 00182100	1. 44924400	-2. 18903500
C	3. 44830200	0. 99574800	-3. 54461600
C	5. 16636800	2. 43139600	-2. 36774900
H	4. 22461600	0. 51204900	-4. 14766300
H	3. 08051700	1. 85877100	-4. 10937000
H	2. 62331700	0. 28961000	-3. 41560000
H	4. 84817900	3. 30027200	-2. 95335300
H	6. 00201700	1. 95817900	-2. 89472500
H	5. 53537800	2. 78345300	-1. 39928100
C	6. 93962600	-2. 60158500	-1. 69572900
C	8. 20492300	-2. 61711600	-0. 83084800
C	6. 39370500	-4. 02134800	-1. 88556600
H	7. 99324600	-3. 02600500	0. 16340200
H	8. 60746400	-1. 60837400	-0. 70106200
H	8. 97761800	-3. 24225800	-1. 29034300
H	7. 14736200	-4. 66692300	-2. 34840700
H	5. 50221100	-4. 01971400	-2. 51933800

H	6.12052500	-4.46373000	-0.92090700
C	3.83884300	-1.42230800	2.09203600
C	4.79025400	-0.92435200	3.18982200
C	3.62706200	-2.93031200	2.27994200
H	4.93115900	0.15841000	3.15859400
H	5.77445100	-1.39203700	3.07231800
H	4.40228200	-1.18902000	4.17890400
H	3.05650300	-3.12030100	3.19186400
H	4.58373000	-3.45598500	2.36839000
H	3.07656900	-3.37546500	1.44575000
C	-3.01173100	-0.91598200	-2.93468000
C	-2.66253400	-2.31347200	-3.44692100
C	-3.80130300	-0.14100900	-3.99974100
H	-3.54796400	-2.82726100	-3.83937300
H	-2.21779100	-2.92712700	-2.65955400
H	-1.93244500	-2.23490900	-4.25683400
H	-3.24985700	-0.11967400	-4.94553200
H	-3.98735600	0.89151000	-3.68789000
H	-4.77005800	-0.62182600	-4.17645100
C	-6.22698300	-3.18647400	0.24920000
C	-7.13266500	-3.69001500	-0.87767400
C	-5.28892800	-4.29945900	0.73487400
H	-6.54310000	-4.05170000	-1.72693900
H	-7.79355500	-2.89687600	-1.23932900
H	-7.75122200	-4.52293400	-0.52798700
H	-5.85684300	-5.17610300	1.06401700
H	-4.66852200	-3.95586800	1.56831200
H	-4.61865200	-4.61185000	-0.07443600
C	-4.48676500	1.41560900	1.36209600
C	-5.82497100	1.70238800	2.04939000
C	-3.39269400	1.19102000	2.41717100
H	-6.08368300	0.92327700	2.77415900
H	-6.64164000	1.77889200	1.32497000
H	-5.76263600	2.64618100	2.60002400
H	-3.32032400	2.06123300	3.07883400
H	-2.40859500	1.01986600	1.96920900
H	-3.63285600	0.31634200	3.03121800
H	3.20338800	1.99106300	-1.67483300
H	7.21048100	-2.20839700	-2.68415000
H	2.87030500	-0.92333500	2.22335000
H	-4.21822500	2.31359400	0.79761300
H	-2.06637400	-0.38765000	-2.77173900
H	-6.86641600	-2.89062200	1.09104800
H	1.19646900	-2.67193400	0.06222200

NH tautomer-I-4

C	-1.81720200	6.02056400	-1.74219600
C	-0.54503100	5.85995700	-1.14576800
C	-0.14397600	4.63668500	-0.67079900
C	-0.99498200	3.50421800	-0.77353900
C	-2.26560800	3.66292000	-1.39269800
C	-2.65599600	4.94351800	-1.86264000
C	-3.13705700	2.54644500	-1.49117000
C	-2.75417600	1.29114900	-1.09381800
C	-1.42614000	1.14200700	-0.60507200
C	-0.60056000	2.20242500	-0.31316300
C	0.64349400	2.00020000	0.47528400
C	1.60005600	1.11377500	0.04826700
C	2.87023700	0.94250300	0.65940300
C	3.11244900	1.68732700	1.78676100
C	2.12770500	2.53627700	2.35621400
C	0.87156100	2.69512800	1.70855300
C	-0.11246000	3.51389300	2.32345100
C	0.15438000	4.16131600	3.50328300
C	1.41615600	4.03108600	4.12879400
C	2.37806700	3.23331700	3.56689100
H	-3.63320100	5.04922500	-2.32597900
H	-2.12205800	6.99538600	-2.10910800
H	0.12278000	6.71200900	-1.06802900
H	0.83834600	4.52197000	-0.22505900
H	-4.15037700	2.69816200	-1.85669900
O	-1.00656900	-0.16091400	-0.32073000
H	-1.08769900	3.61143500	1.85842600
H	-0.61252700	4.77500000	3.96514600
H	1.61368200	4.55392800	5.05909200
H	3.34581900	3.10890700	4.04532100
O	1.35181400	0.38253400	-1.11117300
H	4.08866400	1.63246700	2.25948500
P	0.27628000	-0.80000400	-1.04963900
N	0.72824700	-1.84728300	0.20804600
S	-0.01719000	-2.02063500	1.69030900
O	-0.12194900	-0.73893500	2.34083500
O	0.60227300	-3.17323100	2.30481500
C	-1.75472900	-2.57804200	1.23648900
F	-2.61659000	-1.61884900	1.48889000
F	-1.80244300	-2.91202500	-0.04645000
F	-2.03882500	-3.63883200	1.97425300

O	0.14910600	-1.47295900	-2.34222600
C	-3.71097800	0.15123500	-0.95572800
C	-5.31706000	-2.09378400	-0.47258500
C	5.96973000	-1.48931100	-1.09651300
C	3.91163500	0.06520900	0.04143100
C	4.45259800	0.41700700	-1.21191200
C	4.38695400	-1.07937200	0.71862600
C	5.41282000	-1.82411200	0.13601900
H	5.78692200	-2.70034700	0.66006600
C	5.46972700	-0.37087100	-1.75341300
H	5.89331700	-0.09723400	-2.71784900
C	-5.35554700	-0.99529200	0.38202700
H	-5.99758500	-1.02724200	1.25708700
C	-4.56474600	0.13535700	0.16611600
C	-3.70036100	-0.91887800	-1.86744600
C	-4.50439600	-2.02567800	-1.60364700
H	-4.48905900	-2.87265600	-2.28527000
C	4.01638400	1.64968700	-1.99190900
C	3.50561100	1.28289700	-3.39007500
C	5.16141400	2.66778600	-2.07291200
H	4.30694800	0.86004700	-4.00570900
H	3.13218100	2.17629700	-3.90116900
H	2.69435500	0.55224900	-3.33280200
H	4.83297600	3.57114000	-2.59734700
H	6.01717300	2.25492800	-2.61786000
H	5.50462900	2.95342500	-1.07370300
C	7.07984700	-2.32470400	-1.70448000
C	8.32352700	-2.33929900	-0.80880500
C	6.60402800	-3.75212500	-1.99773400
H	8.10424500	-2.81475500	0.15352500
H	8.67812900	-1.32407800	-0.60893900
H	9.13361700	-2.90286500	-1.28296900
H	7.39706300	-4.33212100	-2.48089000
H	5.72846300	-3.74892400	-2.65325200
H	6.32903400	-4.26737400	-1.07071800
C	3.83498600	-1.53881500	2.06257500
C	4.76284700	-1.12425800	3.21394900
C	3.63443000	-3.05906200	2.11820300
H	4.90000200	-0.04160000	3.26697200
H	5.75152000	-1.57817200	3.08103600
H	4.35729500	-1.46457700	4.17222300
H	3.06170500	-3.33138200	3.00754000
H	4.59448200	-3.58386100	2.16286600
H	3.09007300	-3.43226700	1.24563900

C	-2.88658200	-0.83150500	-3.14725300
C	-2.49132300	-2.19120200	-3.72285900
C	-3.66179200	-0.01425100	-4.19116800
H	-3.35649000	-2.70948900	-4.15233400
H	-2.03751600	-2.82913400	-2.96043200
H	-1.75470400	-2.05203400	-4.51859700
H	-3.08448400	0.07054000	-5.11766200
H	-3.87772900	0.99525600	-3.82769500
H	-4.61473900	-0.50307400	-4.42269300
C	-6.05282200	-3.38204400	-0.15657500
C	-5.14767400	-4.27348500	0.70637400
C	-7.40762100	-3.17191400	0.52142900
H	-4.92513600	-3.77533200	1.65728300
H	-4.19624900	-4.47166600	0.20291400
H	-5.63060500	-5.23156800	0.92587400
H	-7.93854200	-4.12502000	0.60675000
H	-8.03466500	-2.47667800	-0.04451300
H	-7.28897400	-2.77525400	1.53539000
C	-4.58989700	1.27489300	1.18064800
C	-5.96929200	1.48882200	1.81158800
C	-3.53753000	1.06443700	2.27973700
H	-6.23029700	0.68011500	2.50212500
H	-6.75404700	1.55437600	1.05185300
H	-5.97043500	2.41788100	2.38999200
H	-3.52649900	1.92071600	2.96303500
H	-2.52905300	0.93901300	1.87273600
H	-3.77222400	0.16772200	2.86342500
H	3.19502900	2.13716100	-1.46004600
H	7.35534000	-1.85728400	-2.65851400
H	2.86032700	-1.06019900	2.21845100
H	-4.33340900	2.19996900	0.65642300
H	-1.95881000	-0.29323000	-2.92600900
H	-6.22760600	-3.90025300	-1.10846700
H	1.20639600	-2.69729100	-0.08683300

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C	3.96068600	5.34360600	2.13537200
C	2.58640800	5.66986300	2.06003300
C	1.69516700	4.80892100	1.47157000
C	2.13050500	3.57164400	0.92631500
C	3.50541400	3.22262000	1.04631000
C	4.40511600	4.14447800	1.64380800
C	3.95579000	1.94654200	0.61493400

C	3.09057700	1.00133600	0.12419100
C	1.73875200	1.40411700	-0.03697700
C	1.23494800	2.64368900	0.29661500
C	-0.19063700	2.95393600	-0.00828400
C	-1.18259800	2.06026000	0.33267500
C	-2.55081000	2.19765400	-0.04045000
C	-2.92290300	3.38055100	-0.62318700
C	-1.96420400	4.36133000	-0.98957800
C	-0.57991000	4.11844500	-0.75878100
C	0.35958300	5.03111200	-1.30993500
C	-0.05690700	6.14915900	-1.98785100
C	-1.43387800	6.42003100	-2.15871700
C	-2.36403200	5.53714100	-1.67706600
H	5.45346600	3.86822700	1.71794200
H	4.65573200	6.03729200	2.59751300
H	2.23295500	6.60712500	2.47799900
H	0.64169400	5.06406400	1.42760100
H	5.00866900	1.70105600	0.72210900
O	0.86487100	0.44714600	-0.56685700
H	1.41935100	4.83357500	-1.19941500
H	0.67987600	6.82895400	-2.40380700
H	-1.74814900	7.31325000	-2.68893900
H	-3.42598700	5.71045500	-1.82947300
O	-0.88429800	0.94831600	1.11475700
H	-3.96548300	3.54344500	-0.88609900
P	0.01046800	-0.27132600	0.58728400
N	-1.08182500	-1.22449700	-0.26629200
S	-0.83651500	-2.82724200	-0.59419000
O	0.50186000	-3.01570200	-1.09936000
O	-2.02807900	-3.27215700	-1.28533200
C	-0.88160500	-3.63677700	1.08804100
F	0.33664900	-3.79925100	1.55631100
F	-1.60393500	-2.90008400	1.92282500
F	-1.46324700	-4.81998700	0.94071600
O	0.72743100	-0.99677100	1.63634400
C	3.47923000	-0.40905600	-0.18237800
C	4.08002900	-3.10247900	-0.73222500
C	-4.65876800	-1.54768100	0.14202700
C	-3.42990600	0.99021000	0.04530500
C	-3.73341100	0.39753100	1.28502300
C	-3.79241800	0.33657800	-1.16307800
C	-4.39076300	-0.92076400	-1.07808300
H	-4.63026100	-1.45951900	-1.99083500
C	-4.34719300	-0.85912300	1.31008700

H	-4.55989000	-1.31563800	2.27250600
C	3.70026900	-2.23251700	-1.75106000
H	3.61839100	-2.60683400	-2.76905500
C	3.39205000	-0.89697300	-1.50166100
C	3.85112800	-1.27275800	0.86913500
C	4.15671700	-2.59900000	0.56215100
H	4.43843400	-3.27586300	1.36546000
C	-3.44229400	1.09814700	2.60238100
C	-2.71678400	0.19699400	3.60726900
C	-4.75053800	1.63622300	3.19845000
H	-3.35776500	-0.62449900	3.94486100
H	-2.43881100	0.77720100	4.49269500
H	-1.80511100	-0.23158700	3.18150400
H	-4.55422100	2.17374500	4.13177300
H	-5.44178400	0.81507500	3.41869400
H	-5.24901800	2.31931100	2.50376000
C	-5.31032500	-2.91775000	0.13348800
C	-5.00591200	-3.75281200	1.37641800
C	-6.82637700	-2.76961400	-0.05821800
H	-5.47326400	-3.32558300	2.27061600
H	-3.93031300	-3.82977500	1.55384900
H	-5.40492000	-4.76381100	1.25244300
H	-7.30619600	-3.75177300	-0.11851200
H	-7.06046000	-2.21468000	-0.97174100
H	-7.26295400	-2.22637400	0.78736100
C	-3.44190100	0.89240600	-2.54236100
C	-4.41218300	0.44306100	-3.63927600
C	-2.00399200	0.51599900	-2.93098800
H	-5.45511000	0.59562900	-3.34498600
H	-4.27804600	-0.61318800	-3.89353000
H	-4.22372100	1.01927600	-4.54991500
H	-1.76048100	0.91685900	-3.92029900
H	-1.89394400	-0.57481600	-2.97009600
H	-1.26602100	0.90572000	-2.22112500
C	3.91971300	-0.82919300	2.32436500
C	3.30055300	-1.85307300	3.28423000
C	5.37141900	-0.54830000	2.73727700
H	3.92365400	-2.74962500	3.37383000
H	2.30341300	-2.14488500	2.95048000
H	3.22065300	-1.41472500	4.28452400
H	5.41808900	-0.21003200	3.77800000
H	5.84069000	0.21335100	2.10758300
H	5.97113000	-1.46161200	2.65032300
C	4.31548700	-4.57664000	-0.99529400

C	2.96872800	-5.29339600	-1.16154200
C	5.22238600	-4.83106900	-2.20212300
H	2.43471900	-4.90277200	-2.03452100
H	2.32853600	-5.12860700	-0.28985200
H	3.11535600	-6.37062500	-1.29689000
H	5.43208800	-5.90094400	-2.30162800
H	6.17381700	-4.29987400	-2.10441400
H	4.74552300	-4.50355300	-3.13204600
C	2.98761400	-0.02004200	-2.67763100
C	4.17626100	0.19351600	-3.62371300
C	1.78486700	-0.60026400	-3.43206700
H	4.51475100	-0.75994200	-4.04371600
H	5.02156400	0.64701600	-3.09687200
H	3.89468900	0.84815600	-4.45540700
H	1.44260500	0.10428000	-4.19811700
H	0.95681900	-0.80800400	-2.74897200
H	2.04718000	-1.53702900	-3.93527100
H	-2.79641900	1.95770600	2.39833600
H	-4.90385900	-3.45024500	-0.73591800
H	-3.49564300	1.98231000	-2.49797700
H	2.69715700	0.96512700	-2.29963400
H	3.34188300	0.09443000	2.42627200
H	4.81233500	-4.99013400	-0.10784200
H	-2.05177300	-0.91855000	-0.39407900

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C	3.51792700	5.59212300	2.20716700
C	2.11910700	5.79971300	2.17505900
C	1.29110100	4.88718300	1.57216400
C	1.81791000	3.71448200	0.96811000
C	3.22046300	3.48260900	1.04371500
C	4.05182800	4.45601600	1.65825700
C	3.76866100	2.26885500	0.55006700
C	2.97652100	1.27149400	0.03958800
C	1.59096600	1.55953600	-0.07331700
C	0.99028100	2.73634600	0.32155400
C	-0.46436800	2.93071100	0.06168000
C	-1.36466500	1.94036100	0.38930900
C	-2.74876800	1.96912800	0.05224500
C	-3.23838400	3.13441700	-0.47659800
C	-2.37948700	4.20992800	-0.82452700
C	-0.97382200	4.08326900	-0.63320900
C	-0.13278400	5.09669500	-1.16700400

C	-0.66321900	6.19830600	-1.78993800
C	-2.06256600	6.35121700	-1.92045200
C	-2.89870200	5.37075000	-1.45548400
H	5.12166000	4.26984900	1.69841900
H	4.16191000	6.32570100	2.68148800
H	1.69657800	6.68587900	2.63795400
H	0.21871400	5.05060900	1.56144500
H	4.84144200	2.11345000	0.62249900
O	0.78964900	0.54997900	-0.62046400
H	0.94268500	4.99044000	-1.08716700
H	-0.00004700	6.95686500	-2.19337800
H	-2.46786400	7.23247100	-2.40713200
H	-3.97525800	5.45413100	-1.57825100
O	-0.94961600	0.83102900	1.12010100
H	-4.29759000	3.21346900	-0.70994500
P	0.03518000	-0.28387600	0.52588000
N	-0.98820100	-1.30525500	-0.33427400
S	-0.61549800	-2.87675200	-0.69523900
O	0.72167200	-2.94243300	-1.23404400
O	-1.78000900	-3.41067800	-1.36913300
C	-0.55321800	-3.71703700	0.97198300
F	-1.04310600	-4.93992600	0.81325800
F	0.68424600	-3.79099400	1.40828100
F	-1.31248300	-3.05616300	1.83707700
O	0.84380500	-0.97827500	1.52830600
C	3.47934300	-0.08408300	-0.34000800
C	4.29551200	-2.68760100	-1.02570800
C	-4.50435800	-1.95606200	0.15127600
C	-3.51435200	0.68548700	0.11465700
C	-3.73108700	0.02789900	1.33959500
C	-3.84728200	0.04121300	-1.10711500
C	-4.32547000	-1.26820400	-1.05236500
H	-4.53809300	-1.79670300	-1.97769600
C	-4.22738000	-1.27983800	1.33508500
H	-4.37339900	-1.78472100	2.28562300
C	3.82324900	-1.80888600	-1.99321700
H	3.75725800	-2.15064200	-3.02424800
C	3.40235100	-0.51712200	-1.67674400
C	3.95177700	-0.95929200	0.66350900
C	4.35985300	-2.23859300	0.29180700
H	4.71122200	-2.91920600	1.06348600
C	-3.47362600	0.71126900	2.67289500
C	-2.65342400	-0.15272800	3.63641400
C	-4.81077200	1.11750800	3.30801500

H	-3.21425500	-1.03598000	3.96039400
H	-2.40797800	0.42349500	4.53395900
H	-1.71755000	-0.48811600	3.18086300
H	-4.64246600	1.64229400	4.25397600
H	-5.42499700	0.23396300	3.51456500
H	-5.37931600	1.77538000	2.64343400
C	-5.02781500	-3.37946900	0.10969500
C	-4.63605300	-4.21589700	1.32690400
C	-6.55293900	-3.36631700	-0.06646900
H	-5.13487900	-3.85966900	2.23511100
H	-3.55665000	-4.19527800	1.49674300
H	-4.93846100	-5.25638300	1.17659900
H	-6.94111900	-4.38657700	-0.14943900
H	-6.84623700	-2.81184100	-0.96302100
H	-7.02898800	-2.88771500	0.79668400
C	-3.58782800	0.67398800	-2.47324700
C	-4.54167000	0.17268500	-3.56200600
C	-2.13232800	0.44905000	-2.91056000
H	-5.58596400	0.21790700	-3.23800300
H	-4.31758300	-0.85762900	-3.85623400
H	-4.43158600	0.79341000	-4.45609300
H	-1.95477900	0.90569500	-3.88968000
H	-1.92150800	-0.62431500	-2.99368100
H	-1.41460700	0.88185700	-2.20488900
C	4.01962300	-0.57304000	2.13517700
C	3.52212900	-1.68799900	3.06376200
C	5.45132800	-0.17911700	2.52508300
H	4.22714800	-2.52573800	3.10188500
H	2.54774500	-2.05741600	2.73985300
H	3.42800200	-1.29992500	4.08337700
H	5.49692300	0.11766800	3.57843800
H	5.83271800	0.64782300	1.91885000
H	6.12756400	-1.02989800	2.38257000
C	4.66159100	-4.11512700	-1.37969500
C	6.09056000	-4.46923100	-0.95653300
C	3.64790600	-5.08819400	-0.76379900
H	6.20004500	-4.42265800	0.13239900
H	6.81690400	-3.78011800	-1.39744600
H	6.34327300	-5.48699900	-1.27154800
H	3.86630700	-6.11852700	-1.06458600
H	2.63021800	-4.83487200	-1.07341500
H	3.68584500	-5.03876300	0.33044900
C	2.88360700	0.36616000	-2.80146600
C	4.01528400	0.72687400	-3.77219800

C	1.71455200	-0.29402800	-3.54365700
H	4.42640300	-0.17339000	-4.24170000
H	4.83186800	1.23712300	-3.25204400
H	3.64670700	1.38386800	-4.56722200
H	1.27694100	0.40747000	-4.26254500
H	0.93678100	-0.61283900	-2.84412300
H	2.04741100	-1.17655100	-4.10023300
H	-2.90754000	1.62866000	2.48446200
H	-4.58294700	-3.84886900	-0.77712900
H	-3.74211600	1.75182700	-2.38732300
H	2.51652500	1.30394000	-2.37283600
H	3.36420000	0.28905000	2.29178200
H	4.59886400	-4.20800200	-2.47159400
H	-1.98273000	-1.07966600	-0.44158600

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C	-2.68729200	6.02460500	-2.01608500
C	-1.29510200	6.04519800	-1.76815100
C	-0.67511000	4.97567500	-1.17324100
C	-1.41534300	3.82394600	-0.79489900
C	-2.80880600	3.78630700	-1.08482600
C	-3.42267900	4.91686500	-1.68517200
C	-3.56419600	2.61616700	-0.80202900
C	-2.97809000	1.48187300	-0.30130100
C	-1.59542700	1.56578800	0.00837100
C	-0.81196200	2.68375500	-0.16479300
C	0.60553200	2.66305500	0.29355400
C	1.45331500	1.63964100	-0.07495700
C	2.82847300	1.57396600	0.27909000
C	3.34165900	2.61569200	1.00780100
C	2.51562000	3.66239400	1.49232800
C	1.12851300	3.67117600	1.17475200
C	0.30999700	4.67062800	1.76743600
C	0.85145700	5.62964500	2.58533000
C	2.23928500	5.64827300	2.85737100
C	3.04947600	4.68038300	2.32537500
H	-4.48897700	4.87672800	-1.89060900
H	-3.16565000	6.88048700	-2.48138200
H	-0.71081300	6.91308600	-2.05708800
H	0.39494500	4.99834300	-0.99708700
H	-4.62995000	2.61910800	-1.01301300
O	-0.99895200	0.42653000	0.55335100
H	-0.75728600	4.66293900	1.57736000

H	0.20638800	6.37843300	3.03383300
H	2.65394100	6.41835100	3.49984900
H	4.11363700	4.66319800	2.54525000
O	1.01595200	0.63030500	-0.92813400
H	4.40357100	2.63744900	1.23495700
P	-0.13933800	-0.40296900	-0.51756000
N	0.67516700	-1.48421900	0.50983900
S	-0.11322000	-2.75897900	1.21743000
O	-1.52804200	-2.49747700	1.10661900
O	0.54258300	-3.09603900	2.45861900
C	0.29563800	-4.12988500	0.05546300
F	-0.15811900	-3.85735900	-1.15068800
F	1.61799700	-4.26632100	0.01754400
F	-0.25411300	-5.24568700	0.50718600
O	-0.81938900	-0.99036500	-1.66921900
C	-3.69359600	0.19136600	-0.06066600
C	-4.86382600	-2.31450100	0.42381500
C	5.15826200	-1.81044500	-1.02916400
C	3.65276000	0.40779800	-0.16677200
C	3.99472200	0.27500100	-1.52516500
C	4.05186300	-0.57697200	0.76620200
C	4.80376600	-1.66183200	0.31121000
H	5.10769200	-2.42484700	1.02340700
C	4.74717800	-0.83044300	-1.92628700
H	5.01230300	-0.93703100	-2.97637600
C	-4.54100500	-1.46358100	1.47380000
H	-4.72984400	-1.79329300	2.49370700
C	-3.94616700	-0.22014200	1.25880200
C	-4.02657800	-0.64548300	-1.14727500
C	-4.61138200	-1.88074900	-0.87721300
H	-4.85100500	-2.53919300	-1.70824000
C	3.59279300	1.30314400	-2.57118700
C	2.80220900	0.66924100	-3.72120300
C	4.83070600	2.04322700	-3.09397500
H	3.41780200	-0.04052900	-4.28426300
H	2.47053400	1.44421300	-4.41957400
H	1.91980300	0.14150800	-3.34913300
H	4.54075400	2.80873800	-3.82089500
H	5.51929300	1.35046800	-3.59018500
H	5.37298500	2.52970900	-2.27717700
C	5.92850000	-3.03027100	-1.49546900
C	7.29263400	-3.13837400	-0.80595300
C	5.10479800	-4.30628300	-1.27992000
H	7.17431900	-3.27816800	0.27414300

H	7.88937500	-2.23570700	-0.96535100
H	7.85172400	-3.99612100	-1.19315100
H	5.63542200	-5.17966300	-1.67229600
H	4.13241800	-4.23813600	-1.77635000
H	4.92346200	-4.47494500	-0.21235100
C	3.66868400	-0.51362400	2.24254700
C	4.73498700	0.21368100	3.07405700
C	3.44182800	-1.90845400	2.84889100
H	4.85683900	1.25570100	2.77322500
H	5.70163300	-0.28924300	2.95964600
H	4.46397600	0.19495800	4.13467200
H	2.81166900	-1.84292500	3.73912000
H	4.39464300	-2.36015200	3.14715200
H	2.96412900	-2.60074500	2.15034100
C	-3.78119100	-0.23437600	-2.59229200
C	-3.33448000	-1.39779000	-3.48389000
C	-5.04241600	0.41154800	-3.18390700
H	-4.15645000	-2.09641500	-3.67641600
H	-2.50223600	-1.93872700	-3.03055200
H	-3.00839000	-1.00958500	-4.45427900
H	-4.86625200	0.72531700	-4.21845400
H	-5.36455000	1.28566900	-2.61114000
H	-5.86903400	-0.30820500	-3.18217200
C	-5.40695600	-3.70458900	0.68930500
C	-6.72972000	-3.96389200	-0.03797000
C	-4.35880500	-4.76016700	0.31265000
H	-6.59364900	-3.93174100	-1.12438800
H	-7.48198200	-3.21587000	0.22917800
H	-7.12049600	-4.95442600	0.21727200
H	-4.71151900	-5.76610700	0.56461400
H	-3.41404400	-4.57506200	0.83183700
H	-4.15839800	-4.73057000	-0.76436400
C	-3.59988100	0.63986300	2.46472200
C	-4.87413300	1.08809200	3.19169300
C	-2.64692800	-0.08382600	3.42275200
H	-5.42469100	0.22448300	3.58032900
H	-5.54021700	1.63452300	2.51675200
H	-4.62734600	1.73867100	4.03739700
H	-2.37230000	0.57475300	4.25375600
H	-1.73609700	-0.39443500	2.90445700
H	-3.11436400	-0.97907200	3.84590900
H	2.94444500	2.04664100	-2.09820100
H	6.10111400	-2.91596700	-2.57315600
H	2.73214000	0.05346700	2.32388500

H	-3.09145200	1.54464900	2.11546400
H	-2.97391600	0.50532800	-2.59918400
H	-5.59327000	-3.78240100	1.76823400
H	1.68802700	-1.41311100	0.63910100

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C	-3.04120300	5.91656700	-1.91491800
C	-1.65516700	6.01460700	-1.65136100
C	-0.97658300	4.96856100	-1.07918100
C	-1.64873500	3.76410800	-0.73981200
C	-3.03436400	3.64986000	-1.04678500
C	-3.71058900	4.75731500	-1.62295400
C	-3.71789100	2.42733600	-0.80815400
C	-3.06793800	1.31704800	-0.33256500
C	-1.69716400	1.47651300	-0.00214300
C	-0.98252200	2.64531800	-0.13511100
C	0.43103700	2.69726300	0.33232200
C	1.33725000	1.73430000	-0.05878600
C	2.71043700	1.72798000	0.31076000
C	3.15874500	2.77649200	1.07237500
C	2.27422300	3.76653000	1.57235800
C	0.89091400	3.70893500	1.24372500
C	0.01515300	4.64637600	1.85549600
C	0.49827800	5.61208300	2.70158300
C	1.88119900	5.69896700	2.98489400
C	2.74627200	4.79006200	2.43565700
H	-4.77038300	4.65804000	-1.84159600
H	-3.56650100	6.75450700	-2.36185400
H	-1.12206200	6.92387200	-1.91053700
H	0.08850500	5.05115100	-0.89138900
H	-4.77808600	2.36755800	-1.03869300
O	-1.03997000	0.35867900	0.51584100
H	-1.04876000	4.58563400	1.65664100
H	-0.18945300	6.31306500	3.16382000
H	2.24919100	6.47386500	3.64961200
H	3.80821600	4.82491000	2.66389700
O	0.95864200	0.73192400	-0.94563400
H	4.21354500	2.84419800	1.32146400
P	-0.12247400	-0.38958400	-0.56826200
N	0.76261600	-1.43392000	0.43463200
S	0.11695900	-2.84330300	1.02124000
O	-1.30805100	-2.79049800	0.80471300
O	0.71802800	-3.14531800	2.29915900

C	0.84190700	-4.05749600	-0.16044700
F	0.43698800	-3.79822200	-1.38704800
F	2.16704500	-3.94981200	-0.09419400
F	0.47567500	-5.27830200	0.19171100
O	-0.75655200	-0.99668800	-1.73546200
C	-3.71058500	-0.02051500	-0.15797400
C	-4.82643700	-2.57571600	0.18747300
C	5.16736000	-1.57521400	-0.98355300
C	3.58921000	0.59933100	-0.13041200
C	3.90630500	0.45035000	-1.49424400
C	4.06181200	-0.34350900	0.81441000
C	4.83809000	-1.41262900	0.36172400
H	5.19320300	-2.14447400	1.08310000
C	4.69691900	-0.63002600	-1.88909000
H	4.94980900	-0.74290800	-2.94146600
C	-4.47432800	-1.79504900	1.28646000
H	-4.62464700	-2.19000700	2.28943800
C	-3.91172600	-0.53028800	1.13994400
C	-4.05041900	-0.79142600	-1.28655500
C	-4.61351200	-2.05296000	-1.08345200
H	-4.87523900	-2.66078400	-1.94621900
C	3.45806500	1.44761300	-2.55195500
C	2.70358000	0.76946300	-3.70105300
C	4.66371400	2.23870000	-3.07625800
H	3.35625400	0.09068200	-4.26050000
H	2.33541100	1.52418700	-4.40330300
H	1.84748300	0.19900800	-3.33102300
H	4.34199600	2.98422800	-3.81059000
H	5.38497400	1.57387400	-3.56424600
H	5.17997300	2.75607900	-2.26156400
C	5.99392400	-2.75911500	-1.44714100
C	7.36062300	-2.80252600	-0.75526000
C	5.23328400	-4.07383400	-1.23687200
H	7.24850200	-2.95801000	0.32330900
H	7.91083600	-1.86925800	-0.90592400
H	7.96321400	-3.62739300	-1.14869000
H	5.81540300	-4.92038000	-1.61513200
H	4.26786200	-4.05812500	-1.75008100
H	5.04205600	-4.24518000	-0.17151600
C	3.76453100	-0.23439700	2.30732800
C	4.90327300	0.48802500	3.04279400
C	3.54011000	-1.59861600	2.97625100
H	5.06294800	1.50129300	2.66873800
H	5.83928900	-0.06738100	2.91554100

H	4.68558600	0.54867800	4.11415300
H	3.05917300	-1.46373900	3.94897700
H	4.49238900	-2.11162300	3.15030500
H	2.91155500	-2.27232500	2.38827600
C	-3.83376800	-0.30005300	-2.71105400
C	-3.27659700	-1.38673400	-3.63748000
C	-5.14131800	0.25695700	-3.29135600
H	-4.02093100	-2.16444800	-3.84047900
H	-2.38745700	-1.84682200	-3.20333400
H	-3.00408200	-0.94156000	-4.60013300
H	-4.98403600	0.62949300	-4.30926100
H	-5.54499100	1.07373700	-2.68573000
H	-5.90184700	-0.53133800	-3.33181600
C	-5.37726400	-3.97575700	0.37327700
C	-4.31190900	-4.89375000	0.98522200
C	-6.65591900	-3.98168100	1.21735400
H	-4.03412300	-4.54705900	1.98674300
H	-3.40371200	-4.89863700	0.37622200
H	-4.68642300	-5.91937400	1.07200100
H	-7.06167200	-4.99579000	1.29458200
H	-7.42187300	-3.33462000	0.77986900
H	-6.45529300	-3.62589200	2.23383000
C	-3.56087500	0.25759300	2.39331200
C	-4.83427300	0.65127500	3.15283400
C	-2.59688200	-0.51358100	3.30160200
H	-5.37734400	-0.23894600	3.48867700
H	-5.50704200	1.23410400	2.51601900
H	-4.58760700	1.24981900	4.03618600
H	-2.31930400	0.09890900	4.16606200
H	-1.68728000	-0.78750200	2.76114600
H	-3.05477000	-1.43399600	3.67848700
H	2.77570100	2.16601300	-2.08876400
H	6.16436400	-2.63557400	-2.52420000
H	2.84992000	0.35806000	2.43003300
H	-3.06150400	1.18590100	2.09794000
H	-3.09398100	0.50629400	-2.68266100
H	-5.62789200	-4.36378300	-0.62252100
H	1.74476000	-1.23786500	0.64731500

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C	2.08660300	5.90867200	2.01096900
C	0.75812600	5.80134100	1.53718400
C	0.30198200	4.62789600	0.99271100

C	1. 15147700	3. 49285900	0. 89449500
C	2. 47574400	3. 59089500	1. 40696000
C	2. 92193700	4. 82465600	1. 94969500
C	3. 32721000	2. 45503600	1. 38638800
C	2. 89472300	1. 23433300	0. 93363600
C	1. 57022400	1. 17039400	0. 42622300
C	0. 71840800	2. 24704200	0. 32842000
C	-0. 60823900	2. 09597000	-0. 32935100
C	-1. 47928000	1. 10876700	0. 07287800
C	-2. 80939100	0. 96827300	-0. 40745800
C	-3. 22235700	1. 86296800	-1. 36232300
C	-2. 34330800	2. 83187900	-1. 91247000
C	-1. 01617200	2. 94473200	-1. 41315800
C	-0. 13739500	3. 87430800	-2. 03112800
C	-0. 57042200	4. 67102900	-3. 06074900
C	-1. 90312500	4. 58764000	-3. 52714200
C	-2. 76662100	3. 68401400	-2. 96587300
H	3. 93900200	4. 88488600	2. 32749500
H	2. 43519400	6. 84553900	2. 43354500
H	0. 09127700	6. 65454900	1. 61079100
H	-0. 72210600	4. 55533400	0. 64309900
H	4. 34786800	2. 55696600	1. 74653300
O	1. 14771200	-0. 06312600	-0. 07047800
H	0. 88973900	3. 94001700	-1. 68919300
H	0. 11840100	5. 36878800	-3. 52624700
H	-2. 23296900	5. 23014000	-4. 33719200
H	-3. 78770000	3. 59284100	-3. 32656300
O	-1. 09063100	0. 21665500	1. 06798100
H	-4. 24942900	1. 83123600	-1. 71364300
P	0. 03527400	-0. 87923900	0. 73507900
N	-0. 62245100	-1. 74890300	-0. 58242200
S	0. 27714700	-2. 41810500	-1. 81608100
O	-0. 42370500	-3. 59897200	-2. 26519500
O	1. 67684900	-2. 41009000	-1. 47463200
C	0. 05733500	-1. 14197300	-3. 15107000
F	-1. 06665800	-1. 38381900	-3. 81167400
F	0. 00195700	0. 07577400	-2. 63539600
F	1. 08309200	-1. 23361300	-3. 98034900
O	0. 39673400	-1. 65491900	1. 91948400
C	3. 74713400	0. 00638700	0. 89317100
C	5. 15974900	-2. 40599200	0. 69925600
C	-5. 51537900	-1. 95037400	1. 26165400
C	-3. 72166100	-0. 06846200	0. 16863400
C	-4. 12935300	0. 04130100	1. 51642500

C	-4.19871700	-1.13155600	-0.62618600
C	-5.09116100	-2.04663900	-0.05885800
H	-5.46699000	-2.86608100	-0.66683100
C	-5.01692200	-0.90054600	2.03142800
H	-5.33398100	-0.80720100	3.06836300
C	5.16164600	-1.49250200	-0.35274800
H	5.70250300	-1.73649000	-1.26422900
C	4.47055700	-0.28471400	-0.27858600
C	3.75572000	-0.88150600	1.98496900
C	4.47092700	-2.07365400	1.86254400
H	4.47646000	-2.77862500	2.68926600
C	-3.68047200	1.17474200	2.42825800
C	-2.99322300	0.64745400	3.69299200
C	-4.86875400	2.07883100	2.78170600
H	-3.69133500	0.07721600	4.31548000
H	-2.62104400	1.48296300	4.29464500
H	-2.14914500	-0.00017400	3.44138800
H	-4.53943900	2.91654400	3.40497200
H	-5.63205800	1.52446700	3.33860100
H	-5.33785800	2.48270100	1.87910100
C	-6.48498900	-2.95745800	1.84882100
C	-5.84778000	-3.73373800	3.00691200
C	-7.78555900	-2.28143900	2.29744800
H	-5.59512800	-3.06069700	3.83353700
H	-4.92874100	-4.23438500	2.68937400
H	-6.54003800	-4.49017200	3.39036700
H	-8.49671100	-3.02488400	2.67161300
H	-8.25412100	-1.73827400	1.47173400
H	-7.59345100	-1.56634500	3.10489900
C	-3.78640000	-1.32531200	-2.07980900
C	-4.85376200	-0.78466700	-3.04204800
C	-3.52292600	-2.79794700	-2.42572200
H	-5.04400500	0.28068800	-2.89468700
H	-5.79955000	-1.31670000	-2.89020600
H	-4.54054200	-0.93579800	-4.08041800
H	-3.01572600	-2.87646900	-3.39055200
H	-4.46067200	-3.35816300	-2.50039600
H	-2.89872500	-3.30834900	-1.68587000
C	3.06052400	-0.53397200	3.29396800
C	2.60637200	-1.75654800	4.09451700
C	3.98389500	0.33482000	4.16116000
H	3.46068400	-2.28892300	4.52795600
H	2.03049000	-2.44416100	3.47302300
H	1.97131700	-1.43241500	4.92484800

H	3.49246000	0.59361900	5.10512000
H	4.26382000	1.26330300	3.65614900
H	4.90411000	-0.21301400	4.39364400
C	5.86999300	-3.73924000	0.56904200
C	5.24206900	-4.58182600	-0.54775600
C	7.37451200	-3.56119900	0.33896000
H	5.38958500	-4.10300400	-1.52206200
H	4.16525600	-4.69706700	-0.39527900
H	5.70109700	-5.57525600	-0.58826200
H	7.87526100	-4.53372300	0.28900700
H	7.83121900	-2.97724300	1.14341600
H	7.56442000	-3.03901200	-0.60528100
C	4.48164800	0.66169000	-1.47137700
C	5.86584400	0.78123100	-2.11787200
C	3.44020800	0.23214100	-2.51200800
H	6.15160900	-0.14109900	-2.63396300
H	6.63675200	1.00681900	-1.37497200
H	5.86031700	1.58141100	-2.86485000
H	3.46372200	0.89865800	-3.38165600
H	2.43251700	0.24749000	-2.09051900
H	3.63811000	-0.79048500	-2.85124300
H	-2.95497700	1.79472400	1.89499400
H	-6.73223600	-3.67441900	1.05546900
H	-2.86161200	-0.76195100	-2.24692600
H	4.20571000	1.65984500	-1.11379500
H	2.16428700	0.05136400	3.05614000
H	5.73343900	-4.27624900	1.51645500
H	-1.49103900	-2.25639200	-0.40503400

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C	-2.16050100	5.69878500	-2.49288700
C	-0.81598100	5.63341900	-2.05822200
C	-0.34297200	4.52015200	-1.41137600
C	-1.19084200	3.40659600	-1.16540100
C	-2.53264000	3.45875400	-1.63746900
C	-2.99545100	4.63198300	-2.28945600
C	-3.38526500	2.33628300	-1.46826900
C	-2.93927800	1.16673100	-0.90674400
C	-1.59756800	1.14803400	-0.44274500
C	-0.74030800	2.22383200	-0.48848900
C	0.60927300	2.13459200	0.13294800
C	1.46286700	1.10564900	-0.19535300
C	2.80959200	1.00835900	0.24813800

C	3. 25858700	1. 99467600	1. 08986000
C	2. 40208800	3. 02028700	1. 56796400
C	1. 05805500	3. 08893200	1. 10717100
C	0. 20417200	4. 08275000	1. 65635700
C	0. 67549200	4. 97836400	2. 58263500
C	2. 02372300	4. 93518400	3. 00804700
C	2. 86466800	3. 97380400	2. 51240900
H	-4. 02530800	4. 65870900	-2. 63505800
H	-2. 52196000	6. 58869500	-2. 99807600
H	-0. 15041800	6. 47045000	-2. 24400700
H	0. 69288000	4. 47811400	-1. 09272900
H	-4. 41806900	2. 40630400	-1. 80032200
O	-1. 16064300	-0. 02963900	0. 16482600
H	-0. 83416600	4. 11929900	1. 34529300
H	0. 00545100	5. 72449900	2. 99773000
H	2. 38354500	5. 65536700	3. 73581800
H	3. 89779300	3. 91424600	2. 84425900
O	1. 03561100	0. 11675100	-1. 07654900
H	4. 29739500	1. 99300900	1. 40627400
P	-0. 07962100	-0. 93173800	-0. 58988800
N	0. 62661400	-1. 66106600	0. 78613900
S	-0. 22396900	-2. 19476600	2. 11621800
O	0. 49438800	-3. 32391700	2. 66041400
O	-1. 63548700	-2. 21819800	1. 82824800
C	0. 04391000	-0. 78728500	3. 30161500
F	1. 19247000	-0. 96159000	3. 94090100
F	0. 07745100	0. 36987700	2. 66025000
F	-0. 94978700	-0. 78975000	4. 17399300
O	-0. 48592300	-1. 82469000	-1. 67281300
C	-3. 79252500	-0. 04508300	-0. 70808100
C	-5. 20531600	-2. 41488300	-0. 21765600
C	5. 44014900	-2. 09018500	-1. 20399300
C	3. 69734000	-0. 08874600	-0. 24901500
C	4. 04856900	-0. 12898400	-1. 61658200
C	4. 20654500	-1. 06142500	0. 63659100
C	5. 07222600	-2. 03885000	0. 13570300
H	5. 47225900	-2. 78937300	0. 81323900
C	4. 91206500	-1. 12703900	-2. 06209300
H	5. 18569000	-1. 14904300	-3. 11525800
C	-5. 16679000	-1. 39972300	0. 73097900
H	-5. 67901600	-1. 55095000	1. 67827500
C	-4. 47360300	-0. 20803300	0. 50956200
C	-3. 84186400	-1. 04345300	-1. 70273300
C	-4. 55396800	-2. 21002500	-1. 43478400

H	-4.58438800	-2.99314200	-2.18728400
C	3.56400500	0.90084100	-2.62772900
C	2.82010100	0.24320000	-3.79576400
C	4.73853300	1.75075600	-3.13022000
H	3.48870600	-0.39692200	-4.38161800
H	2.42434900	1.01066300	-4.46878800
H	1.98594100	-0.36644200	-3.43827000
H	4.38447200	2.51781400	-3.82657700
H	5.47431200	1.13266700	-3.65615900
H	5.24892200	2.24725000	-2.29905000
C	6.38289100	-3.16104100	-1.71736500
C	5.70093300	-4.04885200	-2.76445300
C	7.66898600	-2.54541800	-2.28031200
H	5.42202400	-3.46429800	-3.64795900
H	4.79159300	-4.50580700	-2.36399400
H	6.37556900	-4.84703000	-3.09035100
H	8.36242800	-3.32912200	-2.60186700
H	8.17038600	-1.92440200	-1.53243100
H	7.45007900	-1.91511500	-3.14927500
C	3.85848700	-1.09248100	2.11928700
C	4.97264800	-0.46379400	2.96840900
C	3.60104900	-2.51612300	2.63378200
H	5.16580300	0.57619500	2.69612900
H	5.90601000	-1.02201600	2.83470000
H	4.70561200	-0.49583800	4.02991600
H	3.13686800	-2.48423600	3.62263400
H	4.53743900	-3.07568800	2.72777300
H	2.94105900	-3.09614400	1.98162400
C	-3.19154400	-0.83475700	-3.06342800
C	-2.77164700	-2.13506600	-3.75216300
C	-4.14067000	-0.04973000	-3.98126400
H	-3.64315300	-2.70054100	-4.10143100
H	-2.17879800	-2.76226500	-3.08439900
H	-2.16354400	-1.90145800	-4.63158000
H	-3.68186900	0.10833300	-4.96312800
H	-4.39757900	0.92738000	-3.56333400
H	-5.07138600	-0.61022000	-4.12461600
C	-5.90440000	-3.72728500	0.07883600
C	-6.98717300	-4.05149000	-0.95534600
C	-4.88243000	-4.86645500	0.17820200
H	-6.54928000	-4.19665800	-1.94883000
H	-7.72175300	-3.24392800	-1.02593800
H	-7.51150700	-4.97426800	-0.68610700
H	-5.37218800	-5.80409400	0.46178400

H	-4.10985100	-4.63501000	0.91717600
H	-4.38602900	-5.02199500	-0.78604200
C	-4.44077500	0.85518500	1.59887000
C	-5.80248200	1.05130900	2.27369500
C	-3.36739900	0.52612800	2.64375400
H	-6.07660100	0.18784700	2.88834300
H	-6.59571600	1.20835900	1.53666200
H	-5.76813800	1.92232600	2.93587300
H	-3.36038000	1.27768000	3.44136000
H	-2.37414700	0.49250100	2.19027900
H	-3.55720200	-0.45534900	3.09163300
H	2.86493800	1.58208200	-2.13534100
H	6.65595700	-3.79332000	-0.86282100
H	2.94611900	-0.50363900	2.26551500
H	-4.17173400	1.80909200	1.13198400
H	-2.28465500	-0.23608800	-2.91687400
H	-6.39197700	-3.62363800	1.05681100
H	1.49261400	-2.18060800	0.63243300

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C	-2.41429000	5.76858400	-2.17685000
C	-1.05195300	5.72114100	-1.79907900
C	-0.52364600	4.59273500	-1.22537900
C	-1.33085300	3.44515400	-0.99956800
C	-2.69155700	3.48124000	-1.41585400
C	-3.21152600	4.67003200	-1.99217000
C	-3.50631400	2.32811000	-1.26829900
C	-3.00708400	1.14674200	-0.78138600
C	-1.64811700	1.14457500	-0.37023500
C	-0.82207600	2.24529100	-0.39785700
C	0.55389500	2.16579300	0.16451300
C	1.41992300	1.17720200	-0.24523000
C	2.78620000	1.09761200	0.13840900
C	3.24393000	2.05756200	1.00543700
C	2.38146100	3.03599900	1.56483200
C	1.01790800	3.08732200	1.16298800
C	0.16196700	4.03051300	1.79227100
C	0.64809800	4.89631600	2.73910600
C	2.01376500	4.87227400	3.10647100
C	2.85812600	3.95843900	2.53276800
H	-4.25494800	4.68345900	-2.29523200
H	-2.81962300	6.67056800	-2.62400100
H	-0.41685500	6.58445300	-1.97067500

H	0.52503600	4.56564700	-0.95009800
H	-4.55292300	2.38372000	-1.55705200
O	-1.15745700	-0.04741300	0.16377800
H	-0.88924100	4.05171300	1.52624400
H	-0.02345900	5.60348800	3.21549100
H	2.38484700	5.56862300	3.85157000
H	3.90554000	3.91313100	2.81894100
O	0.98231900	0.21762500	-1.15341200
H	4.29470400	2.07111900	1.27915800
P	-0.08140200	-0.88403200	-0.66949800
N	0.70032000	-1.64745700	0.64627700
S	-0.08206100	-2.26304500	1.98271500
O	0.69127100	-3.38936800	2.45244300
O	-1.50202200	-2.32150900	1.74581400
C	0.18622900	-0.89741800	3.21554700
F	1.36780400	-1.05389100	3.79668400
F	0.14871900	0.28619000	2.62453800
F	-0.76705000	-0.97496200	4.12861800
O	-0.50432600	-1.74390200	-1.77256200
C	-3.81922500	-0.09734100	-0.61210900
C	-5.15080400	-2.52688600	-0.19117700
C	5.42406100	-1.86927900	-1.55655400
C	3.67982800	0.04764000	-0.44317300
C	3.97208700	0.07411200	-1.82189300
C	4.25105800	-0.95045700	0.37880900
C	5.11381100	-1.88354500	-0.19797100
H	5.55529500	-2.64998400	0.43467100
C	4.83979300	-0.88517300	-2.34631500
H	5.07223600	-0.86145700	-3.40916500
C	-5.10542400	-1.55805600	0.80445500
H	-5.57939400	-1.76927800	1.76015800
C	-4.45189900	-0.33816000	0.61860300
C	-3.87693400	-1.04781400	-1.65228600
C	-4.54806000	-2.24546500	-1.41798300
H	-4.58382500	-2.99203500	-2.20650800
C	3.42264700	1.13312700	-2.76714700
C	2.65149600	0.50740400	-3.93499300
C	4.55497500	2.03579700	-3.27446500
H	3.31332900	-0.08653900	-4.57456800
H	2.20936200	1.29280500	-4.55646000
H	1.84846500	-0.14094200	-3.57435400
H	4.15487900	2.82241400	-3.92240600
H	5.28553000	1.46128400	-3.85417400
H	5.08364900	2.50953700	-2.44143500

C	6. 36106300	-2. 90088900	-2. 15423400
C	7. 75756200	-2. 81740500	-1. 52808600
C	5. 78726600	-4. 31603800	-2. 01913300
H	7. 72013200	-3. 05699500	-0. 45969800
H	8. 17868200	-1. 81343700	-1. 63326300
H	8. 43692700	-3. 53033800	-2. 00624100
H	6. 44726900	-5. 04672700	-2. 49762400
H	4. 79876300	-4. 38722300	-2. 48169700
H	5. 68689700	-4. 59561900	-0. 96451400
C	3. 96960800	-1. 04975000	1. 87276800
C	5. 10534900	-0. 42668000	2. 69717800
C	3. 76969000	-2. 49870600	2. 34010600
H	5. 26185700	0. 62771300	2. 45899600
H	6. 04458200	-0. 95541300	2. 49967800
H	4. 88719800	-0. 50731200	3. 76721700
H	3. 34647700	-2. 51753800	3. 34757800
H	4. 72297500	-3. 03635400	2. 37403200
H	3. 09786200	-3. 07034400	1. 69269800
C	-3. 28004900	-0. 75653900	-3. 02232500
C	-2. 85047200	-2. 01050700	-3. 78697900
C	-4. 28060400	0. 04450800	-3. 86889700
H	-3. 71849100	-2. 58257400	-4. 13417300
H	-2. 21860400	-2. 65206100	-3. 17059000
H	-2. 27950000	-1. 71841000	-4. 67378700
H	-3. 86064400	0. 26096700	-4. 85699100
H	-4. 54784400	0. 99352400	-3. 39632300
H	-5. 20095200	-0. 53400500	-4. 00746700
C	-5. 80262700	-3. 87175800	0. 06447600
C	-6. 90733400	-4. 18142000	-0. 95070100
C	-4. 74505300	-4. 98242300	0. 08006700
H	-6. 49685000	-4. 26796900	-1. 96252700
H	-7. 66689700	-3. 39421800	-0. 96173900
H	-7. 39595000	-5. 13098900	-0. 70892800
H	-5. 19811600	-5. 94692900	0. 33284200
H	-3. 95753800	-4. 76187500	0. 80651600
H	-4. 27359900	-5. 07733200	-0. 90439200
C	-4. 40672700	0. 67077400	1. 75788700
C	-5. 74770800	0. 79737800	2. 48842800
C	-3. 28839300	0. 31898100	2. 74661900
H	-5. 97888700	-0. 10259200	3. 06731200
H	-6. 57032400	0. 97064100	1. 78814400
H	-5. 71080600	1. 63472800	3. 19256800
H	-3. 26922900	1. 03126700	3. 57929200
H	-2. 31233300	0. 33174500	2. 25642700

H	-3.43857800	-0.68738400	3.15238300
H	2.72578100	1.77230400	-2.21856100
H	6.45555300	-2.67469700	-3.22393000
H	3.05073200	-0.49122700	2.08267000
H	-4.17832000	1.65327400	1.33030400
H	-2.38444700	-0.14058000	-2.87764000
H	-6.26201200	-3.82790900	1.06045700
H	1.57543200	-2.13184100	0.43846600

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C	-2.31877900	5.95347200	-1.72270000
C	-0.97321200	5.86454200	-1.29564000
C	-0.46687700	4.68206400	-0.81930600
C	-1.28055700	3.51928200	-0.74632000
C	-2.62307800	3.60078200	-1.21220000
C	-3.12095800	4.84364000	-1.68460600
C	-3.44185800	2.44086700	-1.21503800
C	-2.96106200	1.21476800	-0.83092300
C	-1.61873700	1.16730300	-0.37069700
C	-0.79455400	2.26290200	-0.25116000
C	0.55624000	2.12148300	0.35771800
C	1.44118800	1.17932900	-0.11600600
C	2.78979600	1.05804900	0.31530800
C	3.20805500	1.92094000	1.29680400
C	2.31989700	2.83680200	1.91846900
C	0.97469400	2.93231300	1.46616400
C	0.09014600	3.80657100	2.15288600
C	0.53318100	4.56848500	3.20436200
C	1.88203500	4.50383800	3.62520800
C	2.75245900	3.65288300	2.99638400
H	-4.15098800	4.89066700	-2.02752400
H	-2.70694200	6.89745500	-2.09156600
H	-0.33340500	6.73956100	-1.35110100
H	0.56964200	4.62422300	-0.50535300
H	-4.47667600	2.52910700	-1.53626800
O	-1.14524300	-0.07413200	0.05535700
H	-0.94888600	3.85687300	1.84598300
H	-0.15981200	5.22377000	3.72239300
H	2.21932700	5.11852200	4.45357300
H	3.78683200	3.57622700	3.32076900
O	1.04624200	0.32189300	-1.13865600
H	4.24699700	1.90534600	1.61260600
P	-0.03902600	-0.81954100	-0.82389100

N	0.68244500	-1.73425700	0.42808500
S	-0.15818000	-2.48166800	1.65877000
O	0.58595100	-3.66372400	2.02824500
O	-1.56882200	-2.49368900	1.36586600
C	0.07739900	-1.26345900	3.04458500
F	1.22398800	-1.51320100	3.66209900
F	0.09591100	-0.02265700	2.58407800
F	-0.92215200	-1.41253600	3.89714800
O	-0.41787100	-1.54732800	-2.03298900
C	-3.77790200	-0.03761100	-0.81108000
C	-5.11328600	-2.49665300	-0.66245300
C	5.53009000	-1.68919400	-1.57338700
C	3.71381400	0.07952800	-0.33879700
C	4.08172400	0.27144800	-1.68551500
C	4.24046600	-1.01234800	0.38730700
C	5.14174400	-1.86852100	-0.24687600
H	5.55064700	-2.70687300	0.31209700
C	4.98414900	-0.61783900	-2.27160400
H	5.27513100	-0.46702100	-3.30933400
C	-5.10121400	-1.62542500	0.42480100
H	-5.60007000	-1.92079900	1.34501100
C	-4.44770000	-0.39578000	0.37390500
C	-3.80277700	-0.88191800	-1.93665600
C	-4.47880300	-2.09866600	-1.83606200
H	-4.49554800	-2.77074000	-2.68959400
C	3.57378800	1.43394800	-2.52633900
C	2.86364900	0.94779300	-3.79497100
C	4.72360300	2.39018500	-2.86923000
H	3.55847100	0.42921200	-4.46442400
H	2.44982900	1.79987500	-4.34385600
H	2.04617800	0.26418900	-3.55065200
H	4.35028600	3.24745300	-3.43878100
H	5.48434700	1.88817500	-3.47678100
H	5.20920300	2.76280400	-1.96191800
C	6.50831600	-2.64008400	-2.23550600
C	7.86624500	-2.62920000	-1.52466500
C	5.94060700	-4.06241200	-2.30352900
H	7.77003800	-2.99360300	-0.49595700
H	8.28415200	-1.61912700	-1.48608800
H	8.57768200	-3.27941600	-2.04380600
H	6.63351400	-4.72944800	-2.82641000
H	4.98095800	-4.08000100	-2.82787700
H	5.78241000	-4.46607200	-1.29732800
C	3.86487300	-1.29491300	1.83648300

C	4. 93023800	-0. 76574800	2. 80710700
C	3. 66120700	-2. 79226100	2. 10962100
H	5. 07580600	0. 31276400	2. 71555000
H	5. 89240100	-1. 25100100	2. 60843900
H	4. 64424000	-0. 98548700	3. 84109900
H	3. 17188100	-2. 93950800	3. 07546200
H	4. 62028400	-3. 31955200	2. 14310700
H	3. 04609200	-3. 28777500	1. 35199200
C	-3. 16716100	-0. 46220700	-3. 25469500
C	-2. 70953200	-1. 63784900	-4. 12078800
C	-4. 14603700	0. 41394600	-4. 05068200
H	-3. 56424900	-2. 17764200	-4. 54410100
H	-2. 09135000	-2. 33226000	-3. 54942600
H	-2. 11556200	-1. 26221100	-4. 95976500
H	-3. 69789100	0. 72494000	-5. 00041000
H	-4. 43175400	1. 31266800	-3. 49733200
H	-5. 05913100	-0. 15022800	-4. 27182000
C	-5. 78054900	-3. 85433600	-0. 56023200
C	-5. 09329900	-4. 71890800	0. 50355100
C	-7. 28122600	-3. 72911200	-0. 27623000
H	-5. 22331800	-4. 28171900	1. 49969400
H	-4. 01909400	-4. 79628100	0. 31358800
H	-5. 52222100	-5. 72639900	0. 52001300
H	-7. 75245500	-4. 71711500	-0. 24675400
H	-7. 78035400	-3. 12997800	-1. 04345700
H	-7. 45461300	-3. 24731000	0. 69236900
C	-4. 43919200	0. 50181000	1. 60389000
C	-5. 80222400	0. 56053700	2. 30166800
C	-3. 35180600	0. 05722300	2. 58965700
H	-6. 04827800	-0. 38901000	2. 78795000
H	-6. 60368600	0. 79740700	1. 59553900
H	-5. 78915000	1. 32918900	3. 08098200
H	-3. 35774500	0. 68995600	3. 48448000
H	-2. 36051800	0. 11060300	2. 13364600
H	-3. 51583900	-0. 98148600	2. 89649300
H	2. 84697500	2. 00433200	-1. 94174000
H	6. 66140300	-2. 28720800	-3. 26331700
H	2. 92426800	-0. 77454500	2. 04929600
H	-4. 19972100	1. 52004700	1. 27814700
H	-2. 27911100	0. 13869800	-3. 02543900
H	-5. 65979300	-4. 35180200	-1. 53107300
H	1. 55322900	-2. 21518300	0. 19602100

OH tautomer-I-1

C	1. 38677100	6. 10720000	2. 08704800
C	0. 06533700	5. 91345000	1. 61934500
C	-0. 29728400	4. 74068600	1. 00729700
C	0. 64533500	3. 69148100	0. 83294700
C	1. 96516800	3. 87383300	1. 33937800
C	2. 31240400	5. 10638300	1. 95231100
C	2. 91192200	2. 82008800	1. 22854700
C	2. 57063900	1. 59669900	0. 71015500
C	1. 25210600	1. 44573800	0. 23457500
C	0. 31373100	2. 44589800	0. 19845800
C	-0. 99491500	2. 22205300	-0. 47542600
C	-1. 79139200	1. 15171000	-0. 12853200
C	-3. 10096200	0. 93308400	-0. 62753500
C	-3. 58056000	1. 85092300	-1. 52825400
C	-2. 78196600	2. 91753500	-2. 01491100
C	-1. 46491500	3. 09880500	-1. 51026600
C	-0. 66163100	4. 12956100	-2. 06826800
C	-1. 15796600	4. 95248300	-3. 04698100
C	-2. 48209300	4. 79592100	-3. 51948900
C	-3. 27243800	3. 79704700	-3. 01554500
H	3. 32621700	5. 23265500	2. 32243600
H	1. 65871600	7. 04399900	2. 56266800
H	-0. 67096400	6. 69980000	1. 75143100
H	-1. 31612900	4. 60173400	0. 66320300
H	3. 93258700	2. 98838700	1. 56268500
O	0. 93546400	0. 18907000	-0. 28127600
H	0. 35914700	4. 25308600	-1. 72333500
H	-0. 52596300	5. 72761900	-3. 46848000
H	-2. 86184600	5. 45859800	-4. 29044700
H	-4. 28412200	3. 64886300	-3. 38332400
O	-1. 33498200	0. 26406400	0. 85657200
H	-4. 59986400	1. 75038200	-1. 89065100
P	-0. 11358700	-0. 69817000	0. 52866900
N	-0. 44518100	-2. 02893200	-0. 19028800
S	0. 40284300	-2. 84722300	-1. 27520100
O	0. 67551500	-2. 07664400	-2. 47435500
O	-0. 09481200	-4. 20283200	-1. 36231900
C	2. 04351700	-3. 00668600	-0. 41772100
F	2. 78419400	-1. 92747200	-0. 62794100
F	1. 85662500	-3. 12352100	0. 91462500
F	2. 68469200	-4. 07933100	-0. 84244500
C	3. 55493900	0. 48385000	0. 54599400
C	5. 46008000	-1. 55379400	0. 22359600

C	-5.64656400	-2.27531300	0.67986200
C	-3.93992200	-0.20935600	-0.15444400
C	-4.54981900	-0.14322200	1.11196100
C	-4.14351000	-1.32221200	-0.99098100
C	-5.00642500	-2.32990200	-0.55484700
H	-5.17412000	-3.19528000	-1.19118300
C	-5.39620800	-1.17873800	1.50336300
H	-5.87421500	-1.12656800	2.48020900
C	5.13995600	-0.69936400	-0.83005700
H	5.62393400	-0.84217700	-1.79431300
C	4.19049100	0.31206800	-0.69875700
C	3.86691400	-0.35591100	1.62827800
C	4.81500000	-1.36412600	1.44197800
H	5.05969300	-2.02525200	2.27062600
C	-4.32743900	1.02334800	2.06263300
C	-3.71139800	0.55456700	3.38579200
C	-5.63207000	1.79253600	2.30213900
H	-4.38961400	-0.11979900	3.91978700
H	-3.51120100	1.41150500	4.03750400
H	-2.77070200	0.02449200	3.21171600
H	-5.45675400	2.65461200	2.95416700
H	-6.38112800	1.15395000	2.78283200
H	-6.05374200	2.15232900	1.35846600
C	-6.57351400	-3.38933600	1.12725400
C	-6.02416000	-4.10298400	2.36772300
C	-7.99253300	-2.86943600	1.38238300
H	-5.96902000	-3.41442900	3.21830500
H	-5.01875500	-4.49226300	2.18438100
H	-6.67372000	-4.93703200	2.65298600
H	-8.66178600	-3.69217300	1.65444300
H	-8.39672400	-2.37281300	0.49556100
H	-8.00012600	-2.14647600	2.20561500
C	-3.44852900	-1.45974000	-2.33869000
C	-4.32677300	-0.93250000	-3.48182600
C	-3.04225700	-2.90623400	-2.63924800
H	-4.55164000	0.13184100	-3.37696200
H	-5.27683600	-1.47838100	-3.50645200
H	-3.82451800	-1.08040100	-4.44344200
H	-2.31223500	-2.92696700	-3.45419800
H	-3.90497600	-3.50415900	-2.95495400
H	-2.59314800	-3.39043900	-1.77032900
C	3.22989000	-0.16791200	2.99618300
C	2.91074300	-1.50131100	3.68579000
C	4.13227600	0.67814300	3.90446300

H	3.80901400	-1.95292000	4.12011700
H	2.49952300	-2.23734700	2.98538900
H	2.19651800	-1.34739300	4.50029400
H	3.67990200	0.79681900	4.89474700
H	4.30050700	1.67368500	3.48490200
H	5.10736200	0.19393200	4.02783700
C	6.45545500	-2.68110900	0.03424300
C	5.94678400	-3.68477600	-1.00797300
C	7.84272300	-2.15375700	-0.34708400
H	5.87819000	-3.21514500	-1.99540000
H	4.95144200	-4.05740100	-0.74802500
H	6.62826800	-4.53768700	-1.08908100
H	8.55682900	-2.97862700	-0.43748000
H	8.21839600	-1.45066500	0.40192500
H	7.80987700	-1.63352100	-1.31059500
C	3.84180500	1.15494000	-1.91595700
C	5.08472500	1.80187900	-2.53751700
C	3.08431100	0.31167600	-2.95086700
H	5.76289500	1.04875900	-2.95227800
H	5.64080100	2.38623600	-1.79794500
H	4.79334500	2.46762600	-3.35607400
H	2.81738900	0.92359400	-3.81886500
H	2.16875800	-0.11685300	-2.53405100
H	3.70961900	-0.51705300	-3.30245600
H	-3.62032900	1.72049800	1.60134800
H	-6.62265900	-4.12085400	0.31075300
H	-2.52986200	-0.86062400	-2.30563200
H	3.18123100	1.96810900	-1.59782400
H	2.28792400	0.37258900	2.86046900
H	6.54436800	-3.20464200	0.99487400
O	0.42222900	-0.90443900	2.00797700
H	0.88724700	-1.75575200	2.10122000

OH tautomer-I-2

C	1.48856400	6.03933300	2.24644100
C	0.14092100	5.86823100	1.85195500
C	-0.25569000	4.73704500	1.18504500
C	0.67748500	3.71025400	0.87827200
C	2.02339300	3.86647700	1.31114200
C	2.40593600	5.05644700	1.98417700
C	2.96122000	2.82778000	1.07810700
C	2.59998300	1.63664000	0.49960000
C	1.25081600	1.51166600	0.07795100

C	0.30934300	2.51008900	0.18146800
C	-1.04749900	2.32380600	-0.39949300
C	-1.80375300	1.22161700	-0.07119600
C	-3.14334200	1.01564900	-0.48631500
C	-3.70261000	1.98590000	-1.27959900
C	-2.95657100	3.09982600	-1.74305600
C	-1.60647900	3.26552900	-1.32742200
C	-0.85931000	4.34666200	-1.86789700
C	-1.43795800	5.23033600	-2.74294600
C	-2.79283100	5.08699900	-3.12401500
C	-3.53149500	4.04147200	-2.63655100
H	3.44091100	5.16361400	2.29744700
H	1.78794000	6.94327900	2.76705500
H	-0.58810100	6.63786700	2.08458700
H	-1.29388800	4.61402700	0.89709700
H	3.99613200	2.97748400	1.37489700
O	0.88040700	0.30039400	-0.52688000
H	0.18330400	4.46165000	-1.59231900
H	-0.84842100	6.04427400	-3.15272900
H	-3.23783400	5.79770000	-3.81295100
H	-4.56681700	3.90419800	-2.93656800
O	-1.27124300	0.27139500	0.80874100
H	-4.74394000	1.89094100	-1.57492000
P	-0.07507900	-0.65426200	0.32713000
N	-0.53737200	-1.93916300	-0.42003600
S	0.24185800	-2.95308300	-1.38650000
O	0.71211700	-2.32199900	-2.60494600
O	-0.45753100	-4.21811700	-1.43251500
C	1.77185900	-3.30002100	-0.41144900
F	2.53626700	-2.21399400	-0.37032100
F	1.44458800	-3.60558900	0.86176900
F	2.44627500	-4.30706500	-0.93004600
C	3.59938000	0.54975500	0.26919700
C	5.58281000	-1.39503700	-0.16295900
C	-5.48793500	-2.37022600	0.74770300
C	-3.91723400	-0.18354800	-0.04411100
C	-4.43687700	-0.23313000	1.26235200
C	-4.14238500	-1.23970200	-0.94567800
C	-4.93632400	-2.31002400	-0.52887000
H	-5.11830800	-3.13317200	-1.21546200
C	-5.21796000	-1.32652300	1.63176500
H	-5.62743300	-1.36397300	2.63994100
C	5.07941300	-0.63921600	-1.21641800
H	5.46397500	-0.81570700	-2.21898100

C	4. 09206900	0. 32994200	-1. 02915500
C	4. 07625500	-0. 21716500	1. 35092500
C	5. 06926200	-1. 16612500	1. 11311600
H	5. 43875100	-1. 76026100	1. 94665900
C	-4. 18540800	0. 86934100	2. 27989200
C	-3. 46834000	0. 32902700	3. 52230000
C	-5. 49308500	1. 57453200	2. 65893100
H	-4. 08832100	-0. 40469200	4. 04870800
H	-3. 24979400	1. 14374700	4. 22053600
H	-2. 52617700	-0. 15435800	3. 24848300
H	-5. 30066000	2. 39156100	3. 36210600
H	-6. 19034100	0. 87705500	3. 13574200
H	-5. 98568700	1. 98860100	1. 77367400
C	-6. 34206100	-3. 54938100	1. 17254600
C	-5. 68736200	-4. 32355100	2. 32223500
C	-7. 75935100	-3. 10626400	1. 55219300
H	-5. 60253900	-3. 69394100	3. 21500400
H	-4. 68246100	-4. 65751100	2. 04911400
H	-6. 28592400	-5. 20140700	2. 58681800
H	-8. 37938000	-3. 97220900	1. 80619800
H	-8. 23802100	-2. 56664200	0. 72990600
H	-7. 73928800	-2. 44235500	2. 42358200
C	-3. 54275500	-1. 24734900	-2. 34496000
C	-4. 52734700	-0. 68247700	-3. 37817000
C	-3. 09262400	-2. 64600300	-2. 78085500
H	-4. 79405900	0. 35709100	-3. 17091800
H	-5. 44968000	-1. 27443300	-3. 37930600
H	-4. 09246500	-0. 72870800	-4. 38205700
H	-2. 42419200	-2. 57141000	-3. 64438800
H	-3. 94686500	-3. 26333900	-3. 08168000
H	-2. 56273900	-3. 16891100	-1. 98239500
C	3. 52511900	-0. 06608500	2. 76097000
C	3. 25793000	-1. 43037500	3. 41462400
C	4. 46955200	0. 75547900	3. 64733400
H	4. 18385800	-1. 88950100	3. 77731600
H	2. 81155600	-2. 13661400	2. 70649300
H	2. 58947100	-1. 31834500	4. 27372400
H	4. 07528400	0. 83023800	4. 66635600
H	4. 60468800	1. 76895600	3. 25928800
H	5. 45563500	0. 28010300	3. 69652300
C	6. 62147300	-2. 47331500	-0. 40112000
C	7. 90243800	-2. 21780000	0. 39956600
C	6. 04477500	-3. 85822900	-0. 08290500
H	7. 70201800	-2. 24826500	1. 47624000

H	8.32724400	-1.23772800	0.16420100
H	8.65352400	-2.98313300	0.17888000
H	6.76300000	-4.64537000	-0.33404900
H	5.12139300	-4.03816800	-0.64051000
H	5.81419500	-3.94354300	0.98516400
C	3.60725600	1.12138500	-2.23354200
C	4.71833800	2.04289900	-2.75180600
C	3.08440600	0.20057000	-3.34120900
H	5.58215000	1.45910400	-3.08839600
H	5.05960000	2.72844200	-1.96941200
H	4.36080600	2.63571800	-3.60004700
H	2.66531500	0.79705000	-4.15815400
H	2.30633400	-0.47084500	-2.96776800
H	3.89000300	-0.41162200	-3.76114800
H	-3.53123200	1.62084000	1.82593700
H	-6.41777700	-4.22469200	0.31091600
H	-2.65389200	-0.60493400	-2.33044500
H	2.77578000	1.76055300	-1.92063200
H	2.56941500	0.46253800	2.69706500
H	6.87761900	-2.45034400	-1.46792800
O	0.63700900	-0.92758300	1.71854000
H	0.92166400	-1.85483900	1.80999100

OH tautomer-I-3

C	-1.68724800	6.10050300	-2.03812600
C	-0.32257800	5.94521500	-1.69951500
C	0.12108400	4.80182500	-1.08513500
C	-0.77938600	3.74638300	-0.77810300
C	-2.14334700	3.88791800	-1.15576300
C	-2.57450100	5.09061400	-1.77462800
C	-3.05048900	2.82216200	-0.92353300
C	-2.64353000	1.62026100	-0.40016100
C	-1.27756200	1.51089900	-0.03168400
C	-0.36143800	2.53269200	-0.13488100
C	1.01819600	2.35843800	0.39348600
C	1.78591100	1.28370800	0.00584800
C	3.14192100	1.09370300	0.37249300
C	3.70742000	2.05247900	1.17530000
C	2.95471600	3.13599500	1.69625000
C	1.58789400	3.28345700	1.33170800
C	0.83655300	4.33010000	1.93121000
C	1.42601200	5.19994800	2.81284700
C	2.79623400	5.07656600	3.14245500

C	3. 53997500	4. 06328600	2. 59806600
H	-3. 62241600	5. 18592900	-2. 04589300
H	-2. 02377300	7. 01419200	-2. 51737900
H	0. 38181000	6. 73702900	-1. 93358800
H	1. 17160400	4. 69119400	-0. 83999400
H	-4. 09855900	2. 95907200	-1. 17725900
O	-0. 86041200	0. 28822400	0. 51754200
H	-0. 21753900	4. 42905600	1. 69632600
H	0. 83339200	5. 98714400	3. 26789700
H	3. 24939100	5. 77631200	3. 83726700
H	4. 58787100	3. 94056800	2. 85810000
O	1. 24527600	0. 35136800	-0. 88818400
H	4. 75966400	1. 97078700	1. 43381200
P	0. 08269600	-0. 61476800	-0. 40382400
N	0. 59449800	-1. 91789400	0. 27618900
S	-0. 13174100	-2. 98786700	1. 22309600
O	-0. 57666400	-2. 41733100	2. 48036300
O	0. 59553900	-4. 23764500	1. 19523800
C	-1. 68381200	-3. 33051000	0. 28231800
F	-2. 47285400	-2. 26181900	0. 30941900
F	-1. 39032500	-3. 57681900	-1. 01187300
F	-2. 31917700	-4. 37306400	0. 77954800
C	-3. 61047600	0. 50329100	-0. 17572900
C	-5. 53824900	-1. 49795100	0. 25000900
C	5. 51359700	-2. 20976000	-1. 02263900
C	3. 92572900	-0. 07642100	-0. 12692500
C	4. 42032500	-0. 07214400	-1. 44064400
C	4. 18404100	-1. 16182700	0. 73472300
C	4. 98378600	-2. 20317600	0. 26843900
H	5. 18541100	-3. 04455100	0. 92701200
C	5. 21255400	-1. 14245600	-1. 86183000
H	5. 60733700	-1. 14466100	-2. 87641600
C	-5. 00977400	-0. 77477800	1. 31410900
H	-5. 35293600	-0. 99907800	2. 32206400
C	-4. 04871100	0. 22098000	1. 13014100
C	-4. 11221700	-0. 23030200	-1. 26924000
C	-5. 07712600	-1. 20840100	-1. 03361100
H	-5. 46554600	-1. 77717000	-1. 87618900
C	4. 13118400	1. 05881100	-2. 41538200
C	3. 39378600	0. 54777300	-3. 65834700
C	5. 41937100	1. 79561000	-2. 80060900
H	4. 01236500	-0. 15889200	-4. 22200100
H	3. 14715400	1. 38109100	-4. 32455400
H	2. 46541200	0. 04133300	-3. 37899700

H	5. 19870500	2. 63197000	-3. 47205300
H	6. 11532100	1. 12484700	-3. 31592400
H	5. 92625500	2. 18837900	-1. 91370800
C	6. 37394300	-3. 36273300	-1. 50317500
C	7. 63993400	-3. 50990600	-0. 65193400
C	5. 57953700	-4. 67366900	-1. 52788000
H	7. 38491400	-3. 75882000	0. 38390500
H	8. 21977400	-2. 58239100	-0. 64196300
H	8. 27517300	-4. 31214000	-1. 04141000
H	6. 19427900	-5. 49000300	-1. 92126000
H	4. 68506500	-4. 58073000	-2. 15019000
H	5. 25651000	-4. 95143500	-0. 51881600
C	3. 60948500	-1. 22373800	2. 14346800
C	4. 59483900	-0. 65706700	3. 17509700
C	3. 20807600	-2. 64549800	2. 55099800
H	4. 82582700	0. 39563800	2. 99337100
H	5. 53454500	-1. 22016800	3. 14320600
H	4. 17972900	-0. 74486900	4. 18455500
H	2. 54927000	-2. 61211900	3. 42443200
H	4. 08485200	-3. 24297000	2. 82642200
H	2. 68394300	-3. 16566000	1. 74690900
C	-3. 61539800	-0. 01407800	-2. 69100700
C	-3. 34223800	-1. 34685500	-3. 40454200
C	-4. 60835500	0. 81734500	-3. 51274800
H	-4. 27045000	-1. 81374400	-3. 75110700
H	-2. 85487900	-2. 06801300	-2. 73984600
H	-2. 70820200	-1. 18766200	-4. 28211300
H	-4. 25239100	0. 93792800	-4. 54143200
H	-4. 75131900	1. 81278000	-3. 08316200
H	-5. 58513100	0. 32175400	-3. 54514000
C	-6. 54639500	-2. 60604200	0. 48237800
C	-7. 86146500	-2. 34514700	-0. 25905000
C	-5. 95561800	-3. 96488000	0. 08679800
H	-7. 70156400	-2. 32751600	-1. 34276100
H	-8. 29597200	-1. 38462100	0. 03246400
H	-8. 58863600	-3. 13439100	-0. 04254300
H	-6. 64843500	-4. 77621900	0. 33224100
H	-5. 00839200	-4. 14763500	0. 60187400
H	-5. 76419200	-4. 00270000	-0. 99171600
C	-3. 53463400	0. 97484600	2. 34643200
C	-4. 63760900	1. 86868700	2. 92685200
C	-2. 97246100	0. 02300200	3. 40770000
H	-5. 48727300	1. 26586100	3. 26597500
H	-5. 00547300	2. 57805800	2. 17844900

H	-4.26135200	2.43476400	3.78520900
H	-2.53017000	0.59675200	4.22864300
H	-2.20347300	-0.63225300	2.98929800
H	-3.76115500	-0.60592300	3.83485500
H	3.47652300	1.78476000	-1.92208900
H	6.68264500	-3.13387600	-2.53146600
H	2.70189600	-0.60786500	2.16062200
H	-2.71741200	1.63115600	2.03157700
H	-2.66965500	0.53367400	-2.64040900
H	-6.76230200	-2.63118200	1.55800900
O	-0.67283900	-0.84853600	-1.77942300
H	-0.93705300	-1.77839800	-1.90056300

OH tautomer-I-4

C	1.68786200	6.13582000	1.95646400
C	0.33391500	5.98499400	1.57549300
C	-0.10210700	4.82771400	0.98197700
C	0.79560400	3.75332200	0.73947300
C	2.14735700	3.89161300	1.15983400
C	2.57136300	5.10836100	1.75572400
C	3.04930400	2.80940700	0.99190800
C	2.64638300	1.59640300	0.49152600
C	1.29245300	1.49040000	0.08021300
C	0.38547100	2.52461600	0.12015200
C	-0.97710000	2.34863300	-0.45026800
C	-1.77028900	1.29472400	-0.05669800
C	-3.11456500	1.10728700	-0.46562400
C	-3.64027500	2.04601300	-1.31764900
C	-2.85735000	3.10484100	-1.84476900
C	-1.50263600	3.24946000	-1.43658200
C	-0.71846400	4.26865000	-2.04134400
C	-1.26633000	5.11636700	-2.97012300
C	-2.62550000	4.99704500	-3.34418400
C	-3.39968800	4.00930300	-2.79526300
H	3.61036100	5.20067000	2.06028300
H	2.01874000	7.06040000	2.41844500
H	-0.36846500	6.79157100	1.76000600
H	-1.14488100	4.72097100	0.70411400
H	4.08963800	2.94284500	1.27734200
O	0.87940600	0.25535200	-0.44407100
H	0.32777400	4.36384000	-1.77208000
H	-0.64896600	5.88252400	-3.42816200
H	-3.04574100	5.67919800	-4.07616200

H	-4.43910400	3.88941900	-3.08852800
O	-1.27231400	0.38556700	0.88465000
H	-4.68344300	1.96667300	-1.61134800
P	-0.10331800	-0.60684900	0.47463800
N	-0.60633700	-1.92743900	-0.17741500
S	0.14099100	-3.04223000	-1.05359600
O	0.64610000	-2.52482800	-2.31105400
O	-0.60689900	-4.27934300	-1.01038500
C	1.64741600	-3.37233600	-0.03710600
F	2.45656300	-2.31921300	-0.07511700
F	1.29716300	-3.56023500	1.25308900
F	2.28331600	-4.44534500	-0.46362100
C	3.60762200	0.46346100	0.33226600
C	5.52841200	-1.56634400	0.02518200
C	-5.56958800	-2.12800700	0.94526200
C	-3.92869200	-0.03871500	0.04120800
C	-4.47098900	0.01224000	1.33497800
C	-4.16712100	-1.14847600	-0.79475700
C	-4.99354800	-2.16725200	-0.32524200
H	-5.18021600	-3.02709800	-0.96408100
C	-5.28874400	-1.03692700	1.76057800
H	-5.72053100	-1.00287800	2.75939000
C	5.03931500	-0.86872800	-1.07855500
H	5.40699300	-1.12053600	-2.07137400
C	4.08396900	0.13744300	-0.95307000
C	4.06735600	-0.24006700	1.45977200
C	5.03059500	-1.23605600	1.28122900
H	5.39263100	-1.78609500	2.14762800
C	-4.20860800	1.17291000	2.28191300
C	-3.53025000	0.69829200	3.57193100
C	-5.50305600	1.93612100	2.58646000
H	-4.18048900	0.01924500	4.13385800
H	-3.30090100	1.55205000	4.21813200
H	-2.59763900	0.17189100	3.34972600
H	-5.30102800	2.79315800	3.23739300
H	-6.22775100	1.29076400	3.09457100
H	-5.96755800	2.30268500	1.66578100
C	-6.45923700	-3.25680800	1.42980300
C	-7.69818700	-3.41367600	0.54121200
C	-5.68290900	-4.57569300	1.51854000
H	-7.41204900	-3.69497800	-0.47809700
H	-8.26568600	-2.48014900	0.48563500
H	-8.35597400	-4.19703100	0.93168300
H	-6.32057600	-5.37276200	1.91489100

H	-4.80806900	-4.47522800	2.16702900
H	-5.33083500	-4.88693100	0.52918800
C	-3.54437300	-1.25969300	-2.17977500
C	-4.48795300	-0.71752900	-3.26237000
C	-3.14260200	-2.69693800	-2.52837000
H	-4.71496700	0.34232400	-3.12180300
H	-5.43354500	-1.27133800	-3.24574200
H	-4.03892100	-0.84074900	-4.25344800
H	-2.45336700	-2.69680900	-3.37864200
H	-4.01491700	-3.29527900	-2.81577800
H	-2.65224900	-3.19587600	-1.69025400
C	3.53280500	0.02336600	2.85941300
C	3.21791500	-1.28456600	3.60104800
C	4.51442700	0.86272100	3.68666400
H	4.12816100	-1.75574600	3.98691400
H	2.73796700	-2.01611800	2.94256800
H	2.56173800	-1.09108500	4.45519900
H	4.12992600	1.01876100	4.70021200
H	4.68637500	1.84284100	3.23306000
H	5.48155800	0.35328800	3.76311600
C	6.53476100	-2.68702200	-0.14621800
C	5.92585100	-3.84045700	-0.95281600
C	7.83235400	-2.19290800	-0.79399900
H	5.70317500	-3.52012800	-1.97657800
H	4.99087400	-4.18668000	-0.50353500
H	6.62078400	-4.68460500	-1.00828400
H	8.55992800	-3.00757000	-0.86828200
H	8.27980300	-1.38062700	-0.21392800
H	7.64496500	-1.82005400	-1.80684800
C	3.61304700	0.85884900	-2.20630700
C	4.74200500	1.72248200	-2.78237400
C	3.07017200	-0.12018900	-3.25280300
H	5.59462200	1.10062900	-3.07692000
H	5.09593800	2.45169000	-2.04642200
H	4.39718700	2.26450300	-3.66898900
H	2.65872600	0.43151900	-4.10433600
H	2.28197700	-0.75330700	-2.83605200
H	3.86320700	-0.77156500	-3.63631800
H	-3.52507300	1.87416600	1.79208500
H	-6.79889700	-2.99464900	2.44022800
H	-2.63117900	-0.65203100	-2.18456300
H	2.79468900	1.53334200	-1.93603700
H	2.59789100	0.58381000	2.76544000
H	6.77829000	-3.06425000	0.85543700

O	0.60430100	-0.79788300	1.88190600
H	0.84381900	-1.72673000	2.05186000

OH tautomer-II-1

C	3.64907000	5.51217000	2.12966900
C	2.27659200	5.74328600	1.87852200
C	1.51632400	4.80462800	1.22808900
C	2.08904500	3.58042000	0.79089200
C	3.45862400	3.32794000	1.08898800
C	4.22170700	4.32744900	1.74845900
C	4.03286100	2.06509500	0.78410400
C	3.29676900	1.05229700	0.22289500
C	1.96179800	1.37146700	-0.14263300
C	1.33880200	2.57444000	0.09298100
C	-0.07707600	2.76118500	-0.33127200
C	-1.03273000	1.82362900	0.00174000
C	-2.41157800	1.92855500	-0.31195800
C	-2.81023900	3.05936700	-0.98032300
C	-1.88113900	4.03564200	-1.42122800
C	-0.49662200	3.87685200	-1.13179800
C	0.41947100	4.81365500	-1.68260200
C	-0.02399600	5.87132200	-2.43478600
C	-1.40524200	6.05432900	-2.68020100
C	-2.30978300	5.15119000	-2.18854200
H	5.26820100	4.12352300	1.95843100
H	4.23958400	6.26708100	2.63874100
H	1.81862600	6.66994500	2.20948700
H	0.46283400	4.98987000	1.05010900
H	5.06977200	1.88517100	1.05511700
O	1.24692500	0.37094900	-0.80656400
H	1.48193700	4.67870500	-1.51335700
H	0.69285500	6.57082700	-2.85287500
H	-1.74133300	6.89993800	-3.27157300
H	-3.37180300	5.26187800	-2.38986700
O	-0.66604500	0.69926400	0.75168400
H	-3.86313900	3.19164400	-1.21601700
P	0.19114200	-0.44569700	0.05914300
N	-0.57284800	-1.40698500	-0.92489000
S	-0.52593800	-2.99859100	-0.82475500
O	0.49232400	-3.45724700	0.13792600
O	-0.59231400	-3.61921800	-2.12671400
C	-2.12923300	-3.36759800	0.00887200
F	-2.29727700	-2.53529700	1.03213400

F	-3.12789100	-3.22929100	-0.84859300
F	-2.11456900	-4.61428100	0.46012600
C	3.77180900	-0.35759100	0.07897800
C	4.41410900	-3.09047600	-0.16450800
C	-5.21651200	-1.18214700	0.69444800
C	-3.36391200	0.83298600	0.04233800
C	-3.66534600	0.56369200	1.39315200
C	-3.96596600	0.07729300	-0.98346900
C	-4.89383600	-0.90506200	-0.62896600
H	-5.36830100	-1.49045000	-1.41390600
C	-4.58678500	-0.43738900	1.69068800
H	-4.81947800	-0.64186400	2.73409600
C	4.17481800	-2.30642600	-1.29176600
H	4.23109200	-2.76430000	-2.27691600
C	3.85230400	-0.95461800	-1.19697300
C	4.02654500	-1.12572200	1.23627700
C	4.34869300	-2.47666500	1.08245000
H	4.54302600	-3.07892500	1.96683800
C	-3.05416900	1.34915400	2.54407700
C	-2.32721700	0.42970300	3.53201200
C	-4.12560000	2.18416200	3.25685700
H	-3.02794400	-0.24937400	4.02964700
H	-1.83287300	1.02264500	4.30844100
H	-1.56969000	-0.17349000	3.02378500
H	-3.67883800	2.77691600	4.06189600
H	-4.89376500	1.53999600	3.69837300
H	-4.62030700	2.86627000	2.55852000
C	-6.19448800	-2.28723400	1.04452200
C	-5.46958500	-3.46830200	1.70213800
C	-7.33274700	-1.78315000	1.93771200
H	-4.96707300	-3.14883500	2.62208400
H	-4.71379800	-3.88931400	1.03453500
H	-6.17836400	-4.26186800	1.96077700
H	-8.06366000	-2.57913900	2.11248800
H	-7.84823000	-0.93387800	1.48005400
H	-6.95429700	-1.46145300	2.91401700
C	-3.66692800	0.29109100	-2.46211000
C	-4.86541700	0.94756000	-3.16098800
C	-3.28275200	-1.00813800	-3.18011300
H	-5.14471200	1.89350600	-2.68621600
H	-5.74011800	0.28852600	-3.12301900
H	-4.63661300	1.14443200	-4.21343700
H	-3.05848100	-0.79442700	-4.23034900
H	-4.09771200	-1.73920400	-3.16072100

H	-2.39907700	-1.46626000	-2.73104600
C	3.97879800	-0.54791900	2.64564600
C	3.24579900	-1.44538900	3.64966100
C	5.40351500	-0.27235300	3.14851400
H	3.78037500	-2.38408700	3.82602300
H	2.23358700	-1.68065300	3.31276100
H	3.16934800	-0.93056700	4.61272700
H	5.38136700	0.19160400	4.14019600
H	5.95548600	0.38587000	2.47101000
H	5.96551400	-1.21014200	3.22396900
C	4.71228900	-4.57076000	-0.29477900
C	3.51991300	-5.31480000	-0.90866400
C	5.98954600	-4.81864900	-1.10483800
H	3.33841300	-4.97548600	-1.93454400
H	2.60456600	-5.13900000	-0.33738300
H	3.71574000	-6.39164500	-0.94141900
H	6.21463900	-5.88915800	-1.14782200
H	6.84687600	-4.30166200	-0.66370000
H	5.87318300	-4.46148500	-2.13394200
C	3.64548900	-0.16767700	-2.48267700
C	4.99120000	0.03601500	-3.19209700
C	2.63039500	-0.83433900	-3.41808500
H	5.43001100	-0.92751100	-3.47375500
H	5.70442200	0.55358900	-2.54298000
H	4.85943400	0.62786700	-4.10385500
H	2.42978600	-0.18530000	-4.27658100
H	1.68329200	-1.03181900	-2.90764600
H	3.01085900	-1.78404800	-3.80842600
H	-2.31611800	2.04917000	2.14128300
H	-6.63553900	-2.64304700	0.10461400
H	-2.81229900	0.96863800	-2.54816100
H	3.26126400	0.82490700	-2.22901700
H	3.43654600	0.40131800	2.61206600
H	4.87290000	-4.96178300	0.71825800
O	0.87804000	-1.10183800	1.30969900
H	1.05771200	-2.06233900	1.13430900

OH tautomer-II-2

C	-3.59008100	5.47661300	-2.23977500
C	-2.20666300	5.68864400	-2.03598600
C	-1.44931500	4.76628100	-1.35940600
C	-2.03604100	3.57828600	-0.84713400
C	-3.41806900	3.34243600	-1.09731400

C	-4.17733400	4.32529300	-1.78560400
C	-4.00962900	2.10865800	-0.71687500
C	-3.28001400	1.10801000	-0.12608700
C	-1.93013200	1.41504300	0.19169700
C	-1.28920200	2.59131100	-0.11905400
C	0.14151300	2.76821300	0.25598000
C	1.06805900	1.79592300	-0.05893900
C	2.45855400	1.89062300	0.20214300
C	2.89898700	3.04552700	0.79948600
C	2.00265300	4.05959900	1.22228100
C	0.60681000	3.91374000	0.98565400
C	-0.27390500	4.89465500	1.51703000
C	0.21288100	5.97913000	2.20112700
C	1.60449200	6.14669800	2.39351000
C	2.47617400	5.20304600	1.91895300
H	-5.23313000	4.13485100	-1.95832700
H	-4.17779300	6.21881900	-2.77033200
H	-1.73813000	6.58721200	-2.42459400
H	-0.38768400	4.93620700	-1.21841200
H	-5.05659200	1.93804100	-0.95296500
O	-1.21973600	0.43445100	0.88971100
H	-1.34357200	4.77238500	1.38806100
H	-0.47716400	6.71249700	2.60605700
H	1.97477600	7.01353400	2.93129200
H	3.54604000	5.30278700	2.08060200
O	0.65472700	0.64216600	-0.73670700
H	3.96157800	3.16981500	0.99195500
P	-0.19772700	-0.44672800	0.04706900
N	0.58242900	-1.35739300	1.06636100
S	0.52989300	-2.95199400	1.04873900
O	-0.53746500	-3.45432600	0.16453600
O	0.66254600	-3.50464600	2.37588500
C	2.08782800	-3.37335300	0.15381100
F	2.22052800	-2.57695100	-0.90292100
F	3.12761600	-3.22489600	0.95884700
F	2.03331800	-4.63318000	-0.25598200
C	-3.78234300	-0.28247200	0.09320900
C	-4.48886000	-2.98335600	0.47206200
C	5.18266500	-1.30645400	-0.75411200
C	3.38142200	0.76421300	-0.13268900
C	3.62883200	0.42624500	-1.47915200
C	4.01361000	0.05143300	0.90566300
C	4.91497500	-0.96007500	0.56518900
H	5.41135400	-1.51375300	1.35952000

C	4. 52567200	-0. 60121800	-1. 76141700
H	4. 71599600	-0. 85931200	-2. 80153700
C	-4. 20825900	-2. 15766300	1. 55496600
H	-4. 25864300	-2. 57533400	2. 55811000
C	-3. 85293200	-0. 81723500	1. 39368500
C	-4. 07771400	-1. 09724900	-1. 02540500
C	-4. 43155300	-2. 42794000	-0. 80604800
H	-4. 65626700	-3. 05910400	-1. 66276200
C	2. 98542800	1. 16388100	-2. 64410800
C	2. 20477200	0. 20881800	-3. 55444000
C	4. 04095500	1. 94161800	-3. 44037700
H	2. 87422100	-0. 50753500	-4. 04289100
H	1. 68996400	0. 77037000	-4. 34088200
H	1. 45811300	-0. 35361000	-2. 98686500
H	3. 57167000	2. 50178200	-4. 25585500
H	4. 77927600	1. 26179200	-3. 87924700
H	4. 57530000	2. 64817000	-2. 79782200
C	6. 13020600	-2. 44310500	-1. 08614400
C	5. 36430700	-3. 63863200	-1. 66658100
C	7. 24603000	-1. 99868600	-2. 03750100
H	4. 84021200	-3. 35202600	-2. 58530900
H	4. 62150800	-4. 01359400	-0. 95807500
H	6. 05021200	-4. 45706100	-1. 90885200
H	7. 95628400	-2. 81508300	-2. 20318000
H	7. 79196000	-1. 14126500	-1. 63351500
H	6. 83982900	-1. 71036700	-3. 01309200
C	3. 77612100	0. 34266200	2. 38230200
C	5. 00970000	1. 01591400	2. 99965200
C	3. 40559800	-0. 91320400	3. 18009500
H	5. 28234700	1. 93270800	2. 46730300
H	5. 87370000	0. 34293400	2. 96113000
H	4. 82525600	1. 26849800	4. 04891400
H	3. 22801100	-0. 64384000	4. 22643300
H	4. 20945500	-1. 65653900	3. 16452400
H	2. 49800300	-1. 38016900	2. 79221000
C	-4. 03794400	-0. 58454400	-2. 46022100
C	-3. 34219000	-1. 54499400	-3. 43196900
C	-5. 46277900	-0. 29586800	-2. 95511800
H	-3. 90272800	-2. 47665000	-3. 55878400
H	-2. 33176600	-1. 79092200	-3. 09731600
H	-3. 26652400	-1. 07637600	-4. 41840100
H	-5. 44445000	0. 12073600	-3. 96767300
H	-5. 98753000	0. 40726700	-2. 30155500
H	-6. 04929100	-1. 22134400	-2. 97819900

C	-4.82510200	-4.44795800	0.67013700
C	-6.23216200	-4.77610600	0.15887800
C	-3.77550500	-5.34527600	0.00323000
H	-6.30210500	-4.60957000	-0.92181300
H	-6.98707600	-4.15131200	0.64519300
H	-6.47529600	-5.82618200	0.35066400
H	-3.98184400	-6.39946600	0.21516700
H	-2.76833600	-5.10576600	0.35515300
H	-3.79153400	-5.21455200	-1.08486900
C	-3.60164600	0.02048900	2.63842300
C	-4.92658800	0.28369400	3.36712100
C	-2.57958500	-0.62567300	3.58044000
H	-5.37778100	-0.65663900	3.70225100
H	-5.64397200	0.78636000	2.71093400
H	-4.76204800	0.91319600	4.24780100
H	-2.35107400	0.05394300	4.40772400
H	-1.64611100	-0.85935800	3.06038900
H	-2.96814200	-1.55205500	4.01595900
H	2.27580600	1.89718100	-2.24954500
H	6.59645500	-2.76510500	-0.14620700
H	2.93390500	1.03564000	2.46747700
H	-3.20336600	0.99261300	2.33226900
H	-3.47170900	0.35098500	-2.47802400
H	-4.80173600	-4.64417000	1.74953400
O	-0.92736800	-1.16697400	-1.14291000
H	-1.11823200	-2.11162100	-0.90533400

OH tautomer-II-3

C	-3.78732500	5.46858300	-2.00834400
C	-2.40225000	5.70348200	-1.84523100
C	-1.60394600	4.77819000	-1.22178900
C	-2.14887700	3.56408300	-0.72478400
C	-3.53377100	3.30669600	-0.93516100
C	-4.33557100	4.29272900	-1.56850100
C	-4.08744300	2.05040800	-0.57163300
C	-3.31839700	1.04891000	-0.03476800
C	-1.96503100	1.37496500	0.24679500
C	-1.35817400	2.57242100	-0.05117800
C	0.08130600	2.76723200	0.27901700
C	1.01457700	1.82308600	-0.09625900
C	2.41197500	1.94042800	0.11398400
C	2.85149300	3.08739600	0.72707700
C	1.95151600	4.06973800	1.21249600

C	0.55093900	3.90145800	1.02331300
C	-0.32863900	4.84868300	1.61426700
C	0.16167700	5.92390200	2.31031900
C	1.55590100	6.11509700	2.45605700
C	2.42785000	5.20320000	1.92345300
H	-5.39266800	4.08527100	-1.71098800
H	-4.40763100	6.21314400	-2.49680300
H	-1.96521300	6.62229300	-2.22305300
H	-0.54171100	4.96632500	-1.11216100
H	-5.13804900	1.86449900	-0.77836300
O	-1.21287000	0.39063600	0.89320100
H	-1.39969800	4.70737100	1.52140500
H	-0.52721700	6.63125400	2.76095300
H	1.92875000	6.97438100	3.00409400
H	3.50081000	5.32091700	2.04834700
O	0.59910400	0.67942900	-0.78967000
H	3.91799100	3.22950100	0.88237000
P	-0.20010800	-0.44711500	-0.00309100
N	0.63603200	-1.35936500	0.96826800
S	0.59860100	-2.95421500	0.94474100
O	-0.46114800	-3.46394500	0.05535900
O	0.73306600	-3.51269400	2.26951500
C	2.16558700	-3.35037300	0.05707800
F	2.28104000	-2.56642800	-1.01060000
F	3.19665600	-3.16115200	0.86466400
F	2.14284800	-4.61643400	-0.33475100
C	-3.78468500	-0.35777400	0.15890500
C	-4.42596200	-3.08246600	0.47818500
C	5.16503700	-1.15659300	-1.06536900
C	3.34339400	0.84610200	-0.29605500
C	3.54142300	0.56301300	-1.66063600
C	4.03496200	0.11025600	0.69062700
C	4.93733300	-0.87132300	0.27949600
H	5.47117100	-1.43949800	1.03869000
C	4.45411200	-0.43042000	-2.01547900
H	4.62112800	-0.64413700	-3.06963400
C	-4.12317000	-2.28448300	1.57584200
H	-4.13052700	-2.73321700	2.56673800
C	-3.79934000	-0.93296400	1.44394500
C	-4.10246400	-1.14430800	-0.97360100
C	-4.42338100	-2.48781000	-0.78337800
H	-4.66534200	-3.09720600	-1.65110500
C	2.83693700	1.32647200	-2.77218400
C	2.04605600	0.38597900	-3.68873400

C	3. 84238500	2. 16031900	-3. 57652500
H	2. 71356200	-0. 29650500	-4. 22570000
H	1. 49086900	0. 96278900	-4. 43568800
H	1. 33283500	-0. 21345200	-3. 11594500
H	3. 32857900	2. 73893000	-4. 35127400
H	4. 57924400	1. 51686300	-4. 06924700
H	4. 38374400	2. 85537700	-2. 92731300
C	6. 13652600	-2. 24182300	-1. 48860500
C	7. 53575700	-2. 01675800	-0. 90672300
C	5. 60953500	-3. 63192300	-1. 11291600
H	7. 52228800	-2. 08832600	0. 18616100
H	7. 92169400	-1. 02909400	-1. 17505700
H	8. 23250300	-2. 77440000	-1. 27964500
H	6. 28465100	-4. 41187800	-1. 48001500
H	4. 61708900	-3. 80650900	-1. 53929000
H	5. 53169100	-3. 73595100	-0. 02570900
C	3. 86895600	0. 36595600	2. 18410400
C	5. 12738900	1. 04097000	2. 74778300
C	3. 55193300	-0. 90568900	2. 97910000
H	5. 36663400	1. 96616200	2. 21381500
H	5. 99316600	0. 37531600	2. 65664100
H	4. 99446900	1. 27896900	3. 80817900
H	3. 44889000	-0. 65694200	4. 04046800
H	4. 35022200	-1. 65021400	2. 89239500
H	2. 61771300	-1. 36249900	2. 64650400
C	-4. 11951200	-0. 58918200	-2. 39299200
C	-3. 42981500	-1. 50350900	-3. 41247000
C	-5. 56529100	-0. 32206800	-2. 83636500
H	-3. 96944300	-2. 44625500	-3. 54785900
H	-2. 40331200	-1. 73081200	-3. 11561000
H	-3. 39758500	-1. 00643200	-4. 38730300
H	-5. 58779800	0. 12354300	-3. 83640700
H	-6. 08620100	0. 34913900	-2. 14706200
H	-6. 13018900	-1. 26061300	-2. 86902900
C	-4. 72678800	-4. 55892300	0. 64223100
C	-6. 14268100	-4. 90122600	0. 16589700
C	-3. 68133500	-5. 41355200	-0. 08460700
H	-6. 25089900	-4. 70390600	-0. 90641600
H	-6. 89399100	-4. 30745300	0. 69480400
H	-6. 35826400	-5. 96149000	0. 33298400
H	-3. 85953000	-6. 47780200	0. 10095100
H	-2. 66851400	-5. 16366600	0. 24311000
H	-3. 73470900	-5. 25017600	-1. 16710500
C	-3. 52054200	-0. 12841900	2. 70461000

C	-4.82429300	0.08813400	3.48501700
C	-2.45572800	-0.78332300	3.59180300
H	-5.24731000	-0.87004000	3.80606500
H	-5.57228900	0.59701500	2.86902900
H	-4.64092600	0.69380000	4.37859900
H	-2.21076900	-0.12409700	4.43079200
H	-1.53636800	-0.98506600	3.03443500
H	-2.81302500	-1.72897100	4.01240900
H	2.12505500	2.02603600	-2.32418300
H	6.21576900	-2.19660400	-2.58247100
H	3.02643100	1.04869500	2.32735400
H	-3.14999500	0.85961900	2.41516800
H	-3.57728100	0.36058500	-2.40002100
H	-4.66467700	-4.78680500	1.71382000
O	-0.95335400	-1.15909000	-1.18306000
H	-1.10819200	-2.11449200	-0.96244500

OH tautomer-II-4

C	-3.87324300	5.48005900	-1.90049500
C	-2.49876700	5.73965400	-1.69181300
C	-1.69269700	4.80411500	-1.09413500
C	-2.21886700	3.55465300	-0.67014700
C	-3.59163500	3.27484300	-0.92678100
C	-4.40232400	4.27142700	-1.53158600
C	-4.12334300	1.98988800	-0.63714000
C	-3.34279800	0.98203300	-0.12977900
C	-2.00435700	1.32624600	0.19847700
C	-1.41954900	2.55026100	-0.02627900
C	0.00617900	2.76090000	0.35164600
C	0.97104700	1.85633300	-0.04099400
C	2.35819800	1.98873200	0.22182100
C	2.75449100	3.11169100	0.90464700
C	1.81925500	4.05205000	1.40658800
C	0.42892800	3.86602500	1.16491800
C	-0.48790900	4.76564500	1.77340800
C	-0.04189200	5.81498800	2.53563800
C	1.34285700	6.02612200	2.73430500
C	2.24961100	5.15837200	2.18625100
H	-5.45029200	4.04630600	-1.71018100
H	-4.50025800	6.23261700	-2.36766600
H	-2.07601400	6.68607300	-2.01359500
H	-0.63840300	5.01165200	-0.94842300
H	-5.16432000	1.79064800	-0.87729900

O	-1.24264900	0.32805000	0.81106300
H	-1.55246000	4.60834300	1.64039700
H	-0.75899100	6.48591900	2.99782400
H	1.68068100	6.86483600	3.33445100
H	3.31552400	5.29059000	2.35069000
O	0.60354400	0.74202800	-0.80539400
H	3.81216400	3.26548100	1.10309700
P	-0.19685000	-0.44074000	-0.10881600
N	0.62827600	-1.39915100	0.82646300
S	0.59934000	-2.99074900	0.71889400
O	-0.41393300	-3.45709300	-0.24552200
O	0.67398400	-3.61902100	2.01702100
C	2.20874300	-3.33029200	-0.11285300
F	2.35791900	-2.50374600	-1.14332000
F	3.20033900	-3.15777500	0.74635800
F	2.22306400	-4.58050400	-0.55308700
C	-3.77424800	-0.44416500	-0.01017600
C	-4.32380600	-3.20169500	0.17553600
C	5.20244500	-1.00665600	-1.00341900
C	3.32252000	0.93024600	-0.20652000
C	3.57676400	0.71914400	-1.57461800
C	3.98504900	0.15291400	0.76818100
C	4.91793100	-0.79396200	0.34412800
H	5.43113800	-1.39246800	1.09416800
C	4.51740300	-0.24296100	-1.94300700
H	4.72806500	-0.40045200	-2.99922700
C	-4.06987000	-2.44220400	1.31631400
H	-4.07779000	-2.92897400	2.28910000
C	-3.79252000	-1.07878800	1.24993300
C	-4.04516300	-1.18741800	-1.17996000
C	-4.32075800	-2.55156300	-1.05462600
H	-4.52666700	-3.13476600	-1.94909100
C	2.90169000	1.52740500	-2.67256400
C	2.16297700	0.62277500	-3.66539200
C	3.92192200	2.41744200	-3.39387800
H	2.86253200	-0.01909800	-4.21150900
H	1.62450200	1.22823200	-4.40178900
H	1.44101300	-0.01803300	-3.15134300
H	3.42802000	3.02589800	-4.15864000
H	4.68923900	1.81197300	-3.88830900
H	4.42467800	3.08775200	-2.68988500
C	6.21088600	-2.05175000	-1.44106200
C	7.58613300	-1.81706100	-0.80762700
C	5.70892500	-3.46854000	-1.13838900

H	7.54085800	-1.93187600	0.28074100
H	7.95526100	-0.81064300	-1.02512400
H	8.31258200	-2.54261300	-1.18767300
H	6.41557700	-4.21549300	-1.51464300
H	4.73527600	-3.65057000	-1.60307100
H	5.60032900	-3.61923500	-0.05929600
C	3.75380100	0.32708700	2.26463500
C	4.97486200	0.99307100	2.91451900
C	3.42911000	-0.99025600	2.97809000
H	5.21671400	1.94957700	2.44029200
H	5.85665300	0.34865900	2.82412500
H	4.79471200	1.17171600	3.97960300
H	3.27584100	-0.79989000	4.04545500
H	4.24548200	-1.71446200	2.88761200
H	2.51964600	-1.44574900	2.58107900
C	-4.06025300	-0.56946300	-2.57284700
C	-3.33837100	-1.41832400	-3.62598500
C	-5.50766200	-0.31805100	-3.02046100
H	-3.85556400	-2.36452400	-3.81383100
H	-2.31049000	-1.63790000	-3.32812500
H	-3.30549200	-0.87366100	-4.57500400
H	-5.53077200	0.17350200	-3.99873900
H	-6.05317500	0.30636200	-2.30672000
H	-6.04761400	-1.26803000	-3.10402000
C	-4.57118800	-4.69377400	0.27347500
C	-3.33692700	-5.41541200	0.82857100
C	-5.81332700	-5.00396200	1.11605400
H	-3.13224700	-5.09770200	1.85702500
H	-2.44656900	-5.19548200	0.23357300
H	-3.49821800	-6.49843500	0.83802300
H	-6.00303100	-6.08195900	1.13703300
H	-6.70021400	-4.50361400	0.71606900
H	-5.67526300	-4.67007700	2.15028300
C	-3.56484000	-0.32193800	2.55001100
C	-4.89149200	-0.17606800	3.30787400
C	-2.50149700	-0.98504400	3.43298300
H	-5.29467800	-1.15915500	3.57481000
H	-5.63931400	0.33984200	2.69752400
H	-4.74586200	0.39289100	4.23202100
H	-2.28839900	-0.35291500	4.30101600
H	-1.56751000	-1.14469000	2.88633500
H	-2.84379600	-1.95413000	3.81081200
H	2.16087900	2.19144100	-2.21742300
H	6.32144800	-1.95927000	-2.52921200

H	2.89319000	0.98707200	2.40767500
H	-3.21663600	0.68767500	2.31211300
H	-3.54170200	0.39255800	-2.52944700
H	-4.75217300	-5.06238600	-0.74452200
O	-0.91019400	-1.08946900	-1.34816000
H	-1.05515600	-2.05858600	-1.18887300

OH tautomer-III-1

C	2.32133400	6.22452900	1.91244100
C	0.93147300	6.19445800	1.65051400
C	0.34905400	5.08667300	1.08925100
C	1.12697500	3.94435600	0.75933400
C	2.51672000	3.95864300	1.06699100
C	3.09227700	5.12783600	1.63082600
C	3.30355900	2.79860600	0.84335100
C	2.75223900	1.62949700	0.38322100
C	1.37434300	1.66305400	0.04599700
C	0.55994600	2.76872500	0.16159300
C	-0.85479000	2.69960300	-0.29969500
C	-1.65199800	1.65314000	0.10288200
C	-2.99794600	1.44670700	-0.30008500
C	-3.55684100	2.42072700	-1.08764900
C	-2.79830400	3.52133200	-1.56732500
C	-1.42275100	3.64585000	-1.21929400
C	-0.66368800	4.68122100	-1.82787800
C	-1.25275300	5.57209000	-2.68906300
C	-2.63057800	5.47819500	-2.99331800
C	-3.38094600	4.46956800	-2.44902100
H	4.15686900	5.12621900	1.84865100
H	2.76913800	7.11085200	2.35025100
H	0.31888300	7.05427900	1.90227200
H	-0.71911300	5.07117000	0.90227000
H	4.36555400	2.83493800	1.06896900
O	0.85252200	0.47723600	-0.48651000
H	0.39648000	4.75798500	-1.61414300
H	-0.65332600	6.35225200	-3.14736600
H	-3.08443000	6.19416600	-3.67095000
H	-4.43421700	4.36594800	-2.69520100
O	-1.12334000	0.71793500	0.99984300
H	-4.59217100	2.32196200	-1.40335300
P	-0.12194200	-0.37873900	0.43659400
N	-0.77924800	-1.50412200	-0.44604600
S	-0.61197900	-3.06462100	-0.18457900

O	-1.71654700	-3.83213000	-0.71078800
O	-0.13159400	-3.34323700	1.18210600
C	0.84425500	-3.45158100	-1.24055400
F	0.56985000	-3.20887700	-2.51348800
F	1.86207200	-2.68038900	-0.85714100
F	1.18330100	-4.72359900	-1.09470000
C	3.52465000	0.35769100	0.23443100
C	4.93977400	-2.05694500	-0.05349100
C	-4.59105300	-2.40741700	0.73434600
C	-3.66033300	0.15505800	0.05093800
C	-3.92877500	-0.15902600	1.39815700
C	-3.87723500	-0.80308200	-0.96088300
C	-4.34838200	-2.06350600	-0.59082200
H	-4.48959400	-2.82240000	-1.35554500
C	-4.39511600	-1.43280500	1.71284700
H	-4.59964900	-1.67700700	2.75351300
C	4.51308800	-1.33888500	-1.16851700
H	4.72181600	-1.72877600	-2.16300700
C	3.79928900	-0.14841900	-1.05185600
C	3.94194500	-0.35015500	1.37981600
C	4.64733200	-1.54325800	1.20612300
H	4.96928000	-2.10143700	2.08214400
C	-3.76585600	0.86171100	2.51456000
C	-2.92733700	0.32930100	3.68105900
C	-5.14384400	1.32864700	3.00243400
H	-3.43252800	-0.49683300	4.19229900
H	-2.76398000	1.12103000	4.41952500
H	-1.95222000	-0.02600500	3.33640700
H	-5.04113500	2.08967700	3.78325700
H	-5.71037000	0.48837000	3.41880200
H	-5.72825300	1.75229900	2.17984500
C	-5.03062500	-3.80929200	1.10678100
C	-3.99094000	-4.48812100	2.00611400
C	-6.41260700	-3.80781800	1.76949800
H	-3.89796400	-3.95744600	2.96056200
H	-3.00893100	-4.50159500	1.52554100
H	-4.28798400	-5.51929400	2.22484800
H	-6.73530300	-4.83062100	1.99003000
H	-7.16187600	-3.33983700	1.12405500
H	-6.38996700	-3.25416100	2.71488700
C	-3.62668900	-0.52246200	-2.43712800
C	-4.95784400	-0.22353600	-3.14227800
C	-2.89685600	-1.65821000	-3.16280700
H	-5.49210700	0.60636800	-2.66913400

H	-5.61226000	-1.10164100	-3.10116000
H	-4.79106500	0.02730300	-4.19521600
H	-2.69222700	-1.35623100	-4.19557900
H	-3.49769400	-2.57201500	-3.20287200
H	-1.94954900	-1.89677400	-2.67616700
C	3.66020000	0.14047900	2.79388700
C	3.24702900	-0.98635300	3.74827600
C	4.88578100	0.86366400	3.37070400
H	4.09218800	-1.63778700	3.99389700
H	2.45446400	-1.60549900	3.32274200
H	2.88231100	-0.56015100	4.68785000
H	4.67893300	1.22476700	4.38365600
H	5.18488600	1.71773600	2.75749500
H	5.73827000	0.17688900	3.42111700
C	5.64866900	-3.38809600	-0.20895200
C	4.68697200	-4.44412600	-0.76878000
C	6.90334600	-3.27493900	-1.08061700
H	4.33798800	-4.15595700	-1.76720600
H	3.80758700	-4.55736900	-0.12909900
H	5.18468000	-5.41580900	-0.85218400
H	7.42831100	-4.23462200	-1.12260000
H	7.59152900	-2.52071700	-0.68817900
H	6.64503400	-2.99403000	-2.10736500
C	3.36094000	0.55886300	-2.32596400
C	4.58083200	1.04990500	-3.11605700
C	2.46917300	-0.33742000	-3.19380800
H	5.20319100	0.20802700	-3.43844900
H	5.20277400	1.71319100	-2.50705800
H	4.26439900	1.59627000	-4.01053000
H	2.14603900	0.20552300	-4.08804200
H	1.57995000	-0.66014800	-2.64687900
H	3.00756000	-1.23223000	-3.52531100
H	-3.24995900	1.73961500	2.11209600
H	-5.09762700	-4.38648900	0.17615200
H	-2.99338100	0.36623700	-2.51834900
H	2.77504500	1.44267700	-2.05464600
H	2.82832200	0.85091400	2.74792500
H	5.96103400	-3.71201700	0.79213900
O	0.62584100	-0.85342800	1.73247900
H	0.54715900	-1.84120700	1.82681900

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C	-2.25637300	6.19940400	-2.01172400
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C	-0.85843300	6.14961600	-1.80081200
C	-0.27705500	5.05112200	-1.22055500
C	-1.06421900	3.93812200	-0.81986900
C	-2.46405500	3.97050700	-1.07593300
C	-3.03757600	5.13031200	-1.66078300
C	-3.26449000	2.83640000	-0.77938100
C	-2.71886400	1.67322600	-0.29792200
C	-1.32884200	1.68967000	-0.01384300
C	-0.49813500	2.77361300	-0.19985700
C	0.93092100	2.69333300	0.21306600
C	1.69292200	1.61692600	-0.17811400
C	3.04814300	1.39699700	0.18493300
C	3.65371200	2.38748500	0.91535400
C	2.93441100	3.52072100	1.37951300
C	1.54981300	3.66091600	1.07589600
C	0.83349300	4.73363000	1.67145000
C	1.47042700	5.64320100	2.47721500
C	2.85619400	5.53195500	2.73598700
C	3.56669100	4.48854800	2.20389700
H	-4.10954400	5.14330400	-1.83834900
H	-2.70293900	7.07843200	-2.46523500
H	-0.23907900	6.98656500	-2.10715200
H	0.79686900	5.02015200	-1.07243900
H	-4.33404300	2.88799100	-0.96217400
O	-0.81100000	0.51337100	0.54336800
H	-0.23194100	4.82457600	1.49227000
H	0.90316500	6.45201700	2.92670800
H	3.34795200	6.26278000	3.36987800
H	4.62591700	4.37219600	2.41652900
O	1.11390800	0.66128100	-1.02066400
H	4.69740500	2.27882100	1.19872400
P	0.11365000	-0.39423400	-0.38196500
N	0.78243100	-1.50005800	0.51647500
S	0.56635900	-3.06448000	0.32426500
O	1.66605600	-3.84019100	0.84861700
O	0.03662900	-3.38467400	-1.01456500
C	-0.86626000	-3.36565200	1.43883000
F	-0.54623800	-3.07574900	2.69100100
F	-1.87546200	-2.58454800	1.05235000
F	-1.24444100	-4.63313300	1.36007800
C	-3.51458600	0.42816000	-0.06624700
C	-4.99763200	-1.92103700	0.37595600
C	4.50721700	-2.53269100	-0.75656000
C	3.66972700	0.07836200	-0.13943000

C	3.87768500	-0.29417800	-1.48253300
C	3.90246200	-0.84556800	0.90026900
C	4.32663600	-2.13146300	0.56237900
H	4.47805700	-2.86415000	1.35035100
C	4.29829600	-1.59126200	-1.76449600
H	4.45515300	-1.88093300	-2.80174800
C	-4.52387500	-1.16251900	1.44016700
H	-4.73021300	-1.49776500	2.45497300
C	-3.77312400	-0.00164100	1.24747400
C	-3.97493600	-0.32845200	-1.16606400
C	-4.71108600	-1.48607600	-0.91792000
H	-5.05969700	-2.07711100	-1.76151200
C	3.69858200	0.68773500	-2.63083200
C	2.80488500	0.13423900	-3.74544000
C	5.06887100	1.10010700	-3.18510900
H	3.27061200	-0.72299500	-4.24276900
H	2.63397900	0.90203400	-4.50711200
H	1.83458700	-0.18272800	-3.35291400
H	4.95640800	1.83396800	-3.99020100
H	5.59877600	0.23038900	-3.58904800
H	5.69323100	1.53874600	-2.40061300
C	4.89311000	-3.95997600	-1.08996400
C	3.80108200	-4.64203000	-1.92242600
C	6.24795300	-4.02400300	-1.80370800
H	3.68483100	-4.14446500	-2.89205000
H	2.83861200	-4.61059300	-1.40451900
H	4.06188000	-5.68845800	-2.11313500
H	6.53360700	-5.06344800	-1.99563000
H	7.03430700	-3.55342200	-1.20603400
H	6.20382600	-3.50673700	-2.76874000
C	3.71595400	-0.50226200	2.37266500
C	5.08032600	-0.21167500	3.01489400
C	2.98598700	-1.58950000	3.16896300
H	5.61644900	0.58477200	2.48920400
H	5.71051100	-1.10773300	2.98404700
H	4.96080200	0.08414500	4.06258000
H	2.82889900	-1.24301300	4.19607400
H	3.56416300	-2.51712700	3.22218100
H	2.01480700	-1.82028600	2.72763400
C	-3.69768400	0.07734800	-2.60784000
C	-3.36416700	-1.11661400	-3.51078600
C	-4.89390700	0.83527500	-3.20125800
H	-4.25355600	-1.71724900	-3.72897200
H	-2.61828700	-1.77246400	-3.05626700

H	-2.97157000	-0.75960500	-4.46769400
H	-4.69119800	1.12280500	-4.23834300
H	-5.12809100	1.74076000	-2.63577400
H	-5.78476900	0.19714100	-3.19201400
C	-5.75120000	-3.21448500	0.61692100
C	-7.11600900	-3.22585600	-0.07859000
C	-4.90494000	-4.41718200	0.18059200
H	-7.00215500	-3.18313200	-1.16720500
H	-7.72529300	-2.37156200	0.23034200
H	-7.66067700	-4.14464900	0.16138100
H	-5.41808300	-5.35665300	0.41059100
H	-3.93286600	-4.41925200	0.68131000
H	-4.72395100	-4.38758300	-0.89975400
C	-3.27557100	0.75049300	2.47254800
C	-4.45267600	1.31688200	3.27652500
C	-2.38361800	-0.13411300	3.35206600
H	-5.08964900	0.51179000	3.65854300
H	-5.07348200	1.97129600	2.65683400
H	-4.08972000	1.89358100	4.13349700
H	-2.00607000	0.44007400	4.20447600
H	-1.52917000	-0.51754200	2.78895600
H	-2.94129300	-0.98975600	3.74846800
H	3.21965500	1.59321900	-2.24403400
H	4.97981600	-4.50290900	-0.14053300
H	3.10857900	0.40523200	2.44247200
H	-2.67145700	1.60098800	2.14117900
H	-2.82859900	0.74364000	-2.61148400
H	-5.92226800	-3.29529000	1.69808200
O	-0.69015100	-0.89994600	-1.63195300
H	-0.63210200	-1.89148800	-1.69461700

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C	-2.48631900	6.19027900	-1.78684300
C	-1.08522500	6.17248200	-1.59248300
C	-0.46658700	5.07009500	-1.06005700
C	-1.21759300	3.92104400	-0.69331300
C	-2.62086400	3.92344500	-0.93228200
C	-3.23323800	5.08724500	-1.46765000
C	-3.38629000	2.75776700	-0.66697700
C	-2.80321000	1.59405800	-0.23314300
C	-1.41015400	1.63820800	0.03205000
C	-0.61216100	2.75055400	-0.12390600
C	0.82398700	2.69486700	0.26739700

C	1. 61283100	1. 65982600	-0. 17927500
C	2. 98308300	1. 47668200	0. 14285000
C	3. 56768500	2. 45502600	0. 90651000
C	2. 81871700	3. 53906600	1. 43576500
C	1. 42559800	3. 64595100	1. 15957700
C	0. 68470800	4. 66934600	1. 80954100
C	1. 30503700	5. 56474900	2. 64348000
C	2. 69769400	5. 48782200	2. 87734400
C	3. 43287400	4. 49169700	2. 29109400
H	-4. 30718600	5. 07651700	-1. 63297500
H	-2. 96243700	7. 07243600	-2. 20262500
H	-0. 49318000	7. 03760400	-1. 87351700
H	0. 60945500	5. 06424200	-0. 92468000
H	-4. 45926500	2. 78630900	-0. 83436900
O	-0. 85208800	0. 45876400	0. 54033800
H	-0. 38578500	4. 73283000	1. 64931200
H	0. 71969600	6. 33547400	3. 13477800
H	3. 17573100	6. 20721400	3. 53440100
H	4. 49867600	4. 40171400	2. 48255900
O	1. 04798400	0. 71643300	-1. 04510300
H	4. 62171300	2. 37521400	1. 15937600
P	0. 09358100	-0. 38882000	-0. 41939000
N	0. 81552700	-1. 48907500	0. 44441300
S	0. 64470400	-3. 05528900	0. 22003600
O	1. 76471800	-3. 80459300	0. 73759400
O	0. 13053500	-3. 36231600	-1. 12772600
C	-0. 78425100	-3. 42195800	1. 31992600
F	-0. 47490100	-3. 15944800	2. 58060900
F	-1. 81102200	-2. 65475700	0. 95135000
F	-1. 13187400	-4. 69535300	1. 20456700
C	-3. 56209600	0. 32140900	-0. 03003000
C	-4. 97264000	-2. 08091500	0. 35941000
C	4. 72306100	-2. 26055700	-1. 08581400
C	3. 66408700	0. 21592000	-0. 27964300
C	3. 87924000	-0. 04364900	-1. 64503100
C	3. 98406800	-0. 75916500	0. 69176700
C	4. 50599400	-1. 97788700	0. 26226500
H	4. 73009900	-2. 74212600	1. 00211800
C	4. 41526400	-1. 27602600	-2. 01961000
H	4. 59330900	-1. 48039600	-3. 07360800
C	-4. 50540400	-1. 34191900	1. 44005900
H	-4. 68773700	-1. 71369900	2. 44672600
C	-3. 79052900	-0. 15467200	1. 27328700
C	-4. 01681300	-0. 41393700	-1. 14629900

C	-4.71712800	-1.59874400	-0.92423500
H	-5.06164000	-2.17311600	-1.78091000
C	3.59450400	0.98993400	-2.72452800
C	2.70893600	0.43525500	-3.84520300
C	4.91163300	1.53794800	-3.28966900
H	3.21792700	-0.36051300	-4.39901800
H	2.46380300	1.22826300	-4.55930400
H	1.77450900	0.03131700	-3.44569600
H	4.71828500	2.30881700	-4.04311200
H	5.49183300	0.73835400	-3.76313100
H	5.52659700	1.97462800	-2.49668300
C	5.26140800	-3.60838500	-1.52434600
C	6.62509700	-3.90589200	-0.89135200
C	4.25910000	-4.72586100	-1.21274700
H	6.53989900	-3.98730500	0.19763300
H	7.34794100	-3.11567100	-1.11508000
H	7.02229300	-4.85526200	-1.26510800
H	4.63385000	-5.68838300	-1.57742600
H	3.28784200	-4.52900500	-1.67602400
H	4.08966900	-4.80802400	-0.13448400
C	3.81741500	-0.51777500	2.18703900
C	5.18137300	-0.17962300	2.80763200
C	3.18148300	-1.69160900	2.93857100
H	5.65639200	0.67177100	2.31007100
H	5.86067300	-1.03459200	2.71439500
H	5.07536000	0.05611400	3.87183300
H	3.06941000	-1.42613900	3.99535000
H	3.79923000	-2.59378900	2.89160200
H	2.19797100	-1.93564600	2.53497600
C	-3.77260200	0.04468200	-2.57808100
C	-3.41448600	-1.10940100	-3.52229000
C	-5.00012900	0.78330600	-3.13039800
H	-4.28616300	-1.73443300	-3.74339000
H	-2.63769800	-1.75077400	-3.10012900
H	-3.05191000	-0.71052500	-4.47452200
H	-4.82135100	1.11118800	-4.15987100
H	-5.25413300	1.66177500	-2.53169100
H	-5.87056600	0.11750700	-3.13060100
C	-5.68650100	-3.40182600	0.57034700
C	-7.06294300	-3.42755800	-0.10143900
C	-4.81632200	-4.56589100	0.07985800
H	-6.97014600	-3.34345500	-1.18964200
H	-7.68979300	-2.60207400	0.24805200
H	-7.57762300	-4.36915600	0.11519700

H	-5.29893900	-5.52621000	0.28883000
H	-3.83501900	-4.55663800	0.56224000
H	-4.65712200	-4.49708400	-1.00211700
C	-3.29712100	0.57341700	2.51456200
C	-4.47793800	1.07231100	3.35686300
C	-2.36031800	-0.30914500	3.34848200
H	-5.08033100	0.23402700	3.72319800
H	-5.13168200	1.72477900	2.76987800
H	-4.11902500	1.63307600	4.22600900
H	-1.99211400	0.24664300	4.21704300
H	-1.50032200	-0.63883700	2.76039600
H	-2.88017600	-1.19942000	3.71920200
H	3.06190000	1.83201600	-2.27100100
H	5.39779700	-3.56587200	-2.61291200
H	3.15802400	0.34413700	2.32737900
H	-2.72805100	1.45472900	2.20208400
H	-2.92507000	0.73816500	-2.57232200
H	-5.83567900	-3.52264600	1.65104200
O	-0.70795900	-0.89356600	-1.67132400
H	-0.60881700	-1.87937300	-1.76351400

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C	-2.56707400	6.21295600	-1.67122800
C	-1.17256700	6.21381700	-1.43356100
C	-0.54879700	5.10321300	-0.92471700
C	-1.28766700	3.92690800	-0.62595500
C	-2.68249700	3.91197600	-0.90988900
C	-3.30114200	5.08421200	-1.41910500
C	-3.43179200	2.72165500	-0.71781300
C	-2.83922300	1.55320800	-0.31049600
C	-1.45749300	1.61490000	0.00593800
C	-0.67704300	2.74682800	-0.08232100
C	0.74783300	2.70107100	0.34927300
C	1.56782400	1.69697100	-0.11229500
C	2.93148900	1.52576800	0.24277200
C	3.47604200	2.48484900	1.05877200
C	2.69273200	3.53526100	1.60559300
C	1.30637400	3.62832000	1.29302200
C	0.52865600	4.61362000	1.95864600
C	1.10846400	5.48782200	2.84273100
C	2.49515400	5.42643700	3.11383900
C	3.26483000	4.46574400	2.51288900
H	-4.36891600	5.05957700	-1.61923600

H	-3.04773900	7.10163400	-2.06740900
H	-0.58939900	7.10011000	-1.66235000
H	0.52248100	5.11227000	-0.75607800
H	-4.49822200	2.73526300	-0.92418300
O	-0.89323100	0.42828600	0.48985600
H	-0.53788000	4.66439300	1.77007700
H	0.49528700	6.22929900	3.34496400
H	2.94115200	6.12901500	3.81044100
H	4.32624400	4.38709800	2.73176400
O	1.04519000	0.77619000	-1.02785700
H	4.52365300	2.41321700	1.33945100
P	0.09669200	-0.36892200	-0.46803200
N	0.81589500	-1.48230800	0.38099100
S	0.69597500	-3.04340600	0.09607800
O	1.82703600	-3.77913900	0.60913500
O	0.21845500	-3.31486200	-1.27288500
C	-0.74349600	-3.49330100	1.15032600
F	-0.47017200	-3.26582600	2.42616100
F	-1.78559600	-2.74533500	0.78531500
F	-1.04633600	-4.77172500	0.98269600
C	-3.57012600	0.25377500	-0.19493600
C	-4.89777500	-2.21595600	0.02977100
C	4.78412200	-2.12883500	-1.06804100
C	3.64869600	0.29428800	-0.20506500
C	3.90398600	0.08714900	-1.57257400
C	3.96638400	-0.70687200	0.74025100
C	4.52717700	-1.89788200	0.28282100
H	4.75054400	-2.68195200	1.00191100
C	4.47673900	-1.11953400	-1.97515000
H	4.68591200	-1.28297400	-3.03057400
C	-4.48686300	-1.51754200	1.16302000
H	-4.67274800	-1.94481000	2.14666500
C	-3.81577100	-0.29986100	1.07730600
C	-3.97212200	-0.43298900	-1.35837700
C	-4.63410800	-1.65470300	-1.21599000
H	-4.94338700	-2.19759000	-2.10605100
C	3.62555400	1.15172500	-2.62328500
C	2.78214500	0.61827900	-3.78594000
C	4.94510400	1.74595200	-3.13348700
H	3.32270700	-0.14692500	-4.35277700
H	2.53880300	1.43048500	-4.47876500
H	1.84654400	0.18128000	-3.42606000
H	4.75516200	2.53871000	-3.86476000
H	5.55430500	0.97542000	-3.61855900

H	5. 52980300	2. 16691500	-2. 30971200
C	5. 36515300	-3. 44783300	-1. 53861800
C	6. 71772400	-3. 73770000	-0. 87878300
C	4. 38099100	-4. 59782000	-1. 29498500
H	6. 60490700	-3. 86140800	0. 20369900
H	7. 42756000	-2. 92362200	-1. 05320600
H	7. 14720900	-4. 66334200	-1. 27560100
H	4. 78871200	-5. 53835100	-1. 68102700
H	3. 41907200	-4. 40694800	-1. 77968000
H	4. 18252400	-4. 72097400	-0. 22563600
C	3. 75807900	-0. 52246500	2. 23850800
C	5. 10127300	-0. 19108400	2. 90622900
C	3. 11760200	-1. 73052600	2. 92970700
H	5. 57805100	0. 68297300	2. 45132900
H	5. 79365800	-1. 03406400	2. 80091600
H	4. 96487900	0. 00545000	3. 97491900
H	2. 98245100	-1. 50856200	3. 99382100
H	3. 74352800	-2. 62541600	2. 85859200
H	2. 14411100	-1. 96580800	2. 49745400
C	-3. 71786200	0. 11156300	-2. 75783500
C	-3. 28910400	-0. 97148100	-3. 75490600
C	-4. 96622500	0. 82491300	-3. 29680100
H	-4. 12192300	-1. 63306400	-4. 01517200
H	-2. 47813300	-1. 58636500	-3. 35889600
H	-2. 94411300	-0. 50437600	-4. 68240200
H	-4. 77965300	1. 22332200	-4. 29966800
H	-5. 27685100	1. 65163900	-2. 65271600
H	-5. 80344400	0. 12064800	-3. 36000600
C	-5. 55798400	-3. 57553300	0. 15012400
C	-4. 55525800	-4. 61270300	0. 67193700
C	-6. 80915700	-3. 53265100	1. 03300900
H	-4. 20830400	-4. 34154100	1. 67582100
H	-3. 67772000	-4. 67618200	0. 02290900
H	-5. 01773800	-5. 60342300	0. 73035400
H	-7. 29929500	-4. 51133400	1. 05044200
H	-7. 52675800	-2. 79251800	0. 66734800
H	-6. 55307300	-3. 27243400	2. 06575000
C	-3. 38720500	0. 38238000	2. 36829300
C	-4. 61311400	0. 79896300	3. 19106100
C	-2. 44789800	-0. 50589400	3. 19330500
H	-5. 19666800	-0. 07665300	3. 49560900
H	-5. 27020700	1. 45568800	2. 61264900
H	-4. 30449600	1. 32918100	4. 09789100
H	-2. 13779500	0. 01732500	4. 10379900

H	-1.55217500	-0.76939300	2.62566600
H	-2.94377800	-1.43470900	3.49650100
H	3.06330900	1.96642100	-2.15583300
H	5.53002400	-3.36311000	-2.62076000
H	3.08474700	0.32600500	2.39314500
H	-2.84035100	1.29709300	2.11815000
H	-2.90222600	0.83963900	-2.69569500
H	-5.86632200	-3.88066600	-0.85809700
O	-0.65663800	-0.84800900	-1.75910500
H	-0.53740700	-1.82897100	-1.87745300

Re1a

C	-1.20059900	0.85547100	0.98378700
C	-2.06587100	-0.34702500	0.58671200
C	-2.30151300	-1.37341200	1.51123800
C	-2.57737200	-0.47623000	-0.70280300
C	-3.04241400	-2.49093500	1.15441600
H	-1.90601500	-1.28063800	2.51566300
C	-3.31974400	-1.59829800	-1.07720300
H	-2.40405600	0.30792600	-1.43247700
C	-3.55639400	-2.61219900	-0.14399900
H	-3.23835400	-3.28722600	1.86539200
H	-3.70677100	-1.66463700	-2.08698500
O	-4.27093600	-3.74821500	-0.39678900
C	-4.80509300	-3.91755600	-1.69804900
H	-5.32496800	-4.87714500	-1.68735900
H	-5.51830900	-3.12088600	-1.94831300
H	-4.01366600	-3.94145300	-2.45897100
C	0.21168100	0.52937800	0.72386700
C	1.37481500	0.24567800	0.53020100
C	2.73562000	-0.11143300	0.30444200
C	3.67294700	0.84094800	-0.12444900
C	3.17336200	-1.43724200	0.50659700
C	5.00408200	0.49542200	-0.34792100
H	3.35058800	1.86527300	-0.28310700
C	4.49466700	-1.78838400	0.28845500
H	2.45856700	-2.18394100	0.83668800
C	5.42091300	-0.82517100	-0.14049500
H	5.70107200	1.25569800	-0.67948900
H	4.84031900	-2.80537200	0.44190100
O	6.69389600	-1.27203000	-0.32551500
C	7.67264500	-0.33874300	-0.75371300
H	8.60562100	-0.89875300	-0.83329500

H	7.41959600	0.08804500	-1.73293600
H	7.79691200	0.47468000	-0.02707300
C	-1.63689100	2.12713500	0.24460200
C	-0.90003200	2.67982900	-0.80399000
C	-2.84085700	2.73001700	0.62922900
C	-1.35956900	3.82303200	-1.46278500
H	0.03405600	2.21420600	-1.10094400
C	-3.29714000	3.87092700	-0.02515200
H	-3.40627500	2.29607500	1.44703900
C	-2.55728500	4.42136500	-1.07557100
H	-0.77688000	4.24494100	-2.27715900
H	-4.23159000	4.33210000	0.28274100
H	-2.91396900	5.31133000	-1.58663900
O	-1.39725700	1.03625000	2.40058500
H	-0.77124500	1.72630700	2.67457300

Re1b

C	-1.20059900	0.85547100	0.98378700
C	-2.06587100	-0.34702500	0.58671200
C	-2.30151300	-1.37341200	1.51123800
C	-2.57737200	-0.47623000	-0.70280300
C	-3.04241400	-2.49093500	1.15441600
H	-1.90601500	-1.28063800	2.51566300
C	-3.31974400	-1.59829800	-1.07720300
H	-2.40405600	0.30792600	-1.43247700
C	-3.55639400	-2.61219900	-0.14399900
H	-3.23835400	-3.28722600	1.86539200
H	-3.70677100	-1.66463700	-2.08698500
O	-4.27093600	-3.74821500	-0.39678900
C	0.21168100	0.52937800	0.72386700
C	1.37481500	0.24567800	0.53020100
C	2.73562000	-0.11143300	0.30444200
C	3.67294700	0.84094800	-0.12444900
C	3.17336200	-1.43724200	0.50659700
C	5.00408200	0.49542200	-0.34792100
H	3.35058800	1.86527300	-0.28310700
C	4.49466700	-1.78838400	0.28845500
H	2.45856700	-2.18394100	0.83668800
C	5.42091300	-0.82517100	-0.14049500
H	5.70107200	1.25569800	-0.67948900
H	4.84031900	-2.80537200	0.44190100
O	6.69389600	-1.27203000	-0.32551500
C	7.67264500	-0.33874300	-0.75371300

H	8.60562100	-0.89875300	-0.83329500
H	7.41959600	0.08804500	-1.73293600
H	7.79691200	0.47468000	-0.02707300
C	-1.63689100	2.12713500	0.24460200
C	-0.90003200	2.67982900	-0.80399000
C	-2.84085700	2.73001700	0.62922900
C	-1.35956900	3.82303200	-1.46278500
H	0.03405600	2.21420600	-1.10094400
C	-3.29714000	3.87092700	-0.02515200
H	-3.40627500	2.29607500	1.44703900
C	-2.55728500	4.42136500	-1.07557100
H	-0.77688000	4.24494100	-2.27715900
H	-4.23159000	4.33210000	0.28274100
H	-2.91396900	5.31133000	-1.58663900
O	-1.39725700	1.03625000	2.40058500
H	-0.77124500	1.72630700	2.67457300
H	-4.63287587	-3.86295891	-1.27851082

Relc

C	-0.73773000	0.43489300	0.89569400
C	-1.52609500	-0.77599800	0.38108000
C	-1.73771700	-1.88097900	1.21330100
C	-1.98939800	-0.82429400	-0.93466400
C	-2.41015100	-3.00556100	0.74780500
H	-1.37818700	-1.84820700	2.23474300
C	-2.65808900	-1.94888900	-1.41331800
H	-1.83511100	0.02394400	-1.59336700
C	-2.87223500	-3.04341200	-0.57114200
H	-2.58585100	-3.86201500	1.39061900
H	-3.01846100	-1.97193600	-2.44011000
O	-3.52702200	-4.17270900	-0.98016800
C	0.69168600	0.22884200	0.60409700
C	1.86917800	0.04769100	0.37958800
C	3.25178500	-0.17663100	0.10885900
C	4.11733800	0.90648100	-0.13133800
C	3.76773800	-1.48541100	0.07474700
C	5.46460600	0.68265200	-0.39945500
H	3.71949000	1.91604300	-0.10390500
C	5.11643200	-1.70044500	-0.19349500
H	3.09925400	-2.32013200	0.25919500
C	5.96821900	-0.61952300	-0.43143500
H	6.12391400	1.52609500	-0.58371900
H	5.50461200	-2.71469900	-0.21754300

C	-1.25961400	1.74104300	0.28266900
C	-0.56702400	2.43846300	-0.70838500
C	-2.49757300	2.22429200	0.72431400
C	-1.10448400	3.60685900	-1.25441000
H	0.39417100	2.06752500	-1.04908600
C	-3.03092900	3.39069600	0.18292000
H	-3.02912200	1.67800100	1.49632700
C	-2.33560200	4.08597900	-0.81040600
H	-0.55584900	4.14192800	-2.02466500
H	-3.99104100	3.75860000	0.53425000
H	-2.75269300	4.99572900	-1.23322000
O	-0.93327900	0.46347000	2.32219800
H	-0.36728500	1.17645800	2.66036600
H	-3.78763200	-4.06264200	-1.90764000
H	7.02016300	-0.79127200	-0.64065200

Re2a

C	1.85174600	-0.94501500	-0.35852300
C	0.93410600	-1.19877800	0.85714500
C	-0.13021300	-0.09631900	0.77558000
C	1.93013700	0.58439700	-0.45780000
H	2.83246500	-1.41658100	-0.25097500
H	1.37537100	-1.35506700	-1.25446400
H	1.50098800	-1.09326800	1.78971900
H	0.48924200	-2.19592500	0.83436000
H	2.13182100	0.98516900	-1.45529500
H	2.70001200	0.98869800	0.21550100
C	0.58083000	1.07889500	0.05530200
O	0.12297900	2.19169900	-0.08045200
C	-1.35202200	-0.49392000	-0.06843200
O	-1.32777300	-1.47345600	-0.78803100
C	-2.54712100	0.42310200	0.04113500
H	-2.22702100	1.46434700	-0.07783000
H	-3.29585300	0.15705600	-0.70724000
H	-2.98605800	0.33508600	1.04335600
H	-0.48739800	0.27036900	1.74428600

Re2b

C	0.46049400	0.23743700	-0.00284900
O	0.80402100	1.39190600	-0.00030100
C	1.40164600	-0.94741500	0.00027700
H	1.18002300	-1.61681400	-0.83740100

H	2.42815900	-0.58370700	-0.07354600
H	1.27850600	-1.51939100	0.92652700
S	-1.29599700	-0.26016900	-0.00086900
H	-1.75573200	1.00723900	0.01616000

Pr3a

C	-1.98531100	3.23407800	1.70173900
C	-2.52876600	1.86135700	2.12687300
C	-1.32917600	0.91020400	1.98591700
C	-0.59664400	3.27973400	2.33861100
H	-1.90655200	3.27901800	0.60910400
H	-2.62991000	4.05525900	2.02285700
H	-3.38797100	1.54550200	1.53180800
H	-2.83253500	1.87309900	3.17895100
H	-0.65597000	3.60257400	3.38635700
H	0.14316700	3.91326500	1.84246300
C	-0.12832400	1.83027100	2.35084000
C	-1.33193900	-0.25859900	2.99294500
O	-2.07917900	-0.24366000	3.94529700
C	-0.34718300	-1.37199300	2.74460500
H	-0.32415400	-2.02994800	3.61373700
H	-0.65526000	-1.94011100	1.85897900
H	0.64376300	-0.95494900	2.53880700
C	1.19676000	0.62912100	-0.63152800
C	2.13394900	-0.50893700	-0.40607600
C	1.66270400	-1.82899400	-0.43990200
C	3.47780400	-0.29260600	-0.10480600
C	2.50677700	-2.89370900	-0.17910000
H	0.61767700	-2.00949000	-0.68100300
C	4.34053500	-1.35497100	0.15879500
H	3.85843400	0.72411900	-0.06248900
C	3.85415200	-2.66281200	0.12131200
H	2.15349500	-3.91906500	-0.20795100
H	5.37744600	-1.14912500	0.39699100
O	4.60571800	-3.76974900	0.35411300
C	5.96245500	-3.57662500	0.68745200
H	6.38087800	-4.57063400	0.84436800
H	6.50554300	-3.07720400	-0.12418800
H	6.06644600	-2.98750600	1.60677700
C	0.00878900	0.56532600	-0.06825200
C	-1.14262300	0.40982900	0.54687900
C	-2.26631500	-0.30492100	-0.12444900
C	-2.29593500	-0.41412300	-1.51714400
C	-3.29519600	-0.92446100	0.60277500

C	-3.29439600	-1.12438600	-2.17550100
H	-1.51734800	0.07304800	-2.09844400
C	-4.29597900	-1.63508700	-0.03963700
H	-3.32364400	-0.85815100	1.68671000
C	-4.30298300	-1.74312000	-1.43311900
H	-3.27939400	-1.18031000	-3.25761000
H	-5.08946200	-2.11976700	0.51922000
O	-5.32521200	-2.45759100	-1.96846300
C	-5.36551000	-2.58417900	-3.37278700
H	-6.24415300	-3.18839700	-3.59777400
H	-5.46229900	-1.60543600	-3.85820500
H	-4.46893700	-3.08862300	-3.75325600
C	1.60082800	1.79377400	-1.46709500
C	0.99485300	3.04260600	-1.28639900
C	2.56764900	1.65528300	-2.46869600
C	1.34043100	4.12301400	-2.08784400
H	0.24633400	3.15512300	-0.50626700
C	2.91570300	2.73904500	-3.27016600
H	3.04083300	0.69035600	-2.62315100
C	2.30510300	3.97562600	-3.08344000
H	0.86192800	5.08519700	-1.93183400
H	3.66544000	2.61310100	-4.04535100
H	2.57980100	4.82121200	-3.70631000
O	0.98156300	1.44967100	2.61903900

Pr3b

C	-1.17307300	-3.52187000	-1.33363700
C	-1.97799400	-2.33587100	-1.88547300
C	-0.98477500	-1.16308400	-1.88213900
C	0.18946900	-3.37108700	-2.01070500
H	-1.07268300	-3.42679300	-0.24588800
H	-1.64962800	-4.48247600	-1.54120600
H	-2.87756900	-2.12629000	-1.30329200
H	-2.28151400	-2.52177100	-2.92126200
H	0.18009000	-3.81658100	-3.01419300
H	1.04565500	-3.78955800	-1.47511900
C	0.36491900	-1.86892400	-2.19730300
C	-1.23516500	-0.12490900	-2.99488500
O	-1.99332900	-0.37480000	-3.90491300
C	-0.47356700	1.17218500	-2.89855100
H	-0.58162900	1.72173500	-3.83400800
H	-0.87876300	1.76832700	-2.07210500
H	0.57944600	0.97349100	-2.67575800

C	1. 48433200	-0. 13895000	0. 60143000
C	2. 20171700	1. 11112800	0. 21909100
C	1. 50729500	2. 32040900	0. 09336700
C	3. 56556000	1. 09164800	-0. 08259600
C	2. 14841200	3. 47640500	-0. 32562400
H	0. 44715600	2. 34461200	0. 33476800
C	4. 21918300	2. 24478400	-0. 50100800
H	4. 11877800	0. 16026100	-0. 00254200
C	3. 51130000	3. 43993500	-0. 62473800
H	1. 61788800	4. 41770500	-0. 42131700
H	5. 27969100	2. 21415800	-0. 74123800
O	4. 09520600	4. 60113600	-1. 02658600
C	0. 29645500	-0. 35575100	0. 07749300
C	-0. 87393400	-0. 49054800	-0. 50610800
C	-2. 10469800	0. 05068700	0. 13900500
C	-2. 13619900	0. 26259200	1. 51966800
C	-3. 24633400	0. 39514500	-0. 60263500
C	-3. 24774900	0. 80991100	2. 15193900
H	-1. 26879100	-0. 01382200	2. 11322300
C	-4. 35996000	0. 94175100	0. 01376700
H	-3. 27719900	0. 23698300	-1. 67704400
C	-4. 36992900	1. 15517600	1. 39510200
H	-3. 22974000	0. 95219800	3. 22604400
H	-5. 24193200	1. 21206800	-0. 55693600
O	-5. 50780700	1. 69036000	1. 90488200
C	-5. 56405300	1. 89773100	3. 29912900
H	-6. 54583000	2. 32552200	3. 50144300
H	-5. 45737900	0. 95316900	3. 84641300
H	-4. 78689400	2. 59712400	3. 63066500
C	2. 10922100	-1. 11435200	1. 53804600
C	1. 76299700	-2. 46941100	1. 49073200
C	3. 03050100	-0. 69001000	2. 50137000
C	2. 31955300	-3. 37691500	2. 38319200
H	1. 04998200	-2. 80332600	0. 74129100
C	3. 58924100	-1. 59973500	3. 39470100
H	3. 30305600	0. 35988200	2. 55256900
C	3. 23788700	-2. 94523200	3. 33872700
H	2. 04159300	-4. 42525000	2. 32946200
H	4. 29959100	-1. 25220400	4. 13878500
H	3. 67630600	-3. 65459000	4. 03376600
O	1. 37306900	-1. 31414800	-2. 55054400
H	5. 02954800	4. 43802800	-1. 21737700

Pr3c

S	-2.08058400	-0.12164600	2.07160600
O	4.04065100	-4.02468600	-1.49534200
C	2.05833900	-3.10255800	-0.46232900
C	1.35132400	-1.97831800	-0.06103400
C	1.86244400	-0.69327100	-0.27446400
C	3.10318800	-0.56872000	-0.91289400
C	3.81892600	-1.68737400	-1.31464300
C	3.29864000	-2.96090500	-1.08695500
H	1.64477000	-4.09395600	-0.29101200
H	0.37742300	-2.09661000	0.40717400
H	3.51027900	0.41886200	-1.10713100
H	4.77887900	-1.59512800	-1.81122700
C	1.07330300	0.50579200	0.11988400
C	1.74034600	1.81508900	0.38104000
C	2.96184700	1.86886700	1.06156600
C	1.12882000	3.01088300	-0.00876100
C	3.55735000	3.09388800	1.34343800
H	3.43763700	0.94558300	1.37938000
C	1.72541300	4.23457500	0.27435600
H	0.18076600	2.97159800	-0.53900800
C	2.94296300	4.27981800	0.94916800
H	4.50219100	3.12129300	1.87769400
H	1.24068400	5.15441500	-0.03834800
H	3.41121600	5.23507500	1.16565700
C	-0.23425500	0.42197900	0.25488600
C	-1.53098800	0.31527700	0.41493500
C	-2.52863600	0.55555100	-0.66165900
C	-2.08945800	0.99543600	-1.91826700
C	-3.89456100	0.34374000	-0.46564300
C	-2.99424200	1.22151200	-2.94569900
H	-1.02662900	1.14913400	-2.08490000
C	-4.80072100	0.57033200	-1.49856200
H	-4.25403400	0.00141700	0.49875000
C	-4.35741500	1.01070600	-2.74038800
H	-2.63417800	1.56217800	-3.91165900
H	-5.85897600	0.39844300	-1.32709600
H	-5.06603800	1.18640500	-3.54372300
C	-2.32062200	-1.89481800	1.85715800
C	-2.77035400	-2.58711200	3.12470300
H	-3.42817300	-1.95260000	3.72254700
H	-1.88600700	-2.82619200	3.72405500
H	-3.27662200	-3.51534900	2.85570000
O	-2.10774700	-2.46266300	0.81941700

H	3. 56301200	-4. 84166300	-1. 29416900
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cat4

C	1. 05324000	6. 28754600	-1. 66706100
C	-0. 24675100	5. 98337200	-1. 20137500
C	-0. 52164300	4. 75993000	-0. 63320500
C	0. 49104500	3. 77339500	-0. 49910600
C	1. 79479600	4. 06505700	-1. 01709100
C	2. 04852700	5. 34291000	-1. 58141500
C	2. 79814300	3. 06267800	-1. 00740900
C	2. 55182800	1. 79050700	-0. 53948600
C	1. 27496000	1. 55786000	0. 03002100
C	0. 25850800	2. 48772400	0. 10067400
C	-1. 05223800	2. 13669600	0. 71283000
C	-1. 76452700	1. 02963000	0. 28394800
C	-3. 11062200	0. 75917300	0. 63308000
C	-3. 70403500	1. 61446700	1. 53646700
C	-2. 99221700	2. 68023700	2. 14134200
C	-1. 64552800	2. 94889700	1. 73759300
C	-0. 93844800	3. 99280400	2. 39088100
C	-1. 54321000	4. 75020600	3. 36802700
C	-2. 88639400	4. 50837900	3. 73979000
C	-3. 59194300	3. 49239100	3. 13943900
H	3. 04568700	5. 55217700	-1. 95957100
H	1. 25732600	7. 25979000	-2. 10565000
H	-1. 03869600	6. 72030300	-1. 29726500
H	-1. 52402600	4. 53983700	-0. 28855600
H	3. 77388100	3. 29722700	-1. 42066400
O	1. 05942400	0. 29196700	0. 59594300
H	0. 09399200	4. 18022100	2. 12110400
H	-0. 98136700	5. 53665200	3. 86321400
H	-3. 35212100	5. 11771300	4. 50860600
H	-4. 61803400	3. 28272800	3. 42931800
O	-1. 16924200	0. 13866100	-0. 63467400
H	-4. 74599400	1. 46311700	1. 79878900
P	0. 07019900	-0. 73507700	-0. 13178800
N	-0. 28671400	-1. 96060700	0. 78205700
S	0. 55790500	-2. 52616900	2. 04261600
O	1. 14436800	-1. 47638900	2. 87550200
O	-0. 16389100	-3. 63438900	2. 65323800
C	2. 02320700	-3. 32411700	1. 18080500
F	3. 01999300	-3. 49745800	2. 04802200
F	2. 47145100	-2. 51346200	0. 18291600

F	1. 69356600	-4. 49186200	0. 63724000
O	0. 66440900	-1. 10879700	-1. 56486300
C	3. 52688200	0. 66469300	-0. 66607600
C	5. 24957800	-1. 55154500	-0. 88763700
C	-5. 39925200	-2. 33881600	-1. 29787000
C	-3. 87207900	-0. 33945000	-0. 03383200
H	1. 46219700	-1. 66335200	-1. 47231000
C	-4. 26577200	-0. 17864500	-1. 38087000
C	-4. 22083700	-1. 50537500	0. 67663400
C	-4. 98976400	-2. 47691700	0. 02707300
H	-5. 26881200	-3. 37751100	0. 56610200
C	-5. 02057100	-1. 18418200	-1. 98581900
H	-5. 32272800	-1. 06003900	-3. 02208900
C	5. 05191100	-0. 91681500	0. 34131900
H	5. 55393800	-1. 30385200	1. 22061600
C	4. 19620800	0. 17592900	0. 47914000
C	3. 72986300	0. 05979300	-1. 92696500
C	4. 59010200	-1. 04273500	-2. 00527100
H	4. 75371600	-1. 52142900	-2. 96671000
C	-3. 91309900	1. 06106000	-2. 19435100
C	-3. 03835300	0. 70763500	-3. 40917300
C	-5. 17837000	1. 82657900	-2. 61715100
H	-3. 57509600	0. 05845500	-4. 11054700
H	-2. 74884400	1. 61655700	-3. 94980100
H	-2. 12821600	0. 18863200	-3. 09503200
H	-4. 91205100	2. 74161800	-3. 15930100
H	-5. 81123300	1. 21988800	-3. 27457400
H	-5. 77712300	2. 10660500	-1. 74351600
C	-6. 22415400	-3. 42039000	-1. 97301000
C	-5. 46914600	-4. 04574200	-3. 15788800
C	-7. 60017000	-2. 89184600	-2. 41091400
H	-5. 28439400	-3. 30330100	-3. 94308200
H	-4. 49981600	-4. 44357100	-2. 83987700
H	-6. 05025200	-4. 86334000	-3. 60025800
H	-8. 20373400	-3. 69612100	-2. 84770000
H	-8. 14907900	-2. 47164700	-1. 56146000
H	-7. 49822700	-2. 10324100	-3. 16565700
C	-3. 78968900	-1. 73108000	2. 12002800
C	-4. 92350700	-1. 37313300	3. 09807900
C	-3. 30857600	-3. 16777900	2. 37154600
H	-5. 80042500	-2. 00599500	2. 91629000
H	-4. 60058300	-1. 53068800	4. 13364900
H	-5. 23972400	-0. 33029700	2. 99572100
H	-2. 84790500	-3. 24205900	3. 36094800

H	-4.13947400	-3.88227200	2.33887800
H	-2.55892200	-3.46932500	1.63799300
C	3.09502300	0.60556800	-3.20347400
C	2.59070100	-0.47852700	-4.16918900
C	4.09605700	1.51971000	-3.93682700
H	3.41065000	-1.07951600	-4.57678500
H	1.87419600	-1.15121800	-3.69141300
H	2.08284500	-0.00716600	-5.01777100
H	3.63738900	1.95695700	-4.83138600
H	4.44288100	2.33648400	-3.29739900
H	4.97791000	0.94873200	-4.25037800
C	6.11117400	-2.79707700	-1.00224000
C	5.39726800	-4.00894500	-0.37528800
C	7.50825700	-2.60594400	-0.39239400
H	5.22224000	-3.84911000	0.69371900
H	4.42391700	-4.18263400	-0.84606100
H	6.00076700	-4.91678100	-0.48944000
H	8.12397300	-3.49701200	-0.55872600
H	8.02008400	-1.74588000	-0.83696900
H	7.45250800	-2.44126100	0.68947200
C	4.03163900	0.86191800	1.82990000
C	4.96986100	2.08092100	1.91307700
C	4.24351400	-0.06842900	3.03112300
H	6.01669000	1.76402500	1.83671600
H	4.77276300	2.79405900	1.10612800
H	4.84034500	2.60238300	2.86860800
H	3.96753100	0.45488900	3.95260100
H	3.62214400	-0.96387300	2.95816700
H	5.29256200	-0.37122400	3.13263600
H	-3.33118400	1.73824600	-1.56320900
H	-6.39226700	-4.21198400	-1.23071900
H	-2.94416600	-1.06538500	2.32372700
H	3.00365300	1.23021500	1.89655600
H	2.23100400	1.21328000	-2.91960400
H	6.24122400	-3.00505200	-2.07287300

cat5

C	-0.86035600	5.03022800	1.98522800
C	0.37780300	4.61867700	1.16571200
C	-0.15670100	3.58647000	0.11317800
C	-1.25079100	2.91841300	0.93208100
C	-1.69682400	3.77209700	1.95507100
C	-0.69462900	4.33024600	-1.14713100

C	0.58254600	4.70281300	-1.93866400
C	1.54236700	3.59243500	-1.56653900
C	1.02175200	2.84354000	-0.50020700
C	-1.85913100	1.68063300	0.80906100
C	-2.91962400	1.26865100	1.63237300
C	-3.37167800	2.16595300	2.60524400
C	-2.75805700	3.40979400	2.77790900
C	2.75923100	3.24088500	-2.13982700
C	3.46340200	2.14035400	-1.64140900
C	2.92278400	1.30884200	-0.65137600
C	1.67042000	1.67438400	-0.13894200
O	-1.44196600	0.80234000	-0.19913400
O	0.98897300	0.74202000	0.68579900
P	-0.11696800	-0.09209400	-0.12692100
O	-0.33920100	-1.28941600	0.88723300
H	-0.61180700	5.34972300	3.00274400
H	-1.39292500	5.86439800	1.50820000
H	0.89125800	5.46048400	0.69423900
H	1.09711300	4.10852100	1.81633300
H	-1.29551800	3.62877300	-1.73353700
H	-1.31500800	5.19353700	-0.88810800
H	0.96939500	5.68636500	-1.63993400
H	0.40378500	4.74207400	-3.01790900
H	-4.20423500	1.87832400	3.23846100
H	-3.10300700	4.08216400	3.55853400
H	3.16656400	3.81473200	-2.96742800
H	4.43408600	1.88730400	-2.05361700
H	-1.27228600	-1.59786100	0.94747200
C	3.64656400	0.11669800	-0.11569400
C	4.05254600	0.11347600	1.24209100
C	4.73787600	-0.99375300	1.74213300
C	5.04397500	-2.09862500	0.94575100
H	5.04574200	-0.99036200	2.78424900
C	-3.46241500	-0.10542800	1.40532000
C	-3.01304100	-1.18531400	2.20702600
C	-3.28400400	-2.49105600	1.78083200
C	-4.01006500	-2.75305700	0.60949000
H	-2.91743400	-3.32296200	2.37285000
C	3.94146300	-0.99248200	-0.93928900
C	4.64172200	-2.07109300	-0.38675500
H	4.87117200	-2.92544300	-1.01752900
C	-4.26429900	-0.34621500	0.27406700
C	-4.52522900	-1.66992800	-0.09714300
H	-5.11270900	-1.86058700	-0.99127800

N	0.32669800	-0.54498500	-1.56026200
S	-0.22913600	-0.05340200	-2.98999100
O	-0.96982200	1.21317100	-2.95692800
O	0.78544500	-0.25540400	-4.01997600
C	-1.51355800	-1.38094800	-3.28642900
F	-0.92758500	-2.55050100	-3.54732600
F	-2.28064600	-1.53095300	-2.18586500
F	-2.29962800	-1.03894400	-4.30831400
C	3.80520300	1.28503700	2.18734900
C	2.90558000	0.87995200	3.36806200
C	5.13124800	1.89034000	2.67958600
H	3.39230000	0.12518900	3.99652200
H	2.68868300	1.74952000	4.00060400
H	1.95862600	0.46552300	3.01147000
H	4.94301300	2.76796100	3.30968600
H	5.70527800	1.16999800	3.27334300
H	5.75703400	2.20141200	1.83615900
C	3.53425600	-1.06359400	-2.40381000
C	2.82257300	-2.38159800	-2.75011500
C	4.75011100	-0.85611000	-3.32432700
H	3.49879000	-3.24213600	-2.68249700
H	1.97452800	-2.55003700	-2.08174100
H	2.43691000	-2.33088100	-3.77223800
H	4.43450600	-0.85386300	-4.37381400
H	5.25941500	0.09227700	-3.12000600
H	5.48601300	-1.65872900	-3.19208800
C	5.78752800	-3.29459900	1.51354400
C	4.98385500	-3.97439400	2.63478600
C	7.19428700	-2.90681900	1.99893400
H	4.84399800	-3.29627600	3.48470800
H	3.99186600	-4.27366400	2.28046000
H	5.50474300	-4.86711200	3.00058700
H	7.73771600	-3.78768200	2.36064000
H	7.77654700	-2.45008100	1.19164800
H	7.14188000	-2.18477000	2.82213600
C	-2.29713200	-0.93357500	3.53133100
C	-1.25980500	-1.99735600	3.92134400
C	-3.34535300	-0.79794800	4.65350100
H	-1.72639400	-2.96784800	4.12569500
H	-0.49874000	-2.13317700	3.14882600
H	-0.75086500	-1.68728400	4.84031200
H	-2.86101900	-0.55621400	5.60649200
H	-4.07653400	-0.01549900	4.43210100
H	-3.89318400	-1.73938100	4.77767500

C	-4.86657400	0.79270400	-0.53927300
C	-4.36932000	0.82552500	-1.99346400
C	-6.40357100	0.72862700	-0.47879500
H	-4.60924700	-0.10346400	-2.52228600
H	-4.85371000	1.64813000	-2.53228900
H	-3.28945700	0.97451100	-2.04714200
H	-6.83991300	1.59104900	-0.99522900
H	-6.78449500	-0.17753600	-0.96349900
H	-6.76060200	0.73009600	0.55695500
C	-4.17743000	-4.16658600	0.08227800
C	-2.85429300	-4.65215600	-0.54074900
C	-4.68551800	-5.15016500	1.14633600
H	-2.06883700	-4.71740700	0.22192800
H	-2.97498700	-5.64691700	-0.98478000
H	-2.50871700	-3.96509300	-1.31920900
H	-4.86793300	-6.13391500	0.69992900
H	-3.95303200	-5.28692600	1.95019100
H	-5.61957800	-4.79939100	1.59795800
H	3.28580700	2.07320300	1.63732300
H	5.90449100	-4.02216700	0.69934500
H	2.82158200	-0.26364600	-2.60374400
H	-4.56483300	1.73358800	-0.06930200
H	-1.77021700	0.02282700	3.44767800
H	-4.92667300	-4.12459800	-0.71922100

S-NH tautomer

O	1.24163600	-1.26659100	0.65428800
O	2.69912200	0.62250800	-0.22873500
P	1.63761600	-0.48100000	-0.66042900
S	-0.98677300	0.88617100	0.02183900
O	-0.42027700	0.96647900	1.35126600
O	-1.68370400	1.98507200	-0.60461500
C	-2.17810300	-0.52059600	0.03621600
F	-3.20922800	-0.19319900	0.79681600
F	-1.59276000	-1.60420300	0.51101000
F	-2.58676000	-0.74040900	-1.20567300
O	2.04410200	-1.25743500	-1.83057500
N	0.17986800	0.35727900	-1.01235800
H	-0.03839500	0.49064200	-1.99790500
C	1.87278700	-1.11417800	1.93069900
H	2.87830700	-0.70259600	1.82217400
H	1.25176900	-0.45850700	2.54418600

H	1.92686300	-2.10820900	2.37344000
C	2.38044300	1.84732100	0.44091200
H	3.32085200	2.38992700	0.52838100
H	1.67156900	2.42895900	-0.15483000
H	1.95502700	1.65983500	1.42869800

S-OH tautomer

O	1.43977900	-1.70806400	0.11750100
O	2.50810800	0.48624100	0.47601800
P	1.53315800	-0.27133600	-0.50834900
S	-0.90276900	0.89032900	0.17044800
O	-0.43552100	0.62276600	1.53307800
O	-1.53841600	2.15174600	-0.14286700
C	-2.15939000	-0.40958900	-0.16115200
F	-3.17778100	-0.26918200	0.67371100
F	-1.60254100	-1.60797900	0.02816000
F	-2.59552100	-0.32935200	-1.40818300
N	0.21826000	0.51707200	-0.91387500
O	2.30762400	-0.52592600	-1.86911500
H	1.76857000	-0.23450500	-2.62360000
C	2.46018700	1.92004100	0.60648700
H	3.38068200	2.20116300	1.11493000
H	2.41241100	2.39646300	-0.37492500
H	1.59142200	2.19506500	1.20676600
C	1.24613600	-1.95118900	1.52749900
H	1.63292800	-2.95325700	1.70468600
H	1.79814300	-1.21587300	2.11367200
H	0.18336100	-1.89483300	1.75656400

Com-NH

O	3.16920600	-0.15892200	-3.05195900
O	2.24737200	1.57430000	-1.44037000
P	1.88224200	0.24343800	-2.21117900
S	2.86759600	-1.57953000	-0.09265500
O	4.02145200	-0.71169400	-0.21366600
O	2.27442500	-1.90874000	1.18078300
C	3.33427600	-3.18452800	-0.86668400
F	4.24251300	-3.77377200	-0.10555000
F	3.83224300	-2.96849400	-2.07274800
F	2.26148400	-3.95722000	-0.96104400
O	0.62965100	0.40524200	-2.98101400
C	-1.29526700	-1.20145900	0.54711400

C	-2.79441500	-1.03378400	0.76220200
C	-3.36989400	0.17031000	1.14542400
C	-3.63074000	-2.13107800	0.50610100
C	-4.75566300	0.30742200	1.25056000
H	-2.73448200	1.02725500	1.35161900
C	-5.00290300	-2.01052200	0.60460500
H	-3.18930800	-3.08135400	0.21837800
C	-5.57821100	-0.78018500	0.95902900
H	-5.17688200	1.27096400	1.51111700
H	-5.66332000	-2.84527700	0.39512700
O	-6.93013700	-0.74896800	0.98482400
C	-7.54656300	0.51449800	1.16936900
H	-8.61807100	0.33813400	1.07541400
H	-7.33404900	0.91272400	2.16912100
H	-7.21260000	1.22383400	0.40456200
C	-0.50240600	-0.01363200	0.94710400
C	0.30745200	0.83847600	1.24070800
C	1.36174600	1.71916400	1.65644700
C	1.38316700	3.07673800	1.32780700
C	2.42524400	1.18824900	2.41159600
C	2.42841200	3.89909400	1.74056600
H	0.57704400	3.49849800	0.73741500
C	3.46826600	1.99868900	2.82231600
H	2.41848800	0.13090900	2.65754100
C	3.47499000	3.36097600	2.49403800
H	2.41322000	4.94907400	1.47334200
H	4.29509100	1.60392300	3.40282800
O	4.53655700	4.07122000	2.94718800
C	4.57383600	5.45154800	2.65614500
H	5.48681300	5.83209900	3.11297300
H	4.60608500	5.62973300	1.57433600
H	3.70768700	5.97143400	3.08223900
C	-0.75997000	-2.40820200	1.32485600
C	-0.64306400	-2.32968700	2.71340100
C	-0.38926800	-3.57745100	0.66677400
C	-0.14328600	-3.40525600	3.43419700
H	-0.93466200	-1.41452700	3.22234000
C	0.11806900	-4.65492200	1.39361700
H	-0.48524600	-3.64157300	-0.41160200
C	0.24523500	-4.57154200	2.77421800
H	-0.04967400	-3.33358000	4.51340800
H	0.41830500	-5.55816000	0.87074100
H	0.64441500	-5.40892400	3.33809200
O	-1.04137800	-1.46868800	-0.84011900

H	-1.53384300	-0.80603200	-1.36928100
C	-1.79246600	3.66322800	-0.39322100
C	-3.30304700	3.57047700	-0.68912400
C	-3.43112500	2.24086200	-1.39349300
C	-1.11672300	2.78241800	-1.45939600
H	-1.41510400	4.68951300	-0.38096900
H	-1.59987300	3.22046700	0.59140100
H	-3.64741700	4.38779000	-1.33590800
H	-3.91514500	3.61176100	0.21721800
H	-0.21369700	2.27364200	-1.10518600
H	-0.83666700	3.34972100	-2.35805200
C	-2.21921700	1.81045900	-1.80035900
C	-4.74343600	1.60748300	-1.56686900
O	-5.74623900	2.18695500	-1.17151900
C	-4.82260900	0.24342500	-2.20922800
H	-4.19333600	-0.46749200	-1.66282600
H	-5.86056700	-0.09343300	-2.19704200
H	-4.44432000	0.28157600	-3.23566900
O	-1.96030400	0.66594200	-2.46352800
H	-1.01460900	0.65678100	-2.75377900
N	1.72393600	-1.05483600	-1.15252100
H	0.73411700	-1.34336100	-0.98265900
C	3.55816400	1.99220600	-1.01802700
H	3.60815800	3.06390900	-1.21329400
H	3.66773400	1.79083600	0.04739400
H	4.33045700	1.45521200	-1.57130300
C	3.45289300	0.61376200	-4.22874600
H	3.65126200	1.65720600	-3.96455000
H	4.34118100	0.17047600	-4.67505800
H	2.61023100	0.55979900	-4.92080000

TSNH-M2

O	2.21970100	-3.53180200	-1.70424100
O	2.62589200	-3.28965400	0.77815900
P	2.25621500	-2.43214500	-0.53069900
S	-0.65601900	-2.38712000	-0.40606900
O	-0.90405400	-3.37720200	0.63741800
O	-1.61378600	-1.26739700	-0.50007500
C	-0.93512200	-3.32650100	-1.97212400
F	-2.24223200	-3.47803900	-2.15979000
F	-0.37465300	-4.52869600	-1.89114200
F	-0.42150300	-2.67393800	-3.00641200
O	3.33831400	-1.41392200	-0.70489200

C	-0.49370500	1.64873300	1.01870300
C	0.23386700	0.59694600	1.70939900
C	-0.44793200	-0.46898500	2.32985400
C	1.63917100	0.57071000	1.68413400
C	0.24859000	-1.48802500	2.94053400
H	-1.53248300	-0.48950100	2.31542000
C	2.34908000	-0.44685000	2.29294000
H	2.17421600	1.35050600	1.15071200
C	1.65250700	-1.48236500	2.93494700
H	-0.26516700	-2.31868400	3.41092600
H	3.43007300	-0.46169000	2.23018100
O	2.24399200	-2.50981400	3.56311700
C	3.66239500	-2.56058600	3.57442300
H	3.91937600	-3.46620200	4.12318800
H	4.05175000	-2.61664900	2.55398800
H	4.07655200	-1.68959100	4.09474900
C	-1.90056400	1.52865800	0.92119400
C	-3.08910800	1.34658900	0.74867100
C	-4.45819200	1.02750100	0.54636500
C	-5.45361600	2.00998800	0.58558200
C	-4.81282200	-0.31277700	0.28895800
C	-6.78684400	1.67515200	0.38920300
H	-5.17726800	3.04166000	0.77735100
C	-6.13510300	-0.64690000	0.08390900
H	-4.02773900	-1.06143500	0.23053600
C	-7.13008500	0.34165300	0.13753800
H	-7.54281000	2.44961100	0.42973000
H	-6.43609400	-1.66768700	-0.12417500
O	-8.39210600	-0.09009900	-0.07006200
C	-9.43379900	0.86441300	-0.03710800
H	-10.35296900	0.31202500	-0.22807500
H	-9.49543200	1.34930100	0.94395800
H	-9.29693100	1.62648900	-0.81286800
C	0.06051300	3.01607600	0.87831200
C	-0.39380100	3.83194300	-0.16898500
C	0.98560900	3.52449400	1.79680300
C	0.11958600	5.10812600	-0.33029900
H	-1.11105900	3.42481000	-0.87425700
C	1.48372200	4.81546000	1.63960600
H	1.29668400	2.92319300	2.64435200
C	1.06951000	5.59840100	0.56776200
H	-0.18505300	5.71269500	-1.17768200
H	2.20530800	5.20157800	2.35295600
H	1.49050100	6.58734900	0.41848800

O	-0.20325200	1.07682800	-0.94857200
H	0.74142100	0.85838000	-1.12176600
C	4.70711800	2.84308900	0.54142000
C	4.24272600	3.90738400	-0.47136900
C	3.18818700	3.18011800	-1.27492500
C	4.45232200	1.50358800	-0.16663500
H	5.74441600	2.96848600	0.86113700
H	4.07099200	2.90037100	1.43460600
H	5.06546200	4.23186700	-1.12285700
H	3.84612600	4.80822000	0.00563600
H	4.23650100	0.65888200	0.49328200
H	5.30583000	1.19948600	-0.78852500
C	3.29301300	1.84524400	-1.07644300
C	2.35371000	3.91094300	-2.23709800
O	2.45922000	5.12609700	-2.32837700
C	1.40040700	3.14279900	-3.12492700
H	0.64166600	2.62664500	-2.52833100
H	0.92296100	3.84367100	-3.81166000
H	1.93640900	2.36994600	-3.68466700
O	2.53202600	0.88369500	-1.61893600
H	2.86202500	-0.02159900	-1.32463900
N	0.78332100	-1.78579800	-0.49779800
H	-0.68397100	0.21567100	-0.94199600
C	1.86142800	-4.44079400	1.15753600
H	2.55011900	-5.11022300	1.67633200
H	1.04787900	-4.14180300	1.81855400
H	1.44457200	-4.94110800	0.27805300
C	3.44623300	-4.18872100	-2.02799300
H	3.79294800	-4.79018800	-1.18127500
H	3.23719400	-4.83593500	-2.87915100
H	4.20975100	-3.45268100	-2.29156900

TSNH-M1

O	-3.61282400	-2.31998300	-1.97038600
O	-3.02803900	-3.26543500	0.22576800
P	-2.65203100	-2.05068400	-0.71893300
S	-4.12363000	-0.19161200	0.90380400
O	-4.63582300	-1.28468300	1.72667900
O	-3.82879900	1.08899000	1.53567800
C	-5.51815600	0.20109600	-0.22918500
F	-6.56320800	0.64628800	0.45353700
F	-5.87985900	-0.89460600	-0.90482100

F	-5.14970300	1.13045100	-1.11113000
O	-1.19667100	-2.16622500	-1.10884600
C	0.80120600	0.76008200	1.30870200
C	0.30967800	2.11249300	1.05208700
C	-1.03588500	2.31242600	0.68313000
C	1.18272800	3.21039900	1.04618600
C	-1.48270200	3.56466900	0.31566100
H	-1.72477300	1.47432900	0.65759100
C	0.73705900	4.47619900	0.70065200
H	2.22226900	3.06476900	1.32655400
C	-0.60378700	4.65647300	0.32660100
H	-2.51083900	3.71677700	0.00683600
H	1.42816700	5.30990000	0.72271600
O	-1.13212400	5.84120200	-0.03754700
C	-0.28182200	6.96959100	-0.07008000
H	-0.90203600	7.80229200	-0.39912800
H	0.12533500	7.18740200	0.92401600
H	0.54154900	6.82379700	-0.77857700
C	2.07326800	0.45512500	0.93946700
C	3.17893400	0.14547000	0.44819800
C	4.58396500	-0.10674700	0.51085000
C	5.04416600	-1.27176900	1.14145300
C	5.52210000	0.79045100	-0.03995800
C	6.40071900	-1.54875500	1.23297600
H	4.32183800	-1.95795000	1.57346500
C	6.87200500	0.52014200	0.04876100
H	5.17770700	1.68460500	-0.54519500
C	7.32180500	-0.64894400	0.68172000
H	6.72877100	-2.45222100	1.73199300
H	7.61131800	1.19541100	-0.36711500
O	8.65829700	-0.81796000	0.71335100
C	9.16825100	-1.97921900	1.33953000
H	10.25178300	-1.91616700	1.24977400
H	8.88957000	-2.01126600	2.39887200
H	8.81143900	-2.88650000	0.83915600
C	-0.04793000	-0.26004100	1.93455700
C	0.18953800	-1.62163700	1.68668200
C	-1.11551500	0.10664300	2.76769400
C	-0.65543300	-2.58748600	2.20550900
H	1.02096700	-1.90529500	1.04756700
C	-1.94914600	-0.86665200	3.30302500
H	-1.30678000	1.15246200	2.98079500
C	-1.73697300	-2.20860300	3.00279600
H	-0.50318600	-3.63184300	1.95416500

H	-2.79959700	-0.56989500	3.90686200
H	-2.42839700	-2.95922400	3.37170100
O	-1.80014500	1.10146600	-2.21737700
H	-0.90373000	1.07794400	-1.85298400
C	3.22990900	-2.74115200	-1.62643100
C	3.83023600	-1.43917500	-2.18847000
C	2.79762700	-0.39485200	-1.84161300
C	1.70967500	-2.52600100	-1.66701600
H	3.54677000	-3.62956400	-2.17639400
H	3.54787400	-2.86490500	-0.58513100
H	3.95146100	-1.48390500	-3.27928400
H	4.81849100	-1.20868000	-1.77806900
H	1.13885200	-3.04411300	-0.89267700
H	1.27227200	-2.83728800	-2.62577900
C	1.57967900	-1.02296300	-1.58293400
C	2.98641900	1.00389900	-2.27634200
O	4.09400800	1.35960800	-2.65059100
C	1.80904200	1.95107900	-2.29631800
H	1.06232000	1.60194100	-3.01873400
H	1.31540100	1.99502100	-1.32263000
H	2.16188400	2.94179600	-2.58516600
O	0.47553300	-0.41980800	-1.30057500
H	-0.33279500	-1.13590300	-1.17251500
N	-2.95284700	-0.58672300	-0.08394100
H	-2.34699000	0.77909900	-1.47928000
C	-4.35006500	-3.81669100	0.30181200
H	-4.37407700	-4.72787300	-0.29926300
H	-4.53839100	-4.03734300	1.35180300
H	-5.10245200	-3.11365000	-0.05361400
C	-3.62451200	-1.36078600	-3.03749700
H	-2.60923200	-1.05583500	-3.30033900
H	-4.10835500	-1.85204400	-3.88119200
H	-4.19481100	-0.47813400	-2.74082600

com-OH

O	3.26058100	-2.89838400	0.06515500
O	1.33547700	-3.74344600	-1.41214900
P	1.85074700	-2.52589700	-0.53340900
N	1.90873600	-1.13788600	-1.32078600
S	3.06289300	-0.70872400	-2.35768400
O	3.90482600	-1.82369300	-2.76813900
O	2.48698800	0.18436400	-3.34572600
C	4.16021900	0.34819700	-1.32034400

F	5.27032300	0.60380400	-1.99528500
F	4.47123600	-0.28574500	-0.19117600
F	3.55595900	1.48929900	-1.02053000
O	0.86232200	-2.47137300	0.66027800
H	-0.10124800	-2.19464500	0.42365900
C	-2.03684700	-0.95603600	1.12835300
C	-3.34246400	-0.32038100	0.67192500
C	-4.41585300	-1.16060000	0.34168900
C	-3.47779800	1.04888000	0.48199900
C	-5.57379000	-0.64088100	-0.20267700
H	-4.32382400	-2.23203400	0.49880300
C	-4.64501000	1.58825100	-0.05975500
H	-2.65210600	1.71060300	0.72805200
C	-5.68741700	0.73951900	-0.43111000
H	-6.40578400	-1.27768800	-0.48386400
H	-4.70175500	2.65465900	-0.24138000
O	-6.83659400	1.14679200	-1.01350300
C	-6.90830600	2.50062400	-1.43215700
H	-7.85853100	2.59787800	-1.95734100
H	-6.90374900	3.17858400	-0.56990300
H	-6.07753300	2.74255500	-2.10391800
C	-1.01092100	0.03490300	1.50869400
C	-0.07850300	0.74282100	1.81428600
C	1.06820800	1.53495100	2.14372900
C	0.94804200	2.77528400	2.77430100
C	2.34915200	1.06536700	1.80517900
C	2.07351800	3.53910200	3.06901700
H	-0.03810700	3.14615800	3.03634400
C	3.47031500	1.82022300	2.08748000
H	2.44604900	0.10479600	1.30760300
C	3.34035900	3.06153700	2.72408400
H	1.95041400	4.49777100	3.55835900
H	4.46294800	1.47583900	1.81879300
O	4.49777500	3.72480500	2.95877600
C	4.41590500	4.98532000	3.58890200
H	5.44027600	5.34599300	3.67712400
H	3.83036900	5.69200600	2.98875600
H	3.97079000	4.90177900	4.58763400
C	-2.26535500	-1.92984700	2.28530400
C	-2.15152800	-3.30732200	2.11827000
C	-2.62916100	-1.41249700	3.53013800
C	-2.39639200	-4.16100400	3.19475000
H	-1.87769700	-3.71563400	1.15151000
C	-2.87269100	-2.26442400	4.59854100

H	-2.71913600	-0.33612500	3.65332700
C	-2.75540800	-3.64475700	4.43344500
H	-2.30543600	-5.23422400	3.05684900
H	-3.15531900	-1.85283000	5.56255300
H	-2.94604700	-4.31162800	5.26864300
O	-1.50345600	-1.73145100	0.02649800
H	-1.42001400	-1.12746400	-0.74847000
C	-0.14449800	3.33214300	-0.87261200
C	-1.42058400	3.47644800	-1.72841700
C	-1.75059700	2.04921700	-2.10334600
C	0.50213100	2.02125300	-1.34774600
H	0.52824900	4.18954900	-0.94682900
H	-0.42424000	3.21712800	0.18146400
H	-1.24500400	4.07929900	-2.62887800
H	-2.24461800	3.95551500	-1.18939600
H	1.03552100	1.48085900	-0.55993700
H	1.21070500	2.17302300	-2.17292200
C	-0.68855900	1.25531500	-1.85620000
C	-3.04757700	1.71067300	-2.69931900
O	-3.85920000	2.59929400	-2.92051200
C	-3.36150000	0.26662900	-3.01396000
H	-3.34588400	-0.32836300	-2.09321400
H	-4.35323400	0.21081600	-3.46580000
H	-2.60815400	-0.15512300	-3.68625700
O	-0.61923600	-0.08309400	-2.05052200
H	0.31325200	-0.37483600	-1.91016000
C	3.40064300	-4.09696700	0.84842800
H	4.45343600	-4.15628200	1.11741200
H	2.78063300	-4.02572300	1.74430900
H	3.11309200	-4.96800300	0.25496800
C	1.72035100	-3.91468000	-2.78940900
H	1.19543400	-4.80585100	-3.12920900
H	1.40530800	-3.04670800	-3.37402100
H	2.80028200	-4.03870900	-2.87218200

TSOH-M2

O	-4.17756800	2.63306900	-0.35173200
O	-2.89931200	2.40032600	-2.46672800
P	-2.88625200	1.92728500	-0.93310600
N	-2.99800600	0.28016700	-0.89597400
S	-4.27894200	-0.48281600	-1.44949100
O	-5.20087400	0.35431200	-2.21034900
O	-3.89569100	-1.78549000	-1.97557800

C	-5.20227900	-0.86937000	0.09291800
F	-6.30492400	-1.55008200	-0.18612000
F	-5.53134000	0.25320200	0.72498400
F	-4.44919200	-1.60987200	0.92023900
O	-1.66613400	2.36797700	-0.19150400
H	-0.12836300	1.85489100	-0.59142500
C	1.48908700	1.15122800	1.19127700
C	0.74947500	-0.01761300	1.65390200
C	1.42678000	-1.16748700	2.10729100
C	-0.65657300	-0.00330200	1.66481500
C	0.71951600	-2.22746000	2.63443200
H	2.51002000	-1.21103200	2.05724400
C	-1.37352800	-1.08495500	2.14513600
H	-1.18886600	0.84969100	1.24928800
C	-0.68375700	-2.19007800	2.66615200
H	1.22170600	-3.10816400	3.01930200
H	-2.45518100	-1.06539700	2.09038300
O	-1.28538400	-3.26556800	3.20631800
C	-2.70304900	-3.31994900	3.17881300
H	-2.97193000	-4.26418200	3.65000700
H	-3.13926500	-2.48832400	3.74245000
H	-3.07686400	-3.30010100	2.14954100
C	2.83822900	0.97524300	0.82252500
C	3.99421800	0.80398000	0.48135700
C	5.33391100	0.59188100	0.06865600
C	5.73067700	-0.67327800	-0.39149500
C	6.26968800	1.64559800	0.10428500
C	7.03820200	-0.88663700	-0.80717000
H	4.99727800	-1.47650100	-0.43257900
C	7.56856600	1.43304900	-0.30286700
H	5.95811600	2.62309700	0.45782400
C	7.96153100	0.16424900	-0.76134300
H	7.32618400	-1.86829900	-1.16297000
H	8.30962500	2.22435300	-0.28315000
O	9.25158200	0.05944500	-1.13802300
C	9.70597100	-1.19421800	-1.61099900
H	10.75869300	-1.05802200	-1.85489600
H	9.60457100	-1.96681500	-0.84071800
H	9.15769100	-1.49927200	-2.50925800
C	1.08138800	2.52120000	1.56998400
C	1.57841900	3.60961900	0.83621900
C	0.23827100	2.74995400	2.66254900
C	1.21285000	4.90116200	1.17578100
H	2.21625300	3.41652300	-0.02089300

C	-0.11335600	4.05104600	3.00699200
H	-0.12103000	1.91592000	3.25465600
C	0.36496500	5.12366400	2.26297000
H	1.58057000	5.73838800	0.59176800
H	-0.76487700	4.22323800	3.85710000
H	0.07911600	6.13691100	2.52750700
O	0.71359700	1.34948800	-0.76604400
H	0.39369100	0.45861000	-1.03079400
C	-0.79966700	-4.33884800	0.02577000
C	0.71843000	-4.14401500	-0.22455900
C	0.83140500	-2.75836200	-0.81126600
C	-1.51445500	-3.14774300	-0.64791700
H	-1.15548400	-5.29166700	-0.37228400
H	-1.00060000	-4.34746200	1.09962800
H	1.12056500	-4.89152500	-0.91923500
H	1.30727100	-4.23006200	0.69445900
H	-2.25787900	-2.65253500	-0.01271300
H	-2.05060000	-3.42047900	-1.56375800
C	-0.39018700	-2.21145900	-0.99884500
C	2.14441800	-2.16385000	-1.06399800
O	3.13340600	-2.60326700	-0.48447700
C	2.30040200	-1.05349600	-2.08558700
H	3.19676500	-1.26806000	-2.67395100
H	1.43512200	-0.96276400	-2.74407100
H	2.46201000	-0.09377200	-1.58458100
O	-0.63590100	-0.97722200	-1.47193300
H	-1.57297400	-0.67688400	-1.28082500
C	-5.34021900	3.03301600	-1.08902900
H	-5.15073900	3.00485100	-2.16118600
H	-6.15422800	2.35111100	-0.84428200
H	-5.57763100	4.04778100	-0.76609000
C	-2.00486100	1.74388600	-3.36557700
H	-2.01229600	2.32193500	-4.28894300
H	-0.98780300	1.72177100	-2.95694800
H	-2.34521500	0.72315100	-3.56388600

TSOH-M1

C	-1.66195900	-1.30126500	1.07206200
C	-2.90416300	-2.01234900	0.75655200
C	-2.90051400	-3.41169900	0.57694700
C	-4.09088900	-1.30769400	0.50939600
C	-4.04608700	-4.06517900	0.17177600
H	-1.96697100	-3.95356700	0.67995900

C	-5.24844400	-1.95748800	0.11187100
H	-4.10567100	-0.22871400	0.62841900
C	-5.22840300	-3.34715400	-0.06141500
H	-4.05566800	-5.13670800	0.00417300
H	-6.14602100	-1.38039600	-0.07227100
O	-6.28968000	-4.07863000	-0.45622500
C	-7.49709900	-3.39896600	-0.74151100
H	-8.20578600	-4.16578500	-1.05239200
H	-7.88034700	-2.88532800	0.14774200
H	-7.36080700	-2.67411000	-1.55189000
C	-1.56173000	-0.00730800	0.67742000
C	-1.64839300	1.17508800	0.27673200
C	-1.90864000	2.56263800	0.48019700
C	-0.94990100	3.37364100	1.10478500
C	-3.14034200	3.12457600	0.08551700
C	-1.20474700	4.71774600	1.33847700
H	-0.00217200	2.93983000	1.40632800
C	-3.39691300	4.46030600	0.31661400
H	-3.86924300	2.49278400	-0.41595000
C	-2.43122600	5.26599300	0.94121000
H	-0.45133100	5.32461700	1.82542700
H	-4.33575400	4.91794100	0.02428300
O	-2.77767700	6.55576700	1.11866000
C	-1.84514500	7.41633800	1.74548200
H	-2.32097600	8.39542200	1.78346600
H	-1.61945700	7.07912600	2.76342800
H	-0.91721300	7.48161000	1.16641800
C	-0.58267700	-1.94510200	1.83256800
C	0.75884500	-1.60714100	1.60687800
C	-0.90004000	-2.87708100	2.83249200
C	1.76361900	-2.21720600	2.34581400
H	1.00576300	-0.90055000	0.81995600
C	0.10758800	-3.46953300	3.58163400
H	-1.93973000	-3.11349100	3.03500000
C	1.43967900	-3.14790200	3.33204700
H	2.79886300	-1.96335400	2.14571300
H	-0.14738300	-4.18118500	4.36057800
H	2.22892800	-3.62129900	3.90866300
O	-0.22836900	-3.39815400	-0.71439100
H	-0.29581400	-3.75084600	-1.61220900
C	-0.29394800	3.22682000	-2.38412000
C	-1.62009500	2.47972700	-2.64543300
C	-1.40993500	1.09711200	-2.08358600
C	0.74345600	2.14714400	-2.01594700

H	0.02094500	3.80811400	-3.25283500
H	-0.41792500	3.92815500	-1.55506300
H	-1.83527400	2.38997700	-3.71897400
H	-2.48463300	2.98655500	-2.21006500
H	1.29590700	2.37454900	-1.10029800
H	1.51430500	1.99033200	-2.78026100
C	-0.05905400	0.88707000	-1.85354500
C	-2.51192900	0.10327300	-2.20032000
O	-3.66338300	0.50937800	-2.19279000
C	-2.17252900	-1.35068500	-2.38155400
H	-1.45446200	-1.70977700	-1.63679200
H	-3.09137900	-1.94053300	-2.34913900
H	-1.68897500	-1.46996100	-3.36001900
O	0.47537000	-0.25771900	-1.52741500
H	1.46708200	-0.16547000	-1.34327600
P	3.55305600	-1.73017000	-0.96147700
N	3.12627400	-0.14844000	-0.93615700
S	3.95712100	1.07864500	-0.35841200
O	5.33364300	0.77801400	0.00210200
O	3.67142100	2.29239000	-1.11112500
C	3.10470200	1.37023700	1.24629400
F	3.51866900	2.50078700	1.80181300
F	3.31919400	0.36806600	2.08900800
F	1.77625400	1.46643100	1.04405900
O	2.38647100	-2.63111800	-1.09892600
H	0.69198300	-3.06576100	-0.68086200
O	4.41964300	-1.97996100	0.37329700
O	4.58264900	-2.01466200	-2.15757800
C	5.74464000	-1.19864500	-2.31496600
H	5.46006100	-0.18908400	-2.62654800
H	6.31006300	-1.13800400	-1.38185000
H	6.34270200	-1.66959600	-3.09545600
C	4.79604400	-3.33358100	0.63584700
H	5.38049200	-3.73599900	-0.19772600
H	5.40667000	-3.31679400	1.53875400
H	3.90516500	-3.94978300	0.78935000

IntOH-M2

O	3.37043700	-3.06977400	0.14377100
O	3.25323900	-2.46191300	-2.23631500
C	-3.35869300	-2.56176700	-1.28245400
C	-3.96477700	-1.31639400	-1.96123200
C	-2.85972200	-0.29378300	-1.84386600

C	-1.83932000	-2.40443400	-1.45084200
H	-3.60213000	-2.53475800	-0.21165100
H	-3.73954500	-3.50436000	-1.68349900
H	-4.89246900	-0.98040300	-1.48335900
H	-4.20880700	-1.50994200	-3.01491900
H	-1.48449400	-2.83531400	-2.39750600
H	-1.23307500	-2.85485800	-0.66068100
C	-1.68344100	-0.90060200	-1.52434000
C	-3.09262200	1.11901800	-2.12815900
O	-4.22472000	1.52042000	-2.37982900
C	-1.92367000	2.08115200	-2.11523000
H	-1.12506300	1.73355200	-2.77684200
H	-2.27779600	3.06548100	-2.42565900
H	-1.48603400	2.13870100	-1.11414500
C	-0.72782900	0.77641700	1.42133400
C	-0.05823200	1.99029300	1.04765300
C	-0.70449200	3.24235200	1.21859900
C	1.19856200	1.96044500	0.40427500
C	-0.09553200	4.40518400	0.82028000
H	-1.67921600	3.27545000	1.69640000
C	1.80602800	3.12553900	-0.02387400
H	1.68255500	1.01335100	0.17309300
C	1.17041200	4.35531000	0.19608200
H	-0.55861100	5.37437000	0.96838900
H	2.76171000	3.04377100	-0.52815700
O	1.68528900	5.53517700	-0.16367600
C	2.96392700	5.54116200	-0.78737700
H	3.19536600	6.58857000	-0.97383100
H	3.71988800	5.10022100	-0.13037900
H	2.93743600	4.99091000	-1.73289400
C	-2.11938600	0.75927500	1.38280500
C	-3.31916700	0.62310900	1.17584300
C	-4.69558800	0.40381400	0.96967700
C	-5.28443400	-0.77798500	1.45440400
C	-5.48430500	1.32003500	0.24035900
C	-6.62239200	-1.05001100	1.22758100
H	-4.67501300	-1.48114100	2.01422200
C	-6.81608600	1.05299900	0.01225200
H	-5.02934600	2.21290800	-0.17124200
C	-7.39442600	-0.12894700	0.50220600
H	-7.05501700	-1.96655800	1.60885200
H	-7.43727500	1.73002400	-0.56284800
O	-8.69910600	-0.29475700	0.22593000
C	-9.33455200	-1.47884900	0.67067800

H	-10.36808200	-1.40633000	0.33511400
H	-8.86658800	-2.36549200	0.22866000
H	-9.30781100	-1.55403100	1.76351700
C	-0.04187100	-0.44565500	1.81346200
C	-0.72860100	-1.67584800	1.76894300
C	1.29633600	-0.42626100	2.24799300
C	-0.08258500	-2.85101000	2.10258200
H	-1.76005000	-1.69253200	1.42810800
C	1.94198700	-1.61035300	2.57028700
H	1.82370200	0.51474400	2.34628100
C	1.25971500	-2.82116400	2.48592400
H	-0.60865200	-3.79754100	2.03278000
H	2.98516300	-1.58901500	2.86548100
H	1.77994300	-3.74703100	2.70904700
P	2.65778200	-2.00897200	-0.81682000
N	3.08635600	-0.47278200	-0.50000300
S	4.51634900	0.16869900	-0.56449000
O	5.51443000	-0.58397400	-1.32376800
O	4.42429100	1.61059000	-0.78180000
C	5.08956300	0.04914700	1.17886800
F	6.29093500	0.59394200	1.31882900
F	5.15341300	-1.22919500	1.56393300
F	4.23929500	0.68201300	1.99437300
O	1.17088100	-2.15387500	-0.71314200
O	-0.52058300	-0.29979400	-1.32063000
H	0.18438000	-0.98339700	-1.08007100
C	3.08948900	-1.58585600	-3.35161200
H	3.25934000	-2.18612700	-4.24567900
H	2.07627600	-1.17085600	-3.37832500
H	3.82617300	-0.78079200	-3.29986700
C	4.66884200	-3.59671400	-0.16491000
H	5.05245900	-4.01760500	0.76524700
H	4.57172200	-4.37813100	-0.92112900
H	5.34124800	-2.81632000	-0.52604900

TSOH-M2

O	3.36715800	-3.07528900	0.21472500
O	3.23357200	-2.52278500	-2.17636800
C	-3.30026700	-2.69367700	-1.30584500
C	-3.84155500	-1.42766000	-1.99434900
C	-2.77640500	-0.39480300	-1.71817400
C	-1.77227300	-2.54873500	-1.36606800

H	-3.61932000	-2.69749800	-0.25689100
H	-3.65852000	-3.61796400	-1.76382900
H	-4.82859700	-1.12341800	-1.63286200
H	-3.94058200	-1.56688100	-3.07980200
H	-1.36053500	-2.95747400	-2.29979100
H	-1.21639300	-3.01888200	-0.55131400
C	-1.58106600	-1.05102000	-1.41031300
C	-2.91073500	0.97014500	-2.26985800
O	-3.99225800	1.30965700	-2.72669000
C	-1.72487100	1.90496400	-2.27473600
H	-2.02337900	2.83848900	-2.75330200
H	-1.37472000	2.10009500	-1.25706200
H	-0.88194600	1.45654600	-2.80912100
C	-0.73749800	0.70000800	1.27619200
C	-0.10685800	1.99287800	0.98880700
C	-0.81094300	3.18922200	1.22886800
C	1.14549500	2.06216800	0.36187800
C	-0.26272600	4.40886800	0.89017400
H	-1.78694200	3.14547000	1.70418400
C	1.69679200	3.28428600	0.00141600
H	1.68195600	1.15361300	0.09874600
C	0.99844500	4.46411100	0.27437800
H	-0.78108100	5.34034400	1.09021900
H	2.66149800	3.27909900	-0.49197800
O	1.45265400	5.69915400	-0.02153100
C	2.72662800	5.79718000	-0.63360900
H	2.90829600	6.86206600	-0.77510700
H	3.50565400	5.36986700	0.00703400
H	2.73826800	5.28832700	-1.60362800
C	-2.06227100	0.57849400	0.99492100
C	-3.18326200	0.34383200	0.49339700
C	-4.60766100	0.22806800	0.51999800
C	-5.19977000	-0.86451100	1.16966800
C	-5.43626900	1.18546200	-0.09977300
C	-6.57863000	-1.01469400	1.20890300
H	-4.56425400	-1.59738600	1.65819800
C	-6.80789800	1.04203800	-0.06325700
H	-4.99089000	2.02795500	-0.61527600
C	-7.38900500	-0.05850900	0.58421300
H	-7.00935800	-1.86546700	1.72248800
H	-7.46415800	1.76561600	-0.53383100
O	-8.73549700	-0.10826300	0.55503500
C	-9.37568300	-1.20739200	1.17337700
H	-10.44349300	-1.05674400	1.01999400

H	-9.06892900	-2.15321600	0.71226000
H	-9.16052400	-1.23701900	2.24765900
C	-0.01238300	-0.44729900	1.84155300
C	-0.63928000	-1.70413400	1.91856400
C	1.31333700	-0.32709200	2.27963500
C	0.05352200	-2.81242400	2.37121300
H	-1.67304800	-1.80266400	1.59731800
C	2.01230000	-1.44635800	2.71680900
H	1.80627000	0.63676200	2.26800200
C	1.39048700	-2.68927000	2.75394100
H	-0.43703300	-3.78009200	2.40771900
H	3.05138000	-1.34387800	3.01029800
H	1.94705300	-3.56435600	3.07379800
P	2.65204100	-2.04279400	-0.76257500
N	3.01599700	-0.49353600	-0.48595500
S	4.41848900	0.20860600	-0.60292900
O	5.42224700	-0.53346900	-1.36596800
O	4.25518400	1.63406800	-0.86311400
C	5.04023800	0.15425700	1.12716600
F	6.23860400	0.71644800	1.20878700
F	5.13243800	-1.11188800	1.54583300
F	4.20875500	0.80118200	1.94660700
O	1.15705600	-2.23202800	-0.65695500
O	-0.45531100	-0.46931400	-1.18734100
H	0.30576400	-1.19025000	-0.92841600
C	3.06855500	-1.67250000	-3.31264400
H	3.81270800	-0.87377200	-3.28528100
H	3.22499700	-2.29772100	-4.19178400
H	2.05872200	-1.24923900	-3.34195000
C	4.68827800	-3.56250300	-0.07034000
H	5.33468700	-2.76734600	-0.44670700
H	5.07752100	-3.94542300	0.87313400
H	4.62329700	-4.36450000	-0.80797200

TSOH-R

C	-6.93549600	-1.72905800	-4.27840500
C	-6.18480200	-2.82853200	-3.80341600
C	-5.21388500	-2.65886600	-2.84908200
C	-4.93155700	-1.37224000	-2.31027500
C	-5.65859100	-0.26656400	-2.82840300
C	-6.66945300	-0.47373700	-3.80070100
C	-5.35173500	1.03190900	-2.36086900
C	-4.32664400	1.26735800	-1.48049900

C	-3.57305800	0.15263800	-1.01106900
C	-3.91988700	-1.15350000	-1.30818400
C	-3.26723600	-2.33734000	-0.68620400
C	-1.90442000	-2.47281400	-0.72740900
C	-1.19973000	-3.64990100	-0.36533700
C	-1.94596800	-4.69178300	0.12450400
C	-3.34684100	-4.57470500	0.32879200
C	-4.02220200	-3.38631400	-0.06316400
C	-5.40908300	-3.27048300	0.21108700
C	-6.09286100	-4.29826000	0.80990900
C	-5.43012800	-5.49662000	1.16151400
C	-4.08584500	-5.62689800	0.92895800
H	-7.22098000	0.38998200	-4.16578900
H	-7.70742600	-1.88119100	-5.02608600
H	-6.37165400	-3.81970200	-4.20505600
H	-4.64062100	-3.51518800	-2.51376500
H	-5.94924500	1.87340800	-2.70632400
O	-2.52902100	0.49025200	-0.17073500
H	-5.92112800	-2.34764100	-0.04074400
H	-7.15104800	-4.18687600	1.02494800
H	-5.98445900	-6.30324400	1.63106000
H	-3.55715800	-6.53246300	1.21493900
O	-1.14910400	-1.39211400	-1.16711600
H	-1.45321200	-5.62492100	0.38645200
C	-4.08852400	2.66947900	-1.01479600
C	-3.86339800	5.36142300	-0.25736500
C	3.06139500	-4.03429000	-0.97006500
C	0.27743100	-3.73353600	-0.56487900
C	0.82135600	-3.62170500	-1.86542000
C	1.12987200	-3.95066900	0.53098400
C	2.49851600	-4.13433400	0.29796700
H	3.13591100	-4.35825800	1.14876900
C	2.19966000	-3.73755400	-2.03187100
H	2.61358600	-3.65351000	-3.03609500
C	-4.35016700	4.40503300	0.63452100
H	-4.64164400	4.72240200	1.62862500
C	-4.48824400	3.06099400	0.27892800
C	-3.56490500	3.60748800	-1.92213100
C	-3.49205900	4.94580400	-1.53306800
H	-3.10652600	5.68982000	-2.22538600
C	-0.04955000	-3.49713200	-3.11034500
C	0.28574500	-2.26313600	-3.95177200
C	0.05359400	-4.77740700	-3.95090700
H	1.32194700	-2.29420300	-4.31126100

H	-0.36417200	-2.21822000	-4.83217300
H	0.13683600	-1.34752600	-3.37194800
H	-0.62238400	-4.72758000	-4.81109400
H	1.07215800	-4.91958000	-4.32929500
H	-0.20890700	-5.65707200	-3.35545400
C	4.53796900	-4.29559100	-1.24227700
C	4.69897900	-5.42881900	-2.26725500
C	5.34865500	-4.63065800	0.00882000
H	4.27969100	-6.35833400	-1.86681900
H	4.18801400	-5.21135200	-3.20929400
H	5.75832200	-5.59739900	-2.48606900
H	6.40374900	-4.74636400	-0.25469900
H	5.28924800	-3.84558100	0.76651100
H	5.00183900	-5.57158800	0.45191200
C	0.63773100	-3.98587700	1.97006400
C	0.69951000	-5.40360900	2.55036700
C	1.43080400	-3.01322400	2.84779500
H	1.73208000	-5.77205500	2.56768900
H	0.32093700	-5.40937400	3.57754300
H	0.10610000	-6.11161000	1.96322900
H	0.96170000	-2.94932300	3.83416500
H	2.47217800	-3.33165600	2.97873500
H	1.42114100	-2.01038700	2.40870700
C	-3.03581800	3.14957400	-3.28014500
C	-1.85469100	2.15183000	-3.10307400
C	-2.63241500	4.29901100	-4.20439900
H	-0.97803000	2.48232600	-3.68939400
H	-1.53585200	2.08135700	-2.05364300
H	-2.12256000	1.13686900	-3.44703700
H	-1.77366500	4.85282500	-3.80179500
H	-2.33139500	3.89686700	-5.17504600
H	-3.45251500	5.00612100	-4.36792700
C	-3.71016300	6.81142900	0.16006400
C	-2.60236900	6.95724600	1.20786600
C	-5.02537900	7.40531700	0.67489800
H	-2.85519900	6.39983800	2.11657600
H	-1.64790100	6.57016600	0.83250400
H	-2.46208100	8.00767400	1.48440500
H	-4.90192900	8.46856600	0.90275800
H	-5.82260200	7.30163500	-0.06688200
H	-5.35307700	6.90472200	1.59179000
C	-5.11642200	2.07169200	1.25755300
C	-6.55832900	1.72847800	0.84728100
C	-5.14111000	2.57687400	2.70277800

H	-7.16923400	2.63838900	0.83014500
H	-6.61165200	1.26099400	-0.13780800
H	-6.99683300	1.03782700	1.57512100
H	-5.43925800	1.76160800	3.36738700
H	-4.16533700	2.93995100	3.03287700
H	-5.87059600	3.38631600	2.82298400
H	-1.09423100	-3.40210600	-2.80240500
H	4.96940900	-3.38344200	-1.67903000
H	-0.40125400	-3.64553200	1.99384400
H	-4.52296100	1.14824600	1.24163000
H	-3.85191200	2.61774800	-3.78366800
H	-3.41035400	7.37780500	-0.73139200
C	3.94990600	0.51569100	-3.12303900
C	4.97843100	-0.32347300	-2.34617400
C	4.45342900	-0.30347600	-0.92962000
C	2.62360000	0.24720500	-2.39911500
H	4.20517500	1.57854600	-3.03451000
H	3.90997500	0.26530800	-4.18559600
H	6.00237100	0.05297100	-2.42080100
H	4.99531600	-1.36205300	-2.70585700
H	2.15412900	-0.68190800	-2.76050600
H	1.86822700	1.03408300	-2.45186200
C	3.06210400	-0.04142800	-0.99084800
C	5.13593800	-1.10471100	0.12193200
O	6.24036100	-1.55884000	-0.13187900
C	4.45286300	-1.33842200	1.44287500
H	3.56228700	-1.95720000	1.28405400
H	5.14640600	-1.84677300	2.11517200
H	4.10646700	-0.40355400	1.88982700
C	2.98146500	2.23711600	1.35553400
C	2.89541900	1.65548600	2.70907100
C	3.94894800	1.80486300	3.62649400
C	1.83413100	0.80699100	3.03441600
C	3.92199700	1.14402200	4.83969300
H	4.78519800	2.45194200	3.37472100
C	1.80513900	0.12353200	4.24464200
H	1.03946300	0.62540600	2.31616800
C	2.85049400	0.29425600	5.15467200
H	4.71829000	1.26079800	5.56424700
H	0.96860000	-0.53565800	4.44322400
O	2.91700900	-0.31729100	6.35757000
C	1.86840500	-1.20827500	6.69130900
H	2.10858800	-1.59597800	7.68097000
H	0.90269200	-0.69136700	6.72155700

H	1. 81086100	-2. 03492500	5. 97398800
C	4. 13427900	2. 05970200	0. 68237100
C	5. 04459700	1. 64217800	-0. 08922200
C	6. 31881500	1. 91153700	-0. 70678900
C	6. 40195600	2. 86208100	-1. 73157200
C	7. 48872100	1. 23531500	-0. 31008900
C	7. 61182500	3. 14930400	-2. 35096200
H	5. 50481800	3. 39416200	-2. 03514700
C	8. 69443300	1. 51483200	-0. 92136600
H	7. 43909500	0. 48954500	0. 47450700
C	8. 76590100	2. 46958200	-1. 94614200
H	7. 64626600	3. 89648400	-3. 13460200
H	9. 60645900	1. 00684900	-0. 62806300
O	9. 99036200	2. 66636400	-2. 47760700
C	10. 11721700	3. 61350400	-3. 51947100
H	11. 16973400	3. 61158400	-3. 80002000
H	9. 50723500	3. 33269900	-4. 38574900
H	9. 83105600	4. 61574800	-3. 18006700
C	1. 85816500	2. 93597400	0. 70069200
C	1. 98200700	3. 32895600	-0. 64480600
C	0. 65095000	3. 18696300	1. 36853000
C	0. 93151900	3. 94365100	-1. 30128800
H	2. 91710900	3. 14487400	-1. 16766900
C	-0. 40746000	3. 79118800	0. 69881400
H	0. 53627400	2. 90193400	2. 40877900
C	-0. 26861300	4. 17672500	-0. 63240700
H	1. 04187700	4. 23831300	-2. 34313300
H	-1. 35005800	3. 96321100	1. 21076500
H	-1. 09774300	4. 65019700	-1. 14100700
P	-1. 05651000	-0. 16596400	-0. 11147300
N	-0. 76029100	-0. 66338800	1. 38115100
S	-1. 82030200	-0. 87225500	2. 54481700
O	-3. 17201600	-1. 20084700	2. 10963200
O	-1. 21596300	-1. 63423100	3. 63134500
C	-1. 99334600	0. 82705800	3. 24145400
F	-3. 02566000	0. 86397000	4. 07462100
F	-2. 19227500	1. 72117300	2. 26595900
F	-0. 89814400	1. 18975400	3. 90938800
O	0. 02489500	0. 73575200	-0. 65104100
O	2. 28203300	-0. 02790900	0. 01725200
H	1. 29180100	0. 30257600	-0. 24613000

TS1OH-S

C	5.86622300	-5.18493100	-2.70372300
C	6.41398500	-3.92036300	-2.38677400
C	5.68147300	-2.99283700	-1.68990700
C	4.35325800	-3.27847500	-1.26981400
C	3.79345300	-4.53554000	-1.62508000
C	4.58061700	-5.48012000	-2.33373600
C	2.44878500	-4.81739900	-1.27746300
C	1.65148300	-3.89342000	-0.65151600
C	2.22890300	-2.63872900	-0.30979900
C	3.55398700	-2.34050000	-0.53116000
C	4.14315100	-1.05855100	-0.07134300
C	3.58923500	0.13754100	-0.46682500
C	4.23774300	1.38681100	-0.28175300
C	5.39634100	1.38966600	0.45833900
C	5.92677200	0.21199100	1.03889900
C	5.30441500	-1.03468700	0.76707100
C	5.83396600	-2.20392500	1.37399500
C	6.93920200	-2.13219600	2.18299700
C	7.57952400	-0.89391000	2.42418500
C	7.08001000	0.25255400	1.86526800
H	4.13600200	-6.44026000	-2.58311100
H	6.46100300	-5.91127800	-3.24864600
H	7.42437700	-3.67841400	-2.70160100
H	6.11326500	-2.02392700	-1.46406200
H	2.03476600	-5.79341700	-1.52325300
O	1.40095100	-1.74329200	0.33379500
H	5.34056200	-3.15613300	1.21092700
H	7.32264300	-3.03404000	2.64999600
H	8.45693300	-0.85586000	3.06210000
H	7.54869900	1.21486800	2.05376200
O	2.34923500	0.12485400	-1.11233200
H	5.92790200	2.32880800	0.59593000
C	0.21970000	-4.18465200	-0.34478500
C	-2.47249600	-4.72166000	0.22935000
C	3.30217500	5.10763100	-2.23137200
C	3.79641600	2.64411600	-0.95746200
C	3.89257500	2.73963800	-2.36616200
C	3.43756400	3.76927300	-0.19367000
C	3.20444600	4.98353100	-0.84967200
H	2.92798100	5.85076800	-0.25409400
C	3.63536800	3.96973300	-2.96989900
H	3.70885700	4.06215800	-4.05069400
C	-1.52712900	-4.65029900	1.25017300
H	-1.85173200	-4.79780100	2.27523900

C	-0.18275300	-4.38725800	0.99359200
C	-0.70825700	-4.27662400	-1.40175200
C	-2.04247000	-4.55439400	-1.08397900
H	-2.78214200	-4.63239000	-1.87685100
C	4.37469800	1.56601600	-3.21329800
C	3.93193000	1.63217500	-4.67666700
C	5.90612400	1.45909700	-3.14829800
H	4.44280800	2.43449800	-5.21997200
H	4.18114800	0.69141100	-5.17664700
H	2.85298900	1.78843000	-4.76989800
H	6.36352300	2.37953400	-3.52856500
H	6.25751100	1.30231900	-2.12451000
H	6.25580700	0.62295200	-3.76339200
C	2.97155200	6.40558600	-2.94317900
C	3.56070700	7.63741700	-2.25253000
C	1.45051000	6.54320300	-3.09489400
H	3.09877900	7.80294700	-1.27346300
H	4.63965200	7.53349400	-2.10464900
H	3.37807200	8.53316600	-2.85472200
H	1.19242800	7.45668900	-3.64135200
H	1.02687700	5.68631900	-3.62858500
H	0.97350800	6.58787300	-2.10849400
C	3.27613700	3.72434900	1.31855900
C	4.30831600	4.61386600	2.02066400
C	1.85447700	4.11546300	1.72854300
H	4.16008800	5.66904100	1.76288500
H	4.21111900	4.51519600	3.10639800
H	5.33273800	4.34574900	1.74300800
H	1.74967100	4.06032100	2.81606400
H	1.59920800	5.13194000	1.40434900
H	1.14170600	3.41022200	1.29396100
C	-0.28755700	-4.06887600	-2.85916300
C	0.16877600	-2.62910500	-3.14637100
C	-1.37281400	-4.45818300	-3.86525500
H	-0.60191600	-1.90481200	-2.86989700
H	1.07648200	-2.35660900	-2.60279000
H	0.38004100	-2.51589700	-4.21545500
H	-2.22871300	-3.77352300	-3.81421500
H	-0.96843000	-4.39794000	-4.87988000
H	-1.73941600	-5.47667100	-3.70485000
C	-3.93280200	-4.99051300	0.53732800
C	-4.44943200	-4.10068100	1.67353700
C	-4.16136500	-6.47163800	0.86183900
H	-4.04188200	-4.42010000	2.63874400

H	-4.15827400	-3.05621000	1.52151600
H	-5.54099900	-4.14249300	1.74399300
H	-5.22086800	-6.66919500	1.05592100
H	-3.83330700	-7.11086500	0.03678800
H	-3.59327700	-6.75568100	1.75474300
C	0.82731400	-4.37596000	2.13753500
C	1.70497500	-5.63800500	2.09758500
C	0.18721400	-4.28011100	3.52509800
H	1.07641200	-6.53104500	2.19196900
H	2.27698500	-5.71881500	1.17090600
H	2.41140600	-5.62974400	2.93420800
H	0.96514700	-4.09794200	4.27185300
H	-0.53798000	-3.46732000	3.59256700
H	-0.31575800	-5.21702200	3.79217700
H	3.95502300	0.64461900	-2.79923600
H	3.40638800	6.34303400	-3.94952700
H	3.42249800	2.69579600	1.65995400
H	1.47157800	-3.49624000	2.01463800
H	0.57044100	-4.72452500	-3.04985600
H	-4.50417900	-4.75391600	-0.37180800
P	1.09955700	-0.22261600	-0.13720900
N	1.09118200	0.71120000	1.16267300
S	1.59768200	0.31909400	2.61456200
O	2.67094600	-0.66369200	2.66166200
O	1.69776200	1.51648600	3.44176000
C	0.12864000	-0.56928300	3.30522300
F	0.48341600	-1.26713200	4.37778900
F	-0.38841900	-1.40560100	2.39891500
F	-0.82448500	0.29255300	3.65502100
O	-0.15961700	-0.12915100	-0.95885600
C	-4.46811500	-1.53176800	-2.11142400
C	-5.30777300	-1.56196600	-0.82102900
C	-4.55688500	-0.64799900	0.11920800
C	-3.03052800	-1.26725000	-1.64033500
H	-4.80455800	-0.70328500	-2.74594800
H	-4.55524500	-2.45250700	-2.69385300
H	-6.34566700	-1.25007900	-0.97192400
H	-5.34635300	-2.56934800	-0.38540800
H	-2.49196500	-2.20042700	-1.42082800
H	-2.40364800	-0.69205500	-2.32642900
C	-3.21869600	-0.56209800	-0.32829500
C	-4.99824300	-0.52967600	1.53508200
O	-6.10801500	-0.94422700	1.82614600
C	-4.07285000	0.07183500	2.56286000

H	-3.14046000	-0.49847900	2.62168700
H	-4.57923100	0.06593500	3.52870000
H	-3.79178100	1.09399700	2.29042400
C	-2.92370300	2.70299700	-0.11893900
C	-2.62398100	3.18758500	1.23874600
C	-3.56877000	3.92501100	1.97354600
C	-1.43966300	2.79446600	1.86916000
C	-3.31918900	4.27497400	3.28694300
H	-4.49681300	4.22815400	1.49663000
C	-1.18044700	3.13714900	3.18916300
H	-0.72287500	2.16457500	1.34786400
C	-2.12295600	3.87733500	3.90507300
H	-4.03217900	4.85305800	3.86497800
H	-0.25416200	2.78590300	3.62925500
O	-1.96900100	4.24143800	5.19660800
C	-0.79553900	3.79580900	5.85378600
H	-0.87553700	4.14889800	6.88142400
H	0.10266300	4.21622900	5.38712900
H	-0.72588800	2.70216100	5.83893300
C	-4.14708900	2.18174900	-0.33598600
C	-5.14083800	1.41673000	-0.47306600
C	-6.51075500	1.25835400	-0.88183100
C	-6.83485600	1.25919500	-2.24438400
C	-7.54175800	1.09439800	0.06404000
C	-8.14842700	1.10946600	-2.67000800
H	-6.04448200	1.39309300	-2.97731900
C	-8.84907500	0.94351200	-0.35180100
H	-7.30411000	1.07909100	1.12117000
C	-9.16250800	0.94735500	-1.71901300
H	-8.37002800	1.12375600	-3.73012800
H	-9.65641600	0.81748500	0.36095000
O	-10.46821900	0.79103500	-2.02058900
C	-10.83641000	0.77259200	-3.38524600
H	-11.91558900	0.62548400	-3.40265100
H	-10.34607400	-0.05169700	-3.91573300
H	-10.58862300	1.72148300	-3.87506200
C	-1.91766700	2.70079800	-1.19808600
C	-2.17026100	2.01475800	-2.39772800
C	-0.67585400	3.32505000	-1.02949700
C	-1.18925700	1.90115600	-3.36891100
H	-3.14472500	1.55824200	-2.55389800
C	0.31452200	3.19363200	-1.99674400
H	-0.47573400	3.91195300	-0.14021700
C	0.06577000	2.47548900	-3.16067500

H	-1.39606100	1.35411900	-4.28400800
H	1.27988000	3.65811700	-1.83604500
H	0.84883800	2.37313700	-3.90588200
O	-2.28368900	0.04880400	0.29293400
H	-1.34885400	0.00504900	-0.23496700

TS1NH-R

C	8.16641500	1.52147200	1.12721700
C	7.90192300	0.16308100	0.83331300
C	6.66445500	-0.23100200	0.39130900
C	5.61500700	0.71382800	0.22085500
C	5.87326600	2.06964600	0.55924200
C	7.16874900	2.45080600	0.99720000
C	4.82402900	3.01499000	0.46631100
C	3.54517200	2.65885400	0.11331900
C	3.30524900	1.29432000	-0.21365800
C	4.30807700	0.34801400	-0.24701200
C	4.04429100	-1.03969400	-0.70300300
C	3.05288900	-1.78210600	-0.10614500
C	2.91373400	-3.18334900	-0.29745600
C	3.70487500	-3.77277900	-1.25190400
C	4.62030900	-3.02421000	-2.03375700
C	4.81090900	-1.64507400	-1.75151700
C	5.72381600	-0.91016200	-2.55267500
C	6.42582100	-1.52426500	-3.55891300
C	6.25826400	-2.90453800	-3.81727500
C	5.37127000	-3.63502700	-3.07057600
H	7.34753000	3.49601700	1.23641300
H	9.15332200	1.81981400	1.46673900
H	8.68537400	-0.57702100	0.96331600
H	6.47577100	-1.27763900	0.17979600
H	5.03748200	4.05934500	0.68586500
O	2.02293500	0.96206400	-0.59830100
H	5.84614700	0.15311900	-2.37429100
H	7.10920600	-0.94258500	-4.16982500
H	6.82219700	-3.37779400	-4.61507100
H	5.21751600	-4.69291900	-3.26705900
O	2.18638600	-1.16594000	0.78540000
H	3.63843800	-4.84790400	-1.40445500
C	2.47345600	3.70000800	0.04536600
C	0.59797400	5.78990200	-0.08979200
C	0.70076000	-5.82775100	2.28774800
C	2.07387500	-4.02465200	0.60700700

C	2. 43439900	-4. 13660700	1. 96577000
C	1. 01750400	-4. 80272100	0. 09458300
C	0. 36499600	-5. 70016200	0. 94135800
H	-0. 44683600	-6. 30275100	0. 53677400
C	1. 73486000	-5. 03382700	2. 77549600
H	2. 01237600	-5. 12470600	3. 82524300
C	1. 02741200	5. 13965200	-1. 24348700
H	0. 62999300	5. 45722000	-2. 20178600
C	1. 96954700	4. 11101400	-1. 20802500
C	2. 04358000	4. 33094400	1. 23221900
C	1. 11927200	5. 37304700	1. 13170000
H	0. 81076600	5. 90028600	2. 03063600
C	3. 58637200	-3. 36095300	2. 59148600
C	3. 09918500	-2. 42495600	3. 70364500
C	4. 67157400	-4. 31390600	3. 10776000
H	2. 65905100	-2. 99280800	4. 53332900
H	3. 93983100	-1. 84993800	4. 10651300
H	2. 35137600	-1. 72294800	3. 32333300
H	5. 52171300	-3. 74413800	3. 49745400
H	4. 29463100	-4. 94832600	3. 91753600
H	5. 03191300	-4. 96767900	2. 30742000
C	-0. 05538800	-6. 77557800	3. 19779300
C	0. 05096000	-8. 22714700	2. 71962400
C	-1. 52206200	-6. 34895800	3. 33019800
H	-0. 41126200	-8. 34897700	1. 73385300
H	1. 09608600	-8. 54029600	2. 64094500
H	-0. 46155400	-8. 90090200	3. 41435400
H	-2. 05617400	-7. 00205400	4. 02852700
H	-1. 60288400	-5. 31720100	3. 68718400
H	-2. 02923600	-6. 40762100	2. 36000400
C	0. 51790000	-4. 66845800	-1. 33460400
C	0. 72324800	-5. 95940800	-2. 13387000
C	-0. 95522900	-4. 24854400	-1. 34482100
H	0. 14895600	-6. 78795100	-1. 70267800
H	0. 39248600	-5. 82005100	-3. 16792500
H	1. 77631500	-6. 25828500	-2. 14862500
H	-1. 29915500	-4. 11643900	-2. 37488500
H	-1. 59147500	-4. 99727900	-0. 85650500
H	-1. 07028400	-3. 29047600	-0. 82520000
C	2. 55875500	3. 89495500	2. 60308100
C	1. 99103500	2. 52747900	3. 00369500
C	2. 28803800	4. 90866900	3. 71657200
H	0. 89886600	2. 56674500	3. 08331800
H	2. 22890900	1. 74922800	2. 27594700

H	2. 39349500	2. 22066000	3. 97552300
H	1. 21716800	4. 97726400	3. 94663200
H	2. 79328000	4. 58924700	4. 63294500
H	2. 64703800	5. 91003900	3. 45866900
C	-0. 43029000	6. 90388100	-0. 14717100
C	-1. 84178500	6. 32095500	-0. 29779400
C	-0. 14818400	7. 92466700	-1. 25318000
H	-1. 92977600	5. 79638400	-1. 25613400
H	-2. 06309600	5. 59706100	0. 49432900
H	-2. 59940400	7. 11189200	-0. 26924200
H	-0. 85441700	8. 75870700	-1. 18860700
H	0. 86746600	8. 32338700	-1. 17586100
H	-0. 26200100	7. 47607200	-2. 24542900
C	2. 49420200	3. 52000600	-2. 51459400
C	3. 91296100	4. 03348400	-2. 81111400
C	1. 61204000	3. 83043200	-3. 72739600
H	3. 89907400	5. 12496600	-2. 91157800
H	4. 62428400	3. 77223900	-2. 02505300
H	4. 27669500	3. 61035000	-3. 75346400
H	1. 95409300	3. 24578200	-4. 58570000
H	0. 56276000	3. 58586000	-3. 54823200
H	1. 67845700	4. 88966200	-4. 00179000
H	4. 05181500	-2. 73677700	1. 82506000
H	0. 40630400	-6. 71175300	4. 19185300
H	1. 07566200	-3. 87009100	-1. 83144400
H	2. 53182600	2. 42916900	-2. 40729000
H	3. 64606600	3. 78511300	2. 53404600
H	-0. 37945100	7. 43952900	0. 81107700
C	-4. 14481600	-1. 56659800	-3. 27216200
C	-5. 13242800	-0. 45166100	-2. 85618900
C	-4. 36795500	0. 36263600	-1. 83784800
C	-3. 12287700	-1. 65975700	-2. 12805400
H	-4. 64084700	-2. 51992300	-3. 46587800
H	-3. 61549100	-1. 27429900	-4. 18365500
H	-6. 06006500	-0. 86413700	-2. 44172600
H	-5. 43373700	0. 18377100	-3. 69417500
H	-2. 11716000	-1. 93966700	-2. 45117500
H	-3. 43571600	-2. 37901800	-1. 35482200
C	-3. 16931600	-0. 27917300	-1. 53706600
C	-4. 67248500	1. 80706100	-1. 67212000
O	-5. 76226800	2. 21826900	-2. 03574800
C	-3. 61808000	2. 73040400	-1. 11415400
H	-2. 71571100	2. 68592100	-1. 73425300
H	-4. 01751200	3. 74523200	-1. 09362500

H	-3.31187500	2.42405500	-0.11104600
C	-3.29473300	0.41672100	1.94103100
C	-3.21286200	1.82400700	2.34974500
C	-4.37852300	2.57635300	2.58019800
C	-1.96382200	2.45814400	2.40903500
C	-4.29485700	3.91249100	2.90858200
H	-5.34788800	2.09001200	2.51689500
C	-1.87479900	3.81117800	2.71727500
H	-1.06787900	1.89415000	2.15189200
C	-3.04046900	4.53713300	2.98714700
H	-5.17833600	4.50540100	3.11844000
H	-0.89992300	4.28771500	2.71427400
O	-3.06777300	5.84381500	3.32374700
C	-1.83112600	6.50587300	3.49936400
H	-2.07458400	7.52316200	3.80486300
H	-1.23088200	6.01937400	4.27799000
H	-1.26261400	6.53069700	2.56386600
C	-4.30938600	0.06135200	1.11938200
C	-5.19216100	-0.18140200	0.26416200
C	-6.48692500	-0.66805600	-0.09252000
C	-6.72053800	-2.05013300	-0.10938300
C	-7.52886500	0.21153000	-0.45029800
C	-7.96588300	-2.55994400	-0.45097500
H	-5.91277400	-2.72489400	0.15834200
C	-8.76786900	-0.29031600	-0.78915600
H	-7.34189600	1.27907800	-0.47554800
C	-8.99669800	-1.67569300	-0.79092300
H	-8.12358600	-3.63147800	-0.44777300
H	-9.58742600	0.36404200	-1.06481500
O	-10.24247200	-2.05837700	-1.13363500
C	-10.53076500	-3.44272100	-1.16611700
H	-11.57379900	-3.52355000	-1.46944000
H	-9.89644300	-3.96114700	-1.89415700
H	-10.40067000	-3.89706100	-0.17737500
C	-2.32768500	-0.56687000	2.43446700
C	-2.06712500	-1.74777600	1.72221100
C	-1.65903700	-0.33572900	3.64499900
C	-1.13820200	-2.66009500	2.19355400
H	-2.57719100	-1.92605300	0.77863500
C	-0.74027900	-1.25926800	4.12382700
H	-1.87498500	0.56105600	4.21555500
C	-0.47577700	-2.41667300	3.39937000
H	-0.91442100	-3.55914200	1.62709200
H	-0.22721600	-1.07357200	5.06226800

H	0.24737400	-3.13877000	3.76375900
P	1.09058300	-0.12812300	0.16813100
N	0.22151700	-0.84241100	-1.02821800
S	0.64074200	-0.90936200	-2.57138500
O	2.05749200	-0.75704800	-2.85315800
O	-0.09966300	-1.97804300	-3.23261200
C	-0.13810000	0.63584700	-3.24838700
F	0.48997800	1.01247100	-4.35258900
F	-0.08763100	1.62486700	-2.35743800
F	-1.42535800	0.41810800	-3.54740000
O	0.25635800	0.41375300	1.25479700
O	-2.24381100	0.23046000	-0.78367200
H	-1.38335300	-0.31574400	-0.76959500

TS1NH-S

C	7.79027700	-2.20438600	2.00845200
C	6.93857600	-3.23561000	1.54869100
C	5.76556500	-2.94148200	0.90073100
C	5.37165800	-1.59291300	0.67767400
C	6.20872800	-0.56221700	1.18246200
C	7.42614300	-0.89600300	1.83200900
C	5.80358100	0.78605300	1.04102300
C	4.59862900	1.13477200	0.48221600
C	3.76933200	0.08702400	-0.00953000
C	4.15622300	-1.23778500	-0.00298600
C	3.32768800	-2.29860300	-0.63297000
C	2.00967600	-2.45435700	-0.26801800
C	1.23095700	-3.59444100	-0.61071500
C	1.81628600	-4.51456700	-1.44769700
C	3.10545000	-4.32302600	-2.00172000
C	3.87838700	-3.20185800	-1.59798800
C	5.15542000	-3.00995700	-2.18904700
C	5.64101800	-3.90072200	-3.11222900
C	4.88427500	-5.03593800	-3.48741300
C	3.64363200	-5.23888400	-2.94341300
H	8.05657100	-0.08848500	2.19552900
H	8.71960800	-2.45292200	2.51132800
H	7.21290900	-4.27276400	1.71506000
H	5.12118500	-3.74606200	0.56563400
H	6.46831200	1.57313200	1.39183100
O	2.57439300	0.46227400	-0.59339500
H	5.73684000	-2.13519600	-1.91703700
H	6.61277700	-3.73064100	-3.56541100

H	5.28449600	-5.73531700	-4.21475100
H	3.04209500	-6.09621400	-3.23423800
O	1.42934100	-1.49860100	0.54602500
H	1.26843500	-5.41829800	-1.70035800
C	4.23702200	2.58342000	0.37508700
C	3.80897800	5.35700000	0.20640900
C	-2.61335900	-4.69724700	1.02422600
C	-0.12358700	-3.86483900	-0.03723400
C	-0.29952000	-3.97901100	1.36193300
C	-1.21006500	-4.13680700	-0.89423900
C	-2.42345300	-4.56652300	-0.34588800
H	-3.24746800	-4.78244700	-1.02037000
C	-1.54038400	-4.37600600	1.85478000
H	-1.67758600	-4.45886200	2.93247500
C	4.06352700	4.60188300	-0.93543900
H	4.10238500	5.11220800	-1.89400900
C	4.28051400	3.22268600	-0.88140300
C	3.98145800	3.32510800	1.55026000
C	3.77068800	4.70053800	1.43545100
H	3.58653000	5.28505300	2.33193000
C	0.81091500	-3.73932700	2.37747200
C	0.46648200	-2.56408100	3.30106900
C	1.09757100	-5.01012100	3.18825500
H	-0.44555600	-2.77604900	3.87337500
H	1.28162900	-2.38830000	4.01368500
H	0.30535700	-1.64861600	2.72432900
H	0.23096200	-5.30441200	3.79025000
H	1.34823300	-5.84740600	2.52985500
H	1.93842100	-4.84426300	3.87022600
C	-3.91193600	-5.19039000	1.63893500
C	-3.73504600	-6.63383500	2.13297300
C	-5.12174700	-5.09912400	0.70887100
H	-3.52563300	-7.29604100	1.28551600
H	-2.90094000	-6.71641500	2.83637600
H	-4.64405500	-6.98951000	2.62971500
H	-6.02794100	-5.39030100	1.24893400
H	-5.27610200	-4.08772400	0.31876400
H	-5.01515800	-5.78366200	-0.14029600
C	-1.16181400	-3.93992200	-2.40434000
C	-1.26281800	-5.26711200	-3.16512800
C	-2.28287800	-2.99351200	-2.84717000
H	-1.21304500	-5.08991900	-4.24442600
H	-0.45925800	-5.95947900	-2.89658900
H	-2.21435300	-5.76669300	-2.94908900

H	-2. 15557600	-2. 71894800	-3. 89829200
H	-3. 27302800	-3. 44628600	-2. 71896600
H	-2. 23633100	-2. 08157600	-2. 24956700
C	3. 93987400	2. 65722500	2. 92518800
C	2. 72291300	1. 73525900	3. 07283700
C	3. 97550600	3. 64841000	4. 09038700
H	1. 79170700	2. 28435800	2. 90058000
H	2. 73820600	0. 91048500	2. 35803800
H	2. 69809800	1. 30764300	4. 08201500
H	3. 05167500	4. 23669100	4. 14561100
H	4. 06733100	3. 10000700	5. 03267600
H	4. 81877500	4. 34238600	4. 01673200
C	3. 62761100	6. 86120100	0. 11711800
C	4. 88262100	7. 58090500	0. 62652400
C	2. 38530400	7. 35310800	0. 86654100
H	5. 05127400	7. 35037200	1. 68459000
H	5. 76948000	7. 26580600	0. 06893800
H	4. 77720200	8. 66665500	0. 52812400
H	2. 24719700	8. 42812300	0. 71170700
H	1. 47979800	6. 83892200	0. 52921500
H	2. 48427300	7. 18809400	1. 94536000
C	4. 64376400	2. 46093800	-2. 15326500
C	6. 15432700	2. 17793600	-2. 20209000
C	4. 24765300	3. 18845600	-3. 44239900
H	6. 71056500	3. 12236400	-2. 19380800
H	6. 49137900	1. 57579900	-1. 35555300
H	6. 40689000	1. 64259400	-3. 12347600
H	4. 35213800	2. 50641800	-4. 29119600
H	3. 21408500	3. 53974200	-3. 41830500
H	4. 90102600	4. 04867100	-3. 62840500
H	1. 73379500	-3. 48642400	1. 85125700
H	-4. 11078000	-4. 55827700	2. 51637600
H	-0. 21674400	-3. 45647700	-2. 67104700
H	4. 11006200	1. 50335500	-2. 14171700
H	4. 83418800	2. 03040400	3. 01567800
H	3. 50230600	7. 11100100	-0. 94466700
P	1. 12183200	-0. 01769300	-0. 05263200
N	0. 18596600	-0. 12301200	-1. 39249800
S	0. 69572000	-0. 31177800	-2. 89432100
O	2. 00836700	-0. 91669000	-3. 03496800
O	-0. 40477700	-0. 78508800	-3. 72314600
C	0. 93717800	1. 43593100	-3. 44032800
F	1. 64507300	1. 47252100	-4. 56128900
F	1. 57260600	2. 14088300	-2. 50560900

F	-0.24465600	2.02256500	-3.66683300
O	0.51841000	0.78477700	1.02492100
C	-4.52902400	0.89033000	-3.20992700
C	-5.41581300	-0.04819600	-2.37087900
C	-4.61155200	-0.25802300	-1.11128500
C	-3.09248700	0.55630600	-2.77871800
H	-4.75608000	1.93047300	-2.95095700
H	-4.68188900	0.77420300	-4.28469000
H	-6.41401700	0.35678500	-2.17756300
H	-5.56354100	-1.01695200	-2.86769800
H	-2.64596400	-0.24183700	-3.38615700
H	-2.38551900	1.38992100	-2.82373800
C	-3.27772800	0.03068900	-1.38072000
C	-5.10698700	-1.14375100	-0.03806000
O	-6.26356700	-1.54052600	-0.09346700
C	-4.18123900	-1.56165800	1.07653200
H	-3.38422800	-2.19881600	0.67549100
H	-4.75759200	-2.11448500	1.82135900
H	-3.68638500	-0.70322300	1.53611600
C	-2.80845800	2.01481800	1.61010600
C	-2.71902100	1.34851200	2.90822900
C	-3.88005000	1.12735400	3.67815300
C	-1.49359700	0.84310400	3.37217300
C	-3.81312500	0.45491000	4.87796900
H	-4.83316400	1.50842400	3.32235300
C	-1.42276000	0.15226700	4.57538700
H	-0.60560200	0.93362800	2.75108400
C	-2.57949200	-0.04021000	5.33625500
H	-4.69334300	0.28991400	5.48979400
H	-0.46735300	-0.24937300	4.89223300
O	-2.61531600	-0.69187300	6.51509200
C	-1.40491200	-1.23762000	7.00603500
H	-1.65765300	-1.72946100	7.94465800
H	-0.66421600	-0.45151300	7.19075500
H	-0.99006700	-1.97096900	6.30538800
C	-3.96065800	1.90000800	0.89588200
C	-4.98029600	1.71859700	0.19952800
C	-6.29169800	2.03223900	-0.26929500
C	-6.47523700	3.09034500	-1.17046200
C	-7.41473000	1.29746800	0.16445900
C	-7.74010100	3.42412200	-1.63304700
H	-5.61133300	3.66112000	-1.49757400
C	-8.67405800	1.62461000	-0.29296400
H	-7.28079600	0.46383200	0.84399600

C	-8.84702800	2.68626900	-1.19437100
H	-7.85465600	4.24975200	-2.32461300
H	-9.55144300	1.07184600	0.02381500
O	-10.11626500	2.92269300	-1.57938700
C	-10.35083100	3.97514900	-2.49500700
H	-11.42571400	3.98484500	-2.67053100
H	-9.82651300	3.79921600	-3.44113700
H	-10.03905500	4.93906400	-2.07681700
C	-1.70327000	2.81148900	1.06963600
C	-0.75935100	3.41237800	1.91414700
C	-1.56965000	2.95974600	-0.31937400
C	0.33309100	4.07803000	1.37391400
H	-0.88412900	3.35266400	2.99067700
C	-0.47193400	3.60899800	-0.85393700
H	-2.32413300	2.52956600	-0.97037800
C	0.50094000	4.14178300	-0.00649300
H	1.07436400	4.52927400	2.02728100
H	-0.35597700	3.68214600	-1.92894800
H	1.38994800	4.60642800	-0.42262900
O	-2.31103200	-0.14792400	-0.53524600
H	-1.37346300	-0.03773100	-0.94621600

TS2OH-R

S	3.63152400	1.20920100	2.06107800
S	-1.79920100	0.71468300	-2.70348000
O	1.45324700	1.97593500	-4.56024300
C	2.10246200	0.84748000	-2.54012700
C	3.13729700	0.45845100	-1.72299100
C	4.48764400	0.75054800	-2.04236900
C	4.75593200	1.37761100	-3.28642600
C	3.73177900	1.75805200	-4.11765900
C	2.38857900	1.53520800	-3.73990400
H	1.07295400	0.64007600	-2.26168900
H	2.92050300	-0.08176100	-0.80752900
H	5.78268400	1.54521500	-3.59395000
H	3.91921700	2.23915900	-5.07108400
C	5.52439100	0.44157000	-1.10328000
C	6.89528600	0.98651100	-1.22386000
C	7.10188800	2.33559900	-1.54482400
C	8.00019300	0.17175300	-0.94415700
C	8.39154300	2.85083600	-1.59827900

H	6.24710500	2.98252900	-1.71625400
C	9.28792100	0.68702300	-1.01639200
H	7.83530500	-0.87164100	-0.69201100
C	9.48560000	2.02727300	-1.34342000
H	8.54184200	3.89988500	-1.83200100
H	10.13833800	0.04394400	-0.81376200
H	10.49186400	2.43137600	-1.39274200
C	5.27155800	-0.32809700	0.00050900
C	4.90505000	-0.80104200	1.09371800
C	4.91038200	-1.83458800	2.09917400
C	6.03148600	-2.68074600	2.10939000
C	3.86856900	-2.05316500	3.00927200
C	6.10367200	-3.73475400	3.01065200
H	6.83506400	-2.50084900	1.40240800
C	3.95959500	-3.10073500	3.91831100
H	3.00190300	-1.40182200	2.99822700
C	5.07100500	-3.94306400	3.92155300
H	6.97187100	-4.38583300	3.00771000
H	3.15794600	-3.25844000	4.63307300
H	5.13262300	-4.75811100	4.63577500
C	2.11408700	0.82751200	1.47332700
C	1.06898600	1.87735900	1.24400400
H	0.64180400	1.75805700	0.24001400
H	0.24473900	1.74927800	1.95830000
H	1.48369300	2.87718400	1.34943100
O	1.81424500	-0.40164500	1.18845300
N	-1.16321100	0.72731500	-1.25586200
O	-1.01341800	1.60838400	-3.56436600
O	-3.24461700	0.82203300	-2.79736700
C	-1.40760700	-0.98394100	-3.38343100
O	-0.63596300	-0.63797000	0.92997900
F	-0.90326500	-0.86471700	-4.60711200
F	-0.50814500	-1.60257200	-2.61840700
F	-2.50994000	-1.71669900	-3.44456400
H	0.54547900	1.83902700	-4.19214200
H	0.80144800	-0.51938900	0.95252400
C	-6.82911900	-1.81296700	1.45332300
C	-6.51316500	-0.35778400	1.07747600
C	-5.43892400	-0.45795700	-0.04856300
C	-4.68135900	-1.69024400	0.41449900
C	-5.50107800	-2.49126700	1.21729100
C	-6.12718400	-0.64409600	-1.42681500
C	-6.62515500	0.77047400	-1.79090700
C	-5.60296800	1.65989000	-1.11863000

C	-4.80331900	0.90529900	-0.25510700
C	-3.39082200	-2.11827100	0.13968500
C	-2.89231200	-3.33485000	0.62732000
C	-3.76197600	-4.13032100	1.38091800
C	-5.05560500	-3.71764900	1.68859600
C	-5.35044700	3.00858200	-1.31129700
C	-4.27839500	3.59973900	-0.64405100
C	-3.38962500	2.84934600	0.13166100
C	-3.66235300	1.48170800	0.27217800
O	-2.58169900	-1.31632900	-0.66204700
O	-2.72600700	0.68289600	0.92836700
P	-1.69153800	-0.13951100	-0.00507400
H	-7.18327000	-1.92299200	2.48255800
H	-7.60138500	-2.23423900	0.79670500
H	-7.38908500	0.21662300	0.76263100
H	-6.06448700	0.15352800	1.93714400
H	-5.36724500	-0.96207800	-2.14927500
H	-6.92272400	-1.39582700	-1.39687100
H	-7.63774600	0.95326000	-1.40931500
H	-6.64857200	0.93717300	-2.87170600
H	-3.40083600	-5.09012200	1.73730700
H	-5.69954100	-4.34307400	2.30045600
H	-5.97245200	3.60142300	-1.97576900
H	-4.09773400	4.66539900	-0.74753600
C	-2.24024800	3.50724000	0.82841000
C	-2.16032100	3.47050800	2.24198400
C	-1.15614600	4.19276000	2.88606300
C	-0.22986000	4.96506800	2.18867600
H	-1.11010500	4.16489000	3.97344700
C	-1.47128600	-3.74058300	0.38416800
C	-0.52088800	-3.60881000	1.41654800
C	0.81671800	-3.90018200	1.13950300
C	1.22801700	-4.32322300	-0.12206700
H	1.55994100	-3.76755000	1.92250000
C	-1.28425200	4.24916500	0.10110400
C	-0.31412000	4.97380900	0.80152800
H	0.41023700	5.56272000	0.24199100
C	-1.08334300	-4.21038700	-0.88692800
C	0.26202100	-4.49431100	-1.11142000
H	0.58257200	-4.83704700	-2.09179100
C	-3.13719800	2.70675600	3.12715500
C	-2.41994700	1.59960400	3.91109400
C	-3.88039000	3.65396800	4.07817300
H	-1.68855800	2.02477000	4.60833000

H	-3.14110500	1.02063700	4.49841800
H	-1.90121900	0.91353200	3.23483500
H	-4.63644600	3.10263800	4.64736000
H	-3.19549300	4.11667900	4.79712300
H	-4.38105600	4.45485800	3.52585400
C	-1.24262700	4.30688200	-1.42117500
C	0.13929900	3.91690800	-1.95968000
C	-1.61813200	5.70339700	-1.93517000
H	0.91608300	4.60769200	-1.61347300
H	0.40636400	2.90419200	-1.64444900
H	0.13294600	3.93901100	-3.05350200
H	-1.61345400	5.71821300	-3.02978900
H	-2.60906600	6.01601700	-1.59297600
H	-0.89761500	6.45139800	-1.58436800
C	0.82214800	5.77846100	2.91775400
C	1.67126800	4.91539200	3.85709400
C	0.17321200	6.93599200	3.68641700
H	1.05387000	4.47024100	4.64491000
H	2.16890700	4.10131000	3.32026100
H	2.44158900	5.52291600	4.34348100
H	0.93359500	7.55007900	4.18046700
H	-0.40895400	7.57546400	3.01643800
H	-0.50511600	6.55263100	4.45702400
C	-0.92045800	-3.19415700	2.82741300
C	0.09751000	-2.29164100	3.53138800
C	-1.14848500	-4.44129100	3.69526400
H	1.01797900	-2.83827100	3.76732600
H	0.35191900	-1.42212700	2.92433800
H	-0.32146300	-1.93861300	4.47977400
H	-1.45352300	-4.15634800	4.70817100
H	-1.91402400	-5.10089600	3.28062600
H	-0.21924200	-5.01869000	3.76875500
C	-2.11846100	-4.46029600	-1.97545500
C	-1.53052600	-4.56081200	-3.38507400
C	-2.90292200	-5.74676400	-1.67385600
H	-0.96879500	-5.49337600	-3.51126100
H	-2.33971900	-4.56271200	-4.12173600
H	-0.86205400	-3.72824900	-3.61437800
H	-3.65691400	-5.92535100	-2.44813700
H	-2.22066000	-6.60416200	-1.65698700
H	-3.41209700	-5.69673900	-0.70847800
C	2.69398900	-4.49194200	-0.47059000
C	3.25576600	-3.11707100	-0.85811700
C	3.52759100	-5.11771500	0.64809600

H	3.10714700	-2.41842300	-0.02698300
H	4.32919500	-3.16767100	-1.07908300
H	2.73440900	-2.71154500	-1.73216900
H	4.54822200	-5.30800700	0.29894200
H	3.60107900	-4.44676800	1.51036900
H	3.09593000	-6.06448300	0.98770600
H	-3.89407200	2.23305400	2.49860900
H	1.48843200	6.20781800	2.15797400
H	-1.96399700	3.58744300	-1.82016500
H	-2.82169600	-3.61995800	-1.96671200
H	-1.85984400	-2.63467400	2.76166700
H	2.75026700	-5.14880900	-1.34878100

TS2OH-S

S	-3.62898400	2.12756500	-0.81841400
O	-1.26086400	-3.63734300	-3.48158600
C	-1.90889400	-2.27026000	-1.61387200
C	-2.94539200	-1.68460400	-0.92364800
C	-4.29805700	-1.89046400	-1.29913000
C	-4.56462200	-2.79936800	-2.35565800
C	-3.54032400	-3.37663200	-3.06217500
C	-2.19762100	-3.08932300	-2.72851100
H	-0.87885500	-2.10369100	-1.30163300
H	-2.72431000	-1.04158400	-0.07630900
H	-5.59104200	-3.04499900	-2.60724900
H	-3.72466100	-4.06402500	-3.88075300
C	-5.33398200	-1.13665900	-0.66332900
C	-6.74195400	-1.14337000	-1.12536600
C	-7.06348500	-0.98562200	-2.48105800
C	-7.77446400	-1.23530100	-0.18144700
C	-8.39525000	-0.94053400	-2.87966000
H	-6.26903100	-0.86069900	-3.21016300
C	-9.10147100	-1.20900800	-0.58888500
H	-7.52019400	-1.35005100	0.86790100
C	-9.41446400	-1.06232900	-1.93928600
H	-8.63583300	-0.80146000	-3.92838300
H	-9.89283400	-1.30182300	0.14807100
H	-10.45124200	-1.03392700	-2.25608900
C	-5.06423700	-0.28143600	0.37418300
C	-4.73656900	0.71855000	1.03938300
C	-4.74039600	1.55234500	2.20972100
C	-3.59303800	2.18861000	2.70459300
C	-5.96380300	1.68914900	2.88818200

C	-3.67182700	2.93500600	3.86864200
H	-2.65599500	2.09045900	2.16352500
C	-6.02916500	2.43533300	4.05686600
H	-6.84631200	1.20196400	2.48599000
C	-4.88502400	3.06010800	4.54695100
H	-2.78219800	3.42126200	4.25312000
H	-6.97512600	2.53328900	4.58099400
H	-4.93878800	3.64908100	5.45855800
C	-2.07500300	1.54163200	-0.63418400
C	-1.08282400	1.52337900	-1.75546400
H	-1.41803200	2.12027800	-2.60139300
H	-0.95846200	0.47854400	-2.07071200
H	-0.11189400	1.88641900	-1.39956200
O	-1.69811100	1.02358300	0.48906100
H	-0.35310100	-3.42326100	-3.15311600
H	-0.66779500	0.80602200	0.52967100
S	1.90919000	-1.83439300	-2.22989000
O	1.26407500	-3.11160600	-2.57398100
O	3.35965200	-1.77270600	-2.29863200
C	1.32133600	-0.73012200	-3.58552100
O	0.71753700	0.71001600	0.73046800
F	1.98421700	-0.98399000	-4.70341500
F	0.01820300	-0.94369400	-3.80135400
F	1.48882200	0.54947400	-3.25811400
N	1.21152000	-1.22768200	-0.95690800
C	7.02895800	1.37056800	1.34960700
C	6.54535600	-0.08407900	1.38820700
C	5.53175400	-0.20002100	0.20836900
C	4.90916100	1.19190500	0.25427000
C	5.79282600	2.08847700	0.86547300
C	6.29946500	-0.52133300	-1.10124500
C	6.63640200	-2.02554500	-0.97971900
C	5.49936300	-2.55303200	-0.13357700
C	4.75002300	-1.49094500	0.37372600
C	3.67058700	1.66691200	-0.17143700
C	3.28755000	2.99980900	0.01533600
C	4.22758700	3.87296300	0.57442800
C	5.47637700	3.43260100	1.00306000
C	5.11159000	-3.85672400	0.12569200
C	3.93271700	-4.09728700	0.83783000
C	3.06984800	-3.06232500	1.21977900
C	3.52462500	-1.75589800	0.95541700
O	2.79412500	0.80312400	-0.81665700
O	2.68454300	-0.68385800	1.23249900

P	1. 77234400	-0. 10227100	0. 04248400
H	7. 37436200	1. 73504500	2. 32010400
H	7. 85679600	1. 49599700	0. 63871700
H	7. 35039200	-0. 82004700	1. 30821300
H	6. 01072900	-0. 26982100	2. 32672200
H	5. 62707700	-0. 36504300	-1. 94932100
H	7. 18212800	0. 11396000	-1. 22957900
H	7. 61270500	-2. 19070800	-0. 50883200
H	6. 66249100	-2. 51762500	-1. 95646600
H	3. 95637300	4. 91967300	0. 68102600
H	6. 17781500	4. 12197100	1. 46228800
H	5. 69720900	-4. 69490000	-0. 23811900
H	3. 65997700	-5. 12267700	1. 05266200
C	1. 68735000	-3. 23334200	1. 77917500
C	1. 27284000	-2. 44747900	2. 87947300
C	-0. 08388600	-2. 35616200	3. 18605600
C	-1. 05613000	-3. 01978300	2. 44423300
H	-0. 38806900	-1. 72641200	4. 02091800
C	1. 92085900	3. 52712800	-0. 30665300
C	1. 00267900	3. 75104500	0. 73826500
C	-0. 22985700	4. 34216200	0. 43838200
C	-0. 57002800	4. 74047500	-0. 84964500
H	-0. 93492700	4. 51093400	1. 24734700
C	0. 72284100	-4. 03428900	1. 11444200
C	-0. 62346700	-3. 89119400	1. 44844600
H	-1. 36938200	-4. 46040800	0. 89987300
C	1. 58072200	3. 87522500	-1. 63195000
C	0. 35232800	4. 48926400	-1. 87194300
H	0. 08357900	4. 75825200	-2. 89121400
C	2. 24899100	-1. 74937800	3. 81763300
C	1. 86730100	-0. 28929500	4. 10735300
C	2. 35132500	-2. 54754500	5. 12611200
H	1. 02114200	-0. 23076200	4. 80263800
H	2. 70898200	0. 23035700	4. 57783900
H	1. 59722600	0. 23972800	3. 18992200
H	3. 05104800	-2. 06501700	5. 81663500
H	1. 37453200	-2. 60615200	5. 61912700
H	2. 69542300	-3. 56893300	4. 93857100
C	1. 10661600	-5. 10353700	0. 10434700
C	0. 03185100	-5. 38560100	-0. 94649400
C	1. 40593800	-6. 41045900	0. 86223000
H	-0. 79255500	-5. 98214400	-0. 53921000
H	-0. 37929400	-4. 45182700	-1. 32540600
H	0. 46176900	-5. 93590900	-1. 78716300

H	1. 75111300	-7. 19123300	0. 17393200
H	2. 14874800	-6. 28094600	1. 65375400
H	0. 48696900	-6. 76486000	1. 34594000
C	-2. 53565400	-2. 85193700	2. 73501600
C	-2. 91720400	-1. 40118200	3. 05012700
C	-2. 97125500	-3. 78637600	3. 87189800
H	-2. 51791600	-1. 08595700	4. 02267900
H	-2. 53176100	-0. 70994900	2. 29284300
H	-4. 00672500	-1. 29356600	3. 09495200
H	-4. 05158500	-3. 71663500	4. 04465500
H	-2. 72263600	-4. 82697100	3. 64576300
H	-2. 45913700	-3. 51229600	4. 80191700
C	1. 32026500	3. 41551400	2. 19103500
C	0. 13308200	2. 82048400	2. 95718600
C	1. 80805500	4. 66696600	2. 93618000
H	-0. 66542800	3. 56176400	3. 09300300
H	-0. 27664600	1. 94739800	2. 44728100
H	0. 46018100	2. 51111800	3. 95466500
H	2. 07182100	4. 41720100	3. 97099800
H	2. 68501900	5. 11305300	2. 46228100
H	1. 01563800	5. 42451400	2. 96076800
C	2. 54965200	3. 61687800	-2. 77799200
C	1. 86425700	3. 49691100	-4. 14080200
C	3. 62166000	4. 71461400	-2. 84518800
H	1. 49234500	4. 46595700	-4. 48849100
H	2. 58242600	3. 13815400	-4. 88447900
H	1. 02382800	2. 79647900	-4. 11576800
H	4. 33387400	4. 50518800	-3. 65042200
H	3. 15255200	5. 68275800	-3. 04595200
H	4. 18150900	4. 79277100	-1. 90906000
C	-1. 88520900	5. 42749200	-1. 18188700
C	-2. 82611200	5. 57090600	0. 01571100
C	-1. 62813900	6. 80637000	-1. 80448000
H	-2. 38828900	6. 23010900	0. 77696500
H	-3. 77138500	6. 01596600	-0. 30645600
H	-3. 05015200	4. 60691500	0. 48249500
H	-2. 57446700	7. 30252500	-2. 04519200
H	-1. 08111200	7. 43982700	-1. 09700700
H	-1. 03584100	6. 73894400	-2. 72079800
H	3. 24323600	-1. 75544900	3. 36579300
H	-3. 07765900	-3. 14976400	1. 82507900
H	2. 00125300	-4. 77404900	-0. 43199000
H	3. 04585600	2. 65933400	-2. 57516800
H	2. 12230000	2. 66892700	2. 20010400

H	-2.39645400	4.80554800	-1.93194600
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TS2NH-R

S	3.03871600	3.01872700	1.46073500
S	-1.18081500	-0.52769300	2.61880900
O	9.96032800	2.19676400	-2.70852300
C	8.27341900	2.40387900	-0.99553000
C	7.06072100	1.97208100	-0.48752000
C	6.32059600	0.97277100	-1.13735300
C	6.84963600	0.39716500	-2.30659300
C	8.06866000	0.81095400	-2.81228800
C	8.78172800	1.82373700	-2.16240000
H	8.82779000	3.19329100	-0.49409200
H	6.65954600	2.42252600	0.41596700
H	6.30523100	-0.40078800	-2.80288900
H	8.49375300	0.36537200	-3.70476200
C	5.04257200	0.52756000	-0.57697900
C	3.93485600	0.05475100	-1.41235500
C	3.76828500	0.54355600	-2.72091000
C	2.93701500	-0.76423700	-0.85576800
C	2.61307100	0.24308000	-3.43198700
H	4.51066400	1.20945700	-3.14870100
C	1.78726100	-1.05727200	-1.56928300
H	3.06891300	-1.15802600	0.14764800
C	1.61719900	-0.54366300	-2.85506500
H	2.47386700	0.65428700	-4.42698600
H	1.01999100	-1.68281300	-1.12198100
H	0.69509000	-0.74248700	-3.39187300
C	4.81787600	0.62935300	0.75505300
C	4.40309000	0.88853100	1.90736800
C	4.29890400	0.68602000	3.32377800
C	5.47387900	0.69090100	4.09274800
C	3.05765000	0.44476900	3.93187500
C	5.40457800	0.44033200	5.45671400
H	6.42607800	0.88228100	3.60790500
C	3.00159100	0.19414800	5.29506400
H	2.14936500	0.44485900	3.33915800
C	4.17041900	0.19278000	6.05726200
H	6.31169200	0.43890800	6.05237800
H	2.03720800	0.00003900	5.75381500
H	4.12053600	-0.00020000	7.12469100
C	1.64630400	2.17179000	1.04983400
C	0.43125400	2.87186000	0.52532700

H	0.25017100	2.54777700	-0.50817900
H	-0.43902100	2.54621700	1.10195200
H	0.53376200	3.95419200	0.57299200
O	1.59663300	0.89398700	1.18427100
N	-0.68623000	-0.29344400	1.11166600
O	-0.04922100	-0.21232000	3.48410800
O	-1.94575700	-1.74260000	2.84136400
C	-2.39547800	0.83381900	3.00801900
O	-0.87834000	0.53304900	-1.35313400
F	-2.25231600	1.17257200	4.28332600
F	-2.15109300	1.90920500	2.25630500
F	-3.64850400	0.44682000	2.81497100
H	10.36157200	2.89818400	-2.17546400
H	0.64456400	0.45137000	1.05466700
C	-6.46334500	-1.93632700	-2.13078900
C	-5.51566000	-2.88559300	-1.37740800
C	-4.87428900	-2.00735900	-0.26028400
C	-4.79496000	-0.67842000	-0.98214700
C	-5.75213000	-0.61010400	-1.99731800
C	-5.80546300	-1.96641300	0.98120700
C	-5.53577300	-3.30369800	1.70160100
C	-4.09648200	-3.59193100	1.33542300
C	-3.67133200	-2.72099100	0.32900300
C	-3.97511200	0.41356600	-0.74888600
C	-4.12480200	1.61480600	-1.45210000
C	-5.12254500	1.66049100	-2.43335300
C	-5.92316100	0.55854200	-2.72598200
C	-3.23350700	-4.54742600	1.85129600
C	-1.94451600	-4.64380900	1.33166900
C	-1.46218700	-3.73188600	0.38866200
C	-2.33596100	-2.72459700	-0.04192600
O	-2.97835500	0.28981700	0.21291600
O	-1.84626600	-1.72988700	-0.88214100
P	-1.53309200	-0.24901200	-0.28855100
H	-6.62035800	-2.22856400	-3.17335200
H	-7.45059600	-1.89748400	-1.65249700
H	-6.01032200	-3.77334100	-0.97208500
H	-4.71927500	-3.21939100	-2.05335200
H	-5.49247300	-1.13335900	1.61981900
H	-6.85570300	-1.81836600	0.70976300
H	-6.20473900	-4.09586200	1.34181300
H	-5.67540800	-3.23080200	2.78423800
H	-5.27143500	2.59388900	-2.96804700
H	-6.66924500	0.61894300	-3.51338100

H	-3.56147000	-5.22844100	2.63145600
H	-1.28029200	-5.43288700	1.67222900
C	-0.10177200	-3.88481300	-0.21299500
C	0.01490600	-4.16448300	-1.59627800
C	1.28108900	-4.35536900	-2.14215300
C	2.44811400	-4.28633700	-1.38053900
H	1.36439400	-4.57670600	-3.20547700
C	-3.29641400	2.82626100	-1.15104100
C	-2.32545400	3.27220400	-2.06529900
C	-1.61176100	4.44157700	-1.77557200
C	-1.81615500	5.15813700	-0.60351100
H	-0.86579000	4.78408000	-2.48695500
C	1.06095500	-3.82315800	0.57888900
C	2.30965300	-4.03075400	-0.02124000
H	3.19444300	-3.98599400	0.60732000
C	-3.53688400	3.54883200	0.04256900
C	-2.78167800	4.69104700	0.29244700
H	-2.94375800	5.24843500	1.21198400
C	-1.18064700	-4.30642700	-2.52936400
C	-1.16386200	-3.23341300	-3.62482100
C	-1.23564200	-5.71297100	-3.13929500
H	-0.26140000	-3.31699600	-4.24228000
H	-2.03112400	-3.34720700	-4.28500800
H	-1.19544600	-2.23241500	-3.18475800
H	-2.13741200	-5.82703000	-3.75035400
H	-0.37000700	-5.90333500	-3.78296400
H	-1.24931100	-6.47918100	-2.35805200
C	1.02431500	-3.54960100	2.07492200
C	1.95838900	-2.40135500	2.47236800
C	1.38943500	-4.81249000	2.86708700
H	3.01290600	-2.66214200	2.31595600
H	1.73622400	-1.49609900	1.89924100
H	1.82586200	-2.15665200	3.53049400
H	1.32176100	-4.62083600	3.94294500
H	0.72965600	-5.65137400	2.62525200
H	2.41621100	-5.12440700	2.64195800
C	3.79202700	-4.48276500	-2.06686500
C	4.97319900	-4.53482400	-1.09998600
C	4.03574500	-3.39564900	-3.12497800
H	5.09544400	-3.57264200	-0.58750500
H	4.84665000	-5.31270600	-0.34086900
H	5.89898500	-4.73975800	-1.64625400
H	4.94657400	-3.61573500	-3.69291400
H	3.20296000	-3.31804800	-3.83005800

H	4.15414100	-2.41747200	-2.64612700
C	-2.05088800	2.55948500	-3.38359500
C	-0.55632800	2.43211600	-3.70379800
C	-2.75249400	3.28812400	-4.53955600
H	-0.10411000	3.40511100	-3.92726000
H	-0.01773800	1.96031600	-2.88030500
H	-0.43025600	1.80758200	-4.59631800
H	-2.56481400	2.77359500	-5.48834300
H	-3.83411100	3.35021500	-4.39433100
H	-2.36987200	4.31164200	-4.62870800
C	-4.65017600	3.14341000	1.00379700
C	-4.53822300	3.76600300	2.39882700
C	-6.02192100	3.51581800	0.41820200
H	-4.76063200	4.83874000	2.37204300
H	-5.27234100	3.29951900	3.06335100
H	-3.54782500	3.63371200	2.83914800
H	-6.82159100	3.21851200	1.10530700
H	-6.08202300	4.60080000	0.27534000
H	-6.20481200	3.03416900	-0.54450900
C	-1.06310900	6.43653700	-0.27512800
C	0.22845200	6.62153600	-1.07171600
C	-1.98017900	7.65191100	-0.47246200
H	0.01407300	6.79626300	-2.13194600
H	0.77704100	7.49278000	-0.70109000
H	0.88559200	5.74846400	-0.99971500
H	-1.46870100	8.57731500	-0.18674200
H	-2.27365600	7.73204300	-1.52510900
H	-2.89305100	7.56343500	0.12389600
H	-2.09887900	-4.17525300	-1.95124500
H	3.74181900	-5.44789600	-2.59132100
H	0.00628200	-3.25565000	2.34889100
H	-4.61176200	2.05529900	1.12748800
H	-2.45223300	1.54458400	-3.30589000
H	-0.79852400	6.38842300	0.79097300

TS2NH-S

S	-3.33375300	3.02283000	0.58789300
O	-10.93483200	1.64760100	-1.29179800
C	-9.24108800	0.94561600	0.27740400
C	-7.93328300	0.54281300	0.48808700
C	-7.03539300	0.40936700	-0.58199900
C	-7.48835800	0.72151600	-1.87712300
C	-8.78835800	1.14007500	-2.09466000

C	-9.67381000	1.24634900	-1.01770800
H	-9.93160000	1.02426200	1.11347500
H	-7.59674900	0.30310600	1.49246200
H	-6.79739800	0.67139600	-2.71219200
H	-9.13990300	1.40301800	-3.08617200
C	-5.63939600	0.03198800	-0.32788500
C	-4.83707500	-0.72485700	-1.29266800
C	-5.43369800	-1.52867600	-2.27935500
C	-3.43424000	-0.64129200	-1.22948000
C	-4.63959100	-2.18068400	-3.21240800
H	-6.51153500	-1.65388200	-2.29963800
C	-2.64198400	-1.30519100	-2.15486800
H	-2.96721500	-0.04999900	-0.44899500
C	-3.25071700	-2.05420400	-3.16260100
H	-5.10263300	-2.79761000	-3.97639600
H	-1.55902600	-1.23963700	-2.07581100
H	-2.63802300	-2.55521900	-3.90568900
C	-5.06889600	0.46016800	0.82258000
C	-4.44825200	1.01024600	1.75873700
C	-4.04577700	1.24494700	3.11259900
C	-2.78774300	0.83026100	3.57281400
C	-4.93020500	1.91631600	3.97371800
C	-2.41605100	1.09763500	4.88336600
H	-2.10852300	0.32606000	2.89697100
C	-4.55616500	2.16157400	5.28570000
H	-5.89392000	2.24338800	3.59577600
C	-3.29756100	1.75879500	5.73659600
H	-1.42890500	0.80334600	5.22090000
H	-5.23652500	2.67748000	5.95566000
H	-3.00141400	1.96961700	6.75980300
C	-1.78855100	2.38806400	0.45178200
C	-0.63640900	3.23117200	-0.00255000
H	-0.94149100	4.25179500	-0.22909300
H	-0.16921200	2.77652200	-0.88501800
H	0.11397800	3.22608800	0.79630500
O	-1.54269200	1.15836700	0.73592800
H	-11.44513500	1.71155800	-0.47159300
H	-0.49270200	0.93444500	0.73755100
S	1.19823000	0.54330300	2.54666300
O	0.24949300	1.45497000	3.17683700
O	2.59068300	0.53622400	2.95645000
C	0.55190000	-1.14367400	3.01783600
O	0.74138900	-0.56107700	-1.34687000
F	1.54294900	-1.98807900	3.25510900

F	-0.18260800	-1.03843000	4.12593300
F	-0.22869900	-1.62018300	2.04861100
N	0.94769800	0.64023200	0.96535600
C	6.74401600	-2.62612800	-0.38526800
C	6.53172900	-1.13229900	-0.11234300
C	5.22037400	-1.06257000	0.73451400
C	4.44156600	-2.20101700	0.10181400
C	5.32279600	-3.12259200	-0.47621100
C	5.55960100	-1.28325900	2.23050800
C	6.20298900	0.05336300	2.66135100
C	5.55281100	1.05305500	1.72921200
C	4.77257300	0.38866700	0.77600400
C	3.07579400	-2.44354400	0.03764500
C	2.56696000	-3.59778300	-0.57143900
C	3.48502800	-4.52049700	-1.08750300
C	4.85609000	-4.29240700	-1.05477900
C	5.64895300	2.43427000	1.71114300
C	4.90210000	3.14560300	0.77356100
C	3.95767000	2.52557900	-0.04780300
C	3.89221100	1.11918100	-0.00472100
O	2.21005000	-1.52674800	0.62200300
O	2.96895600	0.45866800	-0.80596500
P	1.64285300	-0.26161000	-0.21868700
H	7.31597300	-2.81973900	-1.29764000
H	7.27672000	-3.11191900	0.44237000
H	7.37345000	-0.64810900	0.38976800
H	6.35678200	-0.60860000	-1.05934700
H	4.62393300	-1.44218100	2.77734800
H	6.21016100	-2.14957300	2.38772300
H	7.29392200	0.03635600	2.54843000
H	5.98953600	0.29510300	3.70688000
H	3.09359300	-5.43025200	-1.53347200
H	5.54610400	-5.01018500	-1.48926500
H	6.29704700	2.95891800	2.40796300
H	5.00585000	4.22322900	0.70510600
C	3.09797600	3.35236900	-0.95050100
C	3.08683800	3.08482300	-2.34202900
C	2.30563100	3.87298700	-3.18803900
C	1.55775400	4.94729000	-2.72303200
H	2.29522400	3.65041400	-4.25333900
C	1.10715000	-3.88408700	-0.73615500
C	0.52853800	-3.75947700	-2.01269600
C	-0.79288500	-4.17596300	-2.18632000
C	-1.56318800	-4.66485800	-1.13697300

H	-1.23625400	-4.12451600	-3.17832100
C	2.34999000	4.45046900	-0.45454400
C	1.61331200	5.21999000	-1.36132100
H	1.03448700	6.05540900	-0.96608100
C	0.35373200	-4.39110800	0.34242500
C	-0.97271200	-4.75661400	0.12422600
H	-1.55761600	-5.14539800	0.95413900
C	3.96005600	2.03065000	-3.01358600
C	3.13095100	1.02154500	-3.81739700
C	5.01052000	2.70918300	-3.90461200
H	2.64785200	1.50255600	-4.67576000
H	3.78099500	0.23054400	-4.20802200
H	2.35678900	0.56021700	-3.19817200
H	5.67953100	1.95987700	-4.34152300
H	4.53950000	3.25874200	-4.72706300
H	5.61518900	3.41727200	-3.32911900
C	2.19177500	4.92302000	1.00110800
C	3.04507800	6.16569900	1.29818300
C	2.30770200	3.88071300	2.12190800
H	4.11298900	5.93026000	1.31748300
H	2.88617300	6.94554300	0.54696000
H	2.77853900	6.57209100	2.27986800
H	1.58825000	4.10310800	2.91599300
H	2.10017100	2.87803300	1.74903100
H	3.30232800	3.84848900	2.57087700
C	0.70790600	5.78241000	-3.66022100
C	1.18775800	7.23706900	-3.70499400
C	-0.77528800	5.70995400	-3.28019500
H	1.08503700	7.71000000	-2.72183800
H	2.24017500	7.29567500	-3.99750000
H	0.59559900	7.81859000	-4.41954300
H	-1.38858100	6.25663600	-4.00425900
H	-1.12351200	4.67306100	-3.24419000
H	-0.94685900	6.15825700	-2.29469000
C	1.30530500	-3.24222300	-3.21781100
C	0.52099800	-2.21828900	-4.04492900
C	1.73539300	-4.40580800	-4.12228800
H	-0.34705300	-2.67585700	-4.53519500
H	0.19452900	-1.38360400	-3.42255700
H	1.16316000	-1.82104200	-4.83891700
H	2.29324500	-4.03275100	-4.98804900
H	2.36675100	-5.12487400	-3.59395000
H	0.85453300	-4.94301600	-4.49345600
C	1.00527700	-4.64177300	1.69452800

C	0.02698700	-4.63095500	2.87279000
C	1.75025100	-5.98544900	1.67519500
H	-0.59468300	-5.53337000	2.88039600
H	0.58534500	-4.61313600	3.81395300
H	-0.63686000	-3.76381800	2.85057200
H	2.22336400	-6.17475000	2.64499000
H	1.04586700	-6.80042600	1.47283600
H	2.52711300	-6.00660100	0.90647700
C	-2.99284700	-5.11653800	-1.36443000
C	-3.11959800	-6.63645600	-1.20736900
C	-3.97538600	-4.39250400	-0.43922700
H	-2.86991300	-6.93818100	-0.18387900
H	-4.14365500	-6.96525500	-1.41556000
H	-2.44113300	-7.16145700	-1.88642600
H	-5.00824700	-4.65853400	-0.69000200
H	-3.80298300	-4.67128200	0.60647000
H	-3.86581300	-3.30708900	-0.52073300
H	4.50932000	1.47823100	-2.25026400
H	0.81982600	5.35706600	-4.66596000
H	1.15400800	5.27927500	1.03609400
H	1.74099300	-3.84932200	1.86252700
H	2.20360000	-2.73535400	-2.84988900
H	-3.25512800	-4.85999400	-2.39999200

TS3OH-R

C	-7.01333700	-1.78950700	-4.09994700
C	-6.26248000	-2.88513200	-3.61601900
C	-5.27762400	-2.70475000	-2.67779100
C	-4.97943500	-1.41120900	-2.16479300
C	-5.70274800	-0.31011100	-2.69553300
C	-6.72966400	-0.52736900	-3.65099200
C	-5.36709300	0.99772500	-2.27504100
C	-4.32757000	1.24029300	-1.41446000
C	-3.60206600	0.12772200	-0.90067900
C	-3.95557900	-1.18058000	-1.17633300
C	-3.27496200	-2.35368900	-0.56587300
C	-1.91011100	-2.46384100	-0.63618400
C	-1.18141100	-3.63540800	-0.30331600
C	-1.90118300	-4.69455800	0.18970900
C	-3.29778500	-4.60090100	0.42922200
C	-3.99868300	-3.41882300	0.06570800

C	-5.38004600	-3.32513700	0.37439300
C	-6.03503500	-4.36811600	0.97885200
C	-5.34730800	-5.56048100	1.30222800
C	-4.00739300	-5.66957800	1.03612300
H	-7.27632400	0.33429200	-4.02564900
H	-7.79556500	-1.94937200	-4.83524900
H	-6.46147200	-3.88243600	-3.99610000
H	-4.70679800	-3.55946000	-2.33535300
H	-5.94159200	1.84011300	-2.65587100
O	-2.56610000	0.47042400	-0.05087400
H	-5.90994000	-2.40695400	0.14358000
H	-7.08919900	-4.27404300	1.22043800
H	-5.87906500	-6.37926000	1.77681800
H	-3.45955100	-6.57027400	1.30050800
O	-1.17992600	-1.37214800	-1.08237900
H	-1.38890500	-5.62341200	0.42836500
C	-4.01856300	2.65316700	-1.03301200
C	-3.67751200	5.37291100	-0.42371800
C	3.07047000	-3.96165900	-0.99983600
C	0.29197200	-3.69706100	-0.53350100
C	0.81130800	-3.53529900	-1.83907100
C	1.16648100	-3.94743400	0.53808300
C	2.53212800	-4.11030200	0.27391900
H	3.18694700	-4.35804600	1.10459400
C	2.18696400	-3.63455600	-2.03407800
H	2.58126200	-3.51256600	-3.04219200
C	-4.19718600	4.48809400	0.52079600
H	-4.47792300	4.87027500	1.49825900
C	-4.39208200	3.13522600	0.23942600
C	-3.46231100	3.51858000	-1.99572100
C	-3.32621000	4.87177300	-1.67410800
H	-2.91876800	5.56215800	-2.40794500
C	-0.07990800	-3.37438900	-3.06557300
C	0.22944300	-2.10515300	-3.86359900
C	0.02467700	-4.62017500	-3.95624500
H	1.25815400	-2.11474300	-4.24513000
H	-0.43934900	-2.03061400	-4.72782200
H	0.08680900	-1.21485500	-3.24404100
H	-0.66515400	-4.54427500	-4.80345500
H	1.03856000	-4.73655300	-4.35531000
H	-0.21958100	-5.52507500	-3.39156900
C	4.54285900	-4.20530800	-1.30830500
C	4.69104400	-5.29081600	-2.38574100
C	5.37605800	-4.59479900	-0.08819600

H	4. 27776900	-6. 23798600	-2. 02200900
H	4. 16824100	-5. 03225600	-3. 31057700
H	5. 74772800	-5. 44788900	-2. 62531000
H	6. 42589100	-4. 69950700	-0. 37629900
H	5. 33223800	-3. 84331700	0. 70342800
H	5. 03605100	-5. 55349000	0. 32088500
C	0. 70166600	-4. 04128700	1. 98394300
C	0. 81370900	-5. 47399400	2. 51873300
C	1. 48316100	-3. 07272800	2. 87566000
H	1. 85695500	-5. 81139800	2. 51336900
H	0. 44797400	-5. 52397000	3. 54945700
H	0. 23535300	-6. 18145800	1. 91591900
H	1. 04597100	-3. 06307200	3. 87879100
H	2. 53912400	-3. 35840000	2. 96213400
H	1. 42109600	-2. 05688100	2. 47285200
C	-2. 97127700	2. 98857900	-3. 34091800
C	-1. 73434200	2. 09656900	-3. 15053700
C	-2. 65964700	4. 08511100	-4. 35969800
H	-1. 34647100	1. 77250700	-4. 12296500
H	-0. 94250600	2. 63548600	-2. 61956300
H	-1. 95831400	1. 19986200	-2. 56858500
H	-1. 78737000	4. 67622700	-4. 05612100
H	-2. 42503700	3. 63023200	-5. 32663700
H	-3. 50297000	4. 76844400	-4. 50063000
C	-3. 49908400	6. 84368600	-0. 09696700
C	-2. 54251900	7. 04482200	1. 08386100
C	-4. 84674400	7. 52118200	0. 17619800
H	-2. 95058900	6. 59466600	1. 99584600
H	-1. 56727800	6. 58603000	0. 89144700
H	-2. 38804600	8. 11121800	1. 27893600
H	-4. 71161600	8. 59280000	0. 35660200
H	-5. 53017700	7. 39467800	-0. 66851000
H	-5. 32417900	7. 08920400	1. 06255500
C	-5. 06880700	2. 23234900	1. 26557000
C	-6. 54327700	2. 00351800	0. 89448300
C	-5. 01254900	2. 77881400	2. 69513100
H	-7. 07594000	2. 96145300	0. 87981100
H	-6. 65785700	1. 53360900	-0. 08454000
H	-7. 02160800	1. 35906000	1. 63949100
H	-5. 34765100	2. 00703100	3. 39324200
H	-4. 00269500	3. 07872400	2. 98437500
H	-5. 67761800	3. 64210900	2. 81366800
H	-1. 12081800	-3. 30383100	-2. 73979300
H	4. 96407700	-3. 27282500	-1. 71001400

H	-0.34599200	-3.73244400	2.03668700
H	-4.55534700	1.26293000	1.26220800
H	-3.76390200	2.36394000	-3.76905600
H	-3.05307500	7.32250100	-0.97888700
C	3.93429000	0.62192600	-2.98401600
C	4.97223800	-0.24893400	-2.25544700
C	4.44433300	-0.31421400	-0.84220300
C	2.61500300	0.32636400	-2.25721600
H	4.19124700	1.67978700	-2.84994900
H	3.88245100	0.42344800	-4.05654400
H	5.99212600	0.14435300	-2.30829300
H	5.00608000	-1.26338700	-2.67792700
H	2.12996600	-0.57529500	-2.65768800
H	1.86897400	1.12624500	-2.26571600
C	3.07661100	-0.02790600	-0.87009200
C	5.16198900	-1.09813400	0.18612700
O	6.28519100	-1.50516200	-0.07601700
C	4.49633400	-1.38685200	1.50649400
H	3.58666500	-1.97325200	1.33838900
H	5.19161300	-1.94101600	2.13992100
H	4.18593800	-0.46635600	2.00693600
C	2.97826900	2.14904900	1.58796700
C	2.88802800	1.50812100	2.90569300
C	3.95459500	1.59786000	3.81681200
C	1.79933300	0.68127000	3.21418200
C	3.91894800	0.90924100	5.01526400
H	4.80694000	2.22723500	3.57725400
C	1.76437800	-0.02515500	4.40604200
H	1.00052500	0.53212700	2.49217500
C	2.82109400	0.09113300	5.31049300
H	4.72448700	0.98425300	5.73737900
H	0.91615400	-0.67673800	4.60940100
O	2.84135100	-0.56940000	6.49035300
C	4.15728000	2.04244100	0.92264700
C	5.09103200	1.71475000	0.15553900
C	6.35059300	1.91758400	-0.48978400
C	6.44627400	2.83438600	-1.54676500
C	7.50420800	1.21143800	-0.09167600
C	7.65124800	3.05513100	-2.19816400
H	5.56223600	3.38804900	-1.84926300
C	8.70526400	1.42737100	-0.73474900
H	7.44199800	0.49169000	0.71550700
C	8.78857000	2.34501200	-1.79262400
H	7.69773700	3.77435700	-3.00665300

H	9.60403300	0.89478400	-0.44476500
O	10.00600700	2.47923800	-2.35358700
C	10.14629400	3.37914200	-3.43577300
H	11.19227300	3.32647500	-3.73495700
H	9.50907400	3.08618600	-4.27790600
H	9.90437600	4.40395900	-3.13179900
C	1.86329800	2.87270800	0.96139900
C	1.99586300	3.32494400	-0.36412200
C	0.66185100	3.11400400	1.64505900
C	0.95800700	3.98987400	-0.98931400
H	2.92657400	3.14767200	-0.89638100
C	-0.38523900	3.76931400	1.00504100
H	0.54313000	2.79135200	2.67386800
C	-0.23835500	4.21016700	-0.30568700
H	1.07209700	4.33485300	-2.01298100
H	-1.32373900	3.93641700	1.52502800
H	-1.06046600	4.71992900	-0.79533300
P	-1.07385000	-0.15157900	-0.01865700
N	-0.76288400	-0.67186600	1.46700400
S	-1.79986100	-0.91237900	2.64123600
O	-3.14998100	-1.27698200	2.23259500
O	-1.15695200	-1.65500800	3.71863100
C	-2.01036100	0.78540500	3.34408700
F	-3.07726600	0.82179400	4.13200800
F	-2.16696500	1.68334300	2.36616000
F	-0.94353500	1.14703500	4.06076100
O	-0.00865300	0.76451300	-0.54872600
O	2.29687400	-0.04341600	0.15825400
H	1.34290900	0.28384400	-0.09399200
H	2.03568800	-1.10155600	6.57108800

TS3OH-S

C	5.82235000	-5.13765400	-2.75692600
C	6.38638400	-3.89115000	-2.39900000
C	5.66096300	-2.97210000	-1.68388100
C	4.32420100	-3.24865000	-1.28513800
C	3.74910500	-4.48692100	-1.67986000
C	4.52895800	-5.42330500	-2.40743300
C	2.39739700	-4.75740600	-1.35212300
C	1.60656600	-3.83983200	-0.70777800
C	2.20011000	-2.60409100	-0.32504900
C	3.53158900	-2.32034800	-0.52858600
C	4.13239300	-1.05936400	-0.02784100

C	3. 59537300	0. 15403100	-0. 39435400
C	4. 25671800	1. 38945400	-0. 16431500
C	5. 40530000	1. 35696800	0. 59101500
C	5. 91614400	0. 15668500	1. 14149800
C	5. 28420700	-1. 07393800	0. 82349300
C	5. 79549400	-2. 26716600	1. 39933300
C	6. 89190500	-2. 23228200	2. 22262900
C	7. 54149800	-1. 00880400	2. 51020000
C	7. 05986900	0. 15956200	1. 98201400
H	4. 07246000	-6. 36903600	-2. 68847800
H	6. 41139300	-5. 85741500	-3. 31666200
H	7. 40372500	-3. 65655000	-2. 69665000
H	6. 10491400	-2. 01687700	-1. 42562700
H	1. 97213200	-5. 72040900	-1. 62825500
O	1. 38777600	-1. 71357400	0. 34391700
H	5. 29477700	-3. 20873700	1. 20055000
H	7. 26128900	-3. 15235500	2. 66479100
H	8. 41210200	-0. 99929500	3. 15839000
H	7. 53609300	1. 11057000	2. 20584200
O	2. 36500800	0. 17371000	-1. 05518800
H	5. 94553500	2. 28528700	0. 76448200
C	0. 16864200	-4. 12370500	-0. 42051200
C	-2. 53476100	-4. 64893000	0. 11677400
C	3. 36879600	5. 17242600	-2. 02033500
C	3. 83965000	2. 67179800	-0. 80705800
C	3. 92678500	2. 79968700	-2. 21589400
C	3. 50941600	3. 78563300	-0. 01622400
C	3. 28918700	5. 02005800	-0. 64206100
H	3. 03843000	5. 87739300	-0. 02240900
C	3. 68024300	4. 04551700	-2. 78730000
H	3. 74356100	4. 16253200	-3. 86651600
C	-1. 59919300	-4. 60264800	1. 14789500
H	-1. 93492800	-4. 76558100	2. 16687100
C	-0. 24923300	-4. 34951600	0. 90936200
C	-0. 75046000	-4. 18996800	-1. 48776800
C	-2. 08938700	-4. 46337600	-1. 18916600
H	-2. 82057400	-4. 52139200	-1. 99175700
C	4. 38180900	1. 63851500	-3. 09501700
C	3. 96537900	1. 76753300	-4. 56192700
C	5. 90750400	1. 47526800	-3. 01403800
H	4. 50254300	2. 57690800	-5. 06809900
H	4. 20276600	0. 83983200	-5. 09120100
H	2. 89165600	1. 95061200	-4. 66840600
H	6. 40177900	2. 37835600	-3. 38997100

H	6. 24389000	1. 30530300	-1. 98760200
H	6. 23187300	0. 62675500	-3. 62625600
C	3. 04378100	6. 48089900	-2. 71605000
C	3. 40739400	7. 71953100	-1. 89604800
C	1. 55590200	6. 50467500	-3. 09479100
H	2. 76340200	7. 81518200	-1. 01520400
H	4. 44654000	7. 68393600	-1. 55544300
H	3. 27128000	8. 62372200	-2. 49752200
H	1. 30419200	7. 42137200	-3. 63885600
H	1. 29153000	5. 64532300	-3. 71956900
H	0. 93634600	6. 45935100	-2. 19137200
C	3. 35927700	3. 71413400	1. 49625100
C	4. 40789100	4. 57960600	2. 20437800
C	1. 94468100	4. 11479200	1. 92276500
H	4. 27121800	5. 64053700	1. 96479500
H	4. 31907900	4. 46518000	3. 28927300
H	5. 42648300	4. 30345400	1. 91300300
H	1. 84978100	4. 05541000	3. 01062800
H	1. 69504400	5. 13457800	1. 60484800
H	1. 22449300	3. 41447500	1. 49222800
C	-0. 31381600	-3. 95872800	-2. 93596700
C	0. 11013600	-2. 50608500	-3. 20021500
C	-1. 37192200	-4. 36533000	-3. 96368300
H	-0. 71980000	-1. 81650800	-3. 02408100
H	0. 93696000	-2. 18214700	-2. 56405600
H	0. 42962000	-2. 39912300	-4. 24279400
H	-2. 24432100	-3. 70143300	-3. 92312900
H	-0. 95167900	-4. 28840500	-4. 97088100
H	-1. 71734600	-5. 39313600	-3. 81539000
C	-3. 99917900	-4. 92270100	0. 40073600
C	-4. 52146300	-4. 10314600	1. 58556600
C	-4. 23779400	-6. 42018500	0. 63110000
H	-4. 12753300	-4. 48618600	2. 53307900
H	-4. 22355300	-3. 05287500	1. 50323700
H	-5. 61391400	-4. 14386600	1. 64113100
H	-5. 29794500	-6. 62204900	0. 81746100
H	-3. 91804300	-7. 00825700	-0. 23427900
H	-3. 66744400	-6. 76360300	1. 50145900
C	0. 75044600	-4. 37999200	2. 06220900
C	1. 61269200	-5. 65160400	1. 99697400
C	0. 09963200	-4. 31277800	3. 44645800
H	0. 97325000	-6. 53866000	2. 07268100
H	2. 18451800	-5. 72069800	1. 06923500
H	2. 31842800	-5. 66904500	2. 83404900

H	0.87357200	-4.16254800	4.20445900
H	-0.61420300	-3.49162900	3.52994300
H	-0.41920300	-5.24917900	3.68312400
H	3.92141000	0.72011400	-2.72010200
H	3.62833400	6.50680500	-3.64534400
H	3.49669200	2.67828400	1.81850500
H	1.40699700	-3.50622400	1.96791700
H	0.56369900	-4.58917400	-3.11988500
H	-4.56243400	-4.62777100	-0.49624300
P	1.08915000	-0.18564400	-0.11407300
N	1.06958500	0.72968800	1.20307900
S	1.55178700	0.30974200	2.65369200
O	2.63232600	-0.66463400	2.70408000
O	1.62572800	1.49213900	3.50546000
C	0.07482200	-0.59622400	3.30207600
F	0.40470600	-1.29875500	4.37971200
F	-0.41504100	-1.42920500	2.37880400
F	-0.89136500	0.26009100	3.63146600
O	-0.15486700	-0.07628900	-0.94676600
C	-4.45814000	-1.36568000	-2.08648500
C	-5.31695400	-1.44142300	-0.80961000
C	-4.55304200	-0.60108000	0.18499200
C	-3.02402500	-1.13599500	-1.58683500
H	-4.77671900	-0.50495100	-2.68671500
H	-4.54725000	-2.25742000	-2.71247700
H	-6.34365000	-1.09169300	-0.95693600
H	-5.39385600	-2.46946800	-0.43077700
H	-2.49488900	-2.08185400	-1.40420900
H	-2.38326100	-0.53720900	-2.23899200
C	-3.23042300	-0.48763400	-0.24816900
C	-5.02766000	-0.48835000	1.58219700
O	-6.16026400	-0.86483000	1.84357600
C	-4.10457100	0.05368200	2.64596700
H	-3.18206300	-0.53298900	2.68989000
H	-4.62253100	0.01746900	3.60505900
H	-3.80382800	1.08178600	2.41997900
C	-2.86055800	2.77226700	0.10161100
C	-2.57886100	3.21915400	1.47062000
C	-3.54717100	3.94694700	2.18598400
C	-1.39813700	2.83652100	2.12560200
C	-3.32781100	4.31730600	3.49922100
H	-4.46822200	4.23576000	1.68763200
C	-1.17869400	3.19147000	3.44689700
H	-0.66871000	2.20512900	1.62242700

C	-2.13743500	3.93911800	4.13293900
H	-4.05661200	4.89580400	4.05618300
H	-0.26711600	2.85279100	3.93597700
O	-1.97453100	4.31844300	5.42067100
C	-4.11237000	2.31198500	-0.15446500
C	-5.13795200	1.62187700	-0.34644900
C	-6.49304600	1.42202700	-0.75256100
C	-6.81505300	1.40783600	-2.11740100
C	-7.52084300	1.23731400	0.19481100
C	-8.12254500	1.22166600	-2.54261200
H	-6.02706800	1.55762600	-2.84952100
C	-8.82237500	1.05079800	-0.22188400
H	-7.28266900	1.23186200	1.25172300
C	-9.13331600	1.03836400	-1.59005400
H	-8.34412300	1.22346300	-3.60276100
H	-9.62714100	0.90620200	0.49009500
O	-10.43231400	0.84589500	-1.89179700
C	-10.80148400	0.80840700	-3.25651400
H	-11.87640600	0.63301100	-3.27074000
H	-10.29058300	-0.00670800	-3.78130800
H	-10.57953600	1.76026700	-3.75253600
C	-1.85605800	2.78265800	-0.97017500
C	-2.13021700	2.15635900	-2.19925000
C	-0.59867400	3.37058600	-0.77893900
C	-1.15639700	2.06456400	-3.17824600
H	-3.11341900	1.72468700	-2.36804800
C	0.38378000	3.25981800	-1.75556200
H	-0.38521400	3.91845800	0.13134000
C	0.11259400	2.59913500	-2.94837400
H	-1.37675900	1.56125700	-4.11478500
H	1.36055100	3.69347000	-1.58103000
H	0.89179400	2.50992900	-3.69959600
O	-2.28760900	0.10760600	0.40503100
H	-1.39269400	0.07496700	-0.12658400
H	-1.12219700	3.99002500	5.74366800