

Supporting Information

for

A Central Functional Group-Dependent Stereoinduction Mechanism for Chiral Super Brønsted C–H Acid Catalysis

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Computational Details

The enantiomeric excess (% ee) is calculated by using the Boltzmann distribution of diastereomeric transition states with the expression

$$ee = \frac{1 - e^{-\Delta G^\ddagger_{R/S}/RT}}{1 + e^{-\Delta G^\ddagger_{R/S}/RT}} \times 100$$

Where $\Delta G^\ddagger$ is the difference in the Gibbs free energies between the competing diastereomeric transition states.

The activation energy ($\Delta E^\ddagger$) could be written as the sum of the energy required to distort the reactant geometries ($\Delta E_{\text{dist}}^\ddagger$) and the interaction energy ($\Delta E_{\text{int}}^\ddagger$) between the distorted fragments in the TS geometries, which can be described as $\Delta E^\ddagger = \Delta E_{\text{dist}}^\ddagger + \Delta E_{\text{int}}^\ddagger$.

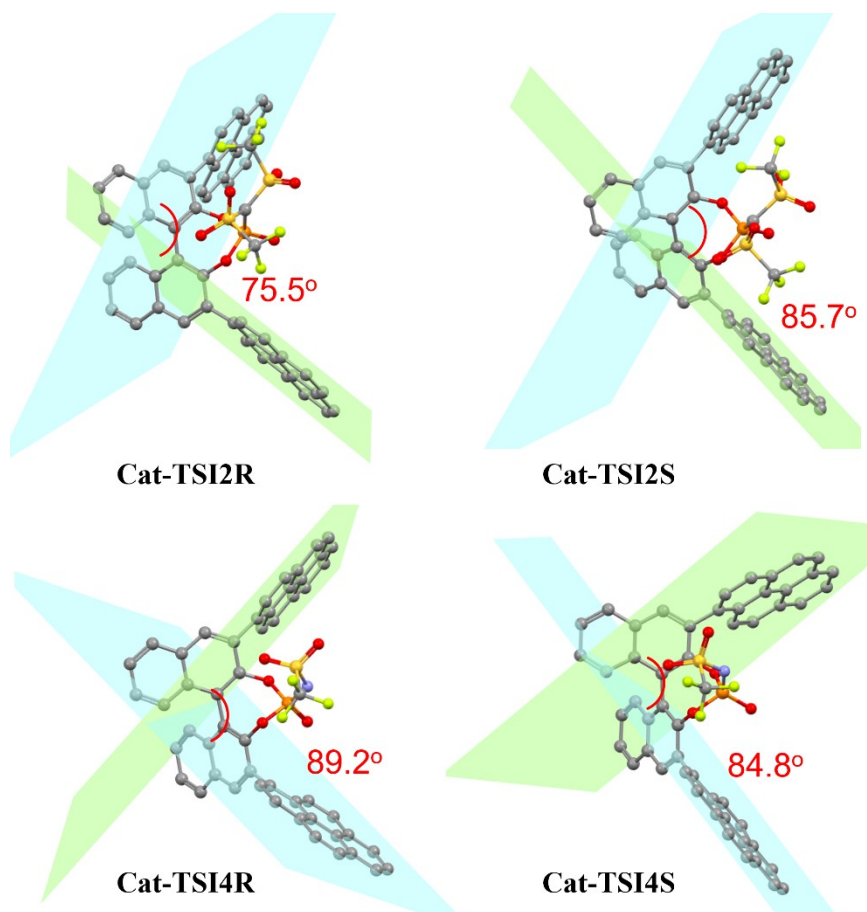


Figure S1. The open angles for the cavity of Cat-TSI2R, Cat-TSI2S, Cat-TSI4R, and Cat-TSI4S.

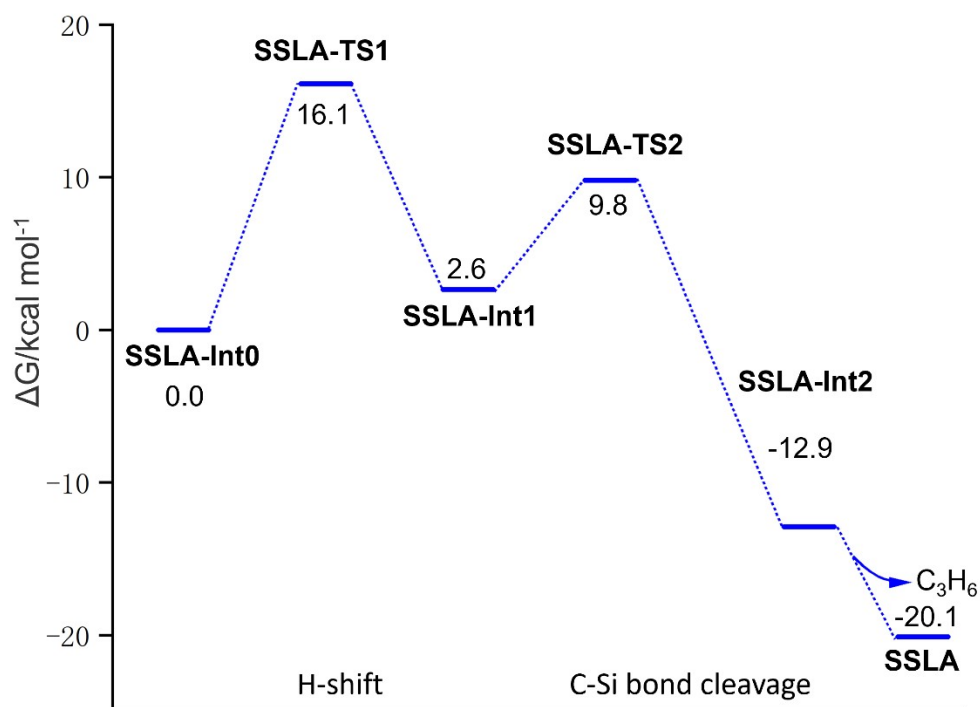


Figure S2. The energy profile for the generation of super silyl Lewis acids in the case of three-component reaction catalyzed by chiral super Brønsted acids using allylsilanes.

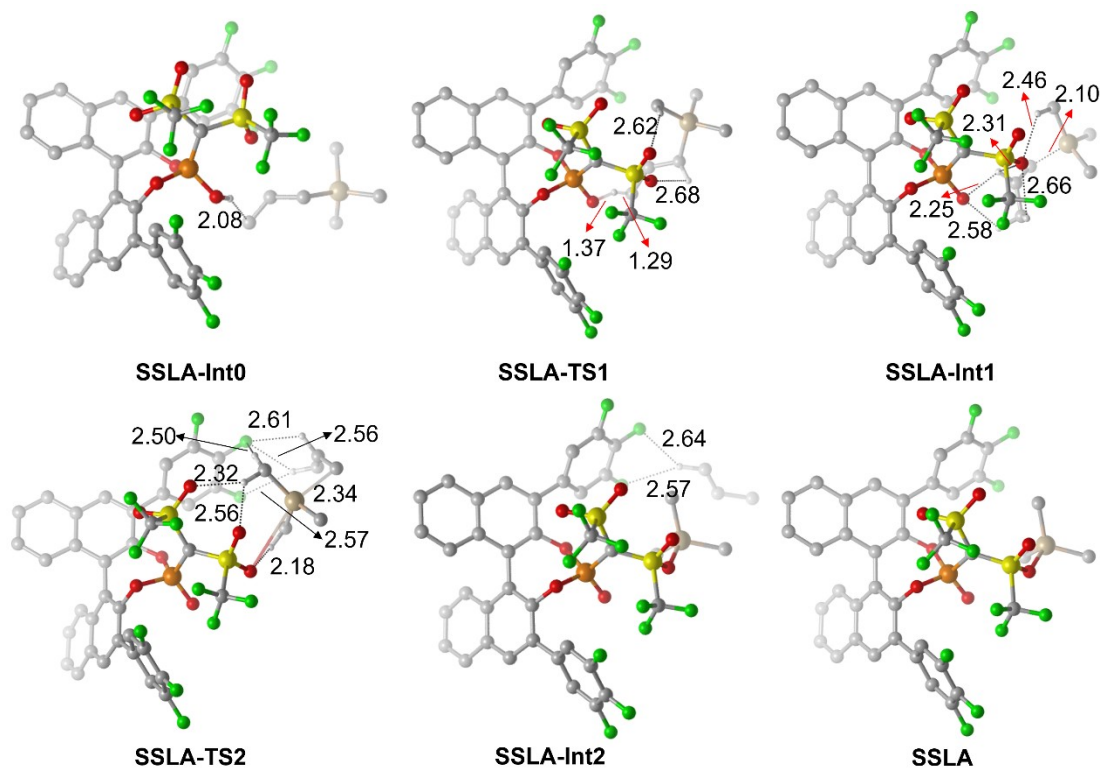


Figure S3. The key intermediates and transition states in the processes of generation of super silyl Lewis acids.

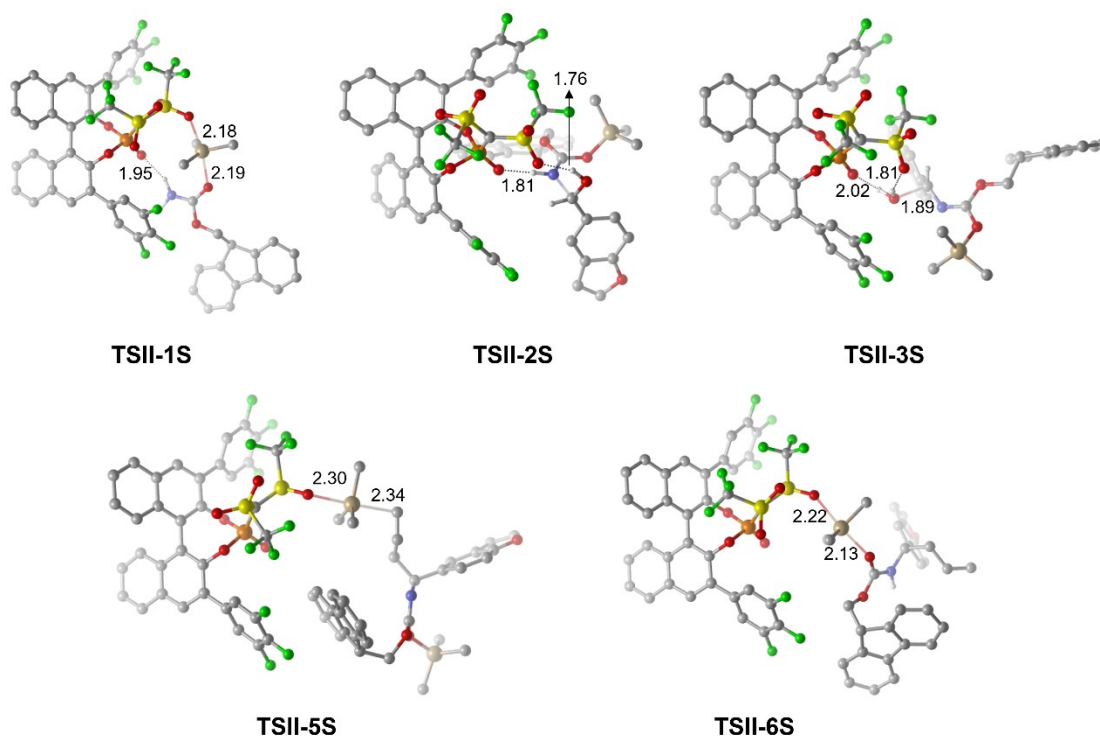


Figure S4. The key transition states in the processes of generation of **Pr-S**.

Brønsted Acid Mechanism

For the Brønsted acid mechanism, both nucleophilic substitution reaction pathways, the S_N1 and the S_N2 , were investigated, differing from each other in the water elimination and the C–C coupling proceeding in a stepwise (S_N1) or a concerted (S_N2) manner. The S_N1 reaction mechanism includes four steps: (Step 1) enantioselective C–N bond formation, (Step 2) water elimination, (Step 3) nucleophilic C–C bond-formation, and (Step 4) TMSOH elimination. The relative free energies on the potential surface of each transition states to the four steps were calculated to be 7.9/10.8, 18.0/10.5, 25.6/27.9, and 18.6/22.4 kcal/mol, to generate the corresponding major/minor product, respectively. These values suggest that the nucleophilic C–C bond formation via **TSIII3S** and **TSIII3R** is the rate-determining and stereo-determining step for both major and minor pathways.

The S_N2 mechanism involves concerted water elimination and C–C bond formation process (**TSIII3S'** and **TSIII3R'**). According to calculations, the transition states in the S_N2 mechanism are less stable than those in the S_N1 mechanism by a free energy difference of 8.5 (major pathway) and 3.5 (minor pathway) kcal/mol, respectively (Figure S5).

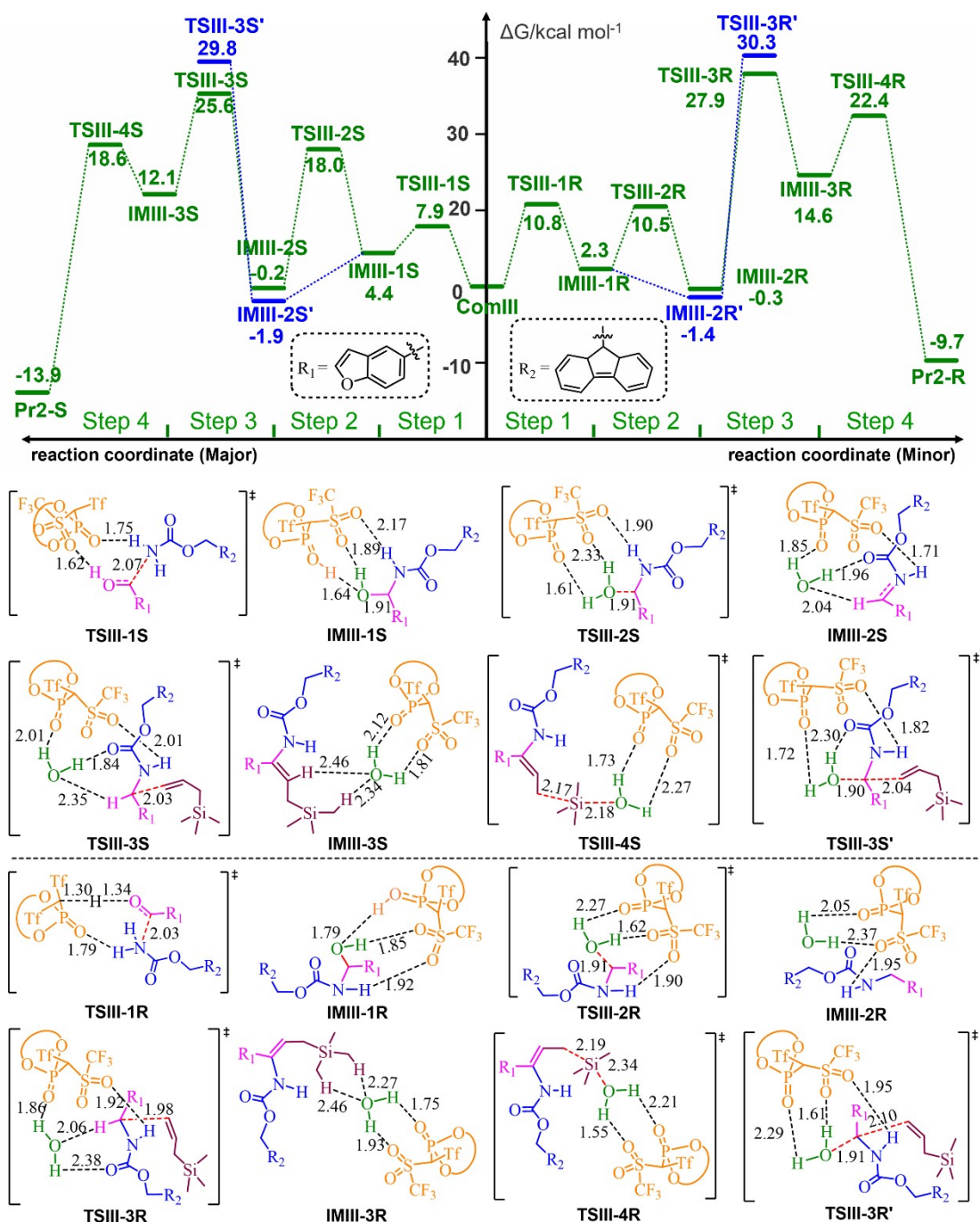
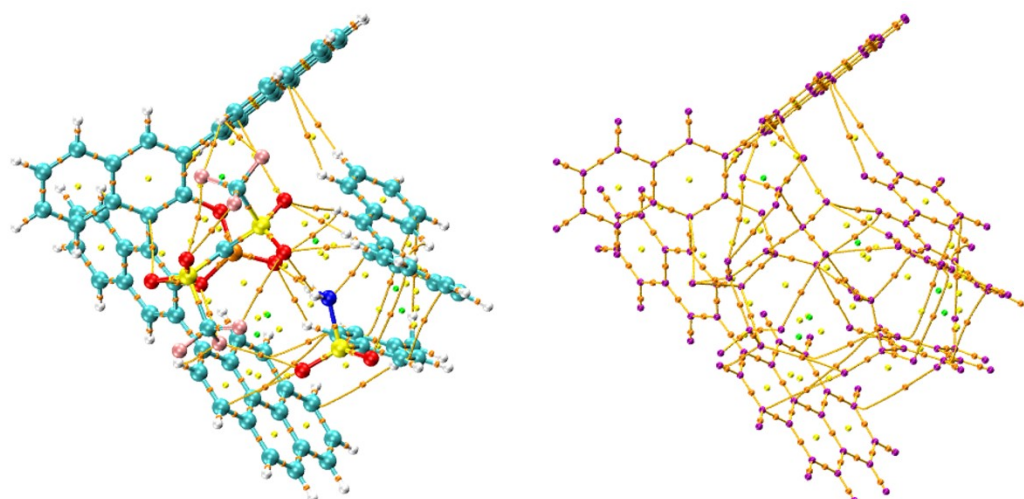


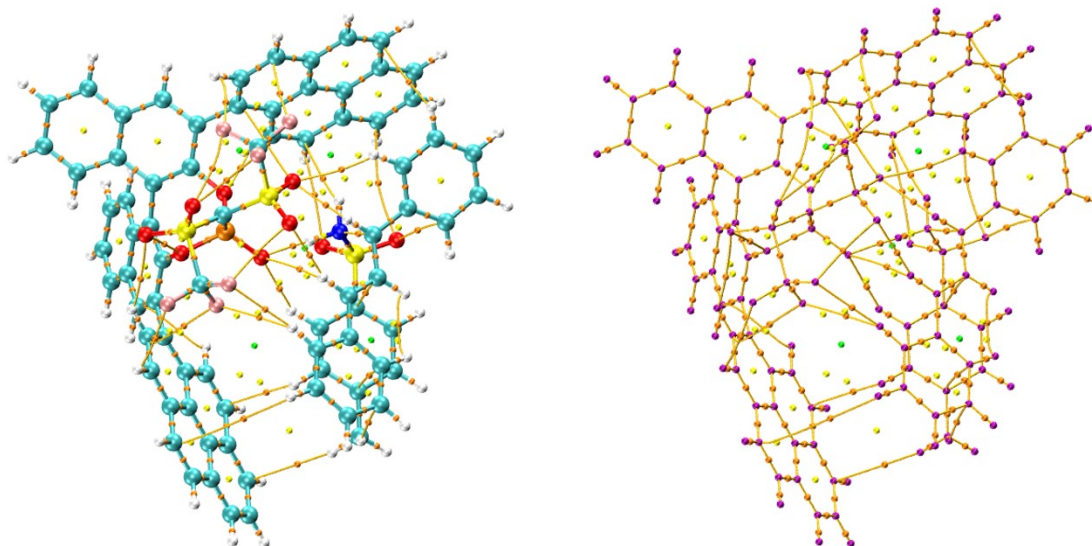
Figure S5. Free energy profiles and schematic elucidation of key transition states and intermediates of the three-component coupling reaction catalyzed by BPTM leading to major product **Pr2-S** and minor product **Pr2-R**, the distances are in Å. Color scheme: in the free energy profiles, S_N1 mechanism in green, and S_N2 mechanism in blue; in the elucidations of stationary points, each structure was partitioned into four fragments with the catalyst in orange, the nascent water in green, the FmocNH₂ and the aldehydes in blue, and the allyltrimethylsilane in brown. R1 = Benzofuran; R2 = fluorenyl.

AIM Analysis



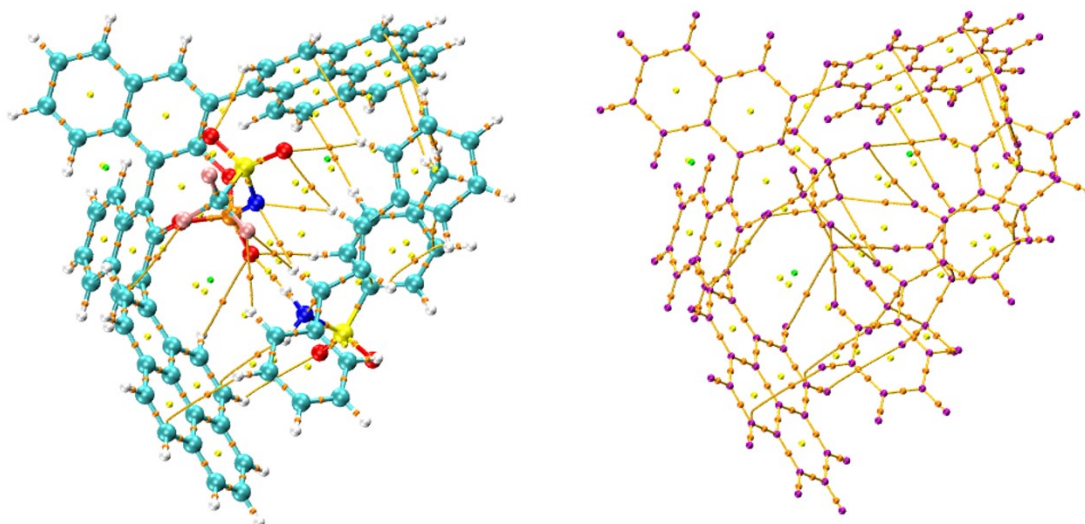
TSI2R

Figure S6. Visualization of QTAIM critical points for the transition states **TSI2R**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.



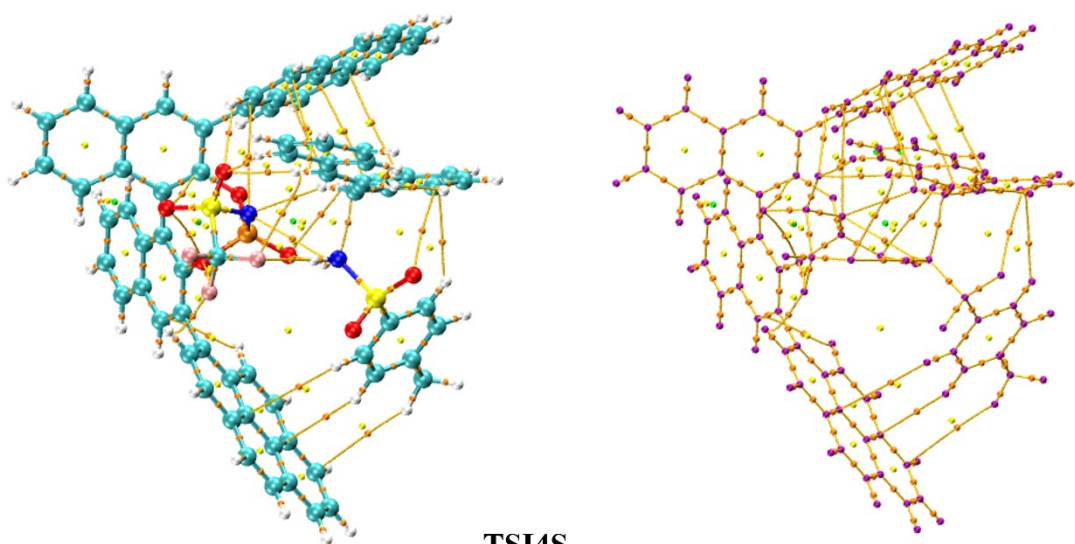
TSI2S

Figure S7. Visualization of QTAIM critical points for the transition states **TSI2S**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.



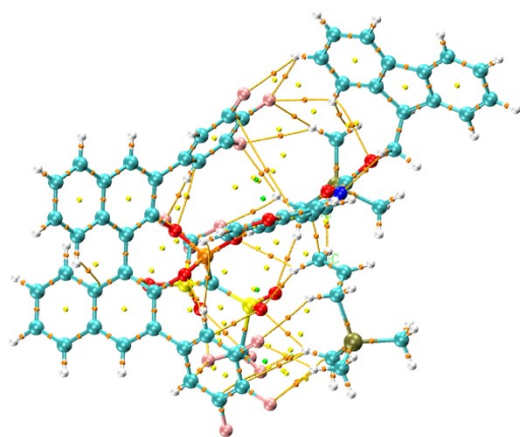
TSI4R

Figure S8. Visualization of QTAIM critical points for the transition states **TSI4R**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.

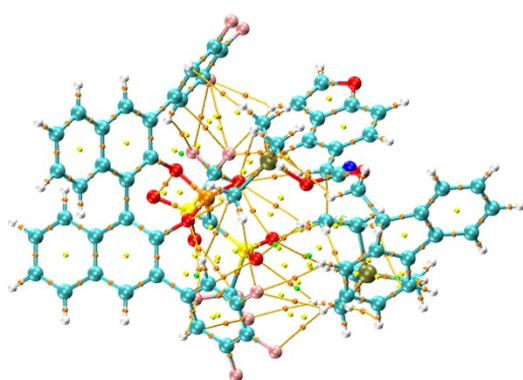
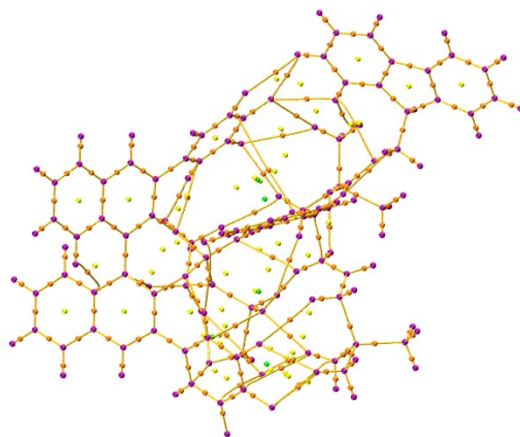


TSI4S

Figure S9. Visualization of QTAIM critical points for the transition states **TSI4S**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.



TSII-4S



TSII-4R

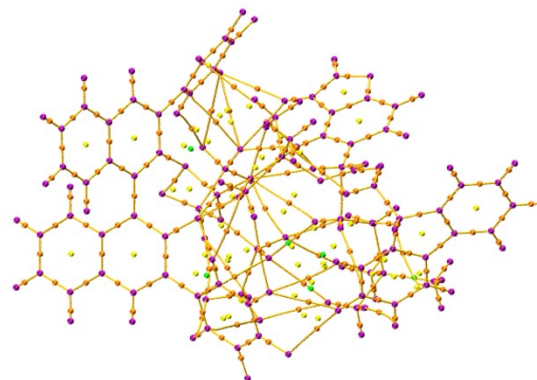


Figure S10. Visualization of QTAIM critical points for the transition states **TSII-4S** and **TSII-4R**. Magenta corresponds to nuclear critical points (NCP), orange to bond critical points (BCP), yellow to ring critical points (RCP), and green to cage critical points (CCP). Yellow lines indicate the bond path.

Hydrogen Bond Energy Strength Analysis by Espinosa's Formulation and Lu's Equation.

E1 is calculated based on Espinosa's formulation $E1 = 1/2 V$

E2 is calculated based on Lu's equation:

The fitted equation for neutral complexes is $E2 = -223.08 \times \rho_{BCP} + 0.7423$ with a mean absolute percentage error (MAPE) of 14.7%, while that for charged complexes is $E2 = -332.34 \times \rho_{BCP} - 1.0661$ with a MAPE of 10.0%.

Table S1. Estimation of Noncovalent Interaction Energies (E_{HB}) Using Espinosa Equation ($E_{\text{HB}} = 1/2V(r_{\text{cp}})$) in the Lower Energy Enantiocontrolling **TSI2R** and **TSI2S**.

Non-covalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	V	E1=1/2 V (kcal/mol)	E2 (kcal/mol)
TSI2R								
N-H $\cdots$ O	1a	1.84	0.034	0.103	0.27 e ⁻¹	-0.28 e ⁻¹	-8.8	-12.4
	1b	2.13	0.019	0.059	0.15 e ⁻¹	-0.15 e ⁻¹	-4.7	-3.5
C-H $\cdots$ O	1c	2.35	0.013	0.040	0.97 e ⁻²	-0.94 e ⁻²	-3.0	-2.2
	1d	2.49	0.009	0.032	0.71 e ⁻²	-0.63 e ⁻²	-2.0	-1.3
	1e	2.53	0.008	0.030	0.66 e ⁻²	-0.56 e ⁻²	-1.8	-3.7
	1f	2.64	0.006	0.024	0.49 e ⁻²	-0.39 e ⁻²	-1.2	-0.6
	1g	2.72	0.006	0.025	0.50 e ⁻²	-0.38 e ⁻²	-1.2	-3.1
E _{Group1}							-22.7	-26.8
C-H $\cdots\pi$	1h	2.95	0.005	0.015	0.28 e ⁻²	-0.21 e ⁻²	-0.7	-0.4
	1i	3.16	0.003	0.010	0.20 e ⁻²	-0.14 e ⁻²	-0.4	0.0
	1j	3.27	0.003	0.008	0.15 e ⁻²	-0.10 e ⁻²	-0.3	0.0
	1k	3.42	0.002	0.007	0.13 e ⁻²	-0.86 e ⁻³	-0.3	0.3
E1/E2 total							-24.4	-26.9
TSI2S								
N-H $\cdots$ O	1a'	1.75	0.040	0.129	0.33 e ⁻¹	-0.34 e ⁻¹	-10.7	-14.4
C-H $\cdots$ O	1b'	2.16	0.018	0.058	0.15 e ⁻¹	-0.15 e ⁻¹	-4.7	-3.3
	1c'	2.38	0.011	0.039	0.88 e ⁻²	-0.79 e ⁻²	-2.5	-4.7
	1d'	2.39	0.012	0.038	0.89 e ⁻²	-0.84 e ⁻²	-2.6	-1.9
E _{Group1}							-20.5	-24.3
C-H $\cdots\pi$	1e'	3.02	0.004	0.014	0.28 e ⁻²	-0.20 e ⁻²	-0.6	-0.2
	1f'	3.06	0.004	0.011	0.22 e ⁻²	-0.16 e ⁻²	-0.5	-0.2
	1g'	3.10	0.004	0.010	0.19 e ⁻²	-0.13 e ⁻²	-0.4	-0.2
N-H $\cdots\pi$	1h'	3.18	0.003	0.010	0.18 e ⁻²	-0.11 e ⁻²	-0.4	0.1
E1/E2 total							-22.4	-24.8

Table S2. Estimation of Noncovalent Interaction Energies (E_{HB}) Using Espinosa Equation ($E_{\text{HB}} = 1/2V(r_{\text{cp}})$) in the Lower Energy Enantiocontrolling **TSI4R** and **TSI4S**.

Non-covalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	V	E1=1/2 V (kcal/mol)	E2 (kcal/mol)
TSI4R								
N-H $\cdots$ O	2a	1.70	0.046	0.145	0.38 e^{-1}	-0.39 e^{-1}	-12.2	-14.4
C-H $\cdots$ O	2b	2.36	0.012	0.042	0.98 e^{-2}	-0.91 e^{-2}	-2.9	-5.1
	2c	2.62	0.007	0.028	0.60 e^{-2}	-0.50 e^{-2}	-1.6	-0.8
C-H $\cdots$ N	2d	2.43	0.012	0.038	0.87 e^{-2}	-0.80 e^{-2}	-2.5	-1.9
	2e	2.56	0.010	0.030	0.69 e^{-2}	-0.62 e^{-2}	-2.0	-1.5
E_{Group1}							-21.2	-23.7
N-H $\cdots\pi$	2f	2.90	0.005	0.016	0.32 e^{-2}	-0.23 e^{-2}	-0.7	-0.4
C-H $\cdots\pi$	2g	3.11	0.004	0.012	0.24 e^{-2}	-0.17 e^{-2}	-0.5	-0.2
	2h	3.16	0.004	0.011	0.22 e^{-2}	-0.16 e^{-2}	-0.5	-0.2
E1/E2 total							-22.9	-24.5
TSI4S								
N-H $\cdots$ O	2a'	1.80	0.036	0.112	0.30 e^{-1}	-0.31 e^{-1}	-9.7	-13.0
N-H $\cdots$ F	2b'	2.28	0.010	0.042	0.96 e^{-2}	-0.86 e^{-2}	-2.7	-4.4
C-H $\cdots$ N	2c'	2.46	0.012	0.036	0.85 e^{-2}	-0.78 e^{-2}	-2.5	-1.9
C-H $\cdots$ O	2d'	2.26	0.015	0.047	0.12 e^{-1}	-0.11 e^{-1}	-3.5	-2.6
	2e'	2.48	0.009	0.030	0.68 e^{-2}	-0.59 e^{-2}	-1.9	-1.3
	2f'	2.68	0.007	0.024	0.51 e^{-2}	-0.41 e^{-2}	-1.3	-0.8
E_{Group1}							-21.6	-24.0
C-H $\cdots\pi$	2g'	2.87	0.005	0.017	0.33 e^{-2}	-0.24 e^{-2}	-0.8	-0.4
E1/E2 total							-22.4	-24.4

Table S3. Estimation of Noncovalent Interaction Energies (E_{HB}) Using Espinosa Equation ($E_{\text{HB}} = 1/2V(r_{\text{cp}})$) in the Lower Energy Enantiocontrolling **TSII-4S** and **TSII-4R**.

Non-covalent Interaction	Bond path	distance	ρ	$\nabla^2\rho$	G	V	E1=1/2 V (kcal/mol)	E2 (kcal/mol)
TSII-4S								
C-H...O	4a	2.17	0.019	0.056	0.14 e^{-1}	-0.14 e^{-1}	-4.4	-7.3
	4b	2.25	0.016	0.050	0.12 e^{-1}	-0.11 e^{-1}	-3.5	-2.8
	4c	2.40	0.011	0.037	0.82 e^{-2}	-0.71 e^{-2}	-2.2	-4.7
	4d	2.47	0.009	0.030	0.68 e^{-2}	-0.60 e^{-2}	-1.9	-1.3
	4e	2.55	0.008	0.028	0.61 e^{-2}	-0.53 e^{-2}	-1.7	-1.0
	4f	2.63	0.007	0.027	0.57 e^{-2}	-0.45 e^{-2}	-1.4	-3.4
C-H...F	4g	2.50	0.007	0.031	0.65 e^{-2}	-0.51 e^{-2}	-1.6	-0.8
E_{Group1}							-16.6	-21.3
C-H...F	4h	2.48	0.007	0.032	0.69 e^{-2}	-0.55 e^{-2}	-1.7	-0.8
	4i	2.50	0.007	0.031	0.64 e^{-2}	-0.50 e^{-2}	-1.6	-0.8
	4j	2.57	0.006	0.029	0.57 e^{-2}	-0.43 e^{-2}	-1.3	-0.6
	4k	2.65	0.005	0.024	0.46 e^{-2}	-0.33 e^{-2}	-1.0	-0.4
	4l	2.65	0.005	0.025	0.48 e^{-2}	-0.34 e^{-2}	-1.1	-0.4
$E_{\text{HB total}}$							-23.3	-24.3
TSII-4R								
C-H...O	4a'	2.24	0.015	0.050	0.12 e^{-1}	-0.12 e^{-1}	-3.8	-2.6
	4b'	2.41	0.010	0.036	0.82 e^{-2}	-0.76 e^{-2}	-2.4	-4.4
	4c'	2.48	0.008	0.031	0.69 e^{-2}	-0.58 e^{-2}	-1.8	-3.7
	4d'	2.56	0.008	0.027	0.59 e^{-2}	-0.50 e^{-2}	-1.6	-3.7
C-H...F	4e'	2.45	0.008	0.035	0.73 e^{-2}	-0.58 e^{-2}	-1.8	-1.0
E_{Group1}							-11.4	-15.4
C-H...F	4f'	2.52	0.007	0.029	0.59 e^{-2}	-0.47 e^{-2}	-1.5	-0.8
	4g'	2.58	0.006	0.026	0.53 e^{-2}	-0.39 e^{-2}	-1.2	-0.6
	4h'	2.68	0.005	0.023	0.44 e^{-2}	-0.30 e^{-2}	-0.9	-0.4
$E_{\text{HB total}}$							-15.0	-17.2

The hydrogen bond energies calculated by Espinosa's formulation are -24.4 and -22.4 kcal/mol (E1) in **TSI2R** and **TSI2S**, by using Lu's Equation (E2), the bond energies are -26.9 and -24.8 kcal/mol, respectively. The energies of E_{Group1} are -22.7 and -20.5 based on Espinosa's formulation, and -26.9 and -24.3 based on Lu's Equation.

For **TSI4R** and **TSI4S**, the hydrogen bond energies are -22.9 and -22.4 kcal/mol (E1) and -24.5 and -24.4 kcal/mol (E2), respectively. E_{Group1} are -21.2 and -21.6 based on Espinosa's formulation, and E_{Group2} are -23.7 and -24.0 based on Lu's Equation.

For **TSII-4S** and **TSII-4R**, the hydrogen bond energies are -23.3 and -15.0 kcal/mol (E1) and -24.3 and -17.2 kcal/mol (E2), respectively. E_{Group1} are -16.6 and -11.4 based on Espinosa's formulation and -20.2 and -15.4 kcal/mol based on Lu's Equation.

The energy differences between E1/E2 are 2.0 and 2.1 kcal/mol (**TSI2R** and **TSI2S**), 1.6 and 2.0 kcal/mol (**TSI4R** and **TSI4S**), 1.0 and 2.2 kcal/mol (**TSII-4S** and **TSII-4R**). Moreover, the E_{Group1} energies in **TSI2R/TSI4R/TSII-4S** are 2.2/2.6, 0.4/0.3, 5.2/4.8 kcal/mol more than those in **TSI2S/TSI4S/TSII-4R** based on Espinosa's formulation/Lu's Equation. Therefore, the above analysis further confirmed that the interactions involved the CFG are responsible for the superior catalytic activity of BPTM (**TSI2R/TSI2S** and **TSII-4S/TSII-4R**), while these effects are weakened or absent in the cases catalyzed by NTPA (**TSI4R/TSI4S**). The two methods of measuring the strength of hydrogen bond can achieve the same conclusion in the asymmetric allylic amination and three-component coupling of allyltrimethylsilane reactions.

S1. Cartesian Coordinates of all reported structures

Rel

C	1.24248000	1.34734400	0.25528700
H	1.14116100	1.68425700	1.30027800
C	2.38334000	0.35107400	0.17789600
C	3.39061200	0.48216100	-0.77526100
C	2.41019400	-0.73097000	1.06053400
C	4.41681700	-0.45852300	-0.84087300
H	3.36808700	1.32706300	-1.45369100

C	3.43523100	-1.66766600	0.99564900
H	1.61821300	-0.83809800	1.79893900
C	4.44324900	-1.53323900	0.04183000
H	5.19979000	-0.34745700	-1.58518700
H	3.44860900	-2.50335500	1.68892600
H	5.24469900	-2.26398500	-0.01026200
O	1.55353700	2.44554900	-0.58706400
H	0.75869600	2.99401800	-0.64399400
C	-0.05548600	0.71605900	-0.17146400
H	-0.05937800	0.29907500	-1.17828700
C	-1.14923400	0.69768400	0.59547300
H	-1.09730100	1.16747200	1.57933300
C	-2.45842700	0.12934700	0.23162900
C	-3.60301900	0.55912400	0.91257200
C	-2.60315300	-0.82697300	-0.78194400
C	-4.86099900	0.07114000	0.57568900
H	-3.50130600	1.29370400	1.70770600
C	-3.85884900	-1.31679900	-1.11828000
H	-1.72213500	-1.20256400	-1.29432300
C	-4.99317200	-0.86686500	-0.44425500
H	-5.73808200	0.42216000	1.11091500
H	-3.95386500	-2.06094400	-1.90322000
H	-5.97298300	-1.25313300	-0.70749300

Re2

C	-0.57884800	-1.23140400	0.01986900
C	0.11419400	-0.02981400	0.05733100
C	-0.54903900	1.19559800	0.06068000
C	-1.93447500	1.20500900	0.01425900
C	-2.66371300	0.00901000	-0.02936500
C	-1.97099700	-1.20134200	-0.02531600
H	-0.03033600	-2.16747300	0.03661700
H	0.01908000	2.11955300	0.10650600
H	-2.46642900	2.15290500	0.01673000

H	-2.52629200	-2.13475600	-0.05332400
C	-4.16964700	0.04388800	-0.06118500
H	-4.58782900	-0.95088200	-0.23170900
H	-4.56904900	0.41946200	0.88685900
H	-4.53034500	0.70724700	-0.85324400
S	1.88640100	-0.04946800	0.13413200
O	2.29992700	-1.43465100	0.30519400
O	2.32606400	0.99867900	1.04160300
N	2.33270700	0.48195300	-1.39378000
H	3.12012100	1.11965200	-1.29645100
H	2.56692500	-0.30578900	-1.99364800

Re3

C	-1.13685700	0.66521700	-0.00003400
C	-0.89708700	-0.71738900	-0.00000400
C	0.42703200	-1.16467700	0.00001200
C	1.44474400	-0.21783800	0.00000000
C	1.16755800	1.16558700	-0.00002900
C	-0.13381300	1.63190400	-0.00004500
C	-3.08678300	-0.30829000	-0.00003700
C	-2.20515600	-1.33084500	0.00001600
H	0.66411300	-2.22606600	0.00004400
H	2.01002400	1.84970300	-0.00003600
H	-0.37525200	2.68869500	-0.00006400
H	-4.16565000	-0.27256500	-0.00006500
H	-2.44263900	-2.38404900	0.00004700
O	-2.46980500	0.91096600	-0.00003900
C	2.85338300	-0.67275000	0.00002000
O	3.81033800	0.06583000	0.00016400
H	2.98700700	-1.77560500	-0.00032300

Re4

C	-3.79741000	-1.72370200	-0.33519000
C	-2.92080700	-2.70033800	0.13917400

C	-1.62119300	-2.36194300	0.52013600
C	-1.21741900	-1.03887600	0.41894000
C	-2.09817500	-0.05703500	-0.06074000
C	-3.39406500	-0.39407600	-0.43927300
H	-4.80505500	-2.00377300	-0.62677200
H	-3.25308300	-3.73115300	0.21286400
H	-0.94261200	-3.12516200	0.89296900
H	-4.08061300	0.36155300	-0.81086800
C	0.12842700	-0.42473200	0.75121600
H	0.36867300	-0.55428100	1.81529600
C	-0.09248900	1.03852700	0.41831100
C	0.79020600	2.10534400	0.51495100
C	0.35447100	3.37469800	0.13108600
C	-0.94401200	3.57088600	-0.34116600
C	-1.83195100	2.50231700	-0.44122200
C	-1.39807700	1.23652900	-0.06002800
H	1.80180700	1.95200800	0.87666500
H	1.03351600	4.21913500	0.19967500
H	-1.26433800	4.56598800	-0.63440400
H	-2.84161400	2.65673300	-0.81169600
C	1.24116600	-1.06834400	-0.06667600
H	1.27020500	-2.15245300	0.08527400
H	1.10401300	-0.87672100	-1.13495500
O	2.47772800	-0.49920900	0.37128200
C	3.56315900	-0.91626400	-0.32023100
O	3.52800400	-1.71461900	-1.22629100
N	4.68266900	-0.28084800	0.13390600
H	4.65080000	0.17351100	1.03340200
H	5.56279000	-0.66676500	-0.17045700

Re5

C	-2.93332600	0.31504600	-0.04402800
C	-1.98741000	-0.56129600	0.29253300
H	-2.89980600	1.34462900	0.30588200

H	-3.77421200	0.03532000	-0.67030700
H	-2.06325200	-1.58245500	-0.08321500
C	-0.76805500	-0.25029600	1.10466800
H	-0.92324900	0.66153700	1.69547500
H	-0.54950700	-1.06312500	1.80865600
Si	0.74320100	0.02331000	-0.01777500
C	2.28525700	0.18698600	1.05325000
H	2.47860000	-0.73428000	1.61285700
H	3.16938300	0.39808800	0.44240900
H	2.17913800	1.00170300	1.77724900
C	0.92239600	-1.44381700	-1.18565300
H	1.01491000	-2.38590100	-0.63447800
H	0.05309100	-1.52413500	-1.84675300
H	1.81178400	-1.33855300	-1.81589500
C	0.46364000	1.59959700	-1.00564100
H	0.43077400	2.47661400	-0.35032200
H	1.26073100	1.75948700	-1.73901400
H	-0.48820700	1.54741600	-1.54447300

BPTM

C	2.48826500	6.22330000	1.92167600
C	1.67310500	5.29083100	1.33139600
C	2.21288100	4.09404400	0.79033000
C	3.61262200	3.86379700	0.91715100
C	4.43139100	4.85747800	1.51586100
C	3.88476200	6.01479700	2.00333200
H	2.05642900	7.12892200	2.33542500
H	0.60321800	5.45992700	1.28358900
C	1.40071300	3.09127800	0.16132300
C	4.16734700	2.62576600	0.50644500
H	5.49909700	4.67148600	1.59354100
H	4.51684000	6.76567600	2.46631700
C	3.38835700	1.62234100	-0.01705400
C	2.01129800	1.91683300	-0.20766700

H	5.23286800	2.46025600	0.64619700
C	-0.06741800	3.24871300	-0.04408800
C	-0.61588300	4.35757700	-0.77412000
C	-0.94134300	2.29081800	0.41903600
C	0.19658800	5.32680800	-1.42008600
C	-2.02848200	4.47307200	-0.89479400
C	-2.35128100	2.36013800	0.27506500
C	-0.36783900	6.37373000	-2.10422900
H	1.27569500	5.22821500	-1.38158900
C	-2.58250700	5.57626200	-1.59497000
C	-2.86507400	3.46472700	-0.35523400
C	-1.77275200	6.51189000	-2.18277000
H	0.27168400	7.09938900	-2.59673100
H	-3.66393500	5.65343100	-1.66685600
H	-3.94189700	3.55776300	-0.47341500
H	-2.20475400	7.34907500	-2.72145600
P	0.41258800	0.04764800	0.32639900
C	-0.36383200	-1.27501800	-0.43645500
O	-0.44960200	1.15734600	1.07844300
O	1.21774600	0.89562600	-0.75411300
S	-0.18158100	-2.88229400	0.16115400
S	-1.41297000	-0.93639300	-1.77022500
O	-0.52152900	-3.85885300	-0.84677300
O	1.09177700	-2.96292500	0.89826400
C	-1.45502900	-2.99126000	1.49654400
F	-1.30557700	-4.11853400	2.16509600
F	-1.26450200	-1.95648000	2.31921900
F	-2.65964600	-2.92645000	0.96718800
C	-0.43091500	-1.39044900	-3.27357600
F	0.77228200	-0.82844700	-3.18519400
F	-0.30758000	-2.69534200	-3.38406000
F	-1.06286600	-0.90459200	-4.33103100
O	-2.59201400	-1.77672300	-1.77884300
O	-1.49713700	0.52177100	-1.82741100

C	-3.22128300	1.23017800	0.68706200
C	-4.14899600	0.72919100	-0.22638100
C	-3.11972400	0.62871900	1.94815600
C	-4.96681700	-0.34472100	0.11611200
H	-4.19114900	1.13974900	-1.23113900
C	-3.93832700	-0.44273300	2.27336900
H	-2.39497100	0.98925400	2.66949300
C	-4.87233300	-0.93713400	1.36473500
H	-5.48776900	-1.79435400	1.61795700
C	3.90345900	0.24550000	-0.23102600
C	3.49576500	-0.55335700	-1.30526200
C	4.75548900	-0.31302500	0.72711500
C	3.88649400	-1.88567800	-1.37703800
H	2.85664900	-0.14848300	-2.08118800
C	5.17333000	-1.63458000	0.61911100
H	5.06924500	0.27651400	1.58319400
C	4.72888600	-2.44159200	-0.42186700
H	5.03138900	-3.48105100	-0.48708600
C	3.30083900	-2.74479000	-2.46402300
C	6.04074200	-2.21692700	1.70142300
C	-3.82819800	-1.11524400	3.61277600
C	-5.96283500	-0.84436400	-0.89395000
F	6.78496300	-3.23107700	1.24563300
F	6.86924800	-1.29321400	2.21022100
F	5.30384900	-2.68636600	2.71711600
F	2.05830400	-3.13949400	-2.13998300
F	4.02866900	-3.84640800	-2.67485900
F	3.21161900	-2.08018700	-3.62322900
F	-2.78785500	-0.66450200	4.32254700
F	-3.67945100	-2.44529000	3.47531300
F	-4.93271300	-0.92852100	4.34823600
F	-6.40239800	-2.07183000	-0.59327100
F	-7.03773600	-0.03815600	-0.94587900
F	-5.44086500	-0.87662200	-2.12312500

O	1.35193900	-0.43799500	1.47556700
H	1.54739200	-1.41537200	1.42178500

NTPA

C	1.52701100	5.54093700	2.72648600
C	0.91775100	4.54475600	2.00664400
C	1.64615700	3.39689200	1.59436100
C	3.01365600	3.29163200	1.97288400
C	3.61899200	4.34539500	2.70639300
C	2.89550200	5.44945000	3.07225500
H	0.95138300	6.40669800	3.03801900
H	-0.13431800	4.62312000	1.75476800
C	1.04520900	2.34019400	0.83050600
C	3.74509100	2.12435500	1.63724400
H	4.66628700	4.25142700	2.98031100
H	3.36478400	6.24912100	3.63609600
C	3.14852200	1.06710600	0.99995600
C	1.78509700	1.19812400	0.61712000
H	4.78940600	2.05179600	1.93107200
C	-0.33140400	2.46040800	0.27390900
C	-0.70897800	3.52978600	-0.60691900
C	-1.26153200	1.48138700	0.53297200
C	0.20563100	4.52026900	-1.05392000
C	-2.04135400	3.56556300	-1.10791600
C	-2.59267900	1.48854200	0.04303400
C	-0.19815100	5.51208400	-1.91160700
H	1.23751100	4.48049100	-0.72416900
C	-2.43202700	4.61486200	-1.98057800
C	-2.95759900	2.54357200	-0.75622000
C	-1.53393700	5.57224100	-2.37114300
H	0.51848600	6.25424100	-2.24880200
H	-3.45651600	4.63282500	-2.34193700
H	-3.97300900	2.59393200	-1.14177900
H	-1.83864600	6.36737800	-3.04383300

P	-0.03918800	-0.68451300	0.38048600
O	-0.85572500	0.35872200	1.27048600
O	1.24589500	0.13515000	-0.10603500
S	-0.45378300	-1.51741700	-2.33290000
C	-0.88573900	0.12750200	-3.04328900
F	-2.18931300	0.36278500	-2.91313000
F	-0.21832100	1.08988000	-2.40849500
F	-0.56729200	0.15080600	-4.32686400
O	0.98175700	-1.64779000	-2.51178100
O	-1.36965000	-2.45148800	-2.94558900
C	-3.53857400	0.39331600	0.37219300
C	-4.30163100	-0.19807700	-0.63218900
C	-3.69333400	-0.04962800	1.69209200
C	-5.21125200	-1.20669500	-0.32072900
H	-4.17030300	0.10506000	-1.66641300
C	-4.60215600	-1.05398200	1.98704800
H	-3.10959800	0.39831900	2.48893200
C	-5.37203900	-1.64194500	0.98473300
H	-6.08294300	-2.42628100	1.22228400
C	3.87548000	-0.19029200	0.68869100
C	4.96122400	-0.21001900	-0.18752300
C	3.43627500	-1.38887900	1.24438100
C	5.56676000	-1.41817000	-0.51910700
H	5.31316500	0.71382200	-0.63610800
C	4.01996700	-2.59323900	0.87173000
H	2.62274000	-1.37988800	1.96299800
C	5.08813900	-2.62425000	-0.01482000
H	5.53415200	-3.56604900	-0.31550800
C	6.77336600	-1.42312700	-1.41806400
C	3.41456000	-3.84967000	1.42332200
C	-4.75629200	-1.55797400	3.39492500
C	-5.99231500	-1.83029400	-1.44465100
F	3.39790600	-3.85035100	2.75977600
F	2.11316800	-3.96066600	1.03385800

F	4.03780600	-4.95008500	1.01011200
F	6.82750100	-2.53327600	-2.16290200
F	7.90787800	-1.37053000	-0.70359700
F	6.77802200	-0.36956000	-2.24415100
F	-4.15451400	-0.75806000	4.28426200
F	-4.22849000	-2.78293800	3.53367300
F	-6.04887000	-1.65195500	3.73873000
F	-6.91693900	-2.68865900	-0.99481200
F	-6.62713800	-0.89282100	-2.16691500
F	-5.19228000	-2.49294000	-2.28490900
N	-0.85711500	-1.30872500	-0.78610900
O	0.37763200	-1.69775800	1.52040500
H	0.66381000	-2.57073700	1.18912400

CPA

C	1.35414100	5.20505900	2.60218000
C	0.74850900	4.26652600	1.80595200
C	1.46826600	3.13086800	1.34732400
C	2.82072200	2.97532700	1.75678900
C	3.42296200	3.96961900	2.57204300
C	2.70920800	5.06386700	2.98326100
H	0.78571500	6.06229800	2.94896000
H	-0.29461400	4.37957100	1.53111200
C	0.87446700	2.12625100	0.51445900
C	3.54084400	1.82284700	1.35784700
H	4.45935000	3.83734100	2.87073500
H	3.17459400	5.81744500	3.61043800
C	2.95315800	0.81183800	0.63606400
C	1.59350500	0.97930900	0.25269200
H	4.57884200	1.72094100	1.66541700
C	-0.48550200	2.29279900	-0.06629300
C	-0.82929400	3.41389500	-0.89375900
C	-1.43176100	1.31532100	0.13579300
C	0.10942200	4.41184000	-1.26910100

C	-2.15727000	3.51356200	-1.39597000
C	-2.75471100	1.37970500	-0.37724900
C	-0.26712800	5.46731700	-2.06037800
H	1.13680600	4.32874800	-0.93333100
C	-2.51974400	4.62670500	-2.19986600
C	-3.09381500	2.48893100	-1.11392200
C	-1.59848600	5.58739700	-2.52194300
H	0.46711700	6.21597200	-2.34101700
H	-3.54165200	4.69258300	-2.56347500
H	-4.10571400	2.58646000	-1.49980900
H	-1.88150700	6.43291900	-3.14048500
P	-0.16426500	-0.91659700	0.15483100
O	-1.08133200	0.19291800	0.87685500
O	1.00785200	-0.03061200	-0.50490600
O	0.20674300	-2.00457100	1.06255700
C	-3.72704800	0.28109200	-0.15496400
C	-4.50482600	-0.17247700	-1.22487600
C	-3.90487800	-0.30364100	1.10323900
C	-5.44125700	-1.18177700	-1.03621300
H	-4.35925100	0.24784800	-2.21467800
C	-4.84471700	-1.31384200	1.27727500
H	-3.30910600	0.02424700	1.94782700
C	-5.61853000	-1.76384200	0.21403100
H	-6.33961500	-2.56314600	0.35506300
C	3.74604900	-0.37429100	0.22035800
C	4.97380500	-0.18182800	-0.41861300
C	3.31033400	-1.67813100	0.46443400
C	5.74418800	-1.27212500	-0.80899400
H	5.31865700	0.82553500	-0.63413700
C	4.08480900	-2.75840800	0.05398400
H	2.37254400	-1.86324200	0.98138200
C	5.30454400	-2.57166100	-0.58416100
H	5.89830400	-3.42097000	-0.90232800
C	7.08420400	-1.02724300	-1.44359100

C	3.54150200	-4.14110700	0.28950300
C	-5.07359700	-1.90130400	2.64374400
C	-6.29865500	-1.65722100	-2.17619100
F	4.43781800	-5.08945700	-0.01667700
F	3.18433000	-4.31447200	1.56728700
F	2.44983800	-4.36387000	-0.45694300
F	7.49755900	-2.07966700	-2.16050200
F	8.02565900	-0.78189800	-0.51923000
F	7.05417500	0.03750600	-2.25863800
F	-4.01384900	-1.73419200	3.44087000
F	-5.33303100	-3.21435400	2.56987200
F	-6.12489900	-1.32797200	3.24841800
F	-6.31266400	-2.99586500	-2.24645300
F	-7.57092400	-1.26262700	-2.02430100
F	-5.87104600	-1.19018400	-3.35603700
O	-0.94339700	-1.33804500	-1.16971000
H	-1.22263300	-2.26670200	-1.12083300

ComI1B

C	0.35362500	3.84516200	-0.60123300
H	0.37753800	4.23311100	-1.62316800
C	1.74345200	3.93439800	-0.00380000
C	1.99624900	3.53400900	1.31674000
C	2.79833700	4.43636900	-0.77717200
C	3.27968500	3.63728000	1.85109100
H	1.19244400	3.13420300	1.92953800
C	4.08265800	4.54448600	-0.23812800
H	2.60964100	4.73397500	-1.80538800
C	4.32568300	4.14635400	1.07702000
H	3.46612900	3.31525900	2.87149000
H	4.89240900	4.93811200	-0.84708600
H	5.32481600	4.22279800	1.49551200
O	0.00361100	2.41978800	-0.72741300
H	-0.96780400	2.29712700	-0.66159600

C	-0.70191700	4.54619500	0.20179600
H	-0.81755800	4.21542500	1.23107200
C	-1.47881900	5.51737500	-0.30300700
H	-1.30772200	5.82838600	-1.33484000
C	-2.54653700	6.24512100	0.39729800
C	-3.06363300	7.41722500	-0.18084600
C	-3.08537700	5.81190700	1.62391900
C	-4.06901700	8.14807500	0.45008100
H	-2.66440500	7.75895500	-1.13337100
C	-4.09104500	6.54102600	2.25165400
H	-2.73386800	4.88923400	2.07684400
C	-4.58509100	7.71340700	1.67142900
H	-4.45015400	9.05426700	-0.01341300
H	-4.49781600	6.18831100	3.19566000
H	-5.37183400	8.27769400	2.16496200
C	3.15269500	-0.36306300	-5.29297500
C	2.91892600	0.98068500	-4.98707200
C	3.53771600	1.99804400	-5.70892500
C	4.41083000	1.66173400	-6.74512200
C	4.66873500	0.32541400	-7.07020800
C	4.02599500	-0.67932200	-6.32746100
H	2.65400600	-1.14493500	-4.72963200
H	3.33013900	3.03374500	-5.46316800
H	4.89563700	2.45350500	-7.31076300
H	4.21187600	-1.72358300	-6.56750400
C	5.59942800	-0.03719900	-8.20285200
H	6.32383300	-0.80037700	-7.89569000
H	5.04274800	-0.44685200	-9.05549000
H	6.15658900	0.83441700	-8.55934100
S	1.77978100	1.39807700	-3.66745800
O	0.62768900	0.49155100	-3.74795300
O	1.60397100	2.85862900	-3.69970300
N	2.63693200	0.93791100	-2.28500400
H	3.08650200	1.74712300	-1.85539700

H	1.99292000	0.50968100	-1.61907200
C	2.53879700	-5.99361200	-2.60667200
C	1.63923200	-5.25468300	-1.87007800
C	2.07698400	-4.39142300	-0.82770700
C	3.48692100	-4.27731200	-0.59991800
C	4.38710600	-5.07078000	-1.36244500
C	3.92631400	-5.91685700	-2.34307800
H	2.17692700	-6.63921700	-3.40209200
H	0.58259900	-5.32213800	-2.09700700
C	1.17810000	-3.60069700	-0.02381500
C	3.96997300	-3.35476700	0.35894900
H	5.45196500	-4.98135500	-1.16241600
H	4.62297700	-6.51401200	-2.92473200
C	3.13098800	-2.51468700	1.06571500
C	1.73501900	-2.67369500	0.83875800
H	5.04103700	-3.29305300	0.52844100
C	-0.30188300	-3.73705000	-0.18406700
C	-0.95565500	-5.00968600	-0.04465700
C	-1.07962900	-2.64573500	-0.54079600
C	-0.31891700	-6.14793000	0.51971700
C	-2.31973300	-5.13017000	-0.46187800
C	-2.42033700	-2.74056700	-1.01919900
C	-0.98828900	-7.34583300	0.64036900
H	0.70150000	-6.06148000	0.87571700
C	-2.97301300	-6.38774800	-0.34756700
C	-2.99013200	-4.00155400	-0.99347600
C	-2.32403600	-7.47396900	0.19141100
H	-0.48710700	-8.19908100	1.08879900
H	-4.00445500	-6.46870000	-0.68149100
H	-3.99068600	-4.13583300	-1.39256400
H	-2.83692700	-8.42709500	0.28460700
P	-0.01444400	-0.72914200	0.89100100
O	-0.49126200	-1.37102000	-0.51213200
O	0.87787200	-1.85052500	1.58993100

S	-2.20780500	1.00550500	1.76998300
S	-1.21298200	-1.04178900	3.72213600
O	-1.90089400	2.17838700	2.59805300
O	-2.14095500	1.14298000	0.29108700
C	-4.03617800	0.60765900	2.14428100
F	-4.74395400	1.10638000	1.13196900
F	-4.23141600	-0.70597000	2.22410500
F	-4.40303400	1.19466700	3.27200000
C	-1.77423100	-2.83963900	3.55739100
F	-2.82372200	-2.94770200	2.73880600
F	-0.78130100	-3.60332900	3.09045900
F	-2.11836900	-3.26591200	4.77362100
O	0.11906000	-1.14408700	4.32119100
O	-2.31113300	-0.36494400	4.42306600
C	-1.22708400	-0.40156800	2.09225100
C	3.67627900	-1.53123400	2.04241100
C	4.67738100	-0.59588600	1.66818300
C	3.23329800	-1.57122200	3.37259200
C	5.26072200	0.23786800	2.67630600
C	5.11880800	-0.41265200	0.30923800
C	3.78100700	-0.74540700	4.34459100
H	2.44472000	-2.26066600	3.65101700
C	6.29703600	1.16211300	2.33754100
C	4.80872600	0.15474300	4.02838900
C	6.10115700	0.47431200	-0.01186300
H	4.63758100	-0.97957200	-0.47941200
H	3.41223500	-0.80053100	5.36513800
C	6.74362900	1.27897500	0.98679600
C	6.88761700	1.98360200	3.34802300
C	5.41387500	0.99901900	5.02079300
H	6.40639800	0.59377200	-1.04876200
C	7.76788000	2.18828000	0.67653300
C	7.90877000	2.87985200	2.99082000
C	6.40955500	1.86937700	4.69820700

H	5.05642300	0.92469300	6.04484400
C	8.34476100	2.97731400	1.67004100
H	8.10558900	2.27292700	-0.35359900
H	8.35971500	3.50063200	3.76126100
H	6.86045800	2.49911600	5.46137600
H	9.13782200	3.67479000	1.41398100
C	-3.12132600	-1.58019000	-1.63579200
C	-4.47896800	-1.27170000	-1.35078100
C	-2.43181800	-0.81593000	-2.59215000
C	-5.12322500	-0.22180700	-2.08399700
C	-5.24739800	-1.94250600	-0.33427500
C	-3.04904400	0.21363600	-3.28624000
H	-1.39196800	-1.03159600	-2.80968300
C	-6.49760400	0.08944500	-1.84389700
C	-4.39862600	0.52309100	-3.06345600
C	-6.55549100	-1.64165700	-0.10522500
H	-4.75656700	-2.68035200	0.28909300
H	-2.47647400	0.77832100	-4.01710700
C	-7.23771400	-0.63069000	-0.85855500
C	-7.14313100	1.12540200	-2.58838000
C	-5.07021500	1.56307400	-3.79066900
H	-7.10284200	-2.16050900	0.67836800
C	-8.58911500	-0.31502900	-0.64365400
C	-8.49690700	1.40487500	-2.34073700
C	-6.38184800	1.84949700	-3.56750300
H	-4.50156800	2.11993400	-4.53140600
C	-9.21061900	0.69127700	-1.37970600
H	-9.14713900	-0.86549300	0.10997600
H	-8.98547500	2.19193600	-2.91012500
H	-6.87763400	2.63842600	-4.12812500
H	-10.25709700	0.92359800	-1.20135000
O	0.90053700	0.44275100	0.43586800
H	0.51225500	1.35138400	0.00215800

TS11

C	2.54239000	-3.51964500	0.49909100
H	2.63930700	-2.94071000	1.41436700
C	3.79399200	-4.09789400	-0.01021400
C	5.01290100	-3.59073200	0.47529200
C	3.81932600	-5.14082000	-0.95406800
C	6.22458000	-4.11119900	0.03322800
H	5.00117600	-2.76964600	1.18563300
C	5.03260600	-5.66187900	-1.39432800
H	2.89489000	-5.55198100	-1.34491600
C	6.23553200	-5.14945600	-0.90193500
H	7.15535700	-3.69728600	0.40770900
H	5.04006700	-6.46768000	-2.12260800
H	7.18078700	-5.55753000	-1.24957500
O	2.53986000	-1.88908700	-0.55646300
H	2.10399900	-2.14537900	-1.40391400
C	1.26583600	-4.15172800	0.30352400
H	1.11245700	-4.73958800	-0.59463100
C	0.27867000	-4.03236600	1.23049300
H	0.47669400	-3.41961300	2.10756000
C	-1.03221400	-4.66243400	1.20582400
C	-1.91297400	-4.40329300	2.27603300
C	-1.46320500	-5.50958700	0.16365900
C	-3.18511600	-4.96819200	2.30012600
H	-1.58932300	-3.74356700	3.07609000
C	-2.73193700	-6.07353000	0.19342200
H	-0.80975800	-5.71673100	-0.67709900
C	-3.59629100	-5.80435300	1.26085500
H	-3.86131400	-4.74377900	3.11907600
H	-3.05399000	-6.71928000	-0.61863800
H	-4.59129400	-6.24048500	1.27604200
C	0.70639800	-0.23395300	6.21778100
C	0.71874400	0.29032500	4.92324900
C	0.96547000	1.64537200	4.70117900

C	1.19967400	2.47936200	5.79349100
C	1.19390200	1.98105100	7.10329500
C	0.94416900	0.61282000	7.29621800
H	0.50043000	-1.28959500	6.36931700
H	0.95192400	2.04757800	3.69400800
H	1.38207800	3.53632000	5.61846600
H	0.93013100	0.20822800	8.30555100
C	1.43879000	2.88775100	8.28441400
H	1.69473700	3.90689400	7.96116300
H	0.54486800	2.95115800	8.92943300
H	2.26375900	2.51174300	8.91210100
S	0.50242300	-0.82890900	3.54262400
O	-0.19792600	-2.01801400	4.06588300
O	1.79505700	-1.01933000	2.85669800
N	-0.45137400	0.03888000	2.49350000
H	-0.15281600	-0.10455000	1.51699500
H	-1.44566500	-0.14683800	2.62049300
C	-0.30225100	5.79660200	3.07626600
C	-0.69796000	5.04878300	1.98909100
C	0.25060300	4.34967800	1.19153600
C	1.62751100	4.41082900	1.58050700
C	2.00714100	5.20857400	2.69539300
C	1.06516100	5.89383100	3.42759200
H	-1.04896000	6.31654200	3.67012800
H	-1.74989500	4.98403400	1.73908400
C	-0.11415800	3.56009100	0.04284300
C	2.59036700	3.66859200	0.85570600
H	3.06050500	5.25955000	2.96046500
H	1.36581000	6.50355300	4.27548000
C	2.24498500	2.82820500	-0.18622100
C	0.86711500	2.78528600	-0.55390800
H	3.63538400	3.75939200	1.13704500
C	-1.51855400	3.54889400	-0.46123300
C	-2.18771400	4.76635100	-0.84046600

C	-2.22117100	2.36170100	-0.57955500
C	-1.51646300	6.01483600	-0.95365600
C	-3.58191900	4.72252400	-1.16473900
C	-3.61792600	2.30210900	-0.84093400
C	-2.19089500	7.15443700	-1.33411600
H	-0.45174800	6.06343900	-0.75676600
C	-4.25240500	5.91868800	-1.53482300
C	-4.26958800	3.48378400	-1.11394000
C	-3.57582500	7.11357200	-1.61645800
H	-1.65017500	8.09257900	-1.42560800
H	-5.31302400	5.86626000	-1.76860800
H	-5.33704300	3.46649800	-1.31764100
H	-4.09684600	8.02050300	-1.91041800
P	-0.30839500	0.57548900	-1.23549600
O	-1.58387500	1.14397900	-0.37675200
O	0.51253200	1.93169100	-1.60296800
S	-0.49070000	-1.81696500	-3.14417800
S	-1.45327100	0.86448900	-4.03460200
O	-0.51131800	-2.06536900	-4.58348400
O	0.59211400	-2.41790400	-2.33579100
C	-2.01679200	-2.67383900	-2.46298800
F	-3.10045100	-2.30152700	-3.13727500
F	-1.85633000	-3.99911100	-2.58610700
F	-2.17304700	-2.37210300	-1.16839600
C	-0.06848800	1.37203000	-5.20878900
F	-0.61515500	2.05110800	-6.22144700
F	0.79987700	2.16867800	-4.57182600
F	0.58582800	0.31653700	-5.68778000
O	-2.40383400	0.11875100	-4.85995900
O	-1.85678400	2.12802900	-3.40152500
O	0.38108700	-0.34682900	-0.27246000
C	-0.70302900	-0.12631100	-2.79866900
H	1.84556800	-1.27436900	-0.19409800
C	3.30355000	2.09150200	-0.93156900

C	4.29943100	1.33689900	-0.25604000
C	3.39029200	2.24479700	-2.32453700
C	5.42444500	0.84655200	-0.99429400
C	4.22628600	1.01451000	1.14557900
C	4.45821700	1.73105100	-3.04743000
H	2.61514600	2.79629700	-2.84411100
C	6.48479100	0.16289400	-0.32277100
C	5.50488800	1.05336800	-2.40424700
C	5.22999600	0.34944400	1.78170100
H	3.33350200	1.28112800	1.69824300
H	4.50059200	1.87805400	-4.12367000
C	6.41237200	-0.07006800	1.08446300
C	7.62935000	-0.28417800	-1.05356400
C	6.65464600	0.57127800	-3.11663800
H	5.13573400	0.11194500	2.83853200
C	7.47999200	-0.71641400	1.73006300
C	8.67443100	-0.92269100	-0.36519100
C	7.67320200	-0.06107500	-2.47197400
H	6.69792400	0.73191500	-4.19113500
C	8.60121700	-1.13073700	1.01159700
H	7.42487100	-0.88520400	2.80298100
H	9.54962900	-1.25092300	-0.92090700
H	8.54248100	-0.41072000	-3.02380800
H	9.42418300	-1.61754000	1.52870000
C	-4.36061500	1.00752100	-0.84058700
C	-4.61181400	0.29540500	0.35834200
C	-4.86273800	0.51715100	-2.05209200
C	-5.38316400	-0.90749300	0.30886400
C	-4.14624200	0.74725300	1.64318600
C	-5.60311000	-0.65981800	-2.10497200
H	-4.64247200	1.05706700	-2.96749500
C	-5.67461100	-1.62710900	1.50871000
C	-5.88245000	-1.38775300	-0.94038200
C	-4.41566800	0.05480400	2.78646800

H	-3.58109200	1.67222000	1.69418500
H	-5.96607700	-1.02453800	-3.06224100
C	-5.19055100	-1.15461100	2.76615900
C	-6.46365900	-2.81822800	1.45873300
C	-6.66099000	-2.59548900	-0.96077700
H	-4.06697700	0.42848600	3.74709500
C	-5.50060700	-1.86902700	3.93501900
C	-6.75272900	-3.49664500	2.65393400
C	-6.94090100	-3.27736900	0.18308600
H	-7.02956500	-2.95217700	-1.91951600
C	-6.27634400	-3.02565300	3.87719800
H	-5.13323500	-1.50463800	4.89136700
H	-7.36262100	-4.39635800	2.61625400
H	-7.53873700	-4.18526600	0.15147400
H	-6.51623100	-3.56093200	4.79223700

IMH

C	-0.30566200	4.07764200	0.79127900
H	-0.43265900	3.31609100	0.02563600
C	-0.33769300	5.43853300	0.32636600
C	-0.67844000	5.66349600	-1.02688100
C	-0.04780800	6.54903500	1.15275800
C	-0.73328900	6.95636200	-1.53394100
H	-0.91194100	4.81137100	-1.65572700
C	-0.09636500	7.83615200	0.63864900
H	0.22798100	6.39710500	2.19154200
C	-0.44105300	8.04193300	-0.70431200
H	-1.00274200	7.11975500	-2.57291000
H	0.13377700	8.68466600	1.27627200
H	-0.47953300	9.05272200	-1.10138000
O	2.36719700	1.46836100	1.70169000
H	2.25232700	0.60014000	1.27704100
C	-0.14304300	3.63733700	2.09130400
H	-0.03315100	4.34530600	2.90674100
C	-0.17367400	2.26576100	2.33981400

H	-0.28767500	1.60572000	1.48346900
C	-0.12418600	1.61611400	3.61798400
C	-0.18611800	0.20255800	3.63462400
C	-0.02468700	2.31270100	4.84473100
C	-0.14515600	-0.49080800	4.83854500
H	-0.25714800	-0.32354500	2.68690200
C	0.01208000	1.61591500	6.04287900
H	0.02031300	3.39688800	4.85454600
C	-0.04680700	0.21525800	6.04092900
H	-0.18489500	-1.57605100	4.84355100
H	0.08713400	2.15470300	6.98288700
H	-0.01474100	-0.32472900	6.98359800
C	-6.25964900	2.94835600	1.61201800
C	-5.51973800	2.60355600	0.48192700
C	-6.13366700	2.48424200	-0.76729800
C	-7.50287500	2.70662100	-0.87314200
C	-8.27309300	3.05404700	0.24781500
C	-7.63106400	3.17172200	1.48630800
H	-5.76418200	3.03277200	2.57332500
H	-5.54634200	2.20230900	-1.63439200
H	-7.98441200	2.60603300	-1.84293700
H	-8.21046600	3.44135800	2.36617200
C	-9.76174400	3.27239500	0.11661000
H	-10.28770500	2.32132900	-0.03887300
H	-10.18016200	3.73923300	1.01370200
H	-9.99809200	3.91321600	-0.74055100
S	-3.74216600	2.44658200	0.63915600
O	-3.46171900	2.12599500	2.05103200
O	-3.11437700	3.63493200	0.03551900
N	-3.38205300	1.16436000	-0.36314100
H	-2.50511100	1.33289300	-0.86895300
H	-3.34740500	0.28794800	0.15706700
C	1.88254400	-4.65172100	4.70362600
C	2.09586000	-4.19865500	3.42003100

C	1.01272200	-4.01033400	2.51795500
C	-0.31273900	-4.28252900	2.98921500
C	-0.49724300	-4.76847800	4.31296800
C	0.57548300	-4.95097100	5.15554700
H	2.72677600	-4.77894200	5.37573800
H	3.10235400	-3.96856100	3.09087400
C	1.18645800	-3.51503300	1.17767600
C	-1.41741700	-4.06748800	2.12777300
H	-1.50837300	-4.98653200	4.64865900
H	0.42211900	-5.31897800	6.16636000
C	-1.27177700	-3.51394600	0.87026300
C	0.05362900	-3.19958300	0.44778400
H	-2.40926300	-4.34705800	2.47207600
C	2.54184900	-3.33988300	0.57883000
C	3.43960100	-4.46125100	0.47397300
C	2.96143300	-2.11248600	0.08855200
C	3.05125900	-5.79713500	0.77227200
C	4.77633200	-4.24128700	0.01316200
C	4.29954500	-1.86856900	-0.33618600
C	3.94114300	-6.84177400	0.65066700
H	2.03245200	-5.99754700	1.08212400
C	5.67513600	-5.33662300	-0.08593300
C	5.17621300	-2.93050000	-0.34618300
C	5.27150600	-6.61311500	0.22916700
H	3.61369600	-7.85366100	0.87374500
H	6.68822200	-5.14508500	-0.43125000
H	6.20222500	-2.76392200	-0.66364300
H	5.96409900	-7.44564100	0.14190400
P	0.59572100	-0.95910800	-0.64682200
O	2.09273600	-1.02538100	0.07830100
O	0.20732600	-2.54272400	-0.77441200
S	0.12874700	1.19974400	-2.74898800
S	1.48533100	-1.34271900	-3.53292700
O	-0.22944300	1.27062000	-4.16418300

O	-0.79465200	1.74864800	-1.73318700
C	1.60003800	2.35704700	-2.55023900
F	1.16849300	3.62372600	-2.66325900
F	2.13364700	2.20216700	-1.32451400
F	2.53263600	2.13823100	-3.46778900
C	0.13163300	-2.27265900	-4.45413100
F	-0.53112600	-3.07746500	-3.61480700
F	-0.73037000	-1.43550900	-5.02506900
F	0.71561400	-3.01848600	-5.39828900
O	2.12893000	-0.51632300	-4.55736000
O	2.24626600	-2.40027200	-2.85003600
O	-0.27869900	-0.17533300	0.26717400
C	0.68803900	-0.38374700	-2.30925600
H	2.96075800	1.93337900	1.09283600
C	-2.44011700	-3.37400100	-0.04249200
C	-3.63209700	-2.71045500	0.34463800
C	-2.38690900	-4.01022000	-1.29194900
C	-4.77814900	-2.77511800	-0.51322100
C	-3.74171300	-1.93502700	1.55411900
C	-3.48672100	-4.05032700	-2.13721400
H	-1.46592900	-4.49571100	-1.59549300
C	-6.00672900	-2.15877000	-0.12254800
C	-4.70366400	-3.46214100	-1.76251400
C	-4.90895800	-1.32868700	1.91366100
H	-2.86248000	-1.81778300	2.17776100
H	-3.41239600	-4.55823600	-3.09526100
C	-6.09168800	-1.43938200	1.10751700
C	-7.15911700	-2.25635800	-0.96283100
C	-5.87279500	-3.53075300	-2.59335100
H	-4.95220700	-0.72938300	2.81935800
C	-7.31194700	-0.85284200	1.47894700
C	-8.36022100	-1.65970200	-0.54652100
C	-7.04792000	-2.96174500	-2.20906000
H	-5.79837800	-4.05588300	-3.54244200

C	-8.43403600	-0.96839900	0.66117400
H	-7.36994800	-0.29834600	2.41173100
H	-9.23801700	-1.74190700	-1.18313400
H	-7.92684700	-3.02781100	-2.84587300
H	-9.37243400	-0.51289700	0.96602400
C	4.77858700	-0.51476600	-0.75942200
C	5.31786500	0.39673800	0.18139000
C	4.76784200	-0.18078700	-2.11808400
C	5.82508700	1.65460300	-0.27738000
C	5.39497000	0.10919200	1.58975900
C	5.25957000	1.04141700	-2.56648200
H	4.36321300	-0.89111000	-2.83009600
C	6.38058800	2.58807400	0.65129600
C	5.78872800	1.97812000	-1.66839600
C	5.93043000	0.99712500	2.47182900
H	5.01433700	-0.84289000	1.94437900
H	5.22555900	1.27549200	-3.62678300
C	6.43997000	2.26818700	2.04205600
C	6.88494100	3.84470500	0.19217100
C	6.30152400	3.24974700	-2.09962400
H	5.97273700	0.75565900	3.53111800
C	6.99164200	3.20043000	2.93631700
C	7.42607700	4.74457100	1.12423500
C	6.82245100	4.14122300	-1.21297000
H	6.26376300	3.48486000	-3.16053400
C	7.47750900	4.42390500	2.48003000
H	7.03633600	2.95481400	3.99465800
H	7.81002200	5.70001200	0.77461000
H	7.20684000	5.09898900	-1.55581600
H	7.90188200	5.13308200	3.18586700

IMH1'

C	-1.62847900	4.13841700	-0.47062100
H	-1.14751300	3.35371700	-1.04350300

C	-2.37787200	5.09270900	-1.23317700
C	-3.04003900	6.20637100	-0.65809700
C	-2.46600300	4.88750300	-2.63235100
C	-3.76097400	7.07796500	-1.45741000
H	-2.98188400	6.38211100	0.41154600
C	-3.19745000	5.76370600	-3.42554400
H	-1.95913700	4.03478900	-3.07366800
C	-3.84267300	6.85588700	-2.84118800
H	-4.26504600	7.93200900	-1.01486400
H	-3.26986100	5.59227300	-4.49468300
H	-4.41517100	7.54043200	-3.46112300
C	-1.44705300	4.09616900	0.90562900
H	-1.88043000	4.85837200	1.54664600
C	-0.72900400	3.03360200	1.44499900
H	-0.35489100	2.28464900	0.74842800
C	-0.43759900	2.79243900	2.82522200
C	0.26835200	1.60514300	3.14271400
C	-0.80731500	3.67559500	3.87139100
C	0.59529800	1.31759300	4.46227400
H	0.53469200	0.92608600	2.33814300
C	-0.47597400	3.37992700	5.18248000
H	-1.34496000	4.59169400	3.64782100
C	0.22743000	2.20167700	5.47892100
H	1.14334600	0.41100000	4.69632500
H	-0.75515700	4.06007700	5.98162000
H	0.48947800	1.97946300	6.50963700
C	-5.61532400	2.55634900	-0.19758800
C	-5.24483000	1.24194000	-0.48676400
C	-5.62148200	0.19001400	0.34741800
C	-6.36488400	0.46595100	1.49486300
C	-6.74710400	1.77594200	1.81229300
C	-6.36225500	2.81330900	0.94930500
H	-5.33027000	3.35697600	-0.87212200
H	-5.34676100	-0.82833900	0.09546000

H	-6.65404000	-0.35395400	2.14768600
H	-6.65841000	3.83510600	1.17686400
C	-7.58452200	2.06026300	3.03708800
H	-7.40763800	3.07108900	3.41989100
H	-8.65594500	1.98217500	2.80897300
H	-7.37186700	1.34819700	3.84125500
S	-4.28242800	0.90297600	-1.96296400
O	-4.55801000	1.94492000	-2.96133500
O	-4.47955200	-0.51396900	-2.29452300
N	-2.71684600	1.22656400	-1.42407200
H	-2.31828600	0.47032000	-0.86096700
H	-2.11536100	1.39540000	-2.23704800
C	4.55151800	-5.67276900	2.16633800
C	4.16981300	-4.64926300	1.32643200
C	2.80734200	-4.46539400	0.95781100
C	1.84072100	-5.35619600	1.52599400
C	2.26807900	-6.41392100	2.37360800
C	3.59692500	-6.57667400	2.68698300
H	5.59918900	-5.78341700	2.43289900
H	4.92054700	-3.96786300	0.94653400
C	2.35836500	-3.41026500	0.08147800
C	0.46663400	-5.15563700	1.25211800
H	1.51612300	-7.08648200	2.77948600
H	3.91319100	-7.38553100	3.33984600
C	0.01471800	-4.09816100	0.48982800
C	0.99398300	-3.22232300	-0.07088800
H	-0.25543200	-5.85453100	1.66554100
C	3.35741700	-2.49488300	-0.54518900
C	4.43395200	-2.98672900	-1.36114600
C	3.31251100	-1.13560700	-0.27820800
C	4.46363600	-4.31049000	-1.87610700
C	5.50133700	-2.09835300	-1.71023300
C	4.41644300	-0.26239800	-0.50719000
C	5.50101300	-4.73537300	-2.67649600

H	3.64158800	-4.98121200	-1.65340300
C	6.56664600	-2.57413800	-2.52058100
C	5.48685800	-0.76916100	-1.21652500
C	6.56984200	-3.86526500	-2.99532100
H	5.49347500	-5.74632400	-3.07450000
H	7.37429600	-1.89019000	-2.77010100
H	6.34870400	-0.13279100	-1.40021800
H	7.38363800	-4.21544800	-3.62426700
P	0.76483100	-0.60382300	-0.58145200
O	2.16370600	-0.59036100	0.29082600
O	0.51370500	-2.18367500	-0.85424100
S	0.83638300	-1.00216400	-3.67749000
S	0.85812400	1.69713000	-2.45525800
O	1.23299700	-0.17615600	-4.82520900
O	1.39763100	-2.33958500	-3.48229500
C	-1.01469900	-1.28990100	-3.93948400
F	-1.18606600	-2.34833500	-4.73558000
F	-1.61592900	-1.52626100	-2.76497200
F	-1.57762300	-0.21860000	-4.49897100
C	2.24953200	2.28429300	-3.62729800
F	3.26029000	1.41448400	-3.65858700
F	1.79207800	2.50287400	-4.84917200
F	2.69608100	3.44639700	-3.12467000
O	-0.37130200	2.15337500	-3.14992500
O	1.17703100	2.32916400	-1.15865200
O	-0.27962900	0.06406900	0.24962200
C	0.96025000	-0.01732000	-2.24350500
C	-1.44253900	-3.93341400	0.22247300
C	-2.38471700	-3.79316400	1.27388900
C	-1.89528400	-3.98270600	-1.10300300
C	-3.78097100	-3.74502100	0.95696200
C	-2.00746200	-3.67066800	2.65800900
C	-3.24645400	-3.91604400	-1.41393100
H	-1.16831800	-4.07324100	-1.90294000

C	-4.75403600	-3.62835700	1.99766500
C	-4.21153500	-3.81021600	-0.40248800
C	-2.93572200	-3.55547800	3.64765300
H	-0.95261100	-3.66045700	2.90814300
H	-3.56408400	-3.94144100	-2.45232500
C	-4.34192300	-3.54231000	3.36207500
C	-6.14808100	-3.59377500	1.67887100
C	-5.61709200	-3.76047400	-0.69430600
H	-2.61856900	-3.46195600	4.68388600
C	-5.31473000	-3.43366300	4.36918000
C	-7.08525800	-3.48541100	2.72055000
C	-6.54320800	-3.66361300	0.29889300
H	-5.92603000	-3.79557400	-1.73552600
C	-6.67100700	-3.40773900	4.04959000
H	-4.99644200	-3.36993600	5.40709600
H	-8.14494700	-3.46735400	2.47685900
H	-7.60387700	-3.62893300	0.06204100
H	-7.41116500	-3.32798200	4.84155400
C	4.46812300	1.12486400	0.03933700
C	4.41127000	1.38386400	1.43437300
C	4.66364700	2.19325600	-0.84352100
C	4.51198600	2.73356900	1.89970800
C	4.30626000	0.34084900	2.41986700
C	4.75202500	3.50597800	-0.39652900
H	4.71807700	1.98725600	-1.90523700
C	4.47100900	3.02054500	3.29968100
C	4.66992900	3.80601800	0.96905800
C	4.28173100	0.61400900	3.75417500
H	4.26550200	-0.68993400	2.08653800
H	4.87444300	4.31277200	-1.11459700
C	4.35347300	1.95936400	4.24747900
C	4.55990100	4.37091200	3.76175300
C	4.75138300	5.15282500	1.46195900
H	4.21911600	-0.19867700	4.47470200

C	4.32337300	2.26260900	5.61913400
C	4.51999400	4.62592700	5.14200000
C	4.69496100	5.42475400	2.79411900
H	4.86337700	5.95747800	0.73906900
C	4.40412300	3.58220100	6.05878100
H	4.24466700	1.45050400	6.33847700
H	4.58872900	5.65352900	5.49119900
H	4.76069100	6.44961400	3.15198600
H	4.38384500	3.79930500	7.12365200

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C	1.46608400	-3.81390900	-1.17329800
H	0.45942900	-3.49733600	-1.43046300
C	2.09206600	-4.72600700	-2.12906500
C	3.28343300	-5.42395500	-1.85158700
C	1.44947600	-4.94042500	-3.36533800
C	3.80681700	-6.31881000	-2.77736600
H	3.80668800	-5.26433500	-0.91473100
C	1.97653300	-5.83731600	-4.28868100
H	0.54502800	-4.38536200	-3.59771200
C	3.15415600	-6.52930300	-3.99572100
H	4.72656800	-6.85144500	-2.55376100
H	1.47193800	-5.99401100	-5.23740100
H	3.56710600	-7.22892300	-4.71727500
C	1.75357400	-3.81848000	0.23032100
H	2.68081700	-4.26198700	0.57590300
C	0.86507600	-3.28520200	1.11558000
H	-0.03484000	-2.82803600	0.70807900
C	0.98147700	-3.25779300	2.56363900
C	-0.07348000	-2.68951200	3.30542700
C	2.09280800	-3.77889400	3.26135200
C	-0.02727400	-2.65075100	4.69667600
H	-0.92926400	-2.27657800	2.77885800
C	2.13815300	-3.73605700	4.64882100

H	2.92360000	-4.21480700	2.71538700
C	1.07716700	-3.17446900	5.37034200
H	-0.85586900	-2.22094100	5.25050500
H	2.99676300	-4.14527100	5.17434700
H	1.11440500	-3.14851000	6.45612800
C	5.32405400	-2.29510300	-0.06839300
C	4.27216300	-1.43510900	-0.38182300
C	3.71821000	-0.57853900	0.57519100
C	4.22523400	-0.60883100	1.86970400
C	5.28424100	-1.46231700	2.21963200
C	5.82263000	-2.30067000	1.23492500
H	5.74613200	-2.93407800	-0.83679600
H	2.89992400	0.08896100	0.32556400
H	3.79874600	0.05422000	2.61684400
H	6.65014900	-2.95968400	1.48586200
C	5.82299600	-1.46077200	3.62937400
H	6.67560600	-2.13845600	3.73643600
H	6.14782000	-0.45492800	3.92025400
H	5.05042900	-1.77165100	4.34387600
S	3.68835600	-1.38260300	-2.06724400
O	4.35243300	-2.42617600	-2.84861500
O	3.65736000	0.00214800	-2.53906700
N	2.04015200	-1.90637600	-1.86764500
H	1.52627500	-1.26329700	-1.22741900
H	1.56973100	-1.87029100	-2.78431100
C	-3.72093900	5.82233700	2.59964000
C	-3.50134800	4.78701900	1.71708800
C	-2.20043100	4.51195200	1.20872400
C	-1.11974300	5.31947400	1.68811200
C	-1.38093300	6.39293700	2.58216600
C	-2.65624900	6.64817300	3.02755300
H	-4.72561300	6.00252000	2.97244500
H	-4.33511700	4.16774500	1.41230500
C	-1.91940500	3.44573500	0.27545600

C	0.20336900	5.01433100	1.29081000
H	-0.54413900	7.00097600	2.91767300
H	-2.84556200	7.46795900	3.71496000
C	0.49935400	3.93845200	0.47956800
C	-0.59406500	3.16307600	-0.01400200
H	1.01388900	5.64117500	1.65240500
C	-3.04532900	2.61354100	-0.24326000
C	-4.17833800	3.19255700	-0.91267300
C	-3.07076700	1.25134000	0.01085200
C	-4.17004500	4.51757200	-1.42418300
C	-5.34729500	2.39155500	-1.11691100
C	-4.26215000	0.47110400	-0.05408700
C	-5.26616400	5.02719300	-2.08446100
H	-3.27480400	5.11882200	-1.31398900
C	-6.46832000	2.95410300	-1.78374100
C	-5.37423900	1.06459400	-0.61666500
C	-6.43182200	4.24485800	-2.25848600
H	-5.23142100	6.03675300	-2.48443400
H	-7.35294300	2.33740800	-1.92334500
H	-6.30267100	0.50210100	-0.67163200
H	-7.29058500	4.66152300	-2.77749400
P	-0.66411500	0.56564000	-0.69691700
O	-1.89355300	0.60424900	0.39292500
O	-0.26215100	2.12417600	-0.87178100
S	-1.23137000	1.25933200	-3.69232500
S	-1.37479900	-1.52831500	-2.68472000
O	-1.94256100	0.58695300	-4.78749900
O	-1.58041700	2.62217000	-3.28809900
C	0.53952700	1.39303200	-4.32193300
F	0.59083500	2.34150200	-5.26113400
F	1.36679400	1.72163300	-3.32230000
F	0.93858600	0.23267000	-4.84608000
C	-3.03233900	-1.84182200	-3.57927800
F	-3.91717100	-0.88265700	-3.30357900

F	-2.86764700	-1.96078200	-4.88530600
F	-3.49556400	-3.00718500	-3.09956900
O	-0.37523800	-2.07205000	-3.63664100
O	-1.51635200	-2.22654200	-1.38865300
O	0.43352200	-0.27689100	-0.12661200
C	-1.18777800	0.15809600	-2.34115700
C	1.91568100	3.65111000	0.11301300
C	2.90613000	3.41830100	1.10314100
C	2.29090600	3.68448300	-1.23655500
C	4.27393500	3.27172000	0.70213700
C	2.60362500	3.29784900	2.50639700
C	3.61175100	3.51580000	-1.62942500
H	1.52763400	3.84750700	-1.98833300
C	5.29658600	3.07122100	1.68062400
C	4.62591500	3.32396900	-0.68035500
C	3.57911500	3.10130200	3.43718000
H	1.56819400	3.35937800	2.82167600
H	3.86707700	3.53627900	-2.68516500
C	4.96181100	2.99534000	3.06680200
C	6.66242100	2.94104300	1.27787700
C	6.00416600	3.17772600	-1.05631300
H	3.31746700	3.01697000	4.48966400
C	5.98322800	2.80499800	4.01265600
C	7.64994600	2.75466400	2.25902300
C	6.97808100	3.00074000	-0.12243300
H	6.25326000	3.21147600	-2.11384000
C	7.31309700	2.68953300	3.61015700
H	5.72466500	2.75569000	5.06792900
H	8.68855300	2.66132400	1.95095600
H	8.01773100	2.89527200	-0.42303300
H	8.09273300	2.55053800	4.35461500
C	-4.36049900	-0.89542200	0.53777300
C	-4.15250000	-1.11954200	1.92495600
C	-4.76580300	-1.96325800	-0.27097200

C	-4.33124400	-2.43755100	2.45475100
C	-3.81426200	-0.06702900	2.84638500
C	-4.92800800	-3.24649400	0.23744300
H	-4.93750400	-1.78252300	-1.32439200
C	-4.15246200	-2.68572000	3.85167300
C	-4.71054700	-3.51404600	1.59511500
C	-3.65330700	-0.30213900	4.17796500
H	-3.69990800	0.94227800	2.46844500
H	-5.22132600	-4.05633200	-0.42579800
C	-3.81116600	-1.61547800	4.73347000
C	-4.32667000	-4.00371100	4.37828800
C	-4.87025900	-4.82916400	2.15105500
H	-3.40627000	0.51728700	4.84891100
C	-3.65312300	-1.87827700	6.10551500
C	-4.15152900	-4.21969400	5.75467300
C	-4.68398600	-5.06539900	3.47813400
H	-5.14956100	-5.63879700	1.48103100
C	-3.82035200	-3.16772600	6.60726000
H	-3.40591200	-1.05792600	6.77550000
H	-4.28357300	-5.22304800	6.15227900
H	-4.81069500	-6.06622400	3.88400200
H	-3.69689200	-3.35369500	7.67090400

TSI2S

C	1.07396100	-3.67671500	0.53079600
H	1.35957800	-2.81035500	1.11924300
C	2.18547900	-4.56306600	0.19003400
C	2.01551500	-5.79322000	-0.47288000
C	3.47791000	-4.17384800	0.59530000
C	3.10933700	-6.61695400	-0.70984500
H	1.03248300	-6.09557000	-0.81775800
C	4.56875800	-5.00581600	0.36265900
H	3.61300600	-3.22001500	1.09904600
C	4.38520200	-6.22749600	-0.28870500

H	2.97203200	-7.56209800	-1.22698200
H	5.55816300	-4.69471100	0.68195400
H	5.23663000	-6.87653500	-0.47451500
C	-0.26570900	-4.14316200	0.74538400
H	-0.58458800	-5.06837900	0.27660100
C	-1.08275100	-3.46607000	1.59970500
H	-0.69113300	-2.55477000	2.04770200
C	-2.41849900	-3.83722400	2.03765700
C	-3.06255200	-2.99966700	2.97125800
C	-3.09279200	-4.99197600	1.58778300
C	-4.33801200	-3.30526200	3.43888100
H	-2.55388200	-2.10676100	3.32243400
C	-4.36427100	-5.29510600	2.05935300
H	-2.62041200	-5.65098900	0.86592900
C	-4.99093000	-4.45277800	2.98641700
H	-4.82115300	-2.64904200	4.15673900
H	-4.87022000	-6.19158800	1.71143900
H	-5.98461000	-4.69468000	3.35345600
C	-1.62658300	-4.48854700	-2.75575800
C	-1.21158000	-3.20203800	-2.40920500
C	-2.10952500	-2.25350300	-1.91009000
C	-3.43962700	-2.62446700	-1.73505200
C	-3.89003100	-3.91228900	-2.06720000
C	-2.96717400	-4.83165900	-2.58439500
H	-0.91140900	-5.19638500	-3.16114300
H	-1.77853500	-1.25524500	-1.64070300
H	-4.14125000	-1.89681000	-1.33909100
H	-3.30128000	-5.82839500	-2.86206100
C	-5.33250700	-4.29663100	-1.84648400
H	-6.01005800	-3.48211700	-2.12305100
H	-5.51260900	-4.51889300	-0.78655200
H	-5.60496800	-5.18554800	-2.42444900
S	0.49388400	-2.76494000	-2.69954600
O	1.24305000	-3.96482900	-3.07826400

O	0.56550100	-1.55284200	-3.51773500
N	1.04096400	-2.35094400	-1.09372300
H	0.53399400	-1.50544600	-0.73933600
H	2.03058600	-2.09460500	-1.18545500
C	0.43439500	5.66166500	-4.54593500
C	0.73298000	5.06226300	-3.34188500
C	-0.28307900	4.46142400	-2.54839300
C	-1.62113200	4.46882100	-3.05603900
C	-1.90079200	5.11556500	-4.29054600
C	-0.89652400	5.70374900	-5.02277500
H	1.23197200	6.10327000	-5.13710000
H	1.76042200	5.03441100	-2.99958600
C	-0.02158200	3.82113700	-1.28415300
C	-2.64527600	3.82561200	-2.32108900
H	-2.92665900	5.12258900	-4.65100000
H	-1.11869200	6.18809500	-5.96956700
C	-2.39138500	3.11388300	-1.16394300
C	-1.04397200	3.09956200	-0.69170700
H	-3.66618200	3.89423800	-2.68559100
C	1.32877500	3.92724900	-0.65709000
C	1.90840100	5.21501600	-0.38434700
C	2.07110100	2.79327700	-0.36020900
C	1.17003600	6.42840300	-0.45183000
C	3.28170200	5.28306600	0.01042500
C	3.46416000	2.83564200	-0.05164600
C	1.76534600	7.63736800	-0.16684500
H	0.11820300	6.39515600	-0.71061200
C	3.87256900	6.54796400	0.27670400
C	4.03030400	4.08683500	0.11410900
C	3.13294400	7.70389200	0.18956500
H	1.17601400	8.54918500	-0.20980700
H	4.92040000	6.58046400	0.56528300
H	5.09232000	4.15718500	0.33203100
H	3.59049000	8.66543100	0.40514600

P	0.21070400	1.10701300	0.50636300
O	1.46381100	1.54548000	-0.45132100
O	-0.78399200	2.38413300	0.47248900
S	-0.16321100	1.95000600	3.48557800
S	1.51717800	-0.35551000	2.70318000
O	0.58649100	1.73994200	4.72968300
O	-0.55607900	3.29332500	3.05885200
C	-1.81239900	1.06667200	3.79477900
F	-2.68866400	1.93485600	4.31487000
F	-2.31361900	0.58341800	2.64599300
F	-1.65752900	0.04776300	4.64493300
C	2.94446200	0.14996700	3.86325900
F	3.29011400	1.42376700	3.68648200
F	2.62455200	-0.06691100	5.12943400
F	3.98218500	-0.63640100	3.54290800
O	0.74861300	-1.32687400	3.50392600
O	2.19745200	-0.85059000	1.48038000
O	-0.35150800	-0.14578200	-0.09337900
C	0.62952300	1.05441000	2.22568100
C	-3.51210400	2.49075100	-0.40602500
C	-4.46121300	1.64075900	-1.03430900
C	-3.68644800	2.82955300	0.94471700
C	-5.60587100	1.20177100	-0.29246700
C	-4.32233300	1.17053800	-2.38883200
C	-4.78549000	2.38884000	1.66927800
H	-2.94764300	3.45621900	1.43329700
C	-6.59647400	0.37701900	-0.91164200
C	-5.77002000	1.58903600	1.07186300
C	-5.26561300	0.38280600	-2.97675200
H	-3.43343500	1.44356400	-2.94572300
H	-4.88574700	2.66903400	2.71429400
C	-6.44478000	-0.03138600	-2.27172900
C	-7.74798100	-0.04320000	-0.17455600
C	-6.93292900	1.14683600	1.78906200

H	-5.12742300	0.04109300	-3.99978700
C	-7.43460100	-0.83419900	-2.86414000
C	-8.71179200	-0.84404300	-0.80892000
C	-7.87984600	0.37030900	1.19487500
H	-7.04259500	1.45315100	2.82663600
C	-8.55614800	-1.23289600	-2.13837800
H	-7.31846100	-1.13672600	-3.90222800
H	-9.58890300	-1.15816300	-0.24822400
H	-8.75768800	0.04803400	1.74988400
H	-9.31546100	-1.84881600	-2.61291900
C	4.34193700	1.63665900	0.08550000
C	4.48038900	0.64204700	-0.91976600
C	5.15525800	1.56456400	1.22656600
C	5.43755600	-0.40908100	-0.73419800
C	3.72806500	0.65014300	-2.14621600
C	6.08286800	0.54823100	1.40914000
H	5.03414900	2.31704100	1.99809600
C	5.60449500	-1.42045000	-1.73208400
C	6.24789500	-0.45095800	0.44183400
C	3.86667700	-0.32908900	-3.08360600
H	3.02626800	1.45384700	-2.32765700
H	6.68547100	0.52116500	2.31346500
C	4.80426600	-1.40219300	-2.91416100
C	6.57502500	-2.45620500	-1.55740200
C	7.21207800	-1.50490800	0.59359400
H	3.25975600	-0.30774500	-3.98436500
C	4.97036100	-2.41309000	-3.87587000
C	6.71530900	-3.43769000	-2.55141800
C	7.37389900	-2.45998200	-0.36300500
H	7.82181600	-1.51649400	1.49394700
C	5.91786300	-3.41749200	-3.69449600
H	4.34873500	-2.40088800	-4.76716600
H	7.45774500	-4.22130200	-2.41843100
H	8.11857900	-3.24349400	-0.24061200

H	6.03633300	-4.18989700	-4.44953700
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C	-2.29989500	2.68695100	-1.03432900
H	-2.30447400	2.86757800	0.04030200
C	-3.53211900	3.26382300	-1.68758200
C	-4.47313500	3.93946900	-0.90290000
C	-3.75305300	3.13927400	-3.06757900
C	-5.61226900	4.49495500	-1.48632600
H	-4.31796800	4.02296700	0.16950300
C	-4.89592100	3.68674000	-3.64741000
H	-3.04592700	2.59740300	-3.69046600
C	-5.82462600	4.37123700	-2.85955600
H	-6.33576600	5.01468700	-0.86467200
H	-5.06114600	3.57852800	-4.71582800
H	-6.71281600	4.80079900	-3.31525700
O	-2.44973000	1.17285700	-1.10239300
H	-2.27836100	0.82351600	-2.04239900
C	-1.00349500	3.11681100	-1.64078700
H	-0.89419500	2.97159700	-2.71241100
C	-0.03805700	3.69694400	-0.90724100
H	-0.20259100	3.78308100	0.16555700
C	1.24014200	4.23813100	-1.38541300
C	2.16757500	4.70056300	-0.43480300
C	1.58336100	4.32848100	-2.74746900
C	3.39758600	5.22641500	-0.82557500
H	1.91730200	4.63799000	0.62163500
C	2.80936900	4.85726400	-3.13782300
H	0.88783600	3.98514000	-3.50657700
C	3.72224900	5.30856500	-2.17976600
H	4.10264000	5.56845400	-0.07286900
H	3.05472700	4.92045300	-4.19472900
H	4.67808100	5.72234600	-2.48952500
C	0.54711800	3.49949200	5.19545400

C	0.77747500	2.79886400	4.01204500
C	2.01560300	2.86635000	3.36722900
C	3.02647700	3.64783000	3.92090100
C	2.81930300	4.37106300	5.10623000
C	1.57064000	4.27898600	5.73398000
H	-0.41481200	3.41937900	5.69026200
H	2.19427300	2.29104500	2.46496800
H	3.99495800	3.68474300	3.42789000
H	1.39576800	4.82022900	6.66062400
C	3.91368500	5.23970200	5.67941500
H	3.92043100	6.22884400	5.20251700
H	3.78081100	5.39662700	6.75456000
H	4.90254900	4.79715100	5.51884900
S	-0.57850800	1.88492800	3.27942400
O	-1.04936000	2.61856000	2.09115800
O	-1.52191400	1.56979600	4.36335100
N	0.16556500	0.50397800	2.71179300
H	0.06856400	-0.26777500	3.36687400
H	-0.14730500	0.25853800	1.76269900
C	0.64229500	-5.77030600	4.20494400
C	0.82462900	-5.25210700	2.94173000
C	-0.24553600	-4.62720400	2.24326800
C	-1.51238500	-4.51982200	2.90600200
C	-1.67042700	-5.07992900	4.20311200
C	-0.61926300	-5.69570300	4.84112300
H	1.47747900	-6.23773700	4.71941800
H	1.79942400	-5.31193300	2.47192500
C	-0.10227500	-4.06175600	0.92898300
C	-2.58320500	-3.84475300	2.26800200
H	-2.64103400	-5.00037800	4.68661600
H	-0.75070000	-6.11459500	5.83488600
C	-2.43938800	-3.23793900	1.03570400
C	-1.17030800	-3.35247000	0.40280200
H	-3.54326500	-3.79218900	2.77443200

C	1.16662400	-4.17443300	0.14762900
C	1.72632800	-5.44994400	-0.21072500
C	1.81883600	-3.03124100	-0.28935900
C	1.06502100	-6.68349600	0.04252400
C	2.98465700	-5.48804300	-0.89532700
C	3.07880700	-3.04335800	-0.94765700
C	1.63207700	-7.88281600	-0.32782400
H	0.09264000	-6.67434600	0.52096000
C	3.54981500	-6.74323400	-1.24830000
C	3.63819500	-4.27383900	-1.22354500
C	2.89265400	-7.91847800	-0.96893100
H	1.10202900	-8.81070200	-0.13119600
H	4.51017600	-6.75382600	-1.75797400
H	4.60360900	-4.31580500	-1.72099800
H	3.33076100	-8.87197800	-1.25032800
P	-0.10501100	-1.34943000	-0.82298800
O	1.24570300	-1.78116700	-0.03945600
O	-0.99459600	-2.71628800	-0.82906800
S	-0.62779900	-0.78442600	-3.61452400
O	-0.96668400	-1.97551800	-4.39015700
O	-1.74881800	0.19169900	-3.40185100
C	0.56939600	0.19234600	-4.65632000
F	-0.02407500	0.49214200	-5.81550900
F	0.91064000	1.32959200	-4.03907600
F	1.67196700	-0.51883700	-4.90462200
O	-0.73812100	-0.27094000	0.03782900
H	-1.73572100	0.66450400	-0.52961900
C	-3.58002300	-2.53572500	0.37903900
C	-4.19700600	-1.40273800	0.96637900
C	-4.07768200	-3.04173500	-0.83045400
C	-5.34657000	-0.82928500	0.33247700
C	-3.70008400	-0.76885600	2.15962700
C	-5.19059700	-2.48576600	-1.44813400
H	-3.58660100	-3.89732000	-1.28426900

C	-5.99300500	0.30757900	0.90816500
C	-5.85278200	-1.38681300	-0.88043700
C	-4.30625400	0.32485300	2.69909300
H	-2.80468400	-1.16391200	2.62579000
H	-5.55877800	-2.90739300	-2.37985700
C	-5.48064500	0.89586700	2.10373600
C	-7.15120800	0.86820800	0.28601700
C	-7.01786800	-0.80216000	-1.48397000
H	-3.88310500	0.79507200	3.58223300
C	-6.12835600	2.01582700	2.65047900
C	-7.76977400	1.98429400	0.87273600
C	-7.64091800	0.27114900	-0.92520400
H	-7.39309400	-1.23939200	-2.40607900
C	-7.26260100	2.55008000	2.04144500
H	-5.73289100	2.46169600	3.55967900
H	-8.65442600	2.40594000	0.40135700
H	-8.52236600	0.70184600	-1.39422900
H	-7.75554200	3.41326400	2.48117000
C	3.77396200	-1.78720100	-1.35840000
C	4.35968200	-0.90973400	-0.41352000
C	3.88711800	-1.50429000	-2.72447900
C	5.06159600	0.24668500	-0.87818400
C	4.30138900	-1.14171500	1.00461600
C	4.56108700	-0.37627500	-3.17967700
H	3.41301700	-2.17117200	-3.43729000
C	5.67377300	1.13944400	0.05416900
C	5.16267800	0.51215500	-2.27806800
C	4.88091900	-0.28770000	1.89283700
H	3.78322200	-2.02339900	1.36651700
H	4.61750400	-0.17486500	-4.24625500
C	5.58653200	0.88340900	1.45604900
C	6.38148200	2.29110100	-0.41094200
C	5.87945900	1.67784200	-2.71574600
H	4.81996100	-0.48586500	2.96026700

C	6.19881500	1.77289400	2.35575300
C	6.97659600	3.15203000	0.52501500
C	6.46249700	2.52635300	-1.82621900
H	5.94659200	1.86792500	-3.78418400
C	6.88547300	2.89408000	1.89237200
H	6.13815000	1.57038100	3.42249100
H	7.51866900	4.02527800	0.16986400
H	7.00413300	3.40288200	-2.17365600
H	7.36069000	3.56763700	2.60092500
N	0.26951200	-1.02641300	-2.33904000

TSI3

C	2.54239000	-3.51964500	0.49909100
H	2.63930700	-2.94071000	1.41436700
C	3.79399200	-4.09789400	-0.01021400
C	5.01290100	-3.59073200	0.47529200
C	3.81932600	-5.14082000	-0.95406800
C	6.22458000	-4.11119900	0.03322800
H	5.00117600	-2.76964600	1.18563300
C	5.03260600	-5.66187900	-1.39432800
H	2.89489000	-5.55198100	-1.34491600
C	6.23553200	-5.14945600	-0.90193500
H	7.15535700	-3.69728600	0.40770900
H	5.04006700	-6.46768000	-2.12260800
H	7.18078700	-5.55753000	-1.24957500
O	2.53986000	-1.88908700	-0.55646300
H	2.10399900	-2.14537900	-1.40391400
C	1.26583600	-4.15172800	0.30352400
H	1.11245700	-4.73958800	-0.59463100
C	0.27867000	-4.03236600	1.23049300
H	0.47669400	-3.41961300	2.10756000
C	-1.03221400	-4.66243400	1.20582400
C	-1.91297400	-4.40329300	2.27603300
C	-1.46320500	-5.50958700	0.16365900

C	-3.18511600	-4.96819200	2.30012600
H	-1.58932300	-3.74356700	3.07609000
C	-2.73193700	-6.07353000	0.19342200
H	-0.80975800	-5.71673100	-0.67709900
C	-3.59629100	-5.80435300	1.26085500
H	-3.86131400	-4.74377900	3.11907600
H	-3.05399000	-6.71928000	-0.61863800
H	-4.59129400	-6.24048500	1.27604200
C	0.70639800	-0.23395300	6.21778100
C	0.71874400	0.29032500	4.92324900
C	0.96547000	1.64537200	4.70117900
C	1.19967400	2.47936200	5.79349100
C	1.19390200	1.98105100	7.10329500
C	0.94416900	0.61282000	7.29621800
H	0.50043000	-1.28959500	6.36931700
H	0.95192400	2.04757800	3.69400800
H	1.38207800	3.53632000	5.61846600
H	0.93013100	0.20822800	8.30555100
C	1.43879000	2.88775100	8.28441400
H	1.69473700	3.90689400	7.96116300
H	0.54486800	2.95115800	8.92943300
H	2.26375900	2.51174300	8.91210100
S	0.50242300	-0.82890900	3.54262400
O	-0.19792600	-2.01801400	4.06588300
O	1.79505700	-1.01933000	2.85669800
N	-0.45137400	0.03888000	2.49350000
H	-0.15281600	-0.10455000	1.51699500
H	-1.44566500	-0.14683800	2.62049300
C	-0.30225100	5.79660200	3.07626600
C	-0.69796000	5.04878300	1.98909100
C	0.25060300	4.34967800	1.19153600
C	1.62751100	4.41082900	1.58050700
C	2.00714100	5.20857400	2.69539300
C	1.06516100	5.89383100	3.42759200

H	-1.04896000	6.31654200	3.67012800
H	-1.74989500	4.98403400	1.73908400
C	-0.11415800	3.56009100	0.04284300
C	2.59036700	3.66859200	0.85570600
H	3.06050500	5.25955000	2.96046500
H	1.36581000	6.50355300	4.27548000
C	2.24498500	2.82820500	-0.18622100
C	0.86711500	2.78528600	-0.55390800
H	3.63538400	3.75939200	1.13704500
C	-1.51855400	3.54889400	-0.46123300
C	-2.18771400	4.76635100	-0.84046600
C	-2.22117100	2.36170100	-0.57955500
C	-1.51646300	6.01483600	-0.95365600
C	-3.58191900	4.72252400	-1.16473900
C	-3.61792600	2.30210900	-0.84093400
C	-2.19089500	7.15443700	-1.33411600
H	-0.45174800	6.06343900	-0.75676600
C	-4.25240500	5.91868800	-1.53482300
C	-4.26958800	3.48378400	-1.11394000
C	-3.57582500	7.11357200	-1.61645800
H	-1.65017500	8.09257900	-1.42560800
H	-5.31302400	5.86626000	-1.76860800
H	-5.33704300	3.46649800	-1.31764100
H	-4.09684600	8.02050300	-1.91041800
P	-0.30839500	0.57548900	-1.23549600
O	-1.58387500	1.14397900	-0.37675200
O	0.51253200	1.93169100	-1.60296800
S	-0.49070000	-1.81696500	-3.14417800
S	-1.45327100	0.86448900	-4.03460200
O	-0.51131800	-2.06536900	-4.58348400
O	0.59211400	-2.41790400	-2.33579100
C	-2.01679200	-2.67383900	-2.46298800
F	-3.10045100	-2.30152700	-3.13727500
F	-1.85633000	-3.99911100	-2.58610700

F	-2.17304700	-2.37210300	-1.16839600
C	-0.06848800	1.37203000	-5.20878900
F	-0.61515500	2.05110800	-6.22144700
F	0.79987700	2.16867800	-4.57182600
F	0.58582800	0.31653700	-5.68778000
O	-2.40383400	0.11875100	-4.85995900
O	-1.85678400	2.12802900	-3.40152500
O	0.38108700	-0.34682900	-0.27246000
C	-0.70302900	-0.12631100	-2.79866900
H	1.84556800	-1.27436900	-0.19409800
C	3.30355000	2.09150200	-0.93156900
C	4.29943100	1.33689900	-0.25604000
C	3.39029200	2.24479700	-2.32453700
C	5.42444500	0.84655200	-0.99429400
C	4.22628600	1.01451000	1.14557900
C	4.45821700	1.73105100	-3.04743000
H	2.61514600	2.79629700	-2.84411100
C	6.48479100	0.16289400	-0.32277100
C	5.50488800	1.05336800	-2.40424700
C	5.22999600	0.34944400	1.78170100
H	3.33350200	1.28112800	1.69824300
H	4.50059200	1.87805400	-4.12367000
C	6.41237200	-0.07006800	1.08446300
C	7.62935000	-0.28417800	-1.05356400
C	6.65464600	0.57127800	-3.11663800
H	5.13573400	0.11194500	2.83853200
C	7.47999200	-0.71641400	1.73006300
C	8.67443100	-0.92269100	-0.36519100
C	7.67320200	-0.06107500	-2.47197400
H	6.69792400	0.73191500	-4.19113500
C	8.60121700	-1.13073700	1.01159700
H	7.42487100	-0.88520400	2.80298100
H	9.54962900	-1.25092300	-0.92090700
H	8.54248100	-0.41072000	-3.02380800

H	9.42418300	-1.61754000	1.52870000
C	-4.36061500	1.00752100	-0.84058700
C	-4.61181400	0.29540500	0.35834200
C	-4.86273800	0.51715100	-2.05209200
C	-5.38316400	-0.90749300	0.30886400
C	-4.14624200	0.74725300	1.64318600
C	-5.60311000	-0.65981800	-2.10497200
H	-4.64247200	1.05706700	-2.96749500
C	-5.67461100	-1.62710900	1.50871000
C	-5.88245000	-1.38775300	-0.94038200
C	-4.41566800	0.05480400	2.78646800
H	-3.58109200	1.67222000	1.69418500
H	-5.96607700	-1.02453800	-3.06224100
C	-5.19055100	-1.15461100	2.76615900
C	-6.46365900	-2.81822800	1.45873300
C	-6.66099000	-2.59548900	-0.96077700
H	-4.06697700	0.42848600	3.74709500
C	-5.50060700	-1.86902700	3.93501900
C	-6.75272900	-3.49664500	2.65393400
C	-6.94090100	-3.27736900	0.18308600
H	-7.02956500	-2.95217700	-1.91951600
C	-6.27634400	-3.02565300	3.87719800
H	-5.13323500	-1.50463800	4.89136700
H	-7.36262100	-4.39635800	2.61625400
H	-7.53873700	-4.18526600	0.15147400
H	-6.51623100	-3.56093200	4.79223700

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C	1.32398200	-3.51359600	-1.27253000
H	0.41142800	-3.28874100	-0.73659700
C	1.96073300	-4.74992200	-0.92942900
C	1.37159100	-5.51990400	0.10364100
C	3.12722100	-5.23121000	-1.57231800
C	1.92990500	-6.73900600	0.46919800
H	0.48324400	-5.14016200	0.60035200

C	3.67510800	-6.44854700	-1.19957800
H	3.60333400	-4.64910100	-2.35452400
C	3.07622900	-7.20408200	-0.18108800
H	1.47480500	-7.32655500	1.26072900
H	4.56938100	-6.81494500	-1.69485000
H	3.51045600	-8.15855000	0.10525000
O	1.67128400	-2.42405100	1.24975300
H	2.59052200	-2.20238700	1.46333500
C	1.70547500	-2.60762900	-2.26241200
H	2.59500500	-2.78022300	-2.86069400
C	0.94257000	-1.46569500	-2.43672800
H	0.10584300	-1.32017600	-1.75609000
C	1.14823600	-0.42005900	-3.40243700
C	0.36541900	0.75212600	-3.27741700
C	2.08578800	-0.50986800	-4.45904600
C	0.52778900	1.80544600	-4.17140000
H	-0.33729800	0.81912800	-2.45175100
C	2.22906200	0.53725800	-5.35684900
H	2.68592800	-1.40632000	-4.57873800
C	1.45442700	1.69739400	-5.21129700
H	-0.05988900	2.71113100	-4.05700700
H	2.94068600	0.45928500	-6.17388300
H	1.57719300	2.51799200	-5.91305900
C	-4.42696100	-5.19133300	0.27005700
C	-4.11082200	-3.86024700	0.00702400
C	-5.09413300	-2.95782200	-0.40720500
C	-6.40408800	-3.40222000	-0.55465300
C	-6.75114800	-4.73796500	-0.29472000
C	-5.74609800	-5.62041900	0.11717500
H	-3.64950100	-5.87219400	0.59873300
H	-4.84012600	-1.91971400	-0.59313300
H	-7.16933500	-2.69755500	-0.87088500
H	-5.99649700	-6.65789000	0.32584100
C	-8.18302400	-5.19852100	-0.43446500

H	-8.25552400	-6.29069700	-0.43301800
H	-8.80109300	-4.82523300	0.39261200
H	-8.63287000	-4.82965200	-1.36338400
S	-2.40094400	-3.33482100	0.12054700
O	-1.91623900	-3.02937500	-1.24109100
O	-1.69202300	-4.36603800	0.90198900
N	-2.48226000	-1.89511600	0.93170100
H	-2.20086100	-1.96493400	1.91439200
H	-1.93408300	-1.17149900	0.44640000
C	1.33091500	6.17709900	-3.17662000
C	1.49847700	5.36395800	-2.07681600
C	0.38147700	4.78270600	-1.41574700
C	-0.92579700	5.04056300	-1.94440800
C	-1.06496900	5.89943300	-3.06952600
C	0.03683200	6.45913500	-3.67472300
H	2.20142300	6.60532600	-3.66639000
H	2.49642800	5.15344300	-1.70959200
C	0.50481300	3.92057400	-0.27294000
C	-2.05664200	4.42704900	-1.34848800
H	-2.06468400	6.09787500	-3.44881300
H	-0.08278100	7.11042000	-4.53623600
C	-1.94486100	3.52384500	-0.30756100
C	-0.63129900	3.27906800	0.19486900
H	-3.04211500	4.67205400	-1.73451400
C	1.81215500	3.67734800	0.40744100
C	2.57390900	4.75969000	0.97214100
C	2.29374500	2.38303800	0.55735200
C	2.09814000	6.09998100	1.01999700
C	3.85104100	4.48144000	1.55840600
C	3.57237400	2.09409300	1.11302300
C	2.85572000	7.10501900	1.57953700
H	1.11593600	6.32756100	0.62329600
C	4.61476500	5.54334100	2.11346500
C	4.32532700	3.14654400	1.58837200

C	4.13311100	6.83133500	2.12211600
H	2.46357700	8.11792100	1.61132500
H	5.58579600	5.31227800	2.54491800
H	5.30662000	2.94825000	2.01188900
H	4.72181500	7.63481200	2.55598300
P	0.13184900	0.90030100	0.84499700
O	1.54193900	1.30902600	0.10107700
O	-0.48255000	2.37151200	1.23165600
S	-0.37279900	0.01029400	3.53858000
O	-1.05292700	1.22603600	3.99903900
O	-1.14110200	-1.25053200	3.53313600
C	0.99211400	-0.30088500	4.77202800
F	0.44931900	-0.58032000	5.95995400
F	1.76096200	-1.33329100	4.39539400
F	1.77230900	0.78349100	4.90296400
O	-0.69236900	0.16689800	-0.16701500
H	1.17088300	-1.68140900	1.64244300
C	-3.14401500	2.89189900	0.30932700
C	-4.14636300	2.25218000	-0.46778700
C	-3.31052000	2.97964600	1.70082100
C	-5.33582300	1.78155500	0.17813400
C	-4.01712900	2.01165300	-1.88158400
C	-4.45326100	2.50635600	2.32907100
H	-2.52778900	3.42843800	2.30135300
C	-6.37750500	1.16588900	-0.58351700
C	-5.49161800	1.92190000	1.59007800
C	-5.00431200	1.41374600	-2.60420300
H	-3.09532400	2.29783500	-2.37439900
H	-4.54713000	2.59187000	3.40818600
C	-6.22973000	0.98680200	-1.99254400
C	-7.57502000	0.72211600	0.06038200
C	-6.69977800	1.45723000	2.21114900
H	-4.86975300	1.23718200	-3.66884000
C	-7.26859100	0.38820500	-2.72410000

C	-8.59004100	0.13418600	-0.71302600
C	-7.69870900	0.89018200	1.48138100
H	-6.79871000	1.57001500	3.28791200
C	-8.43753500	-0.02844100	-2.08955200
H	-7.15028100	0.25253000	-3.79644300
H	-9.50358500	-0.19363900	-0.22251000
H	-8.60955000	0.54623100	1.96558500
H	-9.23518400	-0.48314500	-2.67127400
C	4.10704700	0.70087200	1.19567200
C	4.62860300	0.03824200	0.05834700
C	4.14707900	0.06487500	2.44151900
C	5.19709400	-1.26577600	0.20655300
C	4.62540300	0.63099100	-1.25195400
C	4.69448200	-1.20697000	2.59093800
H	3.71432600	0.56673300	3.29958800
C	5.73443400	-1.95003900	-0.92666000
C	5.23528000	-1.89107700	1.49103100
C	5.13357300	-0.02303600	-2.33269700
H	4.20485200	1.62380500	-1.36970100
H	4.69841000	-1.67974900	3.56961700
C	5.70171000	-1.33662200	-2.21630600
C	6.30884000	-3.25042600	-0.77597800
C	5.82002200	-3.19876700	1.61201800
H	5.11526300	0.44771900	-3.31251200
C	6.22638700	-2.03184500	-3.31937400
C	6.82518800	-3.90432200	-1.90699400
C	6.33439900	-3.84664200	0.53174200
H	5.84183200	-3.66266400	2.59498300
C	6.78073800	-3.30145100	-3.16379300
H	6.20700200	-1.56109000	-4.29961200
H	7.26951900	-4.89005200	-1.79049800
H	6.77436600	-4.83490500	0.64053400
H	7.18925900	-3.82140100	-4.02632200
N	0.53596800	0.18597000	2.22896600

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C	-0.46920000	4.46591900	4.98715000
C	-0.72568900	4.15165200	3.67046500
C	0.29722400	3.63882600	2.82668400
C	1.59829800	3.43474800	3.39079700
C	1.83383000	3.78524500	4.74766400
C	0.82438200	4.29200900	5.53259200
H	-1.27044900	4.84754500	5.61430700
H	-1.72421000	4.28357300	3.26959100
C	0.07268100	3.27525700	1.45378900
C	2.63292000	2.89833100	2.58418200
H	2.82923700	3.63099300	5.15699200
H	1.01372900	4.54861400	6.57123400
C	2.41029000	2.48220900	1.28589900
C	1.09047600	2.63361700	0.77151400
H	3.63174400	2.81759300	3.00415200
C	-1.21008700	3.58026100	0.75426400
C	-1.66302100	4.94262800	0.63998000
C	-1.96633900	2.57701400	0.16214900
C	-0.88080200	6.05788500	1.05153900
C	-2.93938300	5.20496700	0.04935900
C	-3.26316700	2.81756600	-0.38200500
C	-1.34920500	7.34627500	0.91506100
H	0.10634700	5.88979100	1.46500300
C	-3.40172400	6.54351400	-0.06300900
C	-3.71812800	4.11864800	-0.41719500
C	-2.62709800	7.59693300	0.36338100
H	-0.72598200	8.17922800	1.22938700
H	-4.37917600	6.71813800	-0.50650100
H	-4.70552400	4.32045300	-0.82410700
H	-2.98630400	8.61781700	0.26675500
P	-0.09507600	0.73732100	-0.47136400
O	-1.52407500	1.26457300	0.15797200

O	0.81361900	2.10875800	-0.48892400
S	-0.71602000	1.00679000	-3.31318500
C	0.88537000	1.52807100	-4.13564400
F	1.64420100	0.44351400	-4.43170900
F	0.62383300	2.16653600	-5.27900800
F	1.60107200	2.32919800	-3.34292200
O	-1.26204100	0.00631800	-4.25372400
O	-1.44445000	2.26922000	-3.12154200
O	0.42765600	-0.32344000	0.43414400
N	-0.22967700	0.25815600	-2.00569600
C	3.54434100	2.03774700	0.42727200
C	4.43901000	1.01009600	0.81984700
C	3.80017400	2.75090400	-0.75490300
C	5.63604400	0.79808300	0.06104900
C	4.18311400	0.13805400	1.93662900
C	4.94691300	2.53083100	-1.50580400
H	3.09550800	3.51362700	-1.07000100
C	6.58033000	-0.19431000	0.46904000
C	5.89953200	1.58276300	-1.10219300
C	5.07110900	-0.82834200	2.30614000
H	3.24646300	0.23014000	2.47450900
H	5.12682900	3.11916200	-2.40238200
C	6.31109700	-1.01558200	1.60617800
C	7.79904400	-0.37156900	-0.25836700
C	7.12940700	1.38067300	-1.81642000
H	4.83326500	-1.48088500	3.14180000
C	7.25239300	-1.98540400	1.98972000
C	8.71554800	-1.34731000	0.16959900
C	8.04216500	0.45501800	-1.40867300
H	7.32409500	1.99917400	-2.68978500
C	8.44172900	-2.14444500	1.28041100
H	7.04180500	-2.61191800	2.85276200
H	9.64893100	-1.47128600	-0.37509000
H	8.97645500	0.32582700	-1.95067100

H	9.16254100	-2.89360000	1.59738400
C	-4.15815500	1.74206300	-0.90713600
C	-4.78370100	0.79841900	-0.05483000
C	-4.48856400	1.76203900	-2.26909200
C	-5.75405100	-0.10177900	-0.60013400
C	-4.51587100	0.72775100	1.35676800
C	-5.42472200	0.88346800	-2.80357700
H	-3.97772600	2.46685200	-2.91493200
C	-6.41901500	-1.04376400	0.24426200
C	-6.08166200	-0.04983500	-1.98981400
C	-5.14750400	-0.17238000	2.16068200
H	-3.79477300	1.41586000	1.78338400
H	-5.65747100	0.92347100	-3.86493500
C	-6.11724600	-1.09423000	1.63919000
C	-7.39793100	-1.93474400	-0.29829800
C	-7.07705400	-0.94952000	-2.50583600
H	-4.93055300	-0.19786100	3.22618800
C	-6.78267200	-2.02834200	2.45141200
C	-8.03397500	-2.85458100	0.55182200
C	-7.70478100	-1.85139200	-1.70053800
H	-7.32489800	-0.88923500	-3.56323700
C	-7.72698300	-2.89994300	1.91096700
H	-6.55800700	-2.05832200	3.51495500
H	-8.78121300	-3.52760600	0.13787500
H	-8.46072900	-2.52046800	-2.10536800
H	-8.23445500	-3.61285400	2.55542800
C	1.84031100	-2.46375000	-2.74121300
H	1.58211500	-1.64265600	-3.40479400
C	3.24065800	-2.67554600	-2.52517900
C	3.75139900	-3.71240900	-1.70402800
C	4.14899900	-1.78850500	-3.15285700
C	5.11889100	-3.84605800	-1.52175300
H	3.07369400	-4.39039900	-1.19771100
C	5.51695600	-1.92940800	-2.96505200

H	3.75653600	-0.97993600	-3.76292500
C	6.00242500	-2.95595500	-2.14880700
H	5.50515100	-4.63263400	-0.88101000
H	6.20589700	-1.23001900	-3.42626300
H	7.07063600	-3.05277400	-1.98157500
C	0.78252900	-3.15747300	-2.17983800
H	0.96161800	-3.94500500	-1.45717200
C	-0.51393100	-2.77042900	-2.51269700
H	-0.62451200	-1.95481300	-3.22456800
C	-1.73165100	-3.32964500	-2.01964500
C	-2.94647800	-2.79843700	-2.52199200
C	-1.77773500	-4.37463200	-1.06183500
C	-4.16411000	-3.30909400	-2.09424900
H	-2.90387900	-1.97325800	-3.22793500
C	-2.99754300	-4.87506200	-0.63879500
H	-0.86029300	-4.77150700	-0.64057100
C	-4.18932000	-4.34572100	-1.15567300
H	-5.09318900	-2.89469200	-2.46989400
H	-3.02877200	-5.66639500	0.10307800
H	-5.14452900	-4.73219900	-0.81111500
C	-0.15696100	-4.97151400	3.04620900
C	0.14377700	-3.64767400	2.73030600
C	-0.86368500	-2.68993800	2.58306600
C	-2.19007600	-3.08058700	2.75219800
C	-2.52404100	-4.40188500	3.08897100
C	-1.49086400	-5.33890500	3.22482400
H	0.64721900	-5.69139900	3.15649300
H	-0.62249800	-1.66353200	2.32203100
H	-2.97821100	-2.34342400	2.62068600
H	-1.73076600	-6.36812700	3.48255800
C	-3.96234200	-4.79648400	3.32963000
H	-4.65092400	-4.21396800	2.70887100
H	-4.12768000	-5.86013900	3.12602500
H	-4.24469800	-4.62177900	4.37663700

S	1.86582700	-3.16814000	2.60736100
O	2.71301800	-4.36202100	2.73849700
O	2.08496700	-2.03617400	3.52300400
N	1.96787600	-2.69402400	0.98555300
H	1.41799000	-1.83364900	0.81878400
H	2.95257000	-2.47719100	0.81415000

TSI4R

C	0.52571600	6.31897700	-3.54770000
C	0.76983700	5.56055800	-2.42392400
C	-0.26796700	4.81117400	-1.80475400
C	-1.57183800	4.84505600	-2.39936500
C	-1.79371500	5.65153700	-3.54820100
C	-0.76994300	6.37624500	-4.11270800
H	1.33798400	6.87583200	-4.00704700
H	1.76966800	5.52057900	-2.00727600
C	-0.05348700	3.98774100	-0.64540400
C	-2.62021800	4.07780800	-1.83041700
H	-2.79135200	5.67434700	-3.98021800
H	-0.94998600	6.98357300	-4.99544000
C	-2.40770800	3.23642700	-0.75760900
C	-1.09188700	3.17772800	-0.22146300
H	-3.61757400	4.15718100	-2.25521300
C	1.24041100	3.97696200	0.09845700
C	1.76069000	5.18617400	0.68140500
C	1.94327500	2.79523100	0.29029800
C	1.04363600	6.41532500	0.68955100
C	3.04009600	5.15507100	1.32223000
C	3.23566300	2.75539600	0.88872700
C	1.57648100	7.54731500	1.26620600
H	0.05566400	6.45635800	0.24676500
C	3.56856700	6.34276400	1.89518600
C	3.75474600	3.93368800	1.38034900
C	2.85668600	7.51914500	1.86661500

H	1.00275400	8.47025900	1.26536600
H	4.54617300	6.29794700	2.36927700
H	4.74047300	3.92539700	1.83811700
H	3.26679400	8.42060800	2.31348100
P	0.00782400	0.93013600	0.28062500
O	1.43885600	1.59057800	-0.17892200
O	-0.84329700	2.24149800	0.78078800
S	0.57130500	0.21397700	3.03361000
C	-1.07723600	0.29250800	3.91474000
F	-1.75662600	-0.86086000	3.73532900
F	-0.88828800	0.46811100	5.22508400
F	-1.82690500	1.29418200	3.44372100
O	1.21534600	-0.98429500	3.59271300
O	1.18302700	1.53006500	3.27062200
O	-0.57468700	0.27407700	-0.93550500
N	0.12739200	-0.08149700	1.52742200
C	-3.54499200	2.51322600	-0.11571200
C	-4.29434300	1.52235900	-0.79412900
C	-3.93316700	2.90254900	1.17451300
C	-5.48416300	1.00647900	-0.18507900
C	-3.89069300	0.97700600	-2.06428200
C	-5.07613300	2.39189500	1.77679600
H	-3.33577300	3.64113600	1.70044700
C	-6.27909900	0.03595100	-0.86931600
C	-5.88682800	1.46297900	1.10674900
C	-4.63320100	0.02643300	-2.70048500
H	-2.95413700	1.31147200	-2.49657700
H	-5.36183100	2.73028000	2.76972700
C	-5.86436400	-0.46196600	-2.14222600
C	-7.49035400	-0.44559900	-0.28251000
C	-7.10710100	0.95925300	1.67419300
H	-4.28688100	-0.39231500	-3.64122100
C	-6.65901700	-1.41767300	-2.79649200
C	-8.25738400	-1.39334100	-0.97935700

C	-7.87822600	0.05596500	1.00713900
H	-7.40996900	1.32762900	2.65164400
C	-7.84386800	-1.87268700	-2.22116300
H	-6.33739100	-1.79980600	-3.76195000
H	-9.18316700	-1.75285900	-0.53615600
H	-8.80640900	-0.30502300	1.44446800
H	-8.44894100	-2.60841300	-2.74408100
C	4.04522400	1.50420200	1.00616400
C	4.68302000	0.91912200	-0.11541600
C	4.26751400	0.96940300	2.28156600
C	5.56206300	-0.19263000	0.08106700
C	4.51202200	1.41741100	-1.45419500
C	5.10761000	-0.12310200	2.47352700
H	3.75025500	1.40961100	3.12687800
C	6.24894500	-0.77324300	-1.02953300
C	5.77657200	-0.71507400	1.39330500
C	5.15914800	0.85741300	-2.51408200
H	3.85211300	2.26334400	-1.61264100
H	5.25576900	-0.51828900	3.47550300
C	6.05382500	-0.25330200	-2.34559200
C	7.14504500	-1.86993900	-0.82978600
C	6.68044900	-1.81978100	1.56298300
H	5.01327400	1.25605600	-3.51531000
C	6.74568900	-0.83362100	-3.42248600
C	7.81676500	-2.41515400	-1.93603600
C	7.33337100	-2.37242600	0.50379500
H	6.84412300	-2.19854000	2.56962200
C	7.61771000	-1.90146300	-3.21692100
H	6.59805600	-0.43346500	-4.42274000
H	8.50203800	-3.24528100	-1.78181100
H	8.02102900	-3.20205800	0.65072100
H	8.14908800	-2.33421900	-4.06037900
C	-1.91243300	-2.91144800	0.90628200
H	-1.61606000	-1.93430400	1.27971400

C	-3.31925000	-3.26361500	1.11051000
C	-3.87294300	-4.47756500	0.65811700
C	-4.13330200	-2.35867400	1.81882900
C	-5.20502600	-4.77628700	0.91948200
H	-3.27295200	-5.16034700	0.06701600
C	-5.46335700	-2.67003900	2.08882500
H	-3.70873600	-1.42654400	2.17978900
C	-6.00037700	-3.87719000	1.63803000
H	-5.62903600	-5.70828000	0.55714300
H	-6.08154400	-1.96451400	2.63430800
H	-7.04098900	-4.11634000	1.83893000
C	-0.86697300	-3.88819300	0.90545100
H	-1.11326300	-4.91651100	0.66021500
C	0.38608900	-3.52811700	1.30719400
H	0.54900600	-2.47907800	1.54919300
C	1.54123100	-4.39057500	1.47901700
C	2.73249400	-3.80551200	1.95636800
C	1.53277200	-5.77109700	1.18573500
C	3.88166100	-4.57506800	2.12069300
H	2.73733500	-2.74819300	2.20696800
C	2.67926200	-6.53562400	1.35797700
H	0.62616300	-6.24402000	0.82066700
C	3.85810600	-5.93875500	1.82218700
H	4.79521600	-4.10906600	2.47661400
H	2.66071800	-7.59807800	1.13119900
H	4.75388200	-6.54014300	1.95271400
C	0.49308800	-4.56753700	-2.45241500
C	0.03205300	-3.25023000	-2.43448900
C	0.91402600	-2.16574000	-2.47033100
C	2.28257700	-2.42273800	-2.48828300
C	2.78010000	-3.73566700	-2.49518100
C	1.86579900	-4.79807800	-2.48859400
H	-0.21562300	-5.38830800	-2.44233900
H	0.54837800	-1.14399800	-2.45602700

H	2.97577500	-1.58582700	-2.49609800
H	2.23382500	-5.82063200	-2.50473300
C	4.26511000	-3.99670600	-2.47750800
H	4.64864000	-3.96291800	-1.44994400
H	4.50241400	-4.98446600	-2.88597800
H	4.81573500	-3.24370500	-3.04886500
S	-1.72954700	-2.98989300	-2.47570500
O	-2.41352000	-4.27087700	-2.27100400
O	-2.08964000	-2.13945100	-3.61397400
N	-2.01806500	-2.06270500	-1.02648800
H	-1.41863700	-1.19709300	-1.00080800
H	-2.99246700	-1.74675200	-1.09363700

TSI4S

C	1.98322400	7.01352000	1.84149400
C	1.26398500	6.04682500	1.17356800
C	1.90767900	4.91476200	0.60122600
C	3.32383700	4.78988500	0.77561700
C	4.03977500	5.81439500	1.45282600
C	3.38771100	6.90749800	1.97339100
H	1.46477500	7.86483000	2.27433700
H	0.18811900	6.14279200	1.08792700
C	1.19929300	3.88396200	-0.11079600
C	3.98669400	3.63806100	0.28666100
H	5.11654400	5.70808000	1.56182400
H	3.94384900	7.68170700	2.49477700
C	3.30626400	2.59301500	-0.30783500
C	1.89657700	2.74271100	-0.47895600
H	5.06596300	3.57516600	0.39423100
C	-0.25676300	4.01328200	-0.41519900
C	-0.78065900	5.11844300	-1.17186600
C	-1.14135600	3.03539000	0.01121300
C	0.04680500	6.08767000	-1.80270000
C	-2.19817900	5.22850800	-1.34678600

C	-2.55462900	3.14183000	-0.12189100
C	-0.49786800	7.12192500	-2.53115400
H	1.12357000	5.99688700	-1.72246700
C	-2.72892300	6.31753100	-2.08914500
C	-3.05002200	4.24439900	-0.78656500
C	-1.89991800	7.24946700	-2.66806700
H	0.15744000	7.84271800	-3.01268700
H	-3.80788500	6.38938300	-2.20318000
H	-4.12520000	4.35676300	-0.89945400
H	-2.31602800	8.07323100	-3.24148400
P	0.10993100	0.78770900	-0.35362100
O	-0.63852700	1.88493200	0.61362000
O	1.22575500	1.70728300	-1.11271200
S	-1.19639500	0.73298900	-2.97155600
C	-0.08319900	-0.37430200	-3.98746700
F	-0.36212800	-1.67405100	-3.72922400
F	-0.26913000	-0.16106900	-5.29110900
F	1.20456700	-0.16173500	-3.68815900
O	-2.55217900	0.29236700	-3.35959300
O	-0.78642800	2.09952800	-3.30524000
O	0.64755200	-0.28741800	0.53518600
N	-0.88686400	0.22088800	-1.49537000
C	4.03122600	1.39108500	-0.80745000
C	4.91886200	0.65195900	0.01863100
C	3.87210800	1.01098200	-2.14943100
C	5.67035100	-0.42713200	-0.55151700
C	5.08611400	0.91139400	1.42558500
C	4.58266400	-0.04744700	-2.69749700
H	3.17787000	1.56240400	-2.77337600
C	6.59692700	-1.16617300	0.24917700
C	5.50034400	-0.77568800	-1.92571400
C	5.96741300	0.20614100	2.18709300
H	4.47752700	1.67990500	1.88731700
H	4.43562000	-0.31241700	-3.74139400

C	6.76872700	-0.84618500	1.63073200
C	7.35424200	-2.23504200	-0.32539200
C	6.26860300	-1.85835600	-2.47363900
H	6.06680800	0.42548200	3.24768700
C	7.68696800	-1.58262000	2.39848900
C	8.26091700	-2.94253200	0.48139500
C	7.15700900	-2.55371000	-1.71211200
H	6.12322900	-2.11212100	-3.52077600
C	8.42497600	-2.61791600	1.82662000
H	7.81903300	-1.33195700	3.44849900
H	8.83685700	-3.75305600	0.04156100
H	7.73277100	-3.36958100	-2.14224000
H	9.13279000	-3.17584900	2.43384700
C	-3.48578200	2.10214600	0.40931700
C	-3.64880300	1.87628200	1.79929900
C	-4.25920200	1.36966300	-0.50136100
C	-4.59502400	0.89837700	2.24340400
C	-2.91378000	2.60639900	2.79764200
C	-5.17878600	0.41762300	-0.07207300
H	-4.10792100	1.52592300	-1.56448600
C	-4.77775100	0.65427100	3.63957700
C	-5.36732500	0.16212700	1.29350000
C	-3.08754600	2.37183800	4.12758100
H	-2.20791000	3.36296300	2.47309200
H	-5.75857500	-0.14030900	-0.80349600
C	-4.01846400	1.38707800	4.60150900
C	-5.72116300	-0.32456100	4.08214700
C	-6.30937300	-0.81389100	1.76783700
H	-2.51737200	2.93848100	4.85999500
C	-4.21004300	1.12775000	5.96902400
C	-5.87872600	-0.54858900	5.45929200
C	-6.47876200	-1.04734500	3.09780200
H	-6.89092500	-1.36572200	1.03300000
C	-5.13027200	0.16994000	6.39036200

H	-3.63230800	1.68923300	6.69941300
H	-6.59792300	-1.29210900	5.79462100
H	-7.19677300	-1.78866400	3.44063700
H	-5.26804300	-0.01577800	7.45231100
C	-2.27871000	-2.55423600	-0.04994100
H	-2.14842800	-1.49948800	-0.27972200
C	-2.27315000	-2.89362300	1.36748100
C	-2.63309000	-4.16951500	1.84912900
C	-1.94588400	-1.88068300	2.29270600
C	-2.67960700	-4.41398000	3.21692800
H	-2.86065500	-4.96996100	1.15493800
C	-2.00079000	-2.12911200	3.66034900
H	-1.64173100	-0.90368500	1.93088900
C	-2.37053900	-3.39377700	4.12394300
H	-2.96217200	-5.39819700	3.57978100
H	-1.76386900	-1.33532100	4.36166200
H	-2.41955600	-3.58639700	5.19234300
C	-2.94232400	-3.32014000	-1.05752100
H	-3.14845500	-4.36873000	-0.87437300
C	-3.30373400	-2.71974400	-2.22884900
H	-3.04611200	-1.66920800	-2.35972800
C	-4.01086400	-3.31463000	-3.34868500
C	-4.24300200	-2.50585700	-4.48195100
C	-4.46586900	-4.65071400	-3.36257700
C	-4.90800200	-3.01887400	-5.59228600
H	-3.88398600	-1.48022000	-4.47690500
C	-5.12989600	-5.15642800	-4.47234700
H	-4.29797300	-5.29193400	-2.50265200
C	-5.35318300	-4.34226400	-5.58985500
H	-5.07710600	-2.38756400	-6.45982900
H	-5.47510400	-6.18647000	-4.47303200
H	-5.87254300	-4.74331900	-6.45604500
C	2.94192700	-3.46893300	0.73993200
C	1.68929100	-4.06409400	0.89952400

C	1.26170500	-4.54362500	2.13944200
C	2.10938700	-4.41317100	3.23579300
C	3.37119600	-3.81268300	3.11047100
C	3.77345400	-3.34914700	1.85037800
H	3.26591400	-3.11799600	-0.23414500
H	0.29032600	-5.01559600	2.23559800
H	1.78734200	-4.78753400	4.20450400
H	4.75052000	-2.89114300	1.73359400
C	4.27099400	-3.65321000	4.31215600
H	5.30356300	-3.45105800	4.01242800
H	4.26361900	-4.55055200	4.94097800
H	3.93868100	-2.81527200	4.93898000
S	0.63041500	-4.24593100	-0.52396000
O	1.44376800	-4.35084800	-1.73844300
O	-0.39634600	-5.25153100	-0.23375100
N	-0.18469800	-2.71450400	-0.59799000
H	-0.22554500	-2.42608900	-1.58022400
H	0.28873600	-1.94791800	-0.06877900

ComI1C

C	0.99084100	7.80529400	2.03462700
C	0.35167400	6.79615800	1.34893900
C	1.08875000	5.74390400	0.73922000
C	2.51386100	5.74329200	0.88571600
C	3.14340600	6.80887700	1.58515500
C	2.40139200	7.82153000	2.14645400
H	0.40536000	8.59406000	2.49904100
H	-0.73008700	6.79208300	1.28081300
C	0.46533900	4.66372200	0.02644000
C	3.27103400	4.68001300	0.33550800
H	4.22673000	6.79965600	1.67751900
H	2.89262000	8.62716200	2.68496300
C	2.67879600	3.59967000	-0.29058400

C	1.25966300	3.60821700	-0.39466900
H	4.35414700	4.71489200	0.41478000
C	-0.99951900	4.63145300	-0.25359200
C	-1.64693100	5.66091100	-1.02035600
C	-1.75203100	3.54534900	0.16515000
C	-0.94616600	6.74646100	-1.61580700
C	-3.06075500	5.57444600	-1.23624900
C	-3.15190200	3.42656800	-0.06167100
C	-1.61141900	7.70899300	-2.34249400
H	0.12944000	6.80923000	-1.50188500
C	-3.71936600	6.59324600	-1.97747300
C	-3.77511700	4.45900600	-0.73498100
C	-3.01400900	7.64307600	-2.51674800
H	-1.05147000	8.52501600	-2.79109700
H	-4.79458900	6.51686200	-2.12023100
H	-4.84718000	4.40643100	-0.90544300
H	-3.52634700	8.41332000	-3.08645400
P	-0.12829300	1.50117400	0.06219800
O	-1.11422800	2.52053700	0.86557700
O	0.64129900	2.49180400	-0.97160900
O	0.69881000	0.71967600	1.00725100
O	-1.02753500	0.69582300	-0.96844500
H	-1.31561300	-0.18274800	-0.59679100
C	4.75513400	-3.77118400	0.38527800
C	3.42431600	-4.11807000	0.15376900
C	3.07699400	-4.96304700	-0.90096500
C	4.07786000	-5.45729000	-1.73407300
C	5.42350600	-5.12324200	-1.52699800
C	5.74332400	-4.27444000	-0.45871400
H	5.01112800	-3.12335900	1.21672600
H	2.03885800	-5.23705900	-1.05598900
H	3.81012600	-6.11680800	-2.55622600
H	6.77895000	-3.99671800	-0.28169700
C	6.50803000	-5.68566400	-2.41530000

H	6.99150900	-6.55406100	-1.94830600
H	6.10738200	-6.01389000	-3.37977400
H	7.29172500	-4.94458700	-2.60722200
S	2.14131600	-3.48936000	1.23723900
O	2.78901000	-3.08480500	2.48942200
O	1.04880500	-4.47901000	1.22802800
N	1.54967500	-2.14340900	0.42805100
H	0.52788200	-2.16246200	0.41863800
H	1.86662500	-1.26397900	0.83837600
C	3.51212700	2.53025300	-0.90996900
C	4.45518300	1.78294000	-0.16114400
C	3.42353100	2.33208100	-2.29581700
C	5.34999100	0.90162300	-0.84946000
C	4.54238800	1.84804100	1.27453500
C	4.27599300	1.46277500	-2.96286900
H	2.68601800	2.89489200	-2.85990800
C	6.34135900	0.17259300	-0.12332100
C	5.26495700	0.75185400	-2.26659000
C	5.47275500	1.13398600	1.96605100
H	3.82833800	2.46343700	1.81002600
H	4.19398300	1.34393100	-4.04043600
C	6.41896200	0.28639900	1.29782900
C	7.26227800	-0.67377200	-0.81515600
C	6.19510500	-0.11522000	-2.93372300
H	5.50563600	1.18938900	3.05132100
C	7.40244500	-0.43710500	1.99204900
C	8.23876900	-1.36644200	-0.07986400
C	7.15415500	-0.78993200	-2.24269600
H	6.11858900	-0.21781500	-4.01354400
C	8.30434800	-1.25037300	1.30789900
H	7.45449100	-0.35390300	3.07473000
H	8.94939500	-1.99754400	-0.60884700
H	7.85631300	-1.43678500	-2.76353300
H	9.06410300	-1.79685500	1.86020200

C	-3.93874100	2.25370500	0.41758700
C	-4.61791100	1.40246400	-0.49099100
C	-4.05667100	2.02296500	1.79483000
C	-5.45588500	0.36097700	0.02305400
C	-4.48265600	1.51517900	-1.92041500
C	-4.86377700	1.00958300	2.29625600
H	-3.51396800	2.66451600	2.48232400
C	-6.16289200	-0.50245000	-0.87097700
C	-5.58898400	0.17572900	1.43238400
C	-5.14968000	0.68542900	-2.76921400
H	-3.81583300	2.27041600	-2.32011200
H	-4.93563200	0.85493600	3.36920500
C	-6.02183000	-0.34571000	-2.28320600
C	-7.01324800	-1.53060000	-0.35652600
C	-6.45402200	-0.86242100	1.92040700
H	-5.02143000	0.78896300	-3.84413800
C	-6.72337600	-1.20643000	-3.14307400
C	-7.69666100	-2.36586500	-1.25545600
C	-7.13703000	-1.67473300	1.06797500
H	-6.54627500	-0.98855600	2.99580100
C	-7.55162800	-2.20388100	-2.63222700
H	-6.61259900	-1.08548900	-4.21796700
H	-8.34568700	-3.14509500	-0.86304800
H	-7.78965000	-2.45449800	1.45347200
H	-8.08886500	-2.85982800	-3.31200900
C	-2.49858700	-2.62282800	0.58604200
H	-3.46928200	-2.40044300	0.12291000
C	-2.52923000	-2.20278400	2.04712200
C	-1.59225200	-1.33536700	2.61476200
C	-3.53612200	-2.74419900	2.85953800
C	-1.66587300	-1.01278000	3.97329500
H	-0.80108400	-0.90007400	2.01630000
C	-3.60595700	-2.42355200	4.21322000
H	-4.26549300	-3.42450600	2.42735900

C	-2.66807000	-1.55344900	4.77647700
H	-0.92719600	-0.33776400	4.39636700
H	-4.38825100	-2.85862500	4.83017300
H	-2.71706500	-1.30638500	5.83380400
O	-1.47877000	-1.84861900	-0.12958700
H	-1.32588000	-2.32278700	-0.96523500
C	-2.16714700	-4.07903600	0.42344600
H	-1.24532200	-4.39237300	0.90791300
C	-2.92505100	-4.93341000	-0.28357700
H	-3.84594800	-4.55760000	-0.73393100
C	-2.65733600	-6.35994300	-0.51770300
C	-3.61984900	-7.12903000	-1.19416100
C	-1.47053900	-6.99332300	-0.09885000
C	-3.41583300	-8.48608200	-1.44003600
H	-4.53982400	-6.65285100	-1.52667400
C	-1.26845800	-8.34796800	-0.34580500
H	-0.69999200	-6.42475100	0.41397400
C	-2.23826800	-9.10156200	-1.01501200
H	-4.17583200	-9.06090200	-1.96282600
H	-0.34708900	-8.81969600	-0.01452000
H	-2.07428300	-10.15908200	-1.20416000

TSI5

C	2.44233500	7.34599200	1.88085300
C	1.64044200	6.47629200	1.17473800
C	2.16361700	5.26943500	0.63324900
C	3.54388500	4.96771400	0.87031100
C	4.34763900	5.89372800	1.58917000
C	3.81335100	7.06085900	2.08365800
H	2.01633700	8.25837000	2.28992700
H	0.58982400	6.70467800	1.03570200
C	1.36641500	4.32725400	-0.10034200
C	4.08288500	3.75120400	0.38386300
H	5.39614700	5.65363500	1.74983300

H	4.43629700	7.75828900	2.63710200
C	3.30807500	2.80771800	-0.26372200
C	1.92765400	3.11025700	-0.46018500
H	5.14308200	3.55909400	0.52577700
C	-0.05448200	4.59870400	-0.46262200
C	-0.42190600	5.71602600	-1.28747900
C	-1.04301600	3.71703500	-0.04100800
C	0.53268400	6.58455200	-1.88828300
C	-1.80758000	5.95286200	-1.56199400
C	-2.42736500	3.95989600	-0.28695200
C	0.13653800	7.63863000	-2.68121700
H	1.58827000	6.40168000	-1.72549700
C	-2.18450600	7.05736000	-2.37274300
C	-2.77785000	5.07141000	-1.02499400
C	-1.23562200	7.88865900	-2.92027100
H	0.88688100	8.28197200	-3.13305800
H	-3.24256600	7.22530600	-2.56054300
H	-3.82958100	5.27626200	-1.21036500
H	-1.53385600	8.72722500	-3.54360700
P	0.05385000	1.32874200	-0.12763600
O	-0.68419600	2.59746100	0.68041300
O	1.12690100	2.16881000	-1.07503300
O	0.71999400	0.46471700	0.88838500
O	-0.94466400	0.75371300	-1.11790400
H	-1.57447500	-0.48757200	-0.74112800
C	3.62983300	-4.50218500	0.08880100
C	2.27043700	-4.71799800	-0.14696400
C	1.84746900	-5.63376900	-1.10848200
C	2.80134800	-6.33525700	-1.84585200
C	4.17079400	-6.13536800	-1.63422200
C	4.56769500	-5.21085700	-0.65613300
H	3.94576600	-3.79574900	0.84890100
H	0.78740100	-5.80095700	-1.26541700
H	2.47452300	-7.05164300	-2.59593100

H	5.62495200	-5.03815800	-0.47308000
C	5.20367800	-6.90019600	-2.42797700
H	5.77179300	-7.58560400	-1.78611200
H	4.74102900	-7.49491400	-3.22177100
H	5.92828700	-6.22160200	-2.89370000
S	1.05857300	-3.80145800	0.80477900
O	1.66278600	-3.51156300	2.11219800
O	-0.20231500	-4.57512900	0.72728200
N	0.83981700	-2.38125200	-0.02633000
H	-0.10822900	-2.30784400	-0.40246200
H	1.08174800	-1.53294400	0.50311600
C	-3.05260700	-1.84700600	1.10691400
H	-3.87122800	-1.20929800	0.78336500
C	-2.21809900	-1.29507100	2.15240700
C	-2.37139200	0.06801200	2.48397000
C	-1.27405900	-2.07008500	2.86077900
C	-1.60471300	0.64007300	3.48863400
H	-3.08100200	0.67558200	1.93442500
C	-0.50401700	-1.49022500	3.85932400
H	-1.12353400	-3.11460300	2.61899300
C	-0.66838500	-0.13790600	4.17461000
H	-1.71736100	1.69468400	3.71729600
H	0.24271700	-2.08939000	4.36941600
H	-0.05381100	0.31423600	4.94823700
O	-1.98423600	-1.45303800	-0.58948600
H	-2.60875300	-1.58481800	-1.32356400
C	-3.21621900	-3.25535700	0.87420000
H	-2.39790100	-3.91145400	1.14799400
C	-4.34205100	-3.74379900	0.29320500
H	-5.13751100	-3.04207200	0.03805400
C	-4.62098800	-5.14117100	-0.01044200
C	-5.91570400	-5.49440800	-0.43845800
C	-3.64272100	-6.15327000	0.09509100
C	-6.23408800	-6.81675600	-0.73500000

H	-6.67047300	-4.71741300	-0.53341100
C	-3.96458600	-7.47170100	-0.20607300
H	-2.62776400	-5.90348300	0.39035300
C	-5.25911100	-7.80940200	-0.61685800
H	-7.23862800	-7.07335800	-1.05951900
H	-3.20257700	-8.24163900	-0.12487100
H	-5.50316800	-8.84234400	-0.84946300
C	3.93336900	1.57888300	-0.82792200
C	4.71412200	0.69773400	-0.03814100
C	3.83295300	1.35061600	-2.20884300
C	5.45406100	-0.34705300	-0.68000800
C	4.78139000	0.78699900	1.39704000
C	4.53104200	0.32478300	-2.83082200
H	3.21131900	2.01153700	-2.80405400
C	6.29053600	-1.21416200	0.08863400
C	5.37072800	-0.52358400	-2.09384900
C	5.56180500	-0.05422300	2.12977500
H	4.16890600	1.52859200	1.89686500
H	4.44610200	0.18628500	-3.90594100
C	6.36145800	-1.07108800	1.50780500
C	7.06409700	-2.22833400	-0.55813500
C	6.15076000	-1.55626800	-2.71542000
H	5.58166600	0.02638500	3.21398800
C	7.19322400	-1.93126900	2.24363600
C	7.88966200	-3.05869100	0.21900900
C	6.96660100	-2.36499600	-1.98501600
H	6.07915200	-1.67517400	-3.79404000
C	7.95008700	-2.91099700	1.60399300
H	7.24063900	-1.82336000	3.32452300
H	8.48790700	-3.82097600	-0.27527600
H	7.55970900	-3.13565800	-2.47235600
H	8.59198300	-3.56457700	2.18880000
C	-3.51167000	3.11097400	0.30149100
C	-4.17843900	2.10662000	-0.44039800

C	-3.94300900	3.39797400	1.60402100
C	-5.28150600	1.41139600	0.15365900
C	-3.78957000	1.74860200	-1.77928000
C	-5.01512000	2.72848400	2.18556500
H	-3.42940300	4.17553200	2.16223000
C	-5.96693500	0.39086600	-0.57733100
C	-5.70570100	1.73175900	1.47985800
C	-4.44509900	0.77749300	-2.47389200
H	-2.93705600	2.25059900	-2.21903500
H	-5.32995600	2.98084500	3.19521500
C	-5.55445700	0.06184300	-1.90596100
C	-7.06723700	-0.30448700	0.01604300
C	-6.81730900	1.01983700	2.04775200
H	-4.13034400	0.52583100	-3.48398800
C	-6.23986600	-0.94651500	-2.60446500
C	-7.72191600	-1.30543100	-0.72241600
C	-7.46728400	0.04781600	1.35097000
H	-7.13028200	1.27606600	3.05702700
C	-7.31073800	-1.61982400	-2.01775300
H	-5.92920700	-1.19318600	-3.61681100
H	-8.56497900	-1.82635700	-0.27472100
H	-8.30661300	-0.48134200	1.79565800
H	-7.83447800	-2.38985700	-2.57810300

IMI3

C	-1.38636200	7.01545500	2.06632000
C	-1.71948600	5.89776600	1.33282700
C	-0.72837500	5.15501800	0.63304800
C	0.63462700	5.58595100	0.73729700
C	0.94216700	6.75184600	1.48960000
C	-0.04408600	7.45665700	2.14006100
H	-2.16224700	7.56159100	2.59643900
H	-2.75137900	5.56762800	1.29286200
C	-1.02557800	3.97535900	-0.13060400

C	1.65202400	4.84282400	0.08748300
H	1.98025400	7.07082900	1.54849300
H	0.20456100	8.34353700	2.71660900
C	1.38224200	3.67479600	-0.59749700
C	0.02671900	3.23767900	-0.65271800
H	2.67471400	5.20836500	0.13236800
C	-2.42198200	3.50025800	-0.35665400
C	-3.39212100	4.31497200	-1.03526300
C	-2.78280400	2.21855300	0.04177700
C	-3.07827900	5.57795000	-1.61145500
C	-4.73125600	3.82718500	-1.18154000
C	-4.11907400	1.73117600	-0.07825000
C	-4.03810700	6.32408000	-2.25901300
H	-2.06236100	5.94942800	-1.54715400
C	-5.70208000	4.62806000	-1.84193800
C	-5.06075800	2.54765400	-0.67211900
C	-5.36821100	5.85392200	-2.36824600
H	-3.76891900	7.28221800	-2.69555200
H	-6.71571000	4.24422800	-1.93221700
H	-6.08781000	2.20107300	-0.75573600
H	-6.11661900	6.45576600	-2.87649200
P	-0.59765500	0.74093700	-0.30507900
O	-1.84031600	1.39907900	0.62348500
O	-0.24977000	2.03996900	-1.28080800
O	0.50207700	0.46551700	0.67776900
O	-1.15353200	-0.32570200	-1.21004400
H	0.03772900	-1.49916900	-1.80671100
C	5.49593500	-2.56219100	-0.22702500
C	4.51042500	-3.40248900	0.29908800
C	4.63404100	-4.78769900	0.21577200
C	5.75312200	-5.33601000	-0.41270500
C	6.75140500	-4.51848400	-0.95443100
C	6.60476400	-3.12583900	-0.84951800
H	5.38804600	-1.48531000	-0.15851800

H	3.85926800	-5.41957900	0.63543200
H	5.84995900	-6.41697300	-0.48199400
H	7.36928100	-2.46976700	-1.25801000
C	7.95359200	-5.11186000	-1.65048400
H	8.88622700	-4.66348300	-1.28851600
H	8.01551600	-6.19325200	-1.49339600
H	7.91174900	-4.93574700	-2.73323400
S	3.12006200	-2.69383300	1.18240800
O	3.59839200	-1.96204500	2.36556900
O	2.17555100	-3.81770700	1.42210600
N	2.55570500	-1.57672000	0.10946100
H	1.98271900	-1.96224700	-0.66353300
H	2.04530900	-0.80670600	0.56362200
C	-0.88735000	-1.33042600	2.39897000
H	-1.67351900	-0.65089000	2.08062700
C	-0.14111200	-0.91550100	3.55058600
C	-0.44678800	0.34601800	4.11612600
C	0.87996200	-1.70128900	4.13565300
C	0.22880600	0.79739400	5.24002500
H	-1.19914600	0.96575200	3.63728800
C	1.55477200	-1.24034100	5.25716300
H	1.16010700	-2.65170400	3.69681400
C	1.22766800	0.00138300	5.81353900
H	-0.00738200	1.76827100	5.66522900
H	2.34964600	-1.83986400	5.68906600
H	1.76247600	0.35638400	6.69056400
O	0.78140700	-2.08723200	-2.09342300
H	1.21812000	-1.57418600	-2.79042500
C	-0.74164700	-2.50911900	1.67595800
H	0.05248000	-3.20696600	1.91515600
C	-1.56737900	-2.73124900	0.58231800
H	-2.32613600	-1.98293200	0.37061000
C	-1.53162300	-3.85051100	-0.31291400
C	-2.54317000	-3.94150000	-1.29843900

C	-0.53649500	-4.85794600	-0.25177100
C	-2.58564100	-5.02090800	-2.16973600
H	-3.28589900	-3.15352400	-1.36768800
C	-0.58266600	-5.92744400	-1.13344500
H	0.28274300	-4.77441100	0.45453100
C	-1.60744800	-6.01651400	-2.08475500
H	-3.37474500	-5.08669100	-2.91247100
H	0.18594300	-6.69348900	-1.09176900
H	-1.63527300	-6.86059900	-2.76899000
C	2.45940000	2.95954300	-1.33939300
C	3.62109100	2.46498400	-0.69813600
C	2.35164600	2.85835300	-2.73459700
C	4.69251500	1.94852600	-1.49553700
C	3.76481500	2.43020700	0.73360700
C	3.38023500	2.33946000	-3.50962500
H	1.44762500	3.21828000	-3.21613500
C	5.89301700	1.48661600	-0.87358900
C	4.57314800	1.89823400	-2.91695300
C	4.90113400	1.96967100	1.32473100
H	2.92705100	2.74905900	1.34303800
H	3.27394200	2.29258000	-4.59090500
C	6.01530700	1.50216200	0.54936400
C	6.97795200	1.00494500	-1.67123400
C	5.67504400	1.40137600	-3.69241300
H	4.97607200	1.93289500	2.40850900
C	7.20597800	1.04762700	1.13973000
C	8.15339900	0.56994000	-1.03558400
C	6.82625300	0.98123100	-3.09971300
H	5.57052600	1.37265700	-4.77459900
C	8.26290700	0.59148600	0.35418300
H	7.29299700	1.05206500	2.22329400
H	8.98338600	0.21712100	-1.64376900
H	7.65446500	0.61424700	-3.70161600
H	9.17813200	0.24755900	0.82872400

C	-4.53112000	0.41560600	0.49163100
C	-5.06602300	-0.61920500	-0.31561100
C	-4.47371600	0.23375500	1.88166800
C	-5.58148100	-1.80206300	0.30839000
C	-5.09799100	-0.54410300	-1.75349600
C	-4.95507500	-0.91944800	2.49059700
H	-4.06638800	1.03346000	2.49359100
C	-6.15673000	-2.84262100	-0.48537600
C	-5.52806100	-1.94902600	1.72801300
C	-5.64099900	-1.53982600	-2.50736600
H	-4.65995000	0.32299300	-2.23397700
H	-4.91063600	-1.02130200	3.57238900
C	-6.20281000	-2.71791900	-1.90757800
C	-6.68493300	-4.01549500	0.13858100
C	-6.06288400	-3.14006200	2.32696000
H	-5.64653700	-1.45968000	-3.59177100
C	-6.77399700	-3.75174900	-2.66806400
C	-7.24864000	-5.02147100	-0.66313400
C	-6.61805700	-4.12546500	1.56951200
H	-6.01697600	-3.23686900	3.40908400
C	-7.29227100	-4.88849500	-2.04968500
H	-6.81089400	-3.65327700	-3.75035300
H	-7.65280300	-5.91168000	-0.18740000
H	-7.02131800	-5.01983100	2.03827800
H	-7.73363800	-5.67703800	-2.65328700

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C	-1.09791000	-2.48528400	2.38115100
C	-0.51435800	-3.72050600	2.08633400
C	-1.28267300	-4.88187300	2.00843100
C	-2.65559400	-4.80437700	2.23574500
C	-3.27185200	-3.58197000	2.53630100
C	-2.47540600	-2.42829900	2.59053400
H	-0.49916900	-1.57899200	2.42053800

H	-0.80132400	-5.82573900	1.77510700
H	-3.25769800	-5.70869700	2.18156500
H	-2.93728200	-1.46695300	2.80233700
C	-4.75331900	-3.51820200	2.82470900
H	-4.95755400	-3.75989200	3.87655100
H	-5.31095600	-4.23664600	2.21387500
H	-5.16077600	-2.52059800	2.63360300
S	1.26322100	-3.87585400	1.90509100
O	1.88687100	-3.43491500	3.16500400
O	1.57449400	-5.21943700	1.39654000
N	1.57229600	-2.79989800	0.64123900
H	2.55790300	-2.91299500	0.39597000
C	0.52214100	-2.32493900	-2.25538200
H	0.39964200	-1.32693200	-1.82382500
C	1.78998500	-2.62661700	-2.84617100
C	2.10880500	-3.88202000	-3.42077200
C	2.76239400	-1.59656100	-2.86309400
C	3.35314400	-4.09187900	-3.99215100
H	1.38313100	-4.68863800	-3.40218700
C	4.00538100	-1.81209100	-3.44469500
H	2.52464900	-0.63637300	-2.41225400
C	4.30084100	-3.05762700	-4.00566800
H	3.59785400	-5.05801500	-4.42321400
H	4.74585800	-1.02039000	-3.44349300
H	5.27805800	-3.22981700	-4.44807800
C	-0.61120000	-3.13539700	-2.22347700
H	-0.59356900	-4.13883000	-2.63831200
C	-1.76846000	-2.61182000	-1.67076300
H	-1.69295800	-1.59542500	-1.27751100
C	-3.05099500	-3.25432400	-1.58932000
C	-3.27554600	-4.59130200	-1.99978200
C	-4.14124700	-2.50264700	-1.09292000
C	-4.54410000	-5.14395100	-1.92369400
H	-2.45115800	-5.19321100	-2.36791900

C	-5.41470700	-3.05771200	-1.02852700
H	-3.97347400	-1.47874800	-0.77252600
C	-5.61523900	-4.37680700	-1.44311800
H	-4.70875300	-6.17071600	-2.23694300
H	-6.24640100	-2.46662700	-0.66010000
H	-6.60935100	-4.81292900	-1.39312200
C	2.01273100	7.02300800	2.40834500
C	1.38169200	6.05520700	1.65819300
C	2.09772100	4.93471900	1.15045600
C	3.49020700	4.83368600	1.46314000
C	4.11579300	5.85518200	2.22692200
C	3.39622900	6.93192100	2.69045400
H	1.43961800	7.86248000	2.79315500
H	0.31847600	6.13512300	1.46339200
C	1.47810600	3.89282600	0.37801800
C	4.21781200	3.71475600	0.99021300
H	5.17673900	5.76159600	2.44717400
H	3.88201100	7.70473000	3.27996400
C	3.61377600	2.67062000	0.32000200
C	2.20577200	2.74364600	0.08221700
H	5.28918200	3.67475500	1.17039500
C	0.06948500	4.03330900	-0.09142400
C	-0.33929600	5.12067700	-0.93782800
C	-0.87197000	3.08913700	0.28396400
C	0.57508000	6.04893500	-1.50806800
C	-1.72855200	5.26350900	-1.25709700
C	-2.26545900	3.23737900	0.01005200
C	0.13725300	7.07163200	-2.32085700
H	1.63400400	5.93718400	-1.30588700
C	-2.14975000	6.34006300	-2.08385600
C	-2.65954800	4.33001200	-0.73893200
C	-1.23955100	7.22951900	-2.60579600
H	0.85792600	7.76251800	-2.75035800
H	-3.21004800	6.43954000	-2.30498700

H	-3.71677200	4.48923600	-0.93401400
H	-1.57191900	8.04510600	-3.24228400
P	0.37496600	0.79523900	0.19400100
O	-0.45453400	1.99101100	1.00129100
O	1.58919800	1.68846000	-0.55223800
O	0.94646500	-0.07955400	1.27361700
O	-0.44124000	0.23682200	-0.93725200
H	1.40566200	-1.81479800	0.93145300
C	4.50101600	1.60151300	-0.24430700
C	4.74100600	0.36529500	0.40072300
C	5.22177200	1.91828300	-1.40450300
C	5.71811600	-0.53028900	-0.14426500
C	4.04670700	-0.02708000	1.59643600
C	6.17855800	1.05697200	-1.93379500
H	5.03499200	2.87299300	-1.88823600
C	5.96743300	-1.78780300	0.48622300
C	6.45254500	-0.17265200	-1.31659300
C	4.27579500	-1.23220900	2.18816700
H	3.29269300	0.63514000	2.00295200
H	6.73263800	1.34326400	-2.82519700
C	5.23472200	-2.15915300	1.65458500
C	6.94115900	-2.68506400	-0.05269200
C	7.43929800	-1.08611000	-1.82601000
H	3.70444100	-1.52897700	3.06225000
C	5.46478100	-3.41742500	2.23809000
C	7.14955800	-3.92401000	0.57397700
C	7.67129800	-2.28534000	-1.22416900
H	8.00342100	-0.79422100	-2.70939400
C	6.41319900	-4.28606800	1.70123400
H	4.87854200	-3.70843000	3.10504100
H	7.89135000	-4.60572300	0.16410200
H	8.42177700	-2.96506300	-1.62180300
H	6.57745600	-5.25519500	2.16437500
C	-3.28220600	2.33238000	0.61240100

C	-4.32139700	1.74328800	-0.15282900
C	-3.27633600	2.14795100	2.00464600
C	-5.38725000	1.05934300	0.51795500
C	-4.34718200	1.77874200	-1.59246100
C	-4.29388600	1.46395600	2.65601400
H	-2.46561200	2.57590500	2.58413100
C	-6.47639800	0.51157700	-0.22962400
C	-5.37708000	0.93069400	1.93981100
C	-5.37733700	1.24220600	-2.30403900
H	-3.50834900	2.22862700	-2.11097100
H	-4.27064500	1.36386000	3.73859400
C	-6.49146200	0.61081700	-1.65485000
C	-7.55816100	-0.13907200	0.44435200
C	-6.47338900	0.26800500	2.58909700
H	-5.36552100	1.27782800	-3.39084100
C	-7.57458600	0.07208000	-2.36878800
C	-8.62184100	-0.65988600	-0.31297400
C	-7.51801900	-0.23963900	1.87717800
H	-6.45605300	0.18767200	3.67351400
C	-8.62783400	-0.55262200	-1.70303100
H	-7.58303600	0.14884500	-3.45331500
H	-9.44775100	-1.14589100	0.20105700
H	-8.34497600	-0.73036400	2.38488200
H	-9.46034800	-0.95859900	-2.27156000

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C	-0.81302700	-2.23746600	2.52015600
C	-0.23472500	-3.46784100	2.18931100
C	-0.96951800	-4.65261800	2.23080000
C	-2.31077400	-4.60220900	2.60601700
C	-2.92722600	-3.38654500	2.92618400
C	-2.16028800	-2.21142200	2.86995600
H	-0.24315900	-1.31335100	2.47201800
H	-0.49420300	-5.59231100	1.97131300

H	-2.88831600	-5.52221400	2.64246200
H	-2.62566000	-1.25523900	3.09511800
C	-4.38477400	-3.33185700	3.31412800
H	-4.51590000	-2.84736600	4.28927500
H	-4.82063700	-4.33375300	3.37496100
H	-4.96689400	-2.75364100	2.58661700
S	1.50600800	-3.60095500	1.81448800
O	2.30041500	-3.20830600	2.98430800
O	1.75960000	-4.89563300	1.17025500
N	1.72396900	-2.40794300	0.58379900
H	2.73520300	-2.36167500	0.41994600
C	0.93496400	-2.66602100	-1.42329800
H	0.70345500	-1.60083300	-1.41899500
C	2.16676500	-3.06092200	-2.09970200
C	2.60997400	-4.39760200	-2.16338900
C	2.91667300	-2.05582000	-2.74198200
C	3.76329500	-4.71588000	-2.87034600
H	2.07413900	-5.17270700	-1.62569700
C	4.06202900	-2.38388600	-3.46195000
H	2.58763600	-1.02180300	-2.67759600
C	4.48520600	-3.71279800	-3.52721800
H	4.10736100	-5.74547600	-2.90615900
H	4.63187000	-1.60262300	-3.95361500
H	5.38569400	-3.96739800	-4.07918800
C	-0.20459100	-3.52060400	-1.33049100
H	-0.06988500	-4.59315800	-1.42765100
C	-1.44617900	-2.96359400	-1.22003200
H	-1.49043900	-1.87619100	-1.13560400
C	-2.71983300	-3.66156000	-1.24098000
C	-2.83121800	-5.06764100	-1.30051600
C	-3.90156100	-2.89323300	-1.21165500
C	-4.07907700	-5.67623800	-1.33281300
H	-1.93732100	-5.68334400	-1.31870600
C	-5.15239500	-3.50487400	-1.24640300

H	-3.82681000	-1.81016400	-1.16744500
C	-5.24220100	-4.89690900	-1.30792500
H	-4.15118100	-6.75940500	-1.37932700
H	-6.05219400	-2.89819400	-1.22921900
H	-6.21656600	-5.37738100	-1.33722600
C	1.59212500	7.05861800	2.56022300
C	0.99127700	6.11445100	1.75713500
C	1.74477700	5.05634400	1.17620100
C	3.14450500	4.98890900	1.47094200
C	3.73691200	5.98627000	2.29123000
C	2.98085900	7.00375500	2.82536600
H	0.99164400	7.85085800	2.99949200
H	-0.07585800	6.16435700	1.57351400
C	1.15673000	4.03967200	0.34847800
C	3.91353600	3.93010900	0.92654200
H	4.80292500	5.92203100	2.49698900
H	3.44279400	7.75765600	3.45700800
C	3.34202800	2.91295400	0.19091600
C	1.93345200	2.95168000	-0.03065100
H	4.98712000	3.92120500	1.09814700
C	-0.26435000	4.12507600	-0.09683500
C	-0.74241300	5.23344300	-0.87759600
C	-1.14499800	3.10055700	0.21690000
C	0.11097300	6.25193300	-1.38581000
C	-2.13690400	5.30509500	-1.19799000
C	-2.54406900	3.17843800	-0.05502500
C	-0.39039800	7.29122500	-2.13848800
H	1.17465400	6.19762900	-1.18548100
C	-2.62506000	6.39932200	-1.96229400
C	-3.00618900	4.28325700	-0.74392000
C	-1.77365500	7.37622900	-2.42318800
H	0.28511400	8.05171300	-2.52119600
H	-3.68875800	6.44194300	-2.18510100
H	-4.07076700	4.38082500	-0.94014200

H	-2.15655100	8.20508600	-3.01232700
P	0.28274700	0.89264000	0.06999900
O	-0.67116800	1.98872400	0.87770700
O	1.34849000	1.90916900	-0.71671300
O	0.98658400	0.13926700	1.17701200
O	-0.45240400	0.16080700	-1.01000200
H	1.41031500	-1.43790200	0.88381500
C	4.23385200	1.89726800	-0.45701900
C	4.65718900	0.71601400	0.19505700
C	4.74817100	2.20225500	-1.72435700
C	5.62371200	-0.12741300	-0.44296100
C	4.15116800	0.32218500	1.48276100
C	5.68817600	1.38822900	-2.34829800
H	4.41368600	3.11043700	-2.21780000
C	6.06564300	-1.32477200	0.19911200
C	6.15480600	0.22362800	-1.72167400
C	4.55992600	-0.82992700	2.08431200
H	3.39691800	0.94129600	1.95309200
H	6.08134400	1.66296500	-3.32449000
C	5.52791500	-1.69630100	1.46922800
C	7.04170300	-2.16083800	-0.42738500
C	7.14755200	-0.62660600	-2.32010700
H	4.13633800	-1.12753500	3.03889800
C	5.95202700	-2.89386100	2.07011000
C	7.44728100	-3.33933000	0.21888500
C	7.57222800	-1.76316300	-1.70245300
H	7.55869500	-0.33694300	-3.28482200
C	6.90268400	-3.70221500	1.44991900
H	5.52004900	-3.18514500	3.02347800
H	8.19229600	-3.97313600	-0.25659100
H	8.32667400	-2.39406900	-2.16714300
H	7.22085700	-4.62392000	1.92955500
C	-3.50670300	2.17960500	0.48797600
C	-4.45978200	1.52434800	-0.33150900

C	-3.54346500	1.97063500	1.87571900
C	-5.48776400	0.73558700	0.28009600
C	-4.43248600	1.59768200	-1.76947000
C	-4.52667300	1.19114300	2.47096200
H	-2.79843700	2.45779800	2.49618300
C	-6.49059400	0.11011000	-0.52414700
C	-5.52644200	0.57943400	1.69842500
C	-5.37934100	0.98762800	-2.53492300
H	-3.62069100	2.13837300	-2.24229500
H	-4.54533200	1.07657700	3.55244700
C	-6.45465500	0.23980300	-1.94642200
C	-7.53694500	-0.64816200	0.08938200
C	-6.58680300	-0.19015800	2.28687500
H	-5.32833200	1.05269900	-3.61913100
C	-7.45343900	-0.37760700	-2.71711200
C	-8.51670300	-1.24443800	-0.72278900
C	-7.54946300	-0.77428000	1.52041500
H	-6.61021800	-0.29010200	3.36960300
C	-8.47345400	-1.10844100	-2.10968500
H	-7.42268200	-0.27835300	-3.79935500
H	-9.31606300	-1.81403700	-0.25465900
H	-8.35036600	-1.34674300	1.98229700
H	-9.24065300	-1.57531500	-2.72163700

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C	2.09007000	6.60716800	2.54273000
C	1.35427600	5.79314800	1.70975400
C	1.97246600	4.74825900	0.96792000
C	3.38119300	4.54561400	1.13758200
C	4.11379900	5.41347300	1.99202900
C	3.48664700	6.42608500	2.68019200
H	1.59187800	7.39402900	3.10304000
H	0.28368700	5.93914200	1.62160700
C	1.24357500	3.86807600	0.09796900

C	4.01756900	3.47774500	0.45657600
H	5.18400800	5.25206800	2.09947400
H	4.05657000	7.07939000	3.33530500
C	3.31279200	2.58656300	-0.32776600
C	1.90765700	2.78689700	-0.46502300
H	5.09301000	3.35882000	0.56205600
C	-0.20921300	4.05005700	-0.19019800
C	-0.71687100	5.24386400	-0.80765100
C	-1.08982200	3.01042000	0.08612100
C	0.12033400	6.30445900	-1.25531700
C	-2.12753700	5.36648000	-1.02828100
C	-2.49617900	3.12708400	-0.11603100
C	-0.40931100	7.42886700	-1.84887300
H	1.19364700	6.21656400	-1.13435900
C	-2.64347000	6.54569300	-1.63095600
C	-2.98274800	4.30099900	-0.65405300
C	-1.80636200	7.56083400	-2.03086900
H	0.25417900	8.22077300	-2.18627100
H	-3.71810700	6.62334600	-1.77959100
H	-4.05367300	4.41244600	-0.80508700
H	-2.21112300	8.45575400	-2.49564400
P	0.23691500	0.78849100	-0.41264900
O	-0.59689700	1.83415500	0.60827200
O	1.19084200	1.88213700	-1.21991700
O	1.08186200	-0.03443200	0.52858900
O	-0.68949900	0.17871700	-1.41313800
C	2.47120600	-2.91926500	-0.09983600
C	1.47566700	-3.69536900	0.49906600
C	0.77760700	-4.66769900	-0.21871600
C	1.08048200	-4.85537100	-1.56509600
C	2.06355500	-4.08342900	-2.19902300
C	2.75238200	-3.12002100	-1.44761200
H	3.01102300	-2.16812500	0.46567800
H	0.01965700	-5.26447400	0.27581100

H	0.54202000	-5.61082100	-2.13162900
H	3.51896200	-2.51496400	-1.92207400
C	2.35994000	-4.26192100	-3.66820600
H	2.14645000	-5.28301900	-4.00109800
H	1.74369300	-3.58312600	-4.27239000
H	3.40733000	-4.03706000	-3.89338100
S	1.12792200	-3.50270800	2.23632200
O	2.37274800	-3.45812100	3.01151600
O	0.06895700	-4.44669300	2.61562200
N	0.44068600	-1.91438700	2.31865200
H	0.72799900	-1.52012200	3.21811000
H	0.75591200	-1.25743300	1.54443400
C	-1.72516000	-1.65608400	2.23677700
H	-1.50805100	-0.66191600	1.85623200
C	-2.01807200	-1.72126900	3.66767700
C	-2.30710000	-2.92831800	4.33299300
C	-2.01566900	-0.51910800	4.40244300
C	-2.60119700	-2.92328900	5.69258600
H	-2.25570200	-3.86787200	3.79484100
C	-2.31923800	-0.51821300	5.76091900
H	-1.78470700	0.41260300	3.89264900
C	-2.61461000	-1.72114400	6.40744500
H	-2.81274900	-3.85964600	6.20058700
H	-2.32178800	0.41578800	6.31531000
H	-2.84655400	-1.72419400	7.46894200
C	-2.20224500	-2.59241500	1.27982500
H	-2.56153000	-3.55733600	1.62083200
C	-2.19198500	-2.25689400	-0.04722400
H	-1.77675900	-1.28778700	-0.32923400
C	-2.64247100	-3.05367900	-1.16864200
C	-3.28672100	-4.30311700	-1.03733100
C	-2.40021200	-2.53818800	-2.46117300
C	-3.67139900	-5.01528100	-2.16517500
H	-3.49429500	-4.70721100	-0.05083700

C	-2.78491700	-3.26103100	-3.58711500
H	-1.89652400	-1.57900800	-2.55101300
C	-3.41960200	-4.49644200	-3.44233400
H	-4.17184300	-5.97351100	-2.05709100
H	-2.59211000	-2.86025100	-4.57819300
H	-3.72379900	-5.05783200	-4.32191500
C	4.01548800	1.50298300	-1.07219200
C	4.77783500	0.50705800	-0.41401000
C	3.97200000	1.51586900	-2.47405200
C	5.53763900	-0.42366600	-1.19454200
C	4.79876900	0.36125400	1.01847900
C	4.69603100	0.60795800	-3.23499100
H	3.36579000	2.26696700	-2.97046500
C	6.33432300	-1.42184600	-0.55192900
C	5.50149400	-0.36365100	-2.62120700
C	5.54865000	-0.59879900	1.62793500
H	4.17826400	1.02307100	1.61158700
H	4.65220900	0.65427900	-4.32053200
C	6.35762600	-1.51403100	0.87281500
C	7.10671500	-2.33879800	-1.33108800
C	6.28344800	-1.30164600	-3.37842900
H	5.53555300	-0.69569500	2.71082800
C	7.14883600	-2.50010400	1.48349500
C	7.88671900	-3.30530800	-0.67546000
C	7.05320200	-2.24190200	-2.76356700
H	6.25056400	-1.24002500	-4.46383700
C	7.90671400	-3.38223900	0.71571400
H	7.15965000	-2.57163300	2.56821500
H	8.47628900	-3.99978900	-1.26928200
H	7.64327000	-2.94153000	-3.35101800
H	8.51377800	-4.13887200	1.20550400
C	-3.44418900	2.04900100	0.29549000
C	-4.19493600	1.31216400	-0.65213300
C	-3.66370600	1.82830300	1.66212400

C	-5.19549600	0.39529300	-0.19419600
C	-3.98615700	1.43679600	-2.07086000
C	-4.62141000	0.92600100	2.11292500
H	-3.08592600	2.40363800	2.38052900
C	-5.99236400	-0.32736600	-1.13460100
C	-5.41173700	0.20557100	1.20443000
C	-4.74355000	0.74232600	-2.96379900
H	-3.19084600	2.08509100	-2.41933900
H	-4.77885300	0.78836100	3.17997500
C	-5.78216900	-0.15217500	-2.53587100
C	-7.00640600	-1.22567600	-0.67848400
C	-6.43193900	-0.70999000	1.63420800
H	-4.56333200	0.85056200	-4.03074400
C	-6.58453800	-0.86374200	-3.44218400
C	-7.78521000	-1.91423200	-1.62278400
C	-7.19532600	-1.39127100	0.73623500
H	-6.58635400	-0.84368700	2.70246100
C	-7.57542900	-1.73238700	-2.98839600
H	-6.42370100	-0.72850000	-4.50907000
H	-8.55970800	-2.59383500	-1.27506100
H	-7.96820300	-2.07618100	1.07734500
H	-8.18876600	-2.27258000	-3.70480100

Pr1-R

C	0.92262800	-1.43694400	-0.91739300
H	0.85368900	-2.32675500	-1.55956900
C	1.90843100	-1.78153700	0.19930600
C	1.47929000	-1.95950100	1.51854600
C	3.25447900	-2.02326200	-0.11148900
C	2.37778300	-2.35872500	2.51230400
H	0.43566500	-1.80261700	1.77414500
C	4.14907200	-2.42323400	0.87727700
H	3.60069400	-1.87481800	-1.12895600
C	3.71458900	-2.59106800	2.19501300

H	2.02606700	-2.49137600	3.53217700
H	5.18996800	-2.59946200	0.61979100
H	4.41440500	-2.90218200	2.96614800
C	-0.48015700	-1.11245200	-0.46021400
H	-0.59258700	-0.24262900	0.18143100
C	-1.55176800	-1.82732700	-0.83623700
H	-1.38479800	-2.70878700	-1.45847300
C	-2.95972900	-1.58117300	-0.48890000
C	-3.91324000	-2.57144000	-0.78250900
C	-3.40472500	-0.39367200	0.12211100
C	-5.25909600	-2.39480600	-0.46528900
H	-3.58871200	-3.49307100	-1.26046000
C	-4.74863600	-0.21646900	0.43784100
H	-2.69798200	0.40285000	0.33694900
C	-5.68270100	-1.21594400	0.14886200
H	-5.97595600	-3.17727000	-0.69950600
H	-5.07219800	0.70905400	0.90712500
H	-6.73114700	-1.07254500	0.39546200
C	1.12719500	1.93946200	0.99281400
C	0.91848600	1.97757100	-0.38743700
C	-0.16872400	2.66556100	-0.92968500
C	-1.06163300	3.30771000	-0.07376100
C	-0.88192000	3.27936900	1.31759300
C	0.22320400	2.58658600	1.83362000
H	1.98789100	1.41436000	1.39276000
H	-0.30035000	2.70937400	-2.00591300
H	-1.90655400	3.84868300	-0.49301300
H	0.38311800	2.55947000	2.90880900
C	-1.83231100	4.01038700	2.23578500
H	-1.93925200	3.49488100	3.19594400
H	-1.46775600	5.02368500	2.45010300
H	-2.82653800	4.11033100	1.78854900
S	2.06631300	1.12909200	-1.48187200
O	3.30907300	0.96141600	-0.73181500

O	2.02777800	1.81683700	-2.77715100
N	1.45658700	-0.40695700	-1.85946500
H	0.85729500	-0.29854600	-2.67452800

Pr1-S

C	-1.66414900	0.12613700	-0.90769300
H	-1.55481700	-0.04510700	-1.98557300
C	-3.11694800	-0.17600900	-0.53813000
C	-3.64470400	0.16157300	0.71661300
C	-3.93860200	-0.82561900	-1.46679800
C	-4.96907200	-0.14672900	1.02750100
H	-3.01801900	0.66452600	1.44769700
C	-5.26341500	-1.13493300	-1.15464500
H	-3.53841900	-1.09160500	-2.44314400
C	-5.78245100	-0.79489600	0.09491000
H	-5.36675400	0.12160000	2.00273500
H	-5.88881500	-1.63573200	-1.88905500
H	-6.81454100	-1.03065400	0.34033500
C	-0.71431100	-0.81587700	-0.20633100
H	-0.77175600	-0.82738400	0.87747500
C	0.11622700	-1.63510100	-0.86827900
H	0.14205600	-1.57173500	-1.95711300
C	1.03692200	-2.62431600	-0.28946800
C	1.95038200	-3.27656000	-1.13590400
C	1.05303200	-2.95425200	1.07903200
C	2.85486700	-4.21358100	-0.63870700
H	1.95003900	-3.03835000	-2.19729500
C	1.95550100	-3.88953500	1.57650000
H	0.34747200	-2.48332400	1.75712500
C	2.86248300	-4.52340100	0.72157500
H	3.55167300	-4.70253100	-1.31447000
H	1.94835900	-4.13062100	2.63631300
H	3.56346300	-5.25537400	1.11347200
C	2.03994900	1.33442000	1.05193900

C	1.20406500	2.06528700	0.21110200
C	1.71367200	2.72987500	-0.90783400
C	3.07279300	2.64107100	-1.18755600
C	3.93777800	1.90152400	-0.36421600
C	3.40138500	1.25689700	0.75632800
H	1.62596800	0.83846300	1.92256000
H	1.05389400	3.30975700	-1.54486800
H	3.47313300	3.15798600	-2.05650300
H	4.05536200	0.68555300	1.41016000
C	5.40672700	1.79195600	-0.69637800
H	5.80520300	2.74218900	-1.06843000
H	5.57838600	1.04046400	-1.47838000
H	5.99454900	1.49520200	0.17773100
S	-0.53314600	2.23289300	0.61493800
O	-0.76848100	1.46060300	1.84564800
O	-0.90373700	3.65174900	0.54949300
N	-1.31810200	1.56374000	-0.71784800
H	-2.07442400	2.19778400	-0.96733100

SSLA-Int0

C	-4.80133300	2.11765000	-4.41250900
C	-3.99925000	2.10559000	-3.29282600
C	-3.78974100	0.90821700	-2.55478700
C	-4.40819200	-0.29334400	-3.03036600
C	-5.24490800	-0.24284500	-4.17835300
C	-5.44209900	0.93700900	-4.85611800
H	-4.94004000	3.04392900	-4.96289700
H	-3.51158100	3.01845300	-2.97299100
C	-2.95361400	0.84714700	-1.38465400
C	-4.16404500	-1.51612500	-2.36048500
H	-5.71676600	-1.16173200	-4.51717300
H	-6.07800000	0.96386200	-5.73632300
C	-3.30946700	-1.60632000	-1.27920800

C	-2.70338600	-0.39813800	-0.83295300
H	-4.66571400	-2.41308800	-2.71294800
C	-2.32395500	2.07981000	-0.81967500
C	-3.10126000	3.19200300	-0.34843500
C	-0.94841600	2.15894800	-0.71028200
C	-4.52053600	3.17151100	-0.27791400
C	-2.41571900	4.36060100	0.11961600
C	-0.23920800	3.30892100	-0.27045700
C	-5.22131800	4.25732500	0.19815100
H	-5.05490700	2.28123100	-0.58818700
C	-3.17056700	5.46997700	0.58768100
C	-0.99972200	4.39306700	0.12087700
C	-4.54418300	5.42365000	0.62528000
H	-6.30545800	4.21462700	0.25310000
H	-2.63692200	6.35228300	0.93157500
H	-0.49874700	5.29911300	0.45058600
H	-5.11081400	6.27357000	0.99461600
P	-0.25859500	-0.19718900	0.05348100
O	-0.20014800	1.00398300	-1.03005700
O	-1.81152200	-0.50829600	0.25357400
S	2.15009300	-0.06126300	1.71620500
S	-0.54622900	0.81724600	2.91650400
O	2.62875500	-0.03525100	0.31979700
C	2.49827600	-1.83243000	2.26442900
F	3.76569200	-2.11608300	1.94502200
F	2.33688900	-1.95553500	3.57913900
F	1.68704800	-2.68664000	1.63415100
C	-1.12335400	-0.64610600	3.94409400
F	-1.76438300	-1.53487400	3.17279500
F	-0.07673300	-1.24545300	4.51367600
F	-1.95335000	-0.20441000	4.88727400
O	-1.77112700	1.38166900	2.34257100
C	1.24590700	3.34390100	-0.22074500
C	1.89851800	3.79586500	0.93636800

C	2.00939400	2.93455400	-1.32471700
C	3.28667500	3.82786300	0.97769900
H	1.34519500	4.07069600	1.82737300
C	3.39137000	2.96537800	-1.25027300
H	1.54437700	2.58354000	-2.23799300
C	4.05170000	3.41170600	-0.10948400
C	-3.04864500	-2.92020000	-0.63358900
C	-3.12071800	-3.07668700	0.75926600
C	-2.77096100	-4.03842000	-1.43549700
C	-2.91049300	-4.32658400	1.32250700
H	-3.33599800	-2.24361200	1.41535500
C	-2.56916100	-5.27907300	-0.84698100
H	-2.68401200	-3.95313000	-2.51285700
C	-2.63564400	-5.44238900	0.53395700
C	0.40776700	0.09977000	1.62092900
F	3.92220800	4.25269200	2.07653700
F	5.38788900	3.43029900	-0.05705100
F	4.13023700	2.53922100	-2.29642000
F	-2.29336300	-6.35170000	-1.60613200
F	-2.43378100	-6.64120600	1.09183700
F	-2.97918000	-4.48966700	2.65204500
O	2.76163300	0.77849600	2.73830100
C	2.01015400	-1.25693100	-3.26203900
C	3.09904200	-0.99727000	-2.51527400
H	1.73516700	-2.27382100	-3.53788600
H	1.39936000	-0.45756800	-3.67527500
H	3.33026000	0.04359400	-2.29214000
Si	5.83799200	-1.82366000	-2.67268700
C	6.85750400	-3.27826600	-2.01660000
H	6.45768300	-4.23977300	-2.36068400
H	7.89854200	-3.21368700	-2.35599300
H	6.86923300	-3.29600200	-0.92019100
C	5.78910400	-1.87132300	-4.56454400
H	5.35734000	-2.81100200	-4.93035600

H	5.18769200	-1.05090400	-4.97281800
H	6.79797900	-1.78593900	-4.98627300
C	6.57652800	-0.19169400	-2.06328600
H	6.69973300	-0.20095700	-0.97343500
H	7.56625100	-0.01879600	-2.50370200
H	5.94932000	0.67229200	-2.31027100
O	0.29615300	1.59865800	3.81664600
O	0.37181300	-1.40486900	-0.72920100
H	1.09688400	-1.20982900	-1.39205200
C	4.05605800	-2.00707300	-1.97541800
H	3.69705600	-3.02635900	-2.17121100
H	4.13647500	-1.88807400	-0.88607000

SSLA-TS1

C	3.75691200	-4.91216000	-2.95997000
C	2.93076900	-4.28893100	-2.05033800
C	3.18524200	-2.95803700	-1.61961200
C	4.30732500	-2.27094700	-2.18654300
C	5.15201800	-2.94955400	-3.10644900
C	4.88739100	-4.24453200	-3.48587600
H	3.53500200	-5.92686100	-3.27872800
H	2.06580700	-4.81490100	-1.66462300
C	2.34551900	-2.25975500	-0.67957700
C	4.55406300	-0.92220000	-1.83168200
H	6.00707700	-2.41654800	-3.51494500
H	5.53523200	-4.75154400	-4.19534200
C	3.71008700	-0.21416000	-0.99930000
C	2.59123400	-0.91641500	-0.46565000
H	5.43699400	-0.43240700	-2.23301700
C	1.22280100	-2.95458400	0.01941900
C	1.46828300	-4.12891900	0.81846200
C	-0.08022600	-2.49682500	-0.07589300
C	2.77589000	-4.57643400	1.15128800
C	0.35519800	-4.86046200	1.34324400
C	-1.20407300	-3.24453400	0.38167500

C	2.96767100	-5.69576500	1.93186900
H	3.63430600	-4.01531600	0.80119000
C	0.58599100	-6.02244500	2.12673000
C	-0.96040700	-4.41356400	1.06826600
C	1.86528300	-6.43662300	2.41629700
H	3.97772000	-6.00781400	2.18262100
H	-0.27260900	-6.57010400	2.50744600
H	-1.79872000	-5.01231100	1.41419300
H	2.03116100	-7.32060500	3.02546000
P	0.25461400	0.17804400	-0.30725900
O	-0.36120600	-1.28276300	-0.69993200
O	1.69893200	-0.18891800	0.33228600
S	-1.07528800	2.76094500	0.53252900
S	-0.95592400	0.39505000	2.43494600
O	-1.55902000	2.91542200	-0.84998800
C	0.51134200	3.77916600	0.56178700
F	0.18057700	5.06795300	0.46486800
F	1.17147600	3.57642700	1.70643600
F	1.30816000	3.45332000	-0.46075500
C	0.25182300	1.13639100	3.67524700
F	1.50398600	1.04170500	3.20944400
F	-0.03162700	2.41466900	3.91488000
F	0.15491400	0.44090200	4.81044600
O	-0.52605700	-1.00929200	2.31425700
C	-2.59607300	-2.81086100	0.10040700
C	-3.55965500	-2.81482600	1.11961000
C	-2.97847100	-2.44483800	-1.20100400
C	-4.87189500	-2.46091000	0.83391200
H	-3.29095300	-3.05014800	2.14297200
C	-4.29073800	-2.08563500	-1.45322100
H	-2.26557500	-2.43702900	-2.01639300
C	-5.25675300	-2.09107800	-0.45242900
C	3.98702600	1.21110400	-0.68000200
C	3.90634100	1.69873900	0.63464500

C	4.39104800	2.07966000	-1.70670300
C	4.22612300	3.02204300	0.89815000
H	3.58700100	1.07268300	1.45810400
C	4.70730400	3.39853200	-1.41503100
H	4.43699100	1.75024600	-2.73852000
C	4.63369500	3.88779600	-0.11427900
C	-0.60220000	1.11409500	0.88312100
F	-5.79871200	-2.44444700	1.80213500
F	-6.51342900	-1.70395800	-0.71225800
F	-4.65469300	-1.68542200	-2.69657900
F	5.08450200	4.23754000	-2.39428500
F	4.93558600	5.16359400	0.15515700
F	4.15202700	3.49995000	2.14926500
O	-1.86358400	3.29059200	1.64720800
C	-1.35320600	1.24206100	-3.56630600
C	-2.73556100	1.21001600	-3.37721900
H	-0.91969300	2.21739100	-3.79663000
H	-0.93177100	0.40132100	-4.12146500
H	-3.22831700	0.23702500	-3.45338800
Si	-4.93188300	2.25569600	-1.65009900
C	-5.31470600	4.06996400	-1.30824800
H	-5.65157100	4.59961500	-2.20719400
H	-6.10726900	4.15443500	-0.55474700
H	-4.42928000	4.58277400	-0.91685800
C	-6.43060100	1.38098600	-2.40608800
H	-6.77463700	1.86800900	-3.32682600
H	-6.22450600	0.32885900	-2.63079800
H	-7.26630000	1.39541300	-1.69553800
C	-4.38629700	1.35246000	-0.09213900
H	-3.93176700	2.03144800	0.63341200
H	-5.26413300	0.89667200	0.38228800
H	-3.66677500	0.55153300	-0.28635100
O	-2.28223000	0.72420000	2.95089700
O	0.36545700	0.91598900	-1.63138800

H	-0.70769400	1.05160100	-2.46669200
C	-3.59715000	2.34454300	-3.10826700
H	-4.31505800	2.39232900	-3.94558500
H	-3.03759100	3.28059800	-3.05273200
SSLA-Int1			
C	-5.09903800	2.97841100	-3.58607300
C	-4.15798200	2.80217900	-2.59532800
C	-3.95139900	1.52946700	-1.99516500
C	-4.72236600	0.42524800	-2.48361200
C	-5.70100700	0.64477600	-3.49103600
C	-5.89156700	1.89477500	-4.03139100
H	-5.23122300	3.96053600	-4.03181600
H	-3.55645900	3.64328900	-2.27256700
C	-2.98017000	1.29538800	-0.95729200
C	-4.48004400	-0.87433600	-1.97687000
H	-6.28727000	-0.20315500	-3.83710900
H	-6.63717200	2.05005900	-4.80620600
C	-3.48604000	-1.13062900	-1.05295400
C	-2.74468800	-0.01243500	-0.56713600
H	-5.09218900	-1.69492000	-2.34122300
C	-2.20705200	2.41978300	-0.34884800
C	-2.87256300	3.53518400	0.27400600
C	-0.82184000	2.41045900	-0.35325800
C	-4.27446900	3.56569400	0.50891000
C	-2.09461600	4.65154400	0.72131400
C	-0.03349400	3.52601700	0.05544600
C	-4.87220500	4.64842900	1.11642700
H	-4.87805400	2.71314300	0.22071400
C	-2.74330800	5.76155500	1.32525000
C	-0.68689800	4.62617300	0.56466600
C	-4.10511800	5.76599500	1.51861200
H	-5.94404700	4.63905800	1.29471400
H	-2.13587200	6.60350100	1.64856700
H	-0.11144300	5.49611200	0.87035400

H	-4.58983800	6.61549600	1.99151000
P	-0.19895800	-0.21870500	-0.19635400
O	-0.12579100	1.30593300	-0.81676400
O	-1.73430400	-0.26521400	0.35914300
S	2.01409900	-1.71703900	1.21508600
S	0.57903800	0.48479800	2.67201100
O	2.76690700	-1.75391700	-0.06276200
C	1.12033000	-3.38213900	1.22085300
F	2.01984700	-4.33145300	1.49830100
F	0.16882000	-3.38900500	2.15825800
F	0.56133900	-3.65455100	0.03602400
C	-0.34344100	-0.59163700	3.91079000
F	-1.47816400	-1.05277900	3.36666800
F	0.40059900	-1.62545600	4.30384800
F	-0.64785000	0.15997800	4.97208900
O	-0.39438600	1.53018800	2.32085400
C	1.44841400	3.50086100	-0.04978300
C	2.23498200	3.89680000	1.04243000
C	2.08126200	3.10783100	-1.24218100
C	3.62023100	3.89999700	0.93859300
H	1.78179100	4.15678400	1.99201300
C	3.46236500	3.11191100	-1.31229700
H	1.50849700	2.79659200	-2.10686900
C	4.25213100	3.50909700	-0.23848000
C	-3.20220900	-2.52573100	-0.62310200
C	-2.94478700	-2.85873700	0.71717500
C	-3.21721400	-3.54915400	-1.58596100
C	-2.70547000	-4.17995400	1.06466600
H	-2.90889600	-2.10794600	1.49522400
C	-2.97969900	-4.86266000	-1.21017500
H	-3.37952500	-3.33227400	-2.63554500
C	-2.72047400	-5.19880400	0.11483400
C	0.79670500	-0.48215200	1.23226600
F	4.38198800	4.26816000	1.97787200

F	5.59176200	3.47605700	-0.33261700
F	4.09322300	2.70568300	-2.44619300
F	-2.97928900	-5.84212600	-2.13233200
F	-2.48129500	-6.46925600	0.46597100
F	-2.45425800	-4.50912800	2.34107200
O	2.76521900	-1.72335800	2.47027600
C	2.11533600	-2.43420900	-3.18200100
C	2.71013200	-1.13888300	-2.83262400
H	2.63100100	-2.96951200	-3.98248200
H	1.06866200	-2.22966100	-3.45484800
H	2.21071300	-0.63624200	-2.00949600
Si	5.46399800	-1.12440100	-2.26330400
C	5.35218700	-2.95450700	-1.88012600
H	5.17824700	-3.56718300	-2.77165200
H	6.30395900	-3.27976200	-1.44045500
H	4.56262900	-3.14781900	-1.14791500
C	6.82184500	-0.73418500	-3.51112900
H	6.77213300	-1.37729200	-4.39636400
H	6.79174200	0.31093500	-3.83721700
H	7.79539100	-0.90243400	-3.03264100
C	5.52660500	-0.02276200	-0.75903100
H	6.40395200	-0.30650500	-0.16232100
H	5.62947200	1.03485500	-1.01626200
H	4.64432100	-0.16583400	-0.12926900
O	1.83103000	0.84258500	3.33734300
O	0.12590300	-1.13957200	-1.31858100
H	2.02058700	-3.03762600	-2.27055900
C	3.81839100	-0.55633700	-3.43748700
H	3.92682500	0.52449600	-3.31947200
H	4.12259000	-0.95684800	-4.40688500

SSLA-TS2

C	-5.18456700	4.05965700	-2.83564600
C	-4.18095300	3.63603600	-1.99220200

C	-4.12041700	2.28928100	-1.54045700
C	-5.11405700	1.37445400	-2.01818700
C	-6.14818400	1.84815000	-2.87039200
C	-6.18826300	3.16320000	-3.27111000
H	-5.20237800	5.09252600	-3.17289600
H	-3.41561000	4.33456500	-1.67522200
C	-3.08734300	1.79752400	-0.66739500
C	-5.04241600	0.00891400	-1.64817500
H	-6.90136600	1.14226100	-3.21228900
H	-6.97880700	3.51212900	-3.92973800
C	-4.00725600	-0.49193800	-0.88438400
C	-3.02696000	0.43622300	-0.42543700
H	-5.82467900	-0.66331100	-1.99051900
C	-2.08178400	2.70854500	-0.04405500
C	-2.50649800	3.81017200	0.78372600
C	-0.72032000	2.49615300	-0.20704000
C	-3.86092400	4.00996600	1.17023200
C	-1.53063900	4.73029900	1.28393800
C	0.25954300	3.41536400	0.27502200
C	-4.22747900	5.07368500	1.96579300
H	-4.61430600	3.30237800	0.84603000
C	-1.94175300	5.82835500	2.08554900
C	-0.16293500	4.51431900	0.98800800
C	-3.26431300	6.00393600	2.41952200
H	-5.26861700	5.19371400	2.25296600
H	-1.18323900	6.52015900	2.44435500
H	0.57055200	5.22943400	1.35190400
H	-3.56815000	6.84177200	3.04089500
P	-0.56527100	-0.18826000	-0.61111800
O	-0.23322600	1.40487800	-0.89935900
O	-1.93882100	-0.06274600	0.28760100
S	1.42482800	-2.36882600	0.00339300
S	0.94073500	-0.22721900	2.05111100
O	1.85876100	-2.35303800	-1.40516400

C	0.16381200	-3.76926800	0.08479700
F	0.81300400	-4.92101700	-0.12094200
F	-0.39926300	-3.79628100	1.29873400
F	-0.78770200	-3.63165400	-0.83413700
C	0.08977800	-1.29972500	3.34539400
F	-1.18685000	-1.50867700	3.00372000
F	0.70430700	-2.47506800	3.47888400
F	0.12793700	-0.65053400	4.51325600
O	0.20744700	1.04671200	2.11808500
C	1.71248000	3.19113500	0.05268700
C	2.57715400	3.18085100	1.15815800
C	2.23689400	3.01629200	-1.23929100
C	3.93818300	2.99212000	0.96930400
H	2.18799000	3.24999200	2.16669300
C	3.60086900	2.84037600	-1.39735000
H	1.59566200	3.00183400	-2.11231800
C	4.46181300	2.82671600	-0.30677600
C	-3.93059500	-1.94239500	-0.57055900
C	-3.61499600	-2.40059000	0.71914700
C	-4.21405700	-2.87976900	-1.57671900
C	-3.58413600	-3.76232700	0.97718900
H	-3.37498900	-1.71729300	1.52327000
C	-4.18215000	-4.23629600	-1.28979400
H	-4.42172700	-2.56784200	-2.59373700
C	-3.87071800	-4.69743000	-0.01442800
C	0.61353300	-0.91703000	0.49099000
F	4.78312900	2.92857900	2.01092700
F	5.78542400	2.58504600	-0.47992200
F	4.13821700	2.64537800	-2.62771200
F	-4.44297400	-5.14022800	-2.25052100
F	-3.83336900	-6.01098500	0.24961400
F	-3.28035500	-4.21301600	2.20542500
O	2.42996500	-2.75253800	1.01232500
C	7.31084100	0.89380200	-2.83423100

C	7.45072700	0.07239000	-1.60308800
H	7.18468300	0.28991400	-3.73591700
H	8.22312900	1.49904100	-2.94128500
H	7.50698900	0.62839300	-0.66786200
Si	5.23089300	-1.50114900	-1.04329700
C	5.31508100	-3.36888200	-1.02247500
H	6.06465200	-3.75270200	-0.32395800
H	4.32841400	-3.69851200	-0.67052800
H	5.48730000	-3.79655100	-2.01466200
C	5.13958400	-0.69794600	0.63279900
H	5.34830800	0.37412800	0.61278400
H	4.13660300	-0.84308400	1.05675000
H	5.84454800	-1.17842800	1.32179900
C	4.36095400	-0.77729600	-2.52029100
H	3.31338900	-1.09637000	-2.44370500
H	4.38550600	0.31283300	-2.57113000
H	4.76345300	-1.18733300	-3.45385300
O	2.36111800	-0.26100900	2.42698500
O	-0.69906500	-0.90191200	-1.89748700
H	6.48510300	1.60658800	-2.73665800
C	7.50719100	-1.28721500	-1.54747300
H	7.81647000	-1.78311200	-0.62997600
H	7.55734800	-1.87595600	-2.46193100

SSLA-Int2

C	4.17642400	-4.36237100	-3.42415900
C	3.34311600	-3.87207100	-2.44270700
C	3.48746400	-2.54493300	-1.95363500
C	4.49940400	-1.71832900	-2.54066000
C	5.35662000	-2.26130500	-3.53601500
C	5.20394900	-3.55744400	-3.96891800
H	4.03955800	-5.37763700	-3.78600900
H	2.55724600	-4.50153300	-2.04319900
C	2.64121800	-1.98473700	-0.93139700

C	4.61915400	-0.36625700	-2.13752200
H	6.12810400	-1.62325700	-3.96004900
H	5.85920500	-3.96036300	-4.73598700
C	3.75616500	0.21014600	-1.22615600
C	2.76446000	-0.63638200	-0.65113400
H	5.41227300	0.23586200	-2.57231800
C	1.63484400	-2.82113400	-0.21117100
C	2.04240800	-4.00556600	0.50229500
C	0.29051900	-2.48416100	-0.19825000
C	3.40569500	-4.34146500	0.72705800
C	1.04180000	-4.86830100	1.05227300
C	-0.72298800	-3.35241400	0.30444700
C	3.75354000	-5.47743700	1.42522800
H	4.18263800	-3.68230400	0.35847500
C	1.43201900	-6.04373900	1.74788900
C	-0.32439500	-4.52960900	0.89929800
C	2.76078100	-6.34770400	1.93130300
H	4.80307700	-5.70273300	1.59339900
H	0.65546000	-6.69111300	2.14791500
H	-1.07772500	-5.21728600	1.27412400
H	3.04942800	-7.24338900	2.47398200
P	0.37114500	0.22077100	-0.36673700
O	-0.15229100	-1.28081500	-0.73872300
O	1.85542400	-0.06032300	0.24627300
S	-1.18325700	2.48224300	0.86762300
S	-0.62659800	0.10968900	2.57513400
O	-1.93426600	2.67499300	-0.48363200
C	0.13775500	3.81950200	0.58345300
F	-0.48513300	4.99421100	0.59360300
F	0.98190300	3.74405300	1.61175700
F	0.79124000	3.65883800	-0.55295300
C	0.64261500	0.93238200	3.69884400
F	1.86695500	0.80382500	3.17925000
F	0.36575300	2.22913200	3.85197800

F	0.60018400	0.32575900	4.88378000
O	-0.10117400	-1.24064600	2.34923600
C	-2.16960800	-3.02749200	0.19649200
C	-2.99765000	-3.16860800	1.32125200
C	-2.73868600	-2.64175900	-1.02902600
C	-4.36234700	-2.93404400	1.21391500
H	-2.58511600	-3.42517800	2.29012700
C	-4.10261500	-2.41196900	-1.10619400
H	-2.13588100	-2.52284300	-1.92103700
C	-4.93239100	-2.55289300	0.00245800
C	3.87431700	1.65306600	-0.88927300
C	3.78740100	2.11622400	0.43402100
C	4.11799700	2.57707100	-1.91882900
C	3.94324300	3.46813400	0.70120300
H	3.58964300	1.44731000	1.26158900
C	4.27437100	3.92323800	-1.62306200
H	4.15491100	2.26631500	-2.95654900
C	4.19083500	4.38889800	-0.31404900
C	-0.50489500	0.93251000	1.01829600
F	-5.16089600	-3.05581200	2.28446300
F	-6.24532900	-2.29186700	-0.09118800
F	-4.66291100	-2.02571700	-2.27325900
F	4.49654000	4.81238700	-2.60491900
F	4.33112700	5.69195300	-0.03908800
F	3.85275100	3.92295100	1.96189700
O	-1.92338400	2.91850900	2.04694100
C	-8.19365500	2.24767600	-3.55649800
C	-7.35050200	1.03439400	-3.28279000
H	-8.85308700	2.47768600	-2.71292300
H	-8.81921800	2.09932900	-4.44701000
H	-6.66267500	0.74244400	-4.07817100
Si	-3.52059100	2.05376500	-1.06790200
C	-4.46992800	3.63591600	-1.37701900
H	-4.62591600	4.19836400	-0.45021700

H	-3.94553800	4.28359700	-2.08816300
H	-5.45404500	3.39653300	-1.79846600
C	-4.24432900	1.02521000	0.31616800
H	-4.38394900	1.61695000	1.22668400
H	-5.22328000	0.64217400	0.00355100
H	-3.61430500	0.16848300	0.57288300
C	-3.07015400	1.11589400	-2.62212000
H	-2.05009600	0.72495100	-2.54496500
H	-3.75671400	0.27843700	-2.78593600
H	-3.10810400	1.76980500	-3.50031600
O	-1.91612800	0.31810400	3.22827900
O	0.27426700	1.08452500	-1.56435300
H	-7.57266900	3.13138100	-3.75706400
C	-7.39939300	0.29499600	-2.17175600
H	-6.78010600	-0.58665300	-2.03981700
H	-8.08104200	0.53850800	-1.35832100

SSLA

C	-1.63928600	6.04293900	-2.55236700
C	-1.02055000	5.08978000	-1.77347500
C	-1.72907500	3.94642400	-1.31315800
C	-3.09559800	3.79428300	-1.71511400
C	-3.71075400	4.80694700	-2.50029000
C	-3.00151200	5.91152400	-2.90976400
H	-1.07291400	6.90291800	-2.89889700
H	0.02568800	5.20372300	-1.51640500
C	-1.12611700	2.91947400	-0.50316500
C	-3.80870600	2.62835900	-1.34419100
H	-4.75271700	4.68162700	-2.78434800
H	-3.47878300	6.67555700	-3.51686100
C	-3.21656500	1.59352000	-0.64714600
C	-1.85900400	1.77378100	-0.25399700
H	-4.85324900	2.54624600	-1.63190300
C	0.26060600	3.06307000	0.03307400
C	0.61123400	4.18918700	0.86211400

C	1.24123400	2.12063400	-0.23360700
C	-0.35018100	5.11039400	1.36107300
C	1.97780100	4.37639700	1.24385100
C	2.61350400	2.30930200	0.10612000
C	0.02488600	6.16916800	2.15922500
H	-1.39725900	4.96534000	1.12335500
C	2.33595300	5.48975800	2.05016000
C	2.95042300	3.43933400	0.81853600
C	1.38209000	6.37319000	2.49887600
H	-0.73261600	6.85077500	2.53624500
H	3.38135500	5.61986600	2.31920200
H	3.99175000	3.61458800	1.07521500
H	1.66475500	7.21604700	3.12319700
P	-0.20938700	-0.15071500	-0.52713600
O	0.93928500	0.94297900	-0.91128500
O	-1.22567900	0.71349700	0.40992700
S	0.18015000	-3.04769000	0.19181800
S	1.16816600	-1.00833800	2.12226700
O	0.50027700	-3.34436800	-1.30576700
C	-1.65535100	-3.53993000	0.12273100
F	-1.70252300	-4.84672100	-0.11805500
F	-2.16343200	-3.28111000	1.32639200
F	-2.32502400	-2.87922300	-0.80443500
C	-0.13387400	-1.30071300	3.45232900
F	-1.18837800	-0.50865900	3.23907600
F	-0.53338000	-2.57439900	3.44850100
F	0.40707100	-1.00781900	4.63345500
O	1.35241800	0.44622700	2.10136100
C	3.66320100	1.33003800	-0.27988900
C	4.57733400	0.87854400	0.68459200
C	3.78853300	0.88246400	-1.60567900
C	5.59002900	-0.00098600	0.32424600
H	4.48431000	1.17255400	1.72359100
C	4.80642600	0.00270400	-1.93615500

H	3.10534700	1.20862100	-2.38036600
C	5.71583300	-0.45392300	-0.98595200
C	-3.97920300	0.35395100	-0.34580200
C	-3.91905100	-0.26580900	0.91352900
C	-4.81072400	-0.19565300	-1.33538800
C	-4.67515600	-1.40227000	1.15786000
H	-3.28588200	0.11141900	1.70617800
C	-5.56030600	-1.33057200	-1.06269600
H	-4.85720600	0.22932300	-2.33141500
C	-5.50585000	-1.94945200	0.18288700
C	0.39385300	-1.41080300	0.58766000
F	6.46008000	-0.44976300	1.24109200
F	6.66412600	-1.33951100	-1.32345100
F	4.92819000	-0.45598900	-3.19966600
F	-6.34778900	-1.86686500	-2.00942500
F	-6.22323000	-3.05207000	0.43375600
F	-4.61932200	-2.00693100	2.35589400
O	0.79326200	-3.97053400	1.14106600
Si	2.05125100	-3.48906000	-2.19715400
C	1.96511300	-5.24332200	-2.84544200
H	1.95747300	-5.97240600	-2.02810400
H	1.06620300	-5.39808700	-3.45230900
H	2.83577600	-5.45616300	-3.47857400
C	3.42759400	-3.23890900	-0.95408700
H	3.45146300	-4.04846200	-0.21740300
H	4.39586300	-3.21549200	-1.46952700
H	3.32557000	-2.29900200	-0.40306100
C	1.92329400	-2.18344200	-3.53052500
H	1.25586600	-1.37806500	-3.20598900
H	2.90540800	-1.75397400	-3.75528100
H	1.50955600	-2.60352400	-4.45390900
O	2.27285900	-1.90574300	2.45076400
O	-0.75685900	-0.74757900	-1.76541900

ComII

C	-9.37189100	-2.96065400	-2.72586800
C	-8.00413800	-3.08224800	-2.99323900
C	-7.07960900	-2.22312600	-2.38730100
C	-7.54094000	-1.24318900	-1.51396100
C	-8.92122000	-1.11885200	-1.24646500
C	-9.84083700	-1.97830100	-1.85083900
H	-10.07631300	-3.63719500	-3.20295700
H	-7.65551800	-3.85142600	-3.67748100
H	-6.01919200	-2.31626200	-2.60234900
H	-10.90484700	-1.88865500	-1.64619400
C	-6.75974100	-0.19473800	-0.73910000
H	-6.05402600	-0.65678400	-0.03700900
C	-7.85784200	0.53504300	0.01744100
C	-7.74778700	1.59438700	0.91278400
C	-8.91381400	2.10968000	1.49146800
C	-10.16561000	1.56908600	1.17754400
C	-10.27774000	0.50225400	0.28289500
C	-9.11763000	-0.01402400	-0.29788500
H	-6.77758800	2.01208300	1.16952700
H	-8.84494900	2.93582500	2.19413000
H	-11.06019400	1.98124300	1.63731100
H	-11.25325400	0.08392800	0.04755000
C	-5.94706700	0.76983200	-1.61970800
H	-6.55901900	1.14696600	-2.44213800
H	-5.57894000	1.60570500	-1.02297600
O	-4.82663700	0.12854200	-2.26225300
C	-3.72258700	-0.04066300	-1.47918300
O	-3.68063500	0.23960400	-0.29045300
N	-2.70538500	-0.59778500	-2.19206700
H	-2.77835500	-0.57873700	-3.19952200
H	-1.77606000	-0.50085600	-1.78808800
C	2.64926100	4.17995600	-1.62466700
C	1.53532500	5.07903200	-1.57940600
C	2.60475400	2.98784200	-0.81964100

C	0.40459200	4.75307200	-0.79300300
C	0.30565500	3.56956800	-0.08543400
C	1.43931000	2.70590200	-0.12878000
H	-0.42008200	5.45928600	-0.75776900
C	3.76120900	2.04382200	-0.76694100
C	5.06665200	2.48307500	-0.35148400
C	3.59893600	0.71274800	-1.12348200
C	6.17085600	1.57900100	-0.46742900
C	4.69063700	-0.19125600	-1.29061800
C	5.95186600	0.27599100	-0.97554000
H	6.81021400	-0.37361900	-1.12266200
P	1.17647100	0.11958500	-0.22787900
O	2.32062200	0.22672600	-1.39319600
O	1.37895300	1.50523300	0.58907600
S	1.96956000	-0.60371200	2.75092000
S	1.32896200	-2.65799900	0.75763600
O	1.10005600	0.44357100	3.28783300
O	2.10974900	-1.89014100	3.45240900
C	3.69998300	0.15868400	2.78488300
F	3.65328000	1.44493300	2.44683400
F	4.15484400	0.04316500	4.03176900
F	4.51762400	-0.49089700	1.95242900
C	2.74270700	-3.82634200	1.35806100
F	2.43971900	-4.44089400	2.48191600
F	2.88213300	-4.71850800	0.38040200
F	3.85961100	-3.12188800	1.48676500
O	1.15371100	-2.89046800	-0.67517900
C	4.51530900	-1.57238300	-1.81339900
C	5.25281600	-2.62498500	-1.24647400
C	3.67609600	-1.84248000	-2.90710000
C	5.14356600	-3.90758200	-1.76432300
H	5.88818700	-2.46722300	-0.38282400
C	3.58680200	-3.13267000	-3.40648700
H	3.08675200	-1.06525900	-3.37610300

C	4.31622800	-4.18081100	-2.84927100
C	-0.95014400	3.23436000	0.63777500
C	-0.94809300	2.65487100	1.91687500
C	-2.18052300	3.53256600	0.02576800
C	-2.15347300	2.37845600	2.54630900
H	-0.03270200	2.39304000	2.43090500
C	-3.36630100	3.25422300	0.68476800
H	-2.22860100	3.94577100	-0.97523200
C	-3.37419100	2.67242500	1.94620000
O	-0.12925500	-0.12776700	-0.87775000
C	1.63998400	-1.01900800	1.07788600
F	5.83377300	-4.92048600	-1.21399500
F	4.21556100	-5.42236300	-3.33820300
F	2.79477400	-3.39869300	-4.45624000
F	-4.54992800	3.52013300	0.09642200
F	-4.53061600	2.38645600	2.56070900
F	-2.16638200	1.80607900	3.76143100
O	0.20634300	-3.27313900	1.64831700
Si	-1.57435800	-3.06154000	1.81802200
C	1.56955000	6.27433800	-2.34825900
H	0.72146100	6.95215600	-2.29081300
C	2.64031900	6.56021700	-3.16193000
H	2.65288100	7.47253100	-3.75147400
C	3.72120400	5.65142700	-3.24471400
C	3.72767300	4.49496300	-2.49620900
H	4.56084700	3.80778200	-2.58124800
H	4.55383900	5.86497500	-3.90915500
C	5.30752700	3.76620200	0.21144500
H	4.47776600	4.45040500	0.34444900
C	6.57274500	4.14108500	0.60683100
H	6.72938100	5.12283600	1.04489300
C	7.66850500	3.25926300	0.45476500
C	7.46767600	2.00420600	-0.07034100
H	8.29722500	1.30963300	-0.17770400

H	8.66194900	3.57148400	0.76393700
C	-1.86374600	-4.21780500	3.26196800
H	-2.92872900	-4.23549700	3.52452600
H	-1.55826500	-5.24288200	3.02636300
H	-1.30531800	-3.88820400	4.14463000
C	-2.30773600	-3.66954800	0.20886500
H	-1.94278000	-4.66993200	-0.04811500
H	-3.40018500	-3.72246500	0.29832400
H	-2.07998900	-2.99118500	-0.61978600
C	-1.93555600	-1.27413200	2.19559600
H	-2.97637500	-1.19671900	2.53658700
H	-1.29821400	-0.86486300	2.98577200
H	-1.85569400	-0.64553900	1.30368400

TSII-1S

C	9.50721000	2.75471200	2.15113100
C	8.14118100	2.74249900	2.45120100
C	7.33475600	1.66607500	2.06349900
C	7.91284800	0.60649200	1.37210100
C	9.28935200	0.62160300	1.06419900
C	10.09177700	1.69506500	1.45454300
H	10.11930600	3.59722200	2.46176700
H	7.70060300	3.57660000	2.99046900
H	6.27349400	1.66723700	2.29153000
H	11.15342700	1.71037600	1.22187200
C	7.27170000	-0.66846700	0.84060400
H	6.86634300	-1.27516500	1.66381500
C	8.45136700	-1.37833500	0.18974700
C	8.48590000	-2.60429700	-0.46527400
C	9.70237800	-3.06068100	-0.98633500
C	10.86505900	-2.29554800	-0.84780600
C	10.83491100	-1.06489000	-0.18774700
C	9.62229200	-0.60673500	0.33052200
H	7.58806700	-3.20922900	-0.57014200
H	9.74343900	-4.01714000	-1.50002100

H	11.80236600	-2.66337800	-1.25649300
H	11.74328600	-0.47751500	-0.08193700
C	6.13494600	-0.43758400	-0.16152400
H	6.41823100	0.28992300	-0.92474900
H	5.82949200	-1.37081400	-0.63429600
O	4.98668700	0.14091900	0.51163300
C	3.84241800	-0.55223200	0.57519700
O	3.74991200	-1.72458500	0.14995800
N	2.86622700	0.15968600	1.15303500
H	3.05204300	1.13470000	1.34133200
H	1.88436200	-0.11812700	1.13788900
C	-2.92964500	4.34560700	0.99587000
C	-1.82182000	5.25028400	0.92361500
C	-2.80952100	3.05446400	0.37256100
C	-0.62198200	4.83441300	0.29904900
C	-0.45846300	3.56511300	-0.22325200
C	-1.58762300	2.69439900	-0.16977400
H	0.20131200	5.54120300	0.24230200
C	-3.94803900	2.08896100	0.35948900
C	-5.21680800	2.43121800	-0.22489600
C	-3.79626200	0.82633800	0.91463100
C	-6.30914100	1.51535700	-0.09139200
C	-4.88345200	-0.07687900	1.10510500
C	-6.11555100	0.29960800	0.60781200
H	-6.96967700	-0.35492300	0.75852900
P	-1.33650900	0.13428800	0.27974100
O	-2.53673600	0.42213400	1.35667300
O	-1.45878100	1.41804900	-0.71543800
S	-1.87818300	-0.97532400	-2.59493900
S	-1.43330900	-2.76857200	-0.26306000
O	-1.02083100	0.06435800	-3.17189400
O	-1.87746900	-2.33334000	-3.16127200
C	-3.62407700	-0.32294100	-2.90554800
F	-3.68232800	0.98682500	-2.65737500

F	-3.91171600	-0.53902400	-4.19020300
F	-4.52214500	-0.95257800	-2.14240300
C	-2.71405000	-4.03089200	-0.93005600
F	-2.22998600	-4.74067000	-1.93061900
F	-2.96887200	-4.83832500	0.10201200
F	-3.83478200	-3.41160800	-1.29071800
O	-1.62613800	-2.72509300	1.19236200
C	-4.73248700	-1.35988400	1.83963600
C	-5.32584300	-2.52441300	1.32923000
C	-4.05522900	-1.41823300	3.06759900
C	-5.22621000	-3.71644500	2.03255900
H	-5.82809300	-2.52613100	0.36913100
C	-3.97622400	-2.62010600	3.75255800
H	-3.57944500	-0.54496900	3.49579700
C	-4.55882300	-3.78203800	3.25135500
C	0.86706700	3.14980600	-0.75734700
C	1.00935900	2.40694800	-1.94122400
C	2.02236900	3.53251300	-0.05014900
C	2.27962900	2.06162000	-2.38425500
H	0.15653200	2.06251300	-2.51308500
C	3.27825800	3.17376400	-0.51787200
H	1.95426200	4.08282900	0.88168000
C	3.42669800	2.43192900	-1.68528300
O	-0.05556700	0.02718700	1.03198100
C	-1.71860200	-1.17159000	-0.87022900
F	-5.77181200	-4.84093800	1.53933600
F	-4.46936100	-4.93724200	3.92235000
F	-3.33849100	-2.68743700	4.93221000
F	4.38017800	3.49422900	0.18625600
F	4.64198300	2.05054300	-2.10719100
F	2.43439600	1.32975300	-3.49727400
O	-0.15803300	-3.42238500	-0.75213400
Si	1.87894200	-2.76074800	-0.33500200
C	-1.93089800	6.54049300	1.51055900

H	-1.08491100	7.21907900	1.43286400
C	-3.07179800	6.91737200	2.17884200
H	-3.14270900	7.90265000	2.63079000
C	-4.15032600	6.00901000	2.29309500
C	-4.08327500	4.75948800	1.71704800
H	-4.91671400	4.07567900	1.82293400
H	-5.04034000	6.29793600	2.84514800
C	-5.42791600	3.62101800	-0.97435400
H	-4.60258000	4.30761600	-1.12226000
C	-6.65657100	3.90039800	-1.53103200
H	-6.78964100	4.81048000	-2.10934100
C	-7.74418100	3.01114000	-1.36460700
C	-7.56957900	1.84267200	-0.66071700
H	-8.39153500	1.14145500	-0.53917600
H	-8.70933900	3.24769200	-1.80350200
C	2.66933100	-4.32297200	-1.00285400
H	3.75529300	-4.28881200	-0.86575700
H	2.28527800	-5.20594500	-0.48232200
H	2.46047100	-4.43817600	-2.07119200
C	1.51930500	-2.85407000	1.50916000
H	0.95758300	-3.77177500	1.70516000
H	2.46340700	-2.89771000	2.06044000
H	0.91706100	-2.02643300	1.88853000
C	1.66160800	-1.43264700	-1.64575600
H	2.63156100	-1.22112100	-2.10611600
H	0.98972500	-1.79038800	-2.42810800
H	1.25890400	-0.49748900	-1.25462200

IMII-1S

C	6.40539000	-3.64699500	-0.64465300
C	5.11856500	-3.74507600	-1.20686000
C	4.04227200	-3.15462100	-0.53543400
C	4.27995000	-2.48794200	0.66809500
C	5.57755700	-2.42903800	1.21252500
C	6.66594000	-3.00613200	0.56001300

C	6.60445600	-4.80296200	-2.49506300
C	5.28294200	-4.51429300	-2.41696700
H	3.03557800	-3.23031000	-0.93740200
H	5.71952100	-1.94837300	2.17207000
H	7.66700400	-2.97369100	0.97740700
H	7.19320700	-5.35201800	-3.21481400
H	4.51065900	-4.81425400	-3.11071800
O	7.31766800	-4.29015800	-1.43582400
C	3.08636700	-1.88122400	1.38227600
O	3.33205700	-1.64185400	2.73310700
H	2.22577100	-2.54220800	1.25937700
C	5.24698600	5.73249900	-3.99696500
C	5.99024300	5.06904100	-3.01550900
C	5.43638600	3.99037000	-2.31566700
C	4.13694800	3.59245400	-2.60963400
C	3.38839300	4.25672200	-3.60185000
C	3.94371800	5.33076300	-4.29966400
H	5.68968200	6.56751800	-4.53316700
H	7.00510500	5.38952000	-2.79733800
H	6.02666300	3.47063800	-1.56416000
H	3.37566500	5.84848800	-5.06799600
C	3.31318900	2.46444900	-2.00037900
H	3.80676500	1.49502300	-2.16584000
C	2.00672400	2.55545400	-2.77667000
C	0.85777200	1.77791300	-2.66697500
C	-0.22862000	2.06444500	-3.50311200
C	-0.16294100	3.10965000	-4.43020700
C	0.98698600	3.89387000	-4.53939000
C	2.07206700	3.61353200	-3.70741800
H	0.78743200	0.96407600	-1.95154100
H	-1.12850400	1.46248400	-3.43404900
H	-1.01607500	3.30879300	-5.07296800
H	1.03313600	4.70535600	-5.26109400
C	3.16059100	2.66183300	-0.48706600

H	4.13177600	2.80214600	-0.01579900
H	2.51115400	3.50383300	-0.25266000
O	2.49608600	1.51074500	0.11350100
C	3.18948300	0.53307900	0.67726700
C	-3.31265100	-0.37203700	-3.74195500
C	-2.78172900	-1.44763900	-4.52626600
C	-3.27572200	-0.47002800	-2.30315300
C	-2.17327500	-2.54979900	-3.87859300
C	-2.05704300	-2.61906100	-2.50531000
C	-2.63334100	-1.56205300	-1.74231100
H	-1.77085300	-3.35492400	-4.48758900
C	-3.82754000	0.61718100	-1.44050900
C	-5.19371400	1.05311700	-1.54956900
C	-3.01947400	1.23848400	-0.50087800
C	-5.61718600	2.20456900	-0.81097600
C	-3.40747200	2.40886300	0.21363900
C	-4.69109400	2.87532800	0.02449400
H	-5.01262900	3.77602400	0.54080700
P	-1.42892800	-0.73341500	0.40016000
O	-1.74603000	0.74643700	-0.24753100
O	-2.53668000	-1.65710400	-0.35474900
S	-3.51269000	-0.79710700	2.65218500
S	-0.62876700	-1.11282800	3.31946800
O	-3.62324200	-0.21056300	3.98728300
O	-4.32520000	-0.27760100	1.54604600
C	-4.08580100	-2.58537700	2.83082800
F	-5.29722800	-2.57863100	3.39181000
F	-4.17189700	-3.15482200	1.62012500
F	-3.25198700	-3.29840500	3.58443100
C	0.01920200	0.60541500	3.70387200
F	0.50349600	1.17448000	2.58077700
F	-0.92258600	1.38796800	4.21529900
F	1.03360700	0.49852400	4.58260800
O	0.57576000	-1.76919600	2.76735300

C	-2.47687400	3.10620600	1.14107400
C	-2.92889700	3.49814100	2.41115400
C	-1.15936900	3.41477700	0.75860400
C	-2.08136400	4.18569800	3.26934400
H	-3.92248700	3.23769500	2.75793200
C	-0.33561400	4.09207300	1.64131000
H	-0.76985200	3.12958800	-0.21112900
C	-0.77487900	4.49162000	2.89971500
O	-0.01234100	-1.02560100	0.03429400
C	-1.84518600	-0.89742000	2.10604500
F	-2.50133500	4.55710600	4.48804200
F	0.04702400	5.13967300	3.73745300
F	0.94228300	4.38918100	1.29819600
O	-1.18688300	-1.59779600	4.57761400
O	4.38349700	0.73032800	1.15110500
Si	4.99535500	1.67698300	2.51024900
C	3.55403800	2.60623700	3.26425200
H	3.94120900	3.28984900	4.03083200
H	2.98120300	3.20747900	2.55037100
H	2.85643200	1.92450800	3.75921600
C	5.77413600	0.46571400	3.70056100
H	6.05519000	0.98431500	4.62583200
H	5.07524000	-0.33773500	3.94935400
H	6.68166200	0.01760500	3.28166000
C	6.30082800	2.79514900	1.75128200
H	7.00464200	2.21633200	1.14173500
H	5.88645900	3.59582100	1.12960300
H	6.87923000	3.27155700	2.55291100
N	2.60174600	-0.63262800	0.69844500
H	1.62422900	-0.67147500	0.34876700
H	2.44643600	-1.62156900	3.15227100
C	-1.29569600	-3.72974900	-1.87335100
C	-1.80221700	-4.47201700	-0.79496700
C	-0.02872500	-4.04891300	-2.38804100

C	-1.05100900	-5.51087200	-0.26387100
H	-2.76276700	-4.24721600	-0.34840300
C	0.70541600	-5.08368900	-1.82889000
H	0.40751000	-3.47591200	-3.19841800
C	0.20900100	-5.83296400	-0.76712100
F	-1.52688700	-6.23717900	0.75806300
F	0.92645200	-6.82941400	-0.23494300
F	1.94180500	-5.36424300	-2.29331000
C	-6.96126100	2.65140800	-0.92185200
H	-7.26189800	3.53363900	-0.36190300
C	-7.87023800	1.97305000	-1.69982900
H	-8.89860500	2.31660700	-1.76787900
C	-7.46628600	0.81105900	-2.39757500
H	-8.19172600	0.25896800	-2.98885200
C	-6.16454400	0.36548000	-2.32776200
H	-5.87635400	-0.53516800	-2.85762400
C	-3.81194400	0.76781700	-4.43350900
H	-4.17949900	1.61338500	-3.86567500
C	-3.82921600	0.81608100	-5.81072600
H	-4.21533000	1.70015800	-6.31082900
C	-3.35122400	-0.27085900	-6.57900700
H	-3.38054800	-0.22375100	-7.66393100
C	-2.83395200	-1.37563100	-5.94488800
H	-2.44035300	-2.21015200	-6.52012700

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C	6.98030600	3.15777300	0.84526400
C	5.75095000	3.36932900	1.50171100
C	4.56627400	3.06233400	0.82883600
C	4.64911500	2.55170900	-0.47242700
C	5.89946300	2.36624300	-1.10617300
C	7.08813100	2.66659500	-0.45271500
C	7.44489600	3.96694600	2.82727500
C	6.09259500	3.90356100	2.79844900

H	3.60375300	3.23188900	1.30166400
H	5.92033800	2.00163600	-2.12566400
H	8.05449400	2.53832300	-0.92842700
H	8.14914400	4.29502600	3.57696700
H	5.41334700	4.19836800	3.58566100
O	8.01490700	3.52032400	1.65473300
C	3.39217700	2.27415300	-1.17507800
O	3.41789900	2.17059700	-2.49072800
H	2.49431400	2.71642100	-0.75120500
C	4.76458000	-6.33008600	3.59228500
C	5.55359500	-5.65464900	2.65575400
C	5.06890200	-4.50704300	2.01660700
C	3.79162200	-4.05157000	2.32434200
C	2.99779100	-4.72838400	3.27229800
C	3.48374600	-5.87157400	3.90964700
H	5.15344800	-7.21923800	4.08134900
H	6.55030300	-6.02043600	2.42485200
H	5.69416900	-3.97972200	1.29947600
H	2.87927000	-6.39927800	4.64276800
C	3.04015900	-2.84526200	1.77641900
H	3.58839700	-1.91837500	2.00326900
C	1.72489100	-2.90530100	2.53956300
C	0.62188800	-2.06030800	2.46293100
C	-0.49012100	-2.33665200	3.26850500
C	-0.49488700	-3.43579900	4.13367000
C	0.60927800	-4.28687800	4.20922300
C	1.71913800	-4.01830600	3.40638000
H	0.60850500	-1.20449200	1.79457500
H	-1.35702700	-1.68603200	3.22272900
H	-1.36753500	-3.62520200	4.75298200
H	0.60098400	-5.14126500	4.88133600
C	2.88235400	-2.93236700	0.25068800
H	3.84315700	-3.14102600	-0.21947200
H	2.16702200	-3.70391000	-0.03231200

O	2.32666500	-1.70689100	-0.29223900
C	3.13388700	-0.68897000	-0.63222100
C	-3.52966800	0.06863500	3.69887700
C	-2.94755300	0.99029300	4.63021300
C	-3.42547700	0.33905200	2.28532900
C	-2.22600900	2.10993300	4.14831000
C	-2.05356500	2.33868200	2.79942500
C	-2.67965100	1.43752900	1.89048100
H	-1.78088300	2.79337700	4.86673000
C	-4.01527600	-0.58551500	1.27051500
C	-5.41195200	-0.93091000	1.27416500
C	-3.21418700	-1.13763500	0.28230500
C	-5.88190400	-1.94171200	0.37439500
C	-3.65184700	-2.17196700	-0.59470500
C	-4.97027300	-2.56382500	-0.51392300
H	-5.33140900	-3.35989000	-1.15978000
P	-1.41958500	0.79493500	-0.27599800
O	-1.89974500	-0.72299200	0.13340100
O	-2.51205400	1.69704200	0.53194900
S	-3.35026800	1.31594200	-2.61207200
S	-0.42576000	1.56388700	-3.05929400
O	-3.40271700	0.94239500	-4.02513500
O	-4.25498200	0.68551800	-1.64428300
C	-3.82658700	3.14036400	-2.55336100
F	-4.99677100	3.28377600	-3.17995500
F	-3.96561900	3.53331600	-1.27969000
F	-2.91122700	3.90682400	-3.14347900
C	0.18669500	-0.10693300	-3.65766900
F	0.49403100	-0.89120100	-2.61085100
F	-0.72146900	-0.71595800	-4.40902800
F	1.30827200	0.08235000	-4.38157400
O	0.76550700	2.08632000	-2.34194100
C	-2.72632900	-2.79433000	-1.57920000
C	-3.12842900	-2.93496600	-2.91667200

C	-1.46004300	-3.26557300	-1.19011100
C	-2.27844500	-3.53451300	-3.83680900
H	-4.07901700	-2.54332900	-3.26065900
C	-0.63263700	-3.85251500	-2.13225900
H	-1.10961200	-3.17031200	-0.16946500
C	-1.02161600	-3.99931900	-3.46069900
O	-0.01187800	0.90327200	0.19728700
C	-1.71911100	1.23804100	-1.96289600
F	-2.64777100	-3.66665000	-5.12005000
F	-0.19828800	-4.56334100	-4.35606000
F	0.59320500	-4.30754500	-1.78077300
O	-0.86901400	2.25820200	-4.26409900
O	4.35572600	-0.96342500	-1.06466700
Si	4.89073400	-1.77220800	-2.50906800
C	3.43377100	-2.57678200	-3.37434100
H	3.81019900	-3.16797200	-4.21919800
H	2.84096900	-3.24483700	-2.74216000
H	2.75494300	-1.82305000	-3.78357500
C	5.68203600	-0.46822200	-3.59943900
H	5.95821400	-0.90373200	-4.56785100
H	4.99502500	0.36360200	-3.78662000
H	6.59376100	-0.06613300	-3.14448600
C	6.17995800	-3.00282600	-1.91159400
H	6.92798900	-2.50725400	-1.28171100
H	5.74740800	-3.82998100	-1.33828400
H	6.70798300	-3.43962100	-2.76836100
N	2.70640100	0.51333500	-0.51323400
H	1.71965200	0.65534000	-0.25474700
H	2.47064500	2.12410400	-2.78652900
C	-1.17933600	3.44386400	2.32232700
C	-1.60499000	4.37256600	1.35968800
C	0.11747700	3.54699600	2.84883900
C	-0.74387900	5.38029600	0.94991300
H	-2.58691900	4.31364000	0.90644900

C	0.96083700	4.55540500	2.40934700
H	0.49066500	2.82312500	3.56430300
C	0.54910700	5.48571900	1.46134900
F	-1.13798600	6.28251600	0.03905600
F	1.37757200	6.45143400	1.04262900
F	2.23076600	4.62684600	2.87004700
C	-7.25717000	-2.29755700	0.37861900
H	-7.59302500	-3.07442600	-0.30394400
C	-8.15080200	-1.66095800	1.20801200
H	-9.20243800	-1.93319800	1.19412400
C	-7.69843600	-0.63304200	2.06737300
H	-8.40905300	-0.10976200	2.70137100
C	-6.36697600	-0.28042500	2.10242600
H	-6.04185200	0.52013300	2.75708900
C	-4.14290800	-1.10371700	4.22360100
H	-4.55073200	-1.83824600	3.54068900
C	-4.21935500	-1.32259700	5.58208900
H	-4.69239900	-2.22785600	5.95286500
C	-3.68941100	-0.38352400	6.49718700
H	-3.76560200	-0.56371300	7.56578500
C	-3.06224500	0.74546000	6.02558100
H	-2.62765700	1.46558900	6.71463500

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C	-0.28193100	3.70470500	4.40527900
C	0.55997400	3.20164800	3.38917300
C	0.00843900	2.41502200	2.37904400
C	-1.38197700	2.16721900	2.41875500
C	-2.19791000	2.69418200	3.46463800
C	-1.65917400	3.46902400	4.47189200
C	1.74479600	4.41275000	4.84209000
C	1.88330100	3.68688200	3.70945900
H	0.61101700	1.99658100	1.57835100
H	-3.25934400	2.47399700	3.45031800
H	-2.26055300	3.88008800	5.27545100

H	2.44026900	4.96461300	5.45580900
H	2.79414400	3.51427600	3.15587500
O	0.43379700	4.43782100	5.28925200
C	-1.95186600	1.39327600	1.35977900
H	-1.27285700	1.02026200	0.59046300
C	-9.09511600	-2.61400100	-1.40285800
C	-8.13178900	-3.34825600	-0.70310300
C	-7.37812700	-2.74946800	0.31359300
C	-7.59844700	-1.40914200	0.60642100
C	-8.56287500	-0.66402600	-0.10107800
C	-9.31909300	-1.26709300	-1.10799000
H	-9.67393200	-3.09573300	-2.18621300
H	-7.96389000	-4.39259200	-0.95017000
H	-6.62578500	-3.32447900	0.84467100
H	-10.06838900	-0.70266000	-1.65697200
C	-6.93891500	-0.53562500	1.66467400
H	-7.20155000	-0.91328400	2.66653600
C	-7.60480200	0.81513000	1.43993300
C	-7.39701200	2.02089400	2.09857000
C	-8.15492400	3.13732200	1.72533500
C	-9.11145700	3.03758000	0.70983100
C	-9.32595900	1.82625900	0.04800600
C	-8.56618500	0.71340000	0.41395600
H	-6.66008700	2.10607800	2.89423600
H	-8.00024000	4.08690300	2.22988300
H	-9.69440600	3.91174900	0.43300400
H	-10.07221800	1.75694400	-0.73904900
C	-5.41354600	-0.51931700	1.65554800
H	-5.01189700	0.15797300	2.40976100
H	-5.00398900	-1.51883000	1.81418500
O	-4.93857500	-0.07737600	0.34451800
C	-3.82949000	0.62365700	0.24405100
N	-3.23173400	1.09130000	1.33620100
C	-0.66213200	4.87528900	-1.42546500

C	-0.66225700	6.10365400	-0.89832300
H	-0.23322800	4.02304500	-0.90400000
H	-1.07160500	4.67647900	-2.41243100
H	-1.09308200	6.92090600	-1.48034100
C	-0.06901300	6.49221100	0.42576200
H	0.04978000	5.60673100	1.06497100
H	-0.73921900	7.18294000	0.95864500
Si	1.65016400	7.32694400	0.27043400
C	2.11502300	8.04483900	1.96584900
H	2.13685500	7.26150400	2.73372200
H	1.39959700	8.81009500	2.29155100
H	3.10836700	8.50971700	1.94128500
C	1.56641400	8.72789400	-1.00420800
H	1.31680100	8.34303000	-1.99986600
H	2.53007000	9.24587700	-1.08308000
H	0.81035500	9.47670100	-0.73688000
C	2.92728800	6.03744000	-0.25253600
H	3.13752600	5.33073700	0.55830400
H	3.88135100	6.50102900	-0.52992600
H	2.57617000	5.45395100	-1.11087900
O	-3.43090800	0.89866500	-0.94850300
Si	-4.18256800	0.59851600	-2.54304600
C	-5.85083800	1.45543600	-2.48795700
H	-6.54465700	0.98554200	-1.78532600
H	-5.74484500	2.51164500	-2.21510100
H	-6.30820500	1.42044500	-3.48508800
C	-4.30446200	-1.25308100	-2.78329700
H	-4.90856900	-1.73927800	-2.01150000
H	-4.77892000	-1.45788100	-3.75178000
H	-3.31724200	-1.72262900	-2.79776700
C	-2.98821200	1.44918700	-3.69145900
H	-3.31054700	1.31427000	-4.73182500
H	-2.95047600	2.52536500	-3.48925200
H	-1.97102200	1.06033400	-3.59442600

C	3.18958900	-4.43836400	2.59944500
C	2.07399900	-5.10577100	3.20002400
C	2.97964600	-3.66940600	1.40125700
C	0.79323400	-4.98221900	2.61023500
C	0.56717300	-4.18677200	1.50477900
C	1.68478800	-3.50097700	0.94140900
H	-0.03343900	-5.54027500	3.04209900
C	4.12174900	-3.03461800	0.68174500
C	5.20954200	-3.82856600	0.18161100
C	4.14553100	-1.66125700	0.48690200
C	6.35087200	-3.16190500	-0.36505800
C	5.29297600	-0.97406500	-0.01906600
C	6.37028100	-1.74887800	-0.40882600
H	7.27573000	-1.26092400	-0.75748900
P	1.58867800	-1.03658700	0.08616000
O	3.04049900	-0.91430900	0.86992300
O	1.45654000	-2.65707800	-0.13681700
S	1.65637000	-1.44813600	-2.99715600
S	1.37765000	1.23990400	-1.80291500
O	1.96947300	-0.61253100	-4.16211600
O	2.32078600	-2.73530200	-2.78759100
C	-0.17331100	-1.91617100	-3.27689400
F	-0.90080400	-1.70463100	-2.15847100
F	-0.70802900	-1.18951100	-4.25949300
F	-0.26368000	-3.21119700	-3.59739100
C	2.76309600	1.96220500	-2.90612000
F	2.30374600	2.21255300	-4.12392000
F	3.15152700	3.11629700	-2.34316500
F	3.81450200	1.14700800	-2.97302800
O	0.14247000	1.51379100	-2.55578300
C	5.39872700	0.50722100	-0.09291800
C	6.12115300	1.09375400	-1.14656200
C	4.86531100	1.34223600	0.90398900
C	6.30060800	2.46680300	-1.19651300

H	6.50983000	0.49769000	-1.96368200
C	5.06531000	2.71049500	0.82826000
H	4.29746500	0.94098400	1.73278700
C	5.78183400	3.29793100	-0.20862600
C	-0.79697000	-4.09827000	0.92409900
C	-1.00685900	-4.23783900	-0.45697100
C	-1.90420500	-3.92933300	1.77242900
C	-2.29643800	-4.20647400	-0.96408300
H	-0.18026400	-4.35657500	-1.14591300
C	-3.18158100	-3.91025500	1.23586300
H	-1.77879800	-3.78928800	2.84009000
C	-3.39949400	-4.04558600	-0.12985000
O	0.55131700	-0.44560200	0.97139400
C	1.68911700	-0.45775200	-1.57987200
F	6.97654900	3.02638600	-2.21337100
F	5.95907600	4.62415200	-0.25956500
F	4.57057700	3.52626500	1.78849400
F	-4.25776700	-3.71982200	2.04012600
F	-4.64402300	-4.00257200	-0.63685300
F	-2.51731300	-4.31601300	-2.28374400
O	1.58201300	1.90155100	-0.49832200
C	7.44578500	-3.92835500	-0.84855100
H	8.30889700	-3.40383700	-1.25127700
C	7.40848400	-5.30263200	-0.82692600
H	8.24575300	-5.88024700	-1.20852100
C	6.26547900	-5.96586600	-0.32146600
H	6.22662700	-7.05172000	-0.32952700
C	5.19715100	-5.25033000	0.17263300
H	4.32439000	-5.77571200	0.54251100
C	4.45212400	-4.53695500	3.24683600
H	5.30227300	-4.00922400	2.83151800
C	4.60473500	-5.27697400	4.39876000
H	5.57858400	-5.32875900	4.87787100
C	3.50755900	-5.96572700	4.96702600

H	3.64462300	-6.55226000	5.87118500
C	2.26831100	-5.87704500	4.37766200
H	1.41136800	-6.38764700	4.81070500

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C	2.63832400	-1.44068800	5.24206100
C	2.02383200	-2.03211600	4.11881100
C	2.06368500	-1.35567800	2.89893400
C	2.70275100	-0.10847600	2.84220900
C	3.30252900	0.45885200	3.99116900
C	3.28351100	-0.20629300	5.21147300
C	1.78469000	-3.34808400	5.90238800
C	1.47219700	-3.28090100	4.58662200
H	1.60122700	-1.77669600	2.01150200
H	3.78071600	1.42874800	3.90367400
H	3.74020600	0.21263700	6.10172100
H	1.58644900	-4.08314700	6.66785700
H	0.90941600	-4.00171900	4.00976400
O	2.49622300	-2.24634900	6.33072600
C	2.71888800	0.58721900	1.54655000
O	1.03967000	1.44367700	1.56421800
H	2.47323900	-0.03917500	0.68860600
C	9.28607300	-2.17527300	2.35149900
C	7.94654500	-1.90541500	2.65024400
C	7.07622000	-1.42992900	1.66208000
C	7.56643000	-1.22681600	0.37594400
C	8.91664000	-1.50151300	0.07361500
C	9.78130300	-1.97684900	1.06100800
H	9.94710500	-2.54689100	3.12992500
H	7.57550900	-2.06971900	3.65824300
H	6.03695400	-1.22500600	1.89999600
H	10.82186000	-2.19331300	0.83338500
C	6.84517200	-0.72269600	-0.86721800
H	6.01494200	-1.39000700	-1.13926200

C	7.94360100	-0.76501300	-1.92126800
C	7.87964600	-0.43549800	-3.27050900
C	9.03507900	-0.55334900	-4.05205600
C	10.23380100	-0.99696000	-3.48399500
C	10.30072500	-1.33239900	-2.12976200
C	9.15017800	-1.21442600	-1.34800500
H	6.94905100	-0.10057700	-3.72294700
H	8.99824000	-0.30260200	-5.10845300
H	11.12186000	-1.08539200	-4.10395100
H	11.23485600	-1.68119800	-1.69724500
C	6.27674400	0.69096800	-0.72866100
H	7.02291800	1.38343500	-0.33265400
H	5.91206800	1.06919900	-1.68779100
O	5.15470400	0.61577900	0.19337000
C	4.50183500	1.72899000	0.53509700
C	-6.02925600	1.28037600	2.03761600
C	-5.82021000	2.61065700	2.52805600
C	-5.24959800	0.82042200	0.91647100
C	-4.81069000	3.41904500	1.95120300
C	-3.99258600	2.96031000	0.93807200
C	-4.25220700	1.65126300	0.43415000
H	-4.66811700	4.42480700	2.33747500
C	-5.44825000	-0.54167000	0.33322500
C	-6.72811300	-0.97432000	-0.16404100
C	-4.38788100	-1.43022900	0.24674500
C	-6.89083800	-2.33500900	-0.58194000
C	-4.53591900	-2.79522300	-0.13298300
C	-5.78650300	-3.22141100	-0.52072300
H	-5.93248800	-4.25972300	-0.80704900
P	-2.25031300	0.15555700	-0.16614100
O	-3.10344300	-1.02880500	0.57951600
O	-3.43637600	1.18900900	-0.59829500
S	-2.51633100	-0.81014000	-3.06183300
S	0.18792900	-0.31745400	-1.91292800

O	-1.84769400	-1.79524200	-3.91123100
O	-3.87023300	-1.06332500	-2.55229500
C	-2.70919600	0.72616600	-4.13973800
F	-3.27074600	0.36246800	-5.29479700
F	-3.50780200	1.61401500	-3.53028400
F	-1.53172000	1.30180600	-4.38156300
C	0.75688100	-1.96579000	-1.20916100
F	0.27585800	-2.11603900	0.04464400
F	0.33859600	-2.98099900	-1.95284000
F	2.09778800	-1.98288800	-1.14006700
O	0.86949700	0.65360700	-1.02146900
C	-3.36993700	-3.71957500	-0.13547600
C	-3.08122400	-4.47460400	-1.28197900
C	-2.55644100	-3.86099900	1.00167600
C	-2.00131600	-5.34844500	-1.28057400
H	-3.65918800	-4.35567400	-2.19129100
C	-1.48293500	-4.73554600	0.97283400
H	-2.74326500	-3.29075900	1.90352800
C	-1.18982200	-5.49260200	-0.15868400
O	-1.28897200	0.66867900	0.84525700
C	-1.52714800	-0.30193600	-1.70982800
F	-1.70973300	-6.07130600	-2.37238700
F	-0.14493600	-6.33195200	-0.16828000
F	-0.69159500	-4.88257700	2.05823700
O	0.58112100	-0.34787000	-3.31839200
O	4.99112000	2.86212000	0.07989600
Si	4.01517100	4.30564500	-0.21863300
C	2.80954600	3.82488100	-1.57124300
H	2.10971000	4.64624700	-1.76322600
H	3.33181700	3.60242500	-2.50888800
H	2.21247100	2.94525400	-1.30617000
C	3.17796100	4.89548600	1.35069800
H	2.54738900	5.76374500	1.12192600
H	2.53274200	4.11977500	1.77082900

H	3.90474900	5.19328500	2.11512100
C	5.32739300	5.50829300	-0.80984800
H	6.06530800	5.71341200	-0.02603700
H	5.86175000	5.12462400	-1.68597500
H	4.86777700	6.46340800	-1.09171500
N	3.47882500	1.67586300	1.31155200
H	0.71426600	1.37728100	0.63004800
H	0.33673000	0.93007500	2.01400300
C	-2.85247600	3.78805800	0.45726700
C	-2.54922400	3.93646900	-0.90701700
C	-2.05314800	4.44647300	1.40783500
C	-1.46787300	4.71745200	-1.28987000
H	-3.12163200	3.43635100	-1.67769300
C	-0.97905700	5.22200000	0.99770500
H	-2.23085800	4.32669700	2.47030500
C	-0.67461600	5.37115500	-0.35033700
F	-1.15951500	4.86531700	-2.58792900
F	0.38605000	6.10580600	-0.73548600
F	-0.19269500	5.83426100	1.90212200
C	-6.59995100	3.08693100	3.61710100
H	-6.43755100	4.10448800	3.96448300
C	-7.52403100	2.27625000	4.23306400
H	-8.10920300	2.64794400	5.06955800
C	-7.69727700	0.94596100	3.78501100
H	-8.40709200	0.29631200	4.28971800
C	-6.97269900	0.46206200	2.71788200
H	-7.11520200	-0.56165000	2.39443400
C	-7.83858800	-0.09760600	-0.30483300
H	-7.72557600	0.94660700	-0.03730000
C	-9.04472600	-0.54791900	-0.79569300
H	-9.87303800	0.14703700	-0.90402100
C	-9.21260700	-1.90146200	-1.16840000
H	-10.17047700	-2.24494400	-1.54893700
C	-8.15318100	-2.77261400	-1.06450500

H	-8.25948400	-3.81138700	-1.36774300
IMII-3S			
C	1.66105200	4.79568000	-3.16508600
C	0.59378700	3.95767400	-2.77899100
C	0.87597400	2.79565300	-2.05706300
C	2.22398800	2.48321700	-1.80285200
C	3.27358600	3.34263500	-2.22916300
C	3.00447500	4.52305500	-2.89931900
C	-0.17976500	5.72385400	-3.90351000
C	-0.59842800	4.59364300	-3.28942600
H	0.09019600	2.13206000	-1.70996200
H	4.29776200	3.05961800	-2.00940800
H	3.78903600	5.20087100	-3.21817400
H	-0.69992100	6.51273500	-4.42503900
H	-1.61482100	4.23631500	-3.23571400
O	1.19219700	5.87640000	-3.84007300
C	2.50825700	1.21242800	-1.17679300
H	1.67624200	0.67417000	-0.71650700
C	5.39644300	1.76797900	5.12753500
C	4.58090400	0.63555800	5.23137000
C	4.68032800	-0.40240100	4.29716200
C	5.60143000	-0.28591200	3.26315200
C	6.42596900	0.85076100	3.15853800
C	6.32624100	1.88419400	4.09179800
H	5.30709600	2.56384000	5.86186800
H	3.86293800	0.56035300	6.04294100
H	4.04137800	-1.27728600	4.38369800
H	6.96033600	2.76404400	4.02021600
C	5.92451400	-1.27298600	2.14996700
H	6.30297500	-2.21213800	2.58476100
C	7.03888900	-0.56115900	1.39509200
C	7.76766900	-0.98584400	0.29074800
C	8.77039000	-0.15393200	-0.22353800
C	9.03586600	1.08480100	0.36877300

C	8.31231200	1.51104700	1.48510600
C	7.31287200	0.68312300	1.99904400
H	7.57393900	-1.95294400	-0.16729600
H	9.34963600	-0.47639900	-1.08428500
H	9.81796400	1.71932600	-0.03933800
H	8.53087400	2.47087900	1.94557100
C	4.72883300	-1.70619700	1.29742100
H	5.00756300	-2.45305400	0.55587200
H	3.92806000	-2.09483700	1.92284300
O	4.13832400	-0.55063300	0.61808600
C	4.09783100	-0.46328100	-0.68202500
N	3.68820700	0.67490900	-1.23316800
C	-5.36154600	-0.59726300	2.71447000
C	-5.86778700	0.71096600	3.00201400
C	-4.53848000	-0.78882500	1.54596500
C	-5.52107300	1.79021300	2.15500100
C	-4.67050100	1.63501700	1.08039500
C	-4.16424800	0.32656700	0.81449600
H	-5.94049200	2.77105000	2.36257500
C	-4.03697600	-2.15003100	1.19528900
C	-4.93162700	-3.25318000	0.97266100
C	-2.67380700	-2.38598800	1.12853300
C	-4.38753900	-4.57245700	0.85526000
C	-2.11347400	-3.69927200	1.10056200
C	-2.98887300	-4.76027200	0.97663100
H	-2.60184300	-5.77569600	0.98173900
P	-1.75165900	-0.28281100	-0.15035400
O	-1.79904400	-1.30694400	1.14272000
O	-3.30621800	0.19703500	-0.26443700
S	-2.74445300	-1.14744900	-2.97126400
S	0.04391900	-1.59708000	-2.12305400
O	-2.29277600	-2.09237100	-4.00022200
O	-4.12061500	-1.18210800	-2.47433700
C	-2.59974900	0.55469600	-3.81017500

F	-3.79619300	0.91614400	-4.28304500
F	-2.19977000	1.48742300	-2.91868800
F	-1.72284700	0.51931900	-4.80751800
C	0.02279600	-3.41366000	-2.71514600
F	0.07193300	-3.49540700	-4.03571400
F	1.13816000	-3.99079700	-2.21891600
F	-1.03574400	-4.07693000	-2.24955800
O	0.58819900	-0.86621400	-3.28273900
C	-0.65779500	-3.93551600	1.28016100
C	-0.01333100	-4.95743000	0.56596200
C	0.08381400	-3.18167400	2.20664000
C	1.34000700	-5.19489200	0.75504700
H	-0.53746700	-5.53519400	-0.18493200
C	1.42862900	-3.44833700	2.38073000
H	-0.36591400	-2.38166500	2.77959400
C	2.07960600	-4.44660400	1.66390000
C	-4.30717200	2.80842300	0.24501300
C	-4.37612100	2.75673700	-1.15560100
C	-3.91714200	4.00385300	0.87013000
C	-4.04472600	3.88059600	-1.89394200
H	-4.66734800	1.85472800	-1.67836100
C	-3.59529200	5.11428700	0.10359700
H	-3.83007500	4.07135000	1.94877600
C	-3.65077400	5.06946600	-1.28548400
O	-0.77224200	0.79448700	0.14934800
C	-1.57045000	-1.14672200	-1.68849600
F	1.97038300	-6.14778400	0.04785600
F	3.40040100	-4.65478000	1.82449600
F	2.16097800	-2.71911300	3.25770900
F	-3.19072800	6.25452600	0.69356400
F	-3.30606400	6.13351800	-2.02629500
F	-4.05722000	3.83935500	-3.24113900
C	1.44042000	0.88265400	2.67170000
C	1.86026200	2.14717600	2.79007400

H	0.54088100	0.63358500	2.11514400
H	1.99657700	0.05939100	3.11197200
H	2.78180800	2.34300300	3.34111800
C	1.14187200	3.35528000	2.25651900
H	0.37606700	3.04676900	1.53265500
H	1.84420400	4.01436700	1.72357200
Si	0.29845100	4.38820300	3.62678800
C	-0.30785800	6.03292000	2.90133300
H	-1.08040700	5.89493400	2.13636700
H	0.51748000	6.58972400	2.44018300
H	-0.73556100	6.67220700	3.68416000
C	1.54425100	4.75561600	5.01142400
H	1.08051100	5.34065100	5.81528800
H	2.40245100	5.32972600	4.64011500
H	1.93066100	3.83064000	5.45539200
C	-1.16206400	3.41439100	4.33740200
H	-0.83288400	2.44555600	4.73010900
H	-1.91528600	3.21237300	3.56602800
H	-1.65313400	3.96010500	5.15248800
O	0.85543600	-1.63977900	-0.88620300
O	4.57266800	-1.42994100	-1.39465000
Si	4.84664600	-1.64604200	-3.14234000
C	3.79874000	-0.50899000	-4.18409500
H	3.96684500	-0.76989600	-5.23809900
H	2.72863400	-0.61777600	-3.98138900
H	4.07339300	0.54168700	-4.05117200
C	4.43118400	-3.45715500	-3.35208000
H	4.60953400	-3.76783900	-4.38895700
H	5.04815400	-4.08970900	-2.70405400
H	3.38048100	-3.65607400	-3.12063300
C	6.68096700	-1.29800700	-3.33838600
H	6.95813200	-1.36959500	-4.39765900
H	6.94035800	-0.29110100	-2.99388100
H	7.29587500	-2.01472700	-2.78388600

C	-5.26217600	-5.67125900	0.63957800
H	-4.83474000	-6.66809000	0.56240100
C	-6.61813600	-5.47907500	0.51203600
H	-7.27705800	-6.32467000	0.33577500
C	-7.15441800	-4.17267100	0.59451800
C	-6.33505300	-3.08932500	0.82395200
H	-6.75732300	-2.09220200	0.87057200
H	-8.22280200	-4.02107100	0.46809000
C	-5.66749600	-1.64049700	3.63229900
H	-5.26203500	-2.63079500	3.46617700
C	-6.45690800	-1.40969700	4.73774500
H	-6.66726600	-2.22483500	5.42480200
C	-6.99031500	-0.12502500	4.99160500
C	-6.69440200	0.91303000	4.13992900
H	-7.07814700	1.91251200	4.32999600
H	-7.61788800	0.04039300	5.86283900

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C	-2.02752300	1.15568700	4.84152400
C	-0.96987300	0.66565700	4.05238900
C	-1.12132700	0.61472100	2.66099900
C	-2.32922800	1.05375400	2.10315100
C	-3.37035300	1.54132400	2.93061900
C	-3.23705500	1.59761000	4.31328800
C	-0.41437600	0.60495500	6.21708100
C	0.07265600	0.31151900	4.98761900
H	-0.33348600	0.23635800	2.01494000
H	-4.29935000	1.84983600	2.46424100
H	-4.03578000	1.95667000	4.95404600
H	-0.00266600	0.51359800	7.21110100
H	1.04388700	-0.10617300	4.76215600
O	-1.69026400	1.12081100	6.16459500
C	-2.50382900	0.97510000	0.62635100
H	-1.81884300	0.26434300	0.15575500

C	-11.25315500	0.83377600	1.25626000
C	-10.76283100	1.78309200	0.35377200
C	-9.58515900	1.53810300	-0.36267000
C	-8.91043400	0.33922600	-0.16188300
C	-9.40448100	-0.61898100	0.74608900
C	-10.58008200	-0.37350600	1.45814400
H	-12.16935400	1.03638600	1.80447900
H	-11.30082700	2.71522100	0.20471200
H	-9.21562700	2.27781500	-1.06967300
H	-10.96985700	-1.10753600	2.15856000
C	-7.62795800	-0.16364600	-0.81135300
H	-7.75872700	-0.25234900	-1.89983500
C	-7.45216000	-1.53291700	-0.16711000
C	-6.44703200	-2.47648800	-0.35109400
C	-6.49054800	-3.66746500	0.38343100
C	-7.53329500	-3.91075900	1.28273400
C	-8.54755800	-2.96897900	1.46921400
C	-8.50057300	-1.77683300	0.74490600
H	-5.63337900	-2.30638600	-1.04829000
H	-5.69805300	-4.39694400	0.25646900
H	-7.55372500	-4.84117200	1.84393100
H	-9.35536000	-3.16319300	2.17027600
C	-6.46052400	0.79635300	-0.55974600
H	-6.73362100	1.82488400	-0.81760100
H	-6.12418000	0.76253100	0.47601400
O	-5.36362500	0.42132100	-1.43276400
C	-4.09867500	0.54269300	-1.00625300
N	-3.82654600	0.97091500	0.18198000
C	-1.56063000	2.40641900	-0.23058600
C	-2.08243900	3.53540400	0.39871100
H	-0.52355100	2.13997600	-0.04198700
H	-1.89398900	2.18194800	-1.24018200
H	-3.07513800	3.86985500	0.09202800
C	-1.45534700	4.25794800	1.47396300

H	-0.59249100	3.73951200	1.90461100
H	-2.16805900	4.56281600	2.25085100
Si	-0.76193700	5.99672200	0.81682800
C	-2.25609600	7.01142800	0.25312400
H	-1.93415900	8.01650200	-0.04656100
H	-2.99580200	7.13192200	1.05364300
H	-2.76089400	6.56343500	-0.61087700
C	0.44276000	5.71275500	-0.59719600
H	1.07892300	4.83564500	-0.44320600
H	1.09633000	6.58519700	-0.71645900
H	-0.08786400	5.56086000	-1.54430700
C	0.03275300	6.78975400	2.33019700
H	-0.68143900	6.88670900	3.15611200
H	0.38881300	7.79614000	2.07683800
H	0.89192300	6.21083600	2.67900500
O	-3.21229700	0.19347000	-1.91730300
Si	-3.41552700	-0.06887700	-3.64365300
C	-4.17057800	1.50683200	-4.34302000
H	-5.16350600	1.70786900	-3.92806400
H	-3.52970300	2.37452300	-4.14756900
H	-4.27427000	1.41848300	-5.43160600
C	-4.49711700	-1.57578200	-3.92865300
H	-4.53099600	-1.79969700	-5.00275700
H	-4.08304400	-2.45560900	-3.42542300
H	-5.52467100	-1.42943600	-3.58292500
C	-1.67169900	-0.34871300	-4.23829400
H	-0.97494100	0.42824200	-3.90600700
H	-1.29020800	-1.31411300	-3.89432100
H	-1.65387000	-0.36322700	-5.33597600
C	3.91092100	-3.77527200	2.35076900
C	2.95682700	-4.81707600	2.58517900
C	3.70046500	-2.87199300	1.24690500
C	1.78393800	-4.87328800	1.79761600
C	1.51689500	-3.95375300	0.80209200

C	2.52208100	-2.97734200	0.52204000
H	1.05868000	-5.65522300	2.00584500
C	4.67106300	-1.76898800	0.97609200
C	6.06643900	-2.01289900	0.74316000
C	4.22643200	-0.45535800	0.99444000
C	6.96459200	-0.89877500	0.70873400
C	5.10523700	0.67062800	1.00170800
C	6.45779600	0.41110100	0.88595400
H	7.16537100	1.23465500	0.92426500
P	1.93598400	-0.53345500	-0.28831400
O	2.85872600	-0.21371000	1.04539700
O	2.29811200	-2.11128800	-0.54071400
S	3.54086200	-0.66141400	-2.93818500
S	1.94425000	1.74898100	-2.18250600
O	3.79972100	0.28256500	-4.03425700
O	4.62874400	-1.42380300	-2.32048000
C	2.46906400	-1.99401500	-3.76636700
F	2.68809600	-3.19615000	-3.21318600
F	1.16612200	-1.70188300	-3.64731400
F	2.78375600	-2.06128800	-5.05969600
C	3.39804200	2.85058600	-2.75816400
F	4.57663200	2.38300500	-2.34234900
F	3.40078400	2.99574000	-4.07382900
F	3.19734800	4.05593000	-2.19827300
O	1.00666400	1.78707600	-3.31519800
C	4.60813400	2.06508600	1.14413100
C	5.26241400	3.11040000	0.47005700
C	3.50124500	2.37721800	1.95296700
C	4.80287500	4.41363100	0.58197900
H	6.09252200	2.91749400	-0.19814300
C	3.05803900	3.68479800	2.03700900
H	2.95773800	1.61393300	2.49173800
C	3.69353800	4.72100900	1.36309400
C	0.17924600	-3.96093400	0.14854900

C	0.00003900	-3.81480400	-1.23612100
C	-0.95188300	-4.13319600	0.96659600
C	-1.28176500	-3.83087700	-1.76425000
H	0.83752800	-3.68911100	-1.90675500
C	-2.22086600	-4.15713600	0.40959300
H	-0.85933200	-4.21501500	2.04330200
C	-2.40367200	-4.00164500	-0.95923200
O	0.52101900	-0.26522700	0.08131600
C	2.56420200	0.17189700	-1.77276700
F	5.41263300	5.40903900	-0.08211600
F	3.22755100	5.97951500	1.43936600
F	1.96505900	3.98192800	2.77942200
F	-3.30498700	-4.31731500	1.19066900
F	-3.64100800	-4.00182500	-1.49377600
F	-1.47809200	-3.67379300	-3.08861800
O	1.54322800	2.37208200	-0.90093300
C	8.35135100	-1.12714100	0.49774500
H	9.02236400	-0.27164100	0.48459100
C	8.83369300	-2.39823300	0.29090100
H	9.89388500	-2.56062000	0.11784400
C	7.94175000	-3.49650300	0.28338200
C	6.59563500	-3.31026800	0.50765600
H	5.92153200	-4.15901600	0.48388000
H	8.32137000	-4.49606200	0.09016000
C	5.00456500	-3.66760500	3.25506900
H	5.71457900	-2.85928000	3.13567400
C	5.17128600	-4.56788600	4.28455600
H	6.01494000	-4.45744200	4.96042100
C	4.25612300	-5.62944200	4.47461900
C	3.16793000	-5.74340900	3.64265100
H	2.43829100	-6.53611500	3.78993000
H	4.40617400	-6.33814700	5.28426800

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C	2.22844700	4.95118800	-2.41139000
C	1.10270600	4.16488800	-2.09477000
C	1.26481300	3.05394200	-1.25564300
C	2.54445000	2.77620000	-0.75225000
C	3.65205400	3.59006700	-1.09975800
C	3.51002400	4.69033200	-1.93500300
C	0.51435200	5.86574500	-3.41937400
C	-0.00654900	4.79609100	-2.77349700
H	0.42129100	2.42618200	-0.98042200
H	4.61851300	3.35255000	-0.66950400
H	4.34880300	5.32786700	-2.19483200
H	0.07603800	6.62824500	-4.04552800
H	-1.04287800	4.49585000	-2.76923300
O	1.87306900	5.98760500	-3.22316900
C	2.72241700	1.64926700	0.19528100
H	1.78616600	1.32273800	0.65094600
C	5.77420600	-3.11890000	-0.12376600
C	4.81540800	-3.21408000	0.89124300
C	4.94685600	-2.45361800	2.06058500
C	6.04061900	-1.60452000	2.19698000
C	7.00033100	-1.50164000	1.16861200
C	6.86999500	-2.26039300	0.00364700
H	5.67048000	-3.73003800	-1.01647500
H	3.97275700	-3.88833900	0.78153700
H	4.19737500	-2.54171000	2.84292600
H	7.61458600	-2.19970500	-0.78629500
C	6.44174800	-0.72290200	3.37256400
H	6.65727600	-1.35564300	4.24927500
C	7.72766200	-0.07840700	2.87528000
C	8.55914100	0.83376900	3.51341300
C	9.71074500	1.27900700	2.85419500
C	10.02285700	0.80924600	1.57420400
C	9.19181000	-0.11068300	0.93117900
C	8.04046000	-0.55151600	1.58596800

H	8.32699200	1.20301500	4.50991100
H	10.36758500	1.99432400	3.34137200
H	10.92150900	1.16266800	1.07588400
H	9.44162400	-0.47360800	-0.06252200
C	5.36723800	0.26448500	3.84763500
H	5.74579400	0.86311100	4.68100700
H	4.47489900	-0.26870800	4.17551000
O	5.03796200	1.20415400	2.80968800
C	3.88444700	1.12542600	2.13058400
N	3.86886700	1.70362300	0.97949500
C	2.80474800	-0.10075200	-0.69536400
C	3.68165400	0.17506100	-1.73922800
H	1.76086200	-0.28762700	-0.93118100
H	3.18205300	-0.65054900	0.16122500
H	4.74690900	0.21073800	-1.50570500
C	3.27720500	0.47741800	-3.08901000
H	2.20131300	0.65401100	-3.18526700
H	3.86528600	1.28707200	-3.53915700
Si	3.66188200	-1.06137900	-4.27187300
C	2.62925000	-0.75074400	-5.81507600
H	2.79401800	-1.54471900	-6.55407900
H	1.56401700	-0.73379600	-5.56089300
H	2.88400600	0.20460300	-6.28836600
C	5.51677700	-1.00417600	-4.64496500
H	5.80790100	-0.06070100	-5.12162300
H	6.11984900	-1.12275900	-3.73660500
H	5.79358200	-1.81671300	-5.32817000
C	3.22159800	-2.68666500	-3.43015500
H	3.83848900	-2.85562100	-2.54025500
H	2.17365100	-2.72602000	-3.11902000
H	3.39735100	-3.52181700	-4.12010200
O	2.88789700	0.44170000	2.68983100
Si	1.59737700	0.88811100	3.76583100
C	0.79168600	2.45633800	3.12910700

H	0.10482800	2.84933000	3.88979300
H	0.21018500	2.25776800	2.22274600
H	1.52222800	3.24470100	2.91253500
C	0.48181400	-0.60885400	3.70804400
H	-0.05426400	-0.63310600	2.75399000
H	-0.25949600	-0.57929200	4.51586300
H	1.05462900	-1.53854800	3.80365100
C	2.33752900	1.17122400	5.47639700
H	1.54406300	1.47919000	6.16923200
H	3.09220600	1.96658700	5.47411200
H	2.79660800	0.26560100	5.88863100
C	-5.09524300	-0.09000600	3.28264500
C	-5.24066300	1.21321100	3.85904900
C	-4.47011400	-0.22043800	1.98902500
C	-4.74164000	2.33997700	3.16249600
C	-4.06929400	2.22193100	1.96422200
C	-3.91260100	0.91185000	1.41537200
H	-4.89862800	3.32772100	3.58777800
C	-4.36743600	-1.56108300	1.33733400
C	-5.52901400	-2.36620300	1.07105700
C	-3.12530800	-2.08301500	1.01770800
C	-5.34826500	-3.72250600	0.64653800
C	-2.91553400	-3.45181500	0.67004500
C	-4.03678400	-4.24070600	0.50726000
H	-3.91765000	-5.29431200	0.26884400
P	-1.84560000	-0.02367500	-0.00189600
O	-2.01213800	-1.25503500	1.08153800
O	-3.21813800	0.82464100	0.22304400
S	-3.37514700	0.00374800	-2.71817400
S	-0.71508800	-1.25088000	-2.46217800
O	-3.32089600	-0.78770200	-3.95306800
O	-4.63982300	0.19404900	-2.00613000
C	-2.88672300	1.75318900	-3.27462800
F	-3.99024900	2.48142000	-3.46829000

F	-2.14512300	2.35424400	-2.31903900
F	-2.17891500	1.71589700	-4.39821600
C	-1.27369900	-2.81864700	-3.39955800
F	-2.40375400	-3.31804000	-2.89610900
F	-1.41080700	-2.58704000	-4.69585300
F	-0.29320100	-3.72464900	-3.23395900
O	-0.10947800	-0.41833800	-3.52027000
C	-1.55010800	-4.02649600	0.54863700
C	-1.25943300	-4.95469500	-0.46206900
C	-0.54163200	-3.68097200	1.46400900
C	0.01616200	-5.49000900	-0.56812400
H	-1.99480000	-5.22079100	-1.21108000
C	0.72146800	-4.23018200	1.33646900
H	-0.72229900	-2.97644100	2.26420500
C	1.02184300	-5.13822800	0.32601700
C	-3.54089300	3.43292100	1.28220300
C	-3.76653700	3.65659100	-0.08493100
C	-2.83569900	4.39350100	2.02506200
C	-3.27347400	4.80716700	-0.67928600
H	-4.30981800	2.94589300	-0.69428000
C	-2.36266800	5.54185600	1.40565200
H	-2.62706400	4.24769700	3.07901300
C	-2.56666700	5.76284200	0.04679400
O	-0.59083500	0.69468300	0.36045000
C	-2.08702500	-0.53635400	-1.68019100
F	0.31011200	-6.35423000	-1.55324800
F	2.26234900	-5.64261200	0.20454600
F	1.70280700	-3.89191500	2.20322700
F	-1.67618200	6.45878800	2.10963300
F	-2.08760400	6.86095500	-0.55169200
F	-3.44996800	5.01975700	-1.99750900
O	0.15867800	-1.77755600	-1.39277600
C	-6.48855100	-4.52921200	0.38625900
H	-6.33509500	-5.55954800	0.07467400

C	-7.75899300	-4.01557900	0.50454100
H	-8.62350400	-4.63786800	0.29094500
C	-7.93892300	-2.66618800	0.88838700
C	-6.85453700	-1.86443500	1.16957500
H	-7.00765400	-0.82778300	1.44681800
H	-8.94240700	-2.25501200	0.95443600
C	-5.54292400	-1.20364700	4.04670700
H	-5.40723600	-2.20448200	3.65603400
C	-6.13167100	-1.03309400	5.28081200
H	-6.45710200	-1.90388800	5.84344000
C	-6.31226600	0.25961300	5.82452500
C	-5.86953700	1.35767500	5.12513200
H	-5.98304300	2.35843700	5.53517900
H	-6.78699000	0.38012200	6.79428000

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C	-1.10863900	3.78008000	4.60948700
C	-0.02998000	3.19858200	3.91534600
C	-0.29409300	2.36847500	2.81897200
C	-1.62411900	2.16097900	2.43238100
C	-2.67725200	2.76577900	3.15185600
C	-2.43825000	3.57939600	4.25829300
C	0.72526900	4.45667800	5.59923100
C	1.15961000	3.66472400	4.58964300
H	0.51238400	1.87942100	2.27854800
H	-3.69769200	2.56704200	2.84129300
H	-3.24655500	4.03536600	4.82097400
H	1.24158200	5.02267200	6.36030900
H	2.18673200	3.45335700	4.32736900
O	-0.64870900	4.54792500	5.64395000
C	-1.89136200	1.29632100	1.21630300
H	-1.16273900	0.47825900	1.19927400
C	-8.67811900	-3.55799300	-1.25019700
C	-7.53142200	-4.07235100	-0.63571800

C	-6.86828500	-3.34577600	0.36079000
C	-7.36358500	-2.09817500	0.72095500
C	-8.51578300	-1.57490200	0.09990400
C	-9.17994300	-2.30607500	-0.88709100
H	-9.18257100	-4.13731800	-2.01895200
H	-7.14846500	-5.04433100	-0.93379900
H	-5.97534000	-3.75103200	0.82676800
H	-10.07119000	-1.91169500	-1.36862200
C	-6.84883900	-1.12739100	1.77358300
H	-6.94987400	-1.58503900	2.77113500
C	-7.82483300	0.03403700	1.65099100
C	-7.86204000	1.22998300	2.35752000
C	-8.88118000	2.14995600	2.08346400
C	-9.85071400	1.86733200	1.11555800
C	-9.81951100	0.66457800	0.40583700
C	-8.80119800	-0.25227600	0.67550300
H	-7.11604300	1.45404700	3.11700800
H	-8.92159300	3.08858200	2.62964500
H	-10.63798500	2.58940500	0.91562900
H	-10.57805000	0.45025400	-0.34269900
C	-5.37266500	-0.74604000	1.66776600
H	-5.10273100	-0.01825500	2.43639100
H	-4.72947600	-1.62334100	1.79382800
O	-5.11949800	-0.17209600	0.36794000
C	-3.95646500	0.49846100	0.21018700
N	-3.20232600	0.75876700	1.19627500
C	-1.30211600	2.08673700	-0.16185900
C	-2.06372800	3.27171500	-0.41957600
H	-0.26634500	2.27819000	0.11534000
H	-1.36752100	1.35214900	-0.96073400
H	-2.92554300	3.16061300	-1.07657500
C	-1.83304000	4.55090100	0.14072400
H	-1.20402100	4.55517200	1.03521500
H	-2.73278500	5.16473700	0.23795900

Si	-0.72383700	5.64691800	-1.17538500
C	-1.45998900	7.37218600	-0.96345300
H	-1.41592400	7.70759800	0.07888600
H	-2.50407700	7.41497500	-1.29411700
H	-0.89210400	8.09133600	-1.56709400
C	-0.94637700	5.01091400	-2.92838200
H	-0.49008400	4.02332400	-3.05626700
H	-0.44820700	5.69734400	-3.62504000
H	-2.00098000	4.95885200	-3.22385000
C	1.04245900	5.55682200	-0.55476500
H	1.13285000	5.99426600	0.44629700
H	1.69377400	6.12992800	-1.22746800
H	1.42624500	4.53167900	-0.52037200
O	-3.76243400	0.86740600	-1.06055200
Si	-4.56764800	0.35722700	-2.51614500
C	-6.35746700	0.92482500	-2.47184800
H	-6.92972700	0.39722700	-1.70405900
H	-6.43018500	2.00028800	-2.27098400
H	-6.83458000	0.73759200	-3.44223200
C	-4.38312100	-1.49454900	-2.71593100
H	-4.86986100	-2.04425300	-1.90579100
H	-4.84526700	-1.81509800	-3.65844300
H	-3.33063700	-1.79583300	-2.74905000
C	-3.59916100	1.29549600	-3.82414800
H	-4.01579700	1.09423400	-4.81904000
H	-3.64456500	2.38020200	-3.66832400
H	-2.54595600	0.99746200	-3.84292800
C	3.91408600	-4.07454000	2.32215700
C	2.87886900	-4.90963200	2.85521300
C	3.61134900	-3.21464200	1.20650900
C	1.58026200	-4.85397200	2.29343900
C	1.26053900	-3.98233500	1.27266700
C	2.29951200	-3.14432300	0.77101000
H	0.81719400	-5.52492500	2.67911600

C	4.67016100	-2.36442700	0.58452100
C	5.87061600	-2.93652400	0.03808100
C	4.52822500	-0.98524400	0.55827300
C	6.93488300	-2.06400000	-0.35745300
C	5.60874900	-0.09925800	0.26100800
C	6.78800100	-0.66636000	-0.18143600
H	7.64149900	-0.02672700	-0.38883400
P	1.95215200	-0.64961800	0.01409600
O	3.31308500	-0.41947900	0.91324800
O	1.96779400	-2.25842100	-0.23927800
S	1.93652000	-1.04077000	-3.09021100
S	2.00744300	1.63909200	-1.88250100
O	2.41420500	-0.25477400	-4.23372400
O	2.36372800	-2.42801500	-2.90296900
C	0.06281800	-1.19099200	-3.39166700
F	-0.61663600	-1.15853700	-2.22471000
F	-0.37822300	-0.19409400	-4.16148100
F	-0.19496400	-2.35333000	-3.99461400
C	3.50756100	2.21782800	-2.91007200
F	3.17747100	2.40444200	-4.17965300
F	3.89489800	3.39493200	-2.39373500
F	4.51766200	1.35135000	-2.82179300
O	0.85139300	2.07130700	-2.69220100
C	5.52269800	1.36543800	0.50277500
C	6.15786300	2.26265300	-0.36997800
C	4.88217100	1.87246300	1.64680000
C	6.13624500	3.62418000	-0.10632400
H	6.63172100	1.92150800	-1.28232300
C	4.87872500	3.23542300	1.88647100
H	4.37964000	1.22073500	2.34930900
C	5.50199000	4.13205000	1.02291600
C	-0.11828800	-3.95218600	0.71838000
C	-0.34708000	-3.98530600	-0.66754200
C	-1.21494800	-3.94544800	1.59632500

C	-1.64722400	-4.03270800	-1.14551600
H	0.46895100	-3.96717200	-1.38028600
C	-2.50353000	-3.99123700	1.08710700
H	-1.07623200	-3.87838700	2.66938200
C	-2.73889700	-4.05224400	-0.28109100
O	0.81466900	-0.14445400	0.82613000
C	2.11883000	-0.07372300	-1.65713800
F	6.72713600	4.48780000	-0.94980500
F	5.48314400	5.44985300	1.26877000
F	4.27489900	3.73215000	2.98726000
F	-3.56991100	-3.95395600	1.91904600
F	-3.99315600	-4.11318900	-0.75950200
F	-1.88921100	-4.05656600	-2.46692700
O	2.20965800	2.26523600	-0.55756400
C	8.12720200	-2.61748000	-0.89682600
H	8.92962300	-1.94193000	-1.18328900
C	8.25967500	-3.97549200	-1.07088500
H	9.17131900	-4.38726900	-1.49470500
C	7.19738100	-4.83725000	-0.71064100
H	7.29465400	-5.90736500	-0.87165400
C	6.03665400	-4.33312700	-0.16610600
H	5.22571300	-5.00484300	0.09134300
C	5.18668400	-4.10856600	2.95649500
H	5.97457100	-3.45675700	2.59949400
C	5.42818100	-4.94383200	4.02524700
H	6.40799700	-4.94320100	4.49497100
C	4.41470800	-5.79648600	4.52095900
H	4.62166000	-6.45572900	5.35931300
C	3.16551800	-5.77337200	3.94660500
H	2.36936500	-6.40892500	4.32694900

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C	9.26281100	3.79143200	-0.15483300
C	8.60435500	3.79262600	-1.39925300

C	7.57573200	2.86531900	-1.61847800
C	7.22985800	1.97245200	-0.60037800
C	7.91985000	2.00340900	0.63127600
C	8.94903200	2.91315900	0.87355800
C	10.19095300	5.36773000	-1.35862700
C	9.23884300	4.83876800	-2.16600200
H	7.05089300	2.84000200	-2.57136000
H	7.64216300	1.28780800	1.39774500
H	9.48310500	2.93475200	1.81796400
H	10.90673900	6.16455000	-1.49666500
H	9.01107200	5.14884900	-3.17635300
O	10.23491300	4.75603200	-0.13000500
C	6.07556100	0.99594300	-0.83163100
H	6.11710900	0.66137900	-1.87697100
C	1.57553200	-1.48682600	-1.46737500
C	2.55069500	-2.06720600	-2.28676800
C	3.57836100	-2.84217200	-1.73333600
C	3.62646300	-3.01720900	-0.35463400
C	2.65395400	-2.42330700	0.47600400
C	1.62448100	-1.65946600	-0.07988800
H	0.75156100	-0.92173900	-1.89404900
H	2.49991900	-1.93234900	-3.36402400
H	4.32120400	-3.30206800	-2.38065200
H	0.84684800	-1.22394900	0.53857600
C	4.58703500	-3.85245500	0.48125100
H	4.43574400	-4.91664400	0.23421200
C	4.09035800	-3.60108500	1.89736800
C	4.58658400	-4.08504900	3.10119500
C	3.92632800	-3.75352600	4.29003300
C	2.77588300	-2.95914300	4.26424200
C	2.27005200	-2.47320400	3.05624300
C	2.94040200	-2.78752800	1.87183400
H	5.47227300	-4.71614500	3.12964000
H	4.30555100	-4.12417200	5.23858400

H	2.26411500	-2.72301700	5.19336100
H	1.36401200	-1.87557400	3.04555100
C	6.08246200	-3.59739400	0.25265000
H	6.67298100	-4.25356300	0.89813200
H	6.35088200	-3.80163600	-0.78670000
O	6.48368700	-2.26565600	0.61928300
C	6.44276700	-1.27185100	-0.29839300
N	6.08892200	-0.11828100	0.09672000
C	-6.08450200	-2.67307100	-2.17647500
C	-5.52154700	-3.93885400	-2.53774900
C	-5.38288200	-1.84100600	-1.23263600
C	-4.28128000	-4.33027400	-1.97999800
C	-3.56334800	-3.51162500	-1.13192500
C	-4.13045800	-2.24428000	-0.79979400
H	-3.88432200	-5.31067800	-2.22950700
C	-5.96528100	-0.53913800	-0.79352600
C	-7.24980900	-0.46604700	-0.15421200
C	-5.27671700	0.63898600	-1.03131900
C	-7.83399200	0.82079500	0.07407200
C	-5.86595400	1.93053300	-0.87733800
C	-7.13816400	1.98230300	-0.34004300
H	-7.63241100	2.94446200	-0.23727500
P	-2.77729400	0.00966000	-0.50261800
O	-3.96634100	0.56788000	-1.49174400
O	-3.39266200	-1.40823600	0.03114700
S	-3.15059400	0.26627400	2.60094900
S	-1.85195400	2.37838900	0.99595600
O	-3.03669600	1.35241000	3.58367500
O	-4.33089500	-0.59391100	2.55693500
C	-1.73135900	-0.91353400	3.08345200
F	-2.23189600	-1.98853600	3.69322800
F	-1.04824600	-1.31363400	1.99624200
F	-0.87339200	-0.30389900	3.90983700
C	-2.74276400	3.75118100	1.99493600

F	-2.19075000	3.91387200	3.19116300
F	-2.56219800	4.87651100	1.29186600
F	-4.04356200	3.50926200	2.10780400
O	-0.53816000	2.29245700	1.72794600
C	-5.19016500	3.17677300	-1.32497900
C	-5.32600800	4.35333200	-0.57038100
C	-4.46781500	3.22349200	-2.52922400
C	-4.74034700	5.53180100	-1.00783600
H	-5.84509200	4.35725600	0.38027100
C	-3.89700600	4.41527800	-2.94552000
H	-4.33126700	2.34327600	-3.14368700
C	-4.02346800	5.58380200	-2.19852500
C	-2.25796400	-3.97480000	-0.59263200
C	-1.97786400	-3.91634800	0.78012200
C	-1.31078400	-4.53944200	-1.46173400
C	-0.76839500	-4.39951000	1.25665300
H	-2.68173200	-3.49117000	1.48397000
C	-0.11301100	-5.02470400	-0.95797200
H	-1.48177300	-4.57778700	-2.53162000
C	0.17422300	-4.96662400	0.40227700
O	-1.51117800	-0.07148400	-1.26520600
C	-2.74680300	0.91382800	1.04101400
F	-4.85099800	6.65525500	-0.27680900
F	-3.45934500	6.72754100	-2.61185400
F	-3.21011600	4.47212000	-4.09940300
F	0.80670700	-5.55577800	-1.78270900
F	1.34441500	-5.42387000	0.87241100
F	-0.48187800	-4.32807000	2.56811900
C	4.69012700	1.70518400	-0.66978500
C	4.44521500	2.13607300	0.73541200
H	4.61013800	2.54530600	-1.36728000
H	3.92878200	0.96004000	-0.94107700
H	4.67512500	1.37516200	1.47953400
C	3.94703600	3.33143200	1.14450400

H	3.84182100	4.15804300	0.44371200
H	4.01130200	3.59778100	2.19634400
Si	1.67917700	2.78526500	1.34617100
C	1.36214300	4.54490400	1.95499500
H	1.29826700	5.23981900	1.11027300
H	2.13317600	4.90747400	2.64094300
H	0.40370300	4.56269900	2.48068700
C	1.98549700	1.45554000	2.63868500
H	1.06582800	1.25517000	3.19131700
H	2.76126100	1.75785200	3.35073700
H	2.30692100	0.52062700	2.16765200
C	1.41182500	2.43564600	-0.47693000
H	1.46643200	1.36196900	-0.68238000
H	2.14962200	2.94715900	-1.10225800
H	0.41552800	2.76830200	-0.77606600
O	-1.82432200	2.88631300	-0.38270700
O	6.80879600	-1.61324500	-1.55495800
Si	8.39370900	-1.81628800	-2.18895200
C	8.50126200	-3.58295200	-2.82579000
H	9.44762900	-3.74220000	-3.35750400
H	8.45238800	-4.31793400	-2.01455000
H	7.68878000	-3.80192400	-3.52855500
C	9.63814600	-1.48148200	-0.82163700
H	9.49119000	-2.15471000	0.03021100
H	10.66016600	-1.62714800	-1.19239600
H	9.56023300	-0.45277000	-0.45232600
C	8.54786500	-0.59479900	-3.60753400
H	9.50546000	-0.72026200	-4.12789500
H	7.74867100	-0.74021200	-4.34362300
H	8.49641800	0.43911300	-3.24855400
C	-9.10760600	0.90794300	0.69845900
H	-9.54238600	1.89214000	0.85562800
C	-9.77010900	-0.22427700	1.11166300
H	-10.73872000	-0.14573000	1.59746800

C	-9.17968400	-1.49513900	0.91720100
C	-7.95539700	-1.61406500	0.29728200
H	-7.50912700	-2.59334000	0.16751700
H	-9.69381600	-2.38621900	1.26677100
C	-7.29734800	-2.28095100	-2.80818500
H	-7.72257000	-1.31056300	-2.58367300
C	-7.92937700	-3.10734100	-3.71128600
H	-8.85050200	-2.77874400	-4.18483200
C	-7.39004000	-4.37456200	-4.03321400
C	-6.20739600	-4.77655300	-3.45832400
H	-5.76863200	-5.73953800	-3.70862100
H	-7.90345800	-5.01904300	-4.74134200

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C	1.90045500	1.66260600	5.02668700
C	2.05092000	2.74398800	4.14043600
C	0.96945200	3.10773700	3.32564800
C	-0.22232600	2.38985900	3.42151000
C	-0.33005400	1.30428500	4.32082100
C	0.73027200	0.92220200	5.13672200
C	3.94253000	2.41055000	5.28260700
C	3.40418500	3.21160100	4.33114300
H	1.06954600	3.92532000	2.61881100
H	-1.26015100	0.75038300	4.37995900
H	0.65177800	0.08480800	5.82184100
H	4.91684400	2.37782200	5.74721200
H	3.89233600	4.02538000	3.81584500
O	3.05668500	1.45855300	5.72917500
C	-1.40378800	2.81864000	2.56443500
H	-1.05040300	3.60549500	1.89091700
C	-7.57753100	-1.79774100	-3.66884000
C	-6.24249700	-1.69112900	-4.07365800
C	-5.22753300	-1.46171900	-3.13679300
C	-5.57486000	-1.34567400	-1.79479900
C	-6.91889700	-1.44970000	-1.38315700

C	-7.92700200	-1.67832100	-2.32159800
H	-8.35157100	-1.97810100	-4.41025700
H	-5.98877400	-1.79026600	-5.12551900
H	-4.19096200	-1.37991200	-3.45433800
H	-8.96611900	-1.76555300	-2.01425500
C	-4.67707100	-1.07791800	-0.59422300
H	-3.89864000	-1.84278300	-0.48431000
C	-5.66471500	-1.10328800	0.56249800
C	-5.43203300	-0.96732600	1.92755900
C	-6.52058200	-1.00081400	2.80773900
C	-7.82194600	-1.17441700	2.32524400
C	-8.05885000	-1.32881900	0.95753200
C	-6.97568000	-1.29522600	0.07716200
H	-4.42048000	-0.86927500	2.30932700
H	-6.35129400	-0.90326000	3.87685800
H	-8.65553700	-1.20192500	3.02214000
H	-9.07067000	-1.47972200	0.58983000
C	-3.99400600	0.27781700	-0.78289700
H	-3.41234200	0.31615200	-1.70398200
H	-4.72255900	1.08726700	-0.75747200
O	-3.03278100	0.46680500	0.30521900
C	-2.81350800	1.63828700	0.84742200
C	4.51452100	-2.97104000	1.43265100
C	4.02790300	-4.01586100	2.28183600
C	3.59968800	-2.34230300	0.51633000
C	2.66433700	-4.38988800	2.20997400
C	1.75777000	-3.73320300	1.40096400
C	2.25788400	-2.67009900	0.59205500
H	2.31334100	-5.20044500	2.84289900
C	4.08742200	-1.35141900	-0.48775800
C	5.11024800	-1.70982200	-1.43388900
C	3.58571800	-0.05815000	-0.51425700
C	5.69244800	-0.68486500	-2.24506600
C	4.22098900	0.99897900	-1.23867200

C	5.26313200	0.65308600	-2.07786200
H	5.78870400	1.43506700	-2.61881700
P	1.00543700	-0.43594100	0.05588700
O	2.47597700	0.26107400	0.26119700
O	1.36992900	-1.99447300	-0.24107300
S	-0.67419100	-1.16130700	-2.40899800
S	-0.11580300	1.69102200	-1.70524900
O	-1.11885900	-2.29714400	-1.59434700
O	-1.63766400	-0.46441700	-3.27811600
C	0.56391700	-1.87818000	-3.63380600
F	-0.05820000	-2.80935100	-4.36129500
F	0.99879600	-0.90668200	-4.44478700
F	1.61011300	-2.42829000	-3.01688700
C	0.60586200	2.18635400	-3.38082500
F	-0.20726600	1.84541800	-4.37474500
F	0.76372700	3.51546600	-3.37628100
F	1.79544100	1.60475800	-3.56655400
O	-1.54318600	2.04604900	-1.84029300
C	3.87576100	2.43416400	-1.05583700
C	3.88552100	3.29875800	-2.16191300
C	3.62230800	2.96492800	0.21967800
C	3.63002200	4.65108400	-1.99398000
H	4.04653500	2.92639000	-3.16618300
C	3.37694900	4.32040100	0.35633900
H	3.59641300	2.33747800	1.10145700
C	3.37460700	5.18400100	-0.73487500
C	0.34671300	-4.20464000	1.34818800
C	0.10694200	-5.57389600	1.14518100
C	-0.73951000	-3.33771200	1.53108000
C	-1.19399300	-6.05492000	1.12083100
H	0.92218200	-6.26931000	0.97931400
C	-2.02693400	-3.84755600	1.49586700
H	-0.59979400	-2.27629700	1.69813000
C	-2.27946700	-5.20129200	1.29296500

O	0.23342800	-0.20662400	1.31419300
C	0.21834700	0.01196100	-1.47726700
F	3.61954100	5.47742500	-3.05381300
F	3.12543300	6.49113300	-0.57609800
F	3.12721300	4.85260200	1.57546500
F	-3.08446700	-3.02709800	1.66217300
F	-3.53339300	-5.67063000	1.26259900
F	-1.43156400	-7.36269400	0.91881000
C	-2.56782900	3.41990000	3.40937300
C	-3.41351000	2.45195000	4.19212900
H	-2.10797700	4.14783200	4.08670900
H	-3.22364300	3.98576900	2.73796600
H	-3.97349400	1.71900800	3.61082300
C	-3.55348400	2.46765800	5.51837800
H	-3.02006300	3.18179100	6.14224100
H	-4.20669200	1.76728000	6.03192600
O	0.67010900	2.43230800	-0.70272200
O	-3.59902500	2.64549200	0.62811300
Si	-3.80337900	4.10630400	-0.32808500
C	-2.20390000	5.08013900	-0.27850200
H	-1.34761700	4.46500000	-0.57080500
H	-2.26711000	5.91645200	-0.98637900
H	-2.01333000	5.50424600	0.71350000
C	-5.19749900	4.95241800	0.60061500
H	-5.49789300	5.86503900	0.07077000
H	-6.07875700	4.30478000	0.66829300
H	-4.91107500	5.23981300	1.61798400
C	-4.33625200	3.64475700	-2.06096400
H	-4.50375600	4.56735500	-2.63247500
H	-3.56952100	3.06156000	-2.57715600
H	-5.27627200	3.08213700	-2.06894800
C	6.70552300	-1.02376600	-3.18211500
H	7.14480900	-0.23014000	-3.78166000
C	7.11148700	-2.32820500	-3.34074400

H	7.87957800	-2.57898100	-4.06694500
C	6.51520800	-3.34881100	-2.56354000
C	5.54596600	-3.04866400	-1.63163700
H	5.09173400	-3.84445600	-1.05293900
H	6.82090200	-4.38157300	-2.70649000
C	5.87548000	-2.58123900	1.56612100
H	6.25698500	-1.76885300	0.95913900
C	6.70867000	-3.20773800	2.46680400
H	7.74213100	-2.88431800	2.55634100
C	6.23206800	-4.26167000	3.28106100
C	4.91661700	-4.65205900	3.19017000
H	4.53002800	-5.44862300	3.82123600
H	6.90224000	-4.75038600	3.98270500
N	-1.82746000	1.67085800	1.72238900
H	-1.17250700	0.87032100	1.67714800

TSII-6S

C	-6.76952200	4.52657300	3.35696300
C	-5.61167200	4.85810400	2.62903100
C	-5.31153000	4.12765900	1.47112400
C	-6.16885400	3.10225400	1.06677000
C	-7.32443100	2.80581200	1.82686600
C	-7.64084500	3.51076300	2.98584800
C	-5.80821400	6.18207100	4.41783700
C	-5.00291800	5.94825000	3.35291400
H	-4.41850600	4.35483500	0.89413900
H	-8.00147000	2.02595300	1.49321300
H	-8.52674900	3.28411800	3.56958700
H	-5.76009300	6.89219900	5.22987900
H	-4.09137100	6.47573400	3.10944800
O	-6.89147700	5.33680400	4.45117400
C	-5.82462600	2.31248100	-0.18588800
H	-4.85803900	2.66938300	-0.54793400
C	-8.71420100	-2.01393000	-2.82703400
C	-7.51011900	-1.79765700	-3.50565400

C	-6.29332100	-2.19642400	-2.93804400
C	-6.29984800	-2.80937900	-1.69017600
C	-7.51258200	-3.02782600	-1.00483900
C	-8.72512300	-2.63109600	-1.57288800
H	-9.65089200	-1.70313400	-3.28194500
H	-7.51871300	-1.32128900	-4.48203200
H	-5.36211400	-2.02660200	-3.47351300
H	-9.66528500	-2.80214600	-1.05467100
C	-5.13032300	-3.31825300	-0.85949000
H	-4.58384400	-4.11152500	-1.38926800
C	-5.82547700	-3.87996800	0.37363900
C	-5.27287200	-4.51073600	1.48303300
C	-6.12665100	-4.94503200	2.50397200
C	-7.50936300	-4.75476200	2.40931900
C	-8.06696000	-4.13034400	1.29145000
C	-7.21851500	-3.69277800	0.27268500
H	-4.20255900	-4.67907600	1.56152800
H	-5.70959300	-5.43949600	3.37691300
H	-8.15652200	-5.10136900	3.21060400
H	-9.14304300	-3.99381400	1.21886900
C	-4.08694500	-2.23779100	-0.55205500
H	-3.32574100	-2.61376800	0.13207700
H	-3.60620300	-1.87288500	-1.45985700
O	-4.73062200	-1.13014300	0.12706800
C	-4.74595000	0.07946500	-0.43491700
C	5.43029300	-2.92019100	2.34574800
C	4.76108500	-4.11118300	2.77641500
C	4.81390900	-2.11160000	1.32726900
C	3.49207600	-4.43282800	2.23843300
C	2.84651100	-3.61913700	1.32709800
C	3.54756100	-2.45612500	0.88821500
H	3.01098100	-5.34989400	2.56726700
C	5.48313800	-0.88816300	0.79360700
C	6.78731200	-0.95018300	0.19097200

C	4.85131600	0.34577600	0.87923200
C	7.44955900	0.27154000	-0.15220100
C	5.51801900	1.57803600	0.59986300
C	6.80650900	1.50554500	0.10747700
H	7.35309900	2.42448200	-0.08579200
P	2.29448100	-0.21046400	0.42634800
O	3.53444800	0.41394900	1.31327700
O	2.93546400	-1.63752500	-0.05255500
S	2.35396900	-0.26279200	-2.70172300
S	1.32886500	2.06481500	-1.20350500
O	1.83019500	-1.63418800	-2.72873900
O	1.94851000	0.69381500	-3.74604400
C	4.21338200	-0.48634900	-2.97218100
F	4.40662600	-0.66032800	-4.28187900
F	4.88761600	0.59367900	-2.56869600
F	4.66905300	-1.55678600	-2.31983400
C	2.21960900	3.31235500	-2.35171100
F	1.60280300	3.43648800	-3.51523700
F	2.18408900	4.48491000	-1.71230700
F	3.48795100	2.95112000	-2.53921200
O	-0.02114200	2.03721500	-1.86952300
C	4.89627200	2.90256300	0.86394600
C	5.09719200	3.95496600	-0.04394100
C	4.16783300	3.14832300	2.03945200
C	4.57405600	5.21153700	0.22253200
H	5.62186400	3.80016700	-0.97925300
C	3.65787100	4.41364200	2.28186000
H	3.98010300	2.36771300	2.76513300
C	3.85350000	5.46167000	1.38558300
C	1.46828300	-3.94802500	0.87565800
C	1.05606200	-3.77243800	-0.45643900
C	0.55405800	-4.46047600	1.81435200
C	-0.24257600	-4.09600100	-0.81751900
H	1.70677500	-3.35458200	-1.21308700

C	-0.73262400	-4.79071900	1.42005100
H	0.81820600	-4.56515100	2.86019300
C	-1.14240700	-4.62185600	0.10334600
O	1.08364000	-0.27035700	1.27349500
C	2.16065300	0.55749500	-1.17981000
F	4.74927700	6.21793700	-0.65154400
F	3.35079800	6.67898600	1.63281500
F	2.96679800	4.66210100	3.40651900
F	-1.62845500	-5.25805000	2.31234500
F	-2.40710200	-4.92034200	-0.26342600
F	-0.67638600	-3.89557400	-2.07486500
C	-6.82105500	2.47555700	-1.37070700
C	-8.16318800	1.81260800	-1.21959500
H	-6.94566900	3.54975600	-1.55015900
H	-6.32142300	2.05469800	-2.25465200
H	-8.15396900	0.72551500	-1.13431700
C	-9.33382600	2.45265100	-1.23526600
H	-9.39493000	3.53462900	-1.33352900
H	-10.27729300	1.91884200	-1.15694900
O	1.38957000	2.64011000	0.14582800
O	-4.02981300	0.42084600	-1.40582600
Si	-2.02999800	1.13001700	-1.58894900
C	-1.56550900	-0.27740100	-2.73494200
H	-0.77849700	0.04850400	-3.42005600
H	-1.18968600	-1.15865500	-2.20488900
H	-2.43780800	-0.57652500	-3.32591700
C	8.74193200	0.22499000	-0.74140600
H	9.23535400	1.16298100	-0.98430900
C	9.34994500	-0.97765700	-1.01621000
H	10.33422600	-1.00223500	-1.47542300
C	8.68169400	-2.18743800	-0.71428200
C	7.43707200	-2.17513400	-0.12367600
H	6.93395100	-3.11120100	0.08967700
H	9.15201200	-3.13660100	-0.95609100

C	6.65761700	-2.57920200	2.97781000
H	7.15891900	-1.66012200	2.69993500
C	7.20855500	-3.39081400	3.94514100
H	8.14367900	-3.10311600	4.41772200
C	6.56756700	-4.59034500	4.33406500
C	5.36647200	-4.93753400	3.76200300
H	4.85014500	-5.84486200	4.06620700
H	7.01796000	-5.22462600	5.09240900
N	-5.62569500	0.89272600	0.15981900
H	-6.16816200	0.49304700	0.91489100
C	-2.64037200	2.70139100	-2.42212600
H	-1.93338200	3.00147400	-3.19995400
H	-3.62383800	2.54972200	-2.87553100
H	-2.70678100	3.52782900	-1.70519500
C	-1.84400400	1.03404200	0.27791800
H	-0.81796400	1.17337900	0.62092400
H	-2.47030300	1.79753000	0.75606900
H	-2.17030800	0.05590500	0.64630000
Pr-S			
C	-8.69593300	3.67643800	3.68607700
C	-7.30618100	3.79617800	3.86786300
C	-6.45430500	3.44561000	2.81101000
C	-7.00262000	2.99972600	1.60712200
C	-8.40720600	2.90079900	1.46750200
C	-9.27573000	3.23215400	2.50490500
C	-8.38754000	4.41117700	5.72537600
C	-7.13753600	4.27992200	5.21772900
H	-5.37566800	3.51479800	2.92712200
H	-8.82765400	2.57570100	0.52132900
H	-10.35250500	3.15464100	2.39694200
H	-8.75689400	4.73769200	6.68618700
H	-6.21090000	4.49722200	5.73040100
O	-9.35942600	4.05314100	4.82256900
C	-6.07161500	2.62793100	0.46451300

H	-5.04646900	2.63644600	0.85140700
C	-9.42146600	-2.74630200	-3.79901400
C	-8.26629000	-2.28647500	-4.43975300
C	-7.02606800	-2.34055200	-3.79238600
C	-6.95930900	-2.85516700	-2.50333000
C	-8.12236800	-3.31891000	-1.85683300
C	-9.35832400	-3.26681400	-2.50416900
H	-10.37723100	-2.70054000	-4.31450700
H	-8.33091300	-1.88695900	-5.44827200
H	-6.13173200	-1.98415000	-4.29893700
H	-10.25973800	-3.62541100	-2.01349600
C	-5.74949200	-3.02339300	-1.59503300
H	-5.02197300	-3.71401900	-2.04732300
C	-6.36308700	-3.65247000	-0.35110400
C	-5.74304900	-4.06182700	0.82391200
C	-6.52635600	-4.62492600	1.83858900
C	-7.90672500	-4.77960600	1.67294600
C	-8.53021400	-4.37805300	0.48944900
C	-7.75269000	-3.81267400	-0.52292200
H	-4.66999000	-3.96158700	0.95809900
H	-6.05477900	-4.94846400	2.76265600
H	-8.49897300	-5.22075800	2.47044600
H	-9.60218600	-4.50738100	0.36251600
C	-4.97604300	-1.72763300	-1.33883100
H	-4.12560700	-1.91145400	-0.67641700
H	-4.59385400	-1.30926500	-2.27530800
O	-5.86963700	-0.78391800	-0.72466900
C	-5.39875400	0.47443000	-0.55816200
C	5.04117400	-3.16019900	2.77045600
C	4.12421000	-4.18181800	3.18032200
C	4.68791700	-2.32160300	1.65622400
C	2.88197900	-4.31450100	2.51410100
C	2.49495700	-3.46599200	1.49492000
C	3.43128300	-2.46825300	1.09604300

H	2.20973700	-5.10920400	2.82572900
C	5.61592900	-1.27336400	1.13773100
C	6.93195900	-1.60447400	0.66157300
C	5.21118100	0.05325600	1.09017300
C	7.82034800	-0.54522800	0.28800600
C	6.09375500	1.12536600	0.76346000
C	7.38088300	0.79694100	0.38588500
H	8.08523300	1.59232200	0.15792800
P	2.63637100	-0.07672400	0.48030700
O	3.89914300	0.38313100	1.41981400
O	3.06189100	-1.59458600	0.07039100
S	2.90134100	-0.18855600	-2.66978600
S	2.08617200	2.24490300	-1.23905300
O	2.25703700	-1.50230900	-2.69963600
O	2.62548100	0.79924900	-3.72508300
C	4.74520100	-0.56743700	-2.82559400
F	4.98619000	-0.85621800	-4.10453900
F	5.47696000	0.49120700	-2.46591600
F	5.07678400	-1.61014400	-2.06599800
C	3.01661100	3.38641300	-2.48699200
F	2.37550200	3.50797800	-3.62987200
F	3.06987600	4.56794400	-1.87501800
F	4.24569500	2.92501600	-2.67570000
O	0.69007600	2.33459900	-1.93092900
C	5.68073300	2.55104300	0.84710100
C	6.04620900	3.43653100	-0.17917400
C	4.98350000	3.04606700	1.96081300
C	5.71224200	4.78020000	-0.08629200
H	6.55756600	3.08658400	-1.06826700
C	4.66690400	4.39373900	2.03093400
H	4.67597600	2.39846000	2.77199900
C	5.02516900	5.27862600	1.01604400
C	1.14625600	-3.59361800	0.88190000
C	0.95444100	-3.52432000	-0.50768900

C	0.03827000	-3.81467200	1.71773700
C	-0.32208400	-3.66499200	-1.03168800
H	1.76962400	-3.33100300	-1.19229300
C	-1.22566200	-3.95737900	1.16625100
H	0.14006700	-3.83636000	2.79665200
C	-1.42218900	-3.88794100	-0.20817000
O	1.37124300	0.11768300	1.22045000
C	2.71812900	0.66750600	-1.15478900
F	6.04178200	5.62972800	-1.07418000
F	4.70605300	6.57632200	1.09463400
F	4.01014100	4.88167000	3.09439700
F	-2.29707600	-4.14933800	1.95996700
F	-2.65810200	-4.00295700	-0.73066300
F	-0.52943300	-3.58628300	-2.35463500
C	-6.08695800	3.63205400	-0.72586100
C	-7.34958900	3.67079500	-1.53957800
H	-5.86002700	4.62913600	-0.32948000
H	-5.25085100	3.34266800	-1.37672900
H	-7.64394500	2.72786300	-2.00154600
C	-8.09208300	4.75879900	-1.75100900
H	-7.83480500	5.72148800	-1.31362200
H	-8.98280900	4.73181400	-2.37334900
O	2.14951900	2.89990200	0.06716300
O	-4.27944400	0.84995600	-0.89140100
Si	-0.97090200	1.78079300	-1.46044700
C	-0.97564300	-0.08363700	-1.49000800
H	-0.55136900	-0.50864900	-2.40511600
H	-0.43190900	-0.48546100	-0.62978600
H	-2.02359200	-0.39652900	-1.41093400
C	-1.29030900	2.48792600	0.23788700
H	-0.61793100	2.03900500	0.97645700
H	-1.16648500	3.57563500	0.26598700
H	-2.32334300	2.24578600	0.51440300
C	9.12639500	-0.85839800	-0.17681900

H	9.79186200	-0.04100200	-0.44351200
C	9.53627500	-2.16499400	-0.30314500
H	10.53380300	-2.39398000	-0.66726500
C	8.64772000	-3.21490200	0.02795500
C	7.38231800	-2.94354600	0.49990100
H	6.71125000	-3.76070500	0.73714900
H	8.96436000	-4.24672000	-0.09646200
C	6.24082300	-3.00020300	3.51679000
H	6.92866800	-2.20603100	3.25236900
C	6.53263200	-3.82855700	4.57807200
H	7.45251100	-3.68072100	5.13696400
C	5.64507900	-4.86458200	4.95217300
C	4.46441300	-5.03192800	4.26759900
H	3.76250800	-5.81043300	4.55633900
H	5.89208000	-5.51494300	5.78650200
N	-6.34865200	1.25642200	0.01758300
H	-7.17764000	0.78980400	0.35831200
C	-1.94335700	2.57069000	-2.84791100
H	-1.59529800	2.22177500	-3.82612700
H	-2.99658800	2.28995600	-2.73452700
H	-1.86930000	3.66324100	-2.82700300

ComIII

H	-0.07176900	-0.91663300	-0.60449800
C	-5.88217500	1.81028100	-2.38416800
C	-6.31202600	0.47354100	-2.36948300
C	-5.35956400	-0.52763100	-2.17213700
C	-4.03233700	-0.14829500	-1.98890500
C	-3.62942900	1.20682600	-2.01985900
C	-4.55707300	2.21286000	-2.22792900
C	-8.04736000	1.84005200	-2.62871500
C	-7.74388400	0.52792300	-2.53304300
H	-5.64215500	-1.57751200	-2.14007500
H	-2.57644600	1.43537800	-1.86733500

H	-4.28627000	3.26230100	-2.23866300
H	-8.98151300	2.36566200	-2.75457200
H	-8.43797700	-0.29816500	-2.55996800
O	-6.94115400	2.63819000	-2.54641200
C	-3.02772100	-1.18468900	-1.71480000
O	-1.86903200	-0.94387800	-1.44601000
H	-3.38349000	-2.23449700	-1.74853500
C	-8.02529100	1.39446400	1.83901700
C	-6.94188900	1.76287200	1.03953900
C	-5.87459100	0.88467800	0.84696900
C	-5.91776500	-0.36174500	1.44988400
C	-6.98643100	-0.71885200	2.28539600
C	-8.05256600	0.15514200	2.47764900
H	-8.84844600	2.08852200	1.97975500
H	-6.91777300	2.74051000	0.56669100
H	-5.02549000	1.18281400	0.23988900
H	-8.88704900	-0.11553300	3.11857200
C	-4.90200800	-1.48315700	1.37705500
H	-4.89506700	-1.91781700	0.36530100
C	-5.47014700	-2.49700100	2.35263400
C	-4.96075900	-3.72627200	2.74780000
C	-5.69346400	-4.50137100	3.64905600
C	-6.92173600	-4.05531000	4.13906700
C	-7.43845600	-2.82393900	3.74247500
C	-6.70625700	-2.04763800	2.84996000
H	-4.00602600	-4.07342900	2.36678100
H	-5.30403800	-5.46175400	3.97262800
H	-7.47876600	-4.67322400	4.83674200
H	-8.39321600	-2.47657500	4.12717000
C	-3.50102400	-0.97237000	1.66617600
H	-3.21561800	-0.19991700	0.94516000
H	-3.43850200	-0.53906600	2.66914300
O	-2.58892100	-2.07007600	1.56453200
C	-1.28609300	-1.71402300	1.50478400

O	-0.91268800	-0.55617200	1.38256200
N	-0.47438200	-2.78452500	1.56283400
H	-0.86001700	-3.70803100	1.67396200
H	0.52869500	-2.62397600	1.62268200
C	6.22203400	2.83076300	4.29822300
C	5.35147700	2.71528900	3.23916900
C	5.30566800	1.51538200	2.46036800
C	6.16191500	0.42706900	2.82103800
C	7.06704700	0.58747500	3.92002300
C	7.09805900	1.75904000	4.63794000
H	6.24409300	3.74987300	4.89147900
H	4.67516100	3.53437600	2.98375800
C	4.39147800	1.34629300	1.34567500
C	6.09930300	-0.81296100	2.10058200
H	7.72396800	-0.24832900	4.17841600
H	7.78705400	1.87377200	5.47982300
C	5.20136800	-1.00008700	1.06926900
C	4.36704900	0.11289500	0.72382100
H	6.77699400	-1.62703100	2.38015300
C	3.50237700	2.45411800	0.83749300
C	4.09730000	3.71578200	0.43610000
C	2.12708000	2.30740800	0.71724500
C	5.51522200	3.90455100	0.36019400
C	3.24767900	4.80201600	0.07311700
C	1.24637700	3.40108900	0.38853700
C	6.04326100	5.11351400	-0.02810500
H	6.17452600	3.06781000	0.59997800
C	3.82690800	6.05590900	-0.30806300
C	1.82932600	4.62317000	0.10793600
C	5.19125600	6.20814200	-0.35708000
H	7.12805800	5.24118200	-0.09124000
H	3.15731300	6.88054600	-0.56966600
H	1.19005300	5.49314800	-0.07405100
H	5.63278800	7.16269400	-0.65783600

P	1.97142200	-0.36792500	0.50603300
O	1.49177200	1.06215800	1.02674200
O	3.35072600	-0.09068800	-0.27366300
S	1.46119600	-2.52239900	-1.58526700
S	0.78414200	0.36410900	-2.31579200
O	2.28963200	-2.35944200	-2.76276200
O	1.88858200	-3.32460000	-0.45670800
C	-0.10048200	-3.37388500	-2.15920800
F	0.31369000	-4.58129000	-2.52446900
F	-0.95988600	-3.49501100	-1.16052500
F	-0.66972400	-2.77786300	-3.18114300
C	2.46940200	0.97510700	-2.87763900
F	2.88264300	1.93796900	-2.06652700
F	3.38398100	0.03489600	-2.96736900
F	2.24318600	1.49049900	-4.07735400
O	0.21988800	-0.29403300	-3.47345100
O	0.17709900	1.53561000	-1.71051700
C	-0.23253700	3.31958000	0.40355700
C	-0.94255000	4.10569400	-0.51655400
C	-0.95640000	2.55689000	1.32602100
C	-2.31952000	4.16271400	-0.47426700
H	-0.42677700	4.65222800	-1.29606600
C	-2.34082100	2.62550600	1.34145700
H	-0.47528300	1.88790000	2.02812500
C	-3.04172200	3.43723000	0.46172400
C	5.07173400	-2.29621200	0.37202200
C	5.00830500	-2.37982800	-1.02230300
C	5.00977000	-3.47038500	1.12743900
C	4.89576600	-3.61593300	-1.63509800
H	5.02939700	-1.49607100	-1.64890300
C	4.89174000	-4.69376400	0.49401700
H	5.01129700	-3.43537300	2.21045100
C	4.83683900	-4.78514000	-0.88944300
O	1.99505300	-1.38324300	1.56585200

C	0.96580200	-0.85860700	-0.96995200
F	-2.99855000	4.91737200	-1.35301300
F	-4.37603600	3.51186400	0.49628500
F	-3.04770200	1.92863000	2.23760700
F	4.82214100	-5.82305300	1.20498000
F	4.72514700	-5.97016600	-1.48829700
F	4.84597400	-3.71342800	-2.96262100

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H	0.11308800	2.01421100	-2.25278300
C	-2.54701600	4.24279500	1.31959100
C	-3.60831600	4.01867000	0.42712800
C	-3.34942200	3.31732300	-0.74722200
C	-2.04625500	2.87185400	-0.98229100
C	-0.99702200	3.12043200	-0.06880900
C	-1.23963100	3.82292000	1.09894600
C	-4.31924500	5.15589300	2.20235600
C	-4.76242600	4.63790000	1.03550700
H	-4.13996900	3.11332300	-1.46497500
H	0.00689100	2.76306200	-0.27626500
H	-0.44659000	4.04601500	1.80148200
H	-4.81118200	5.70639100	2.98976900
H	-5.76756500	4.69675100	0.64397500
O	-2.98691600	4.93372100	2.39764800
C	-1.84998100	2.11735200	-2.21967200
O	-0.72864100	1.90874800	-2.80442100
H	-2.69269300	2.10863900	-2.90965700
C	-9.59604800	1.31324900	3.02843600
C	-8.55343200	2.23908200	2.97787400
C	-7.56760300	2.14375500	1.99435600
C	-7.64581900	1.11412100	1.06832400
C	-8.68548700	0.17374100	1.12635700
C	-9.66983000	0.27126700	2.10561100
H	-10.35555800	1.40338000	3.79872500

H	-8.50753200	3.03814100	3.71110800
H	-6.75064400	2.86103000	1.96596200
H	-10.47896600	-0.45169300	2.15640500
C	-6.70510500	0.79162300	-0.07661300
H	-6.69785700	1.60471700	-0.81687200
C	-7.32084400	-0.46693700	-0.65915400
C	-6.87908900	-1.25602500	-1.71213100
C	-7.61263100	-2.39501500	-2.05049800
C	-8.77097600	-2.73149700	-1.34845800
C	-9.21511100	-1.94237100	-0.28948200
C	-8.48124500	-0.81132700	0.05348000
H	-5.97638500	-1.00163900	-2.25645000
H	-7.27523400	-3.02459900	-2.86786400
H	-9.33003000	-3.61884400	-1.62847800
H	-10.11357100	-2.21056000	0.25883300
C	-5.28508700	0.59963900	0.42973300
H	-4.93272000	1.47677600	0.98418300
H	-5.21314200	-0.27524600	1.08246300
O	-4.43271000	0.41475700	-0.71273900
C	-3.13854700	0.24735600	-0.40338900
O	-2.68796900	0.21853600	0.70870000
N	-2.36439800	0.21146300	-1.57348800
H	-2.82666600	-0.25736000	-2.34985100
H	-1.40699400	-0.12511400	-1.37442300
C	0.75065600	-3.90384500	5.36840500
C	1.43327500	-3.23539900	4.37971000
C	0.97446100	-3.26819800	3.02321700
C	-0.22866500	-3.98301700	2.72528000
C	-0.91050600	-4.67733900	3.77816300
C	-0.43117000	-4.64200600	5.06485500
H	1.10996000	-3.86944600	6.40124800
H	2.33317600	-2.66354000	4.61677500
C	1.66311200	-2.57139300	1.95579900
C	-0.74874900	-3.97808600	1.39066500

H	-1.82299600	-5.22819700	3.53201700
H	-0.95611100	-5.17006100	5.86631000
C	-0.11125600	-3.29220300	0.37524800
C	1.10613400	-2.60022900	0.69058200
H	-1.66441400	-4.53801500	1.17134700
C	2.91123100	-1.76206500	2.18967900
C	4.11044000	-2.33306900	2.75686800
C	2.90984400	-0.41895000	1.84505300
C	4.24342900	-3.73288500	3.02623000
C	5.21249900	-1.46865200	3.03582900
C	4.00768500	0.47614100	2.10943200
C	5.40613800	-4.23317700	3.56243400
H	3.40845500	-4.39543100	2.78580700
C	6.40425600	-2.02027300	3.61264800
C	5.11495700	-0.07375900	2.73554400
C	6.49780200	-3.36664700	3.86772900
H	5.50402500	-5.30553300	3.75570500
H	7.23805100	-1.34614600	3.82990900
H	5.95247400	0.56978100	3.02581900
H	7.41190500	-3.78647200	4.29734800
P	1.55372000	-0.28958000	-0.33645600
O	1.72454000	0.08743100	1.22631300
O	1.76550700	-1.88803100	-0.35726700
S	4.26282500	-0.80165600	-1.60412200
S	2.69653600	1.53644200	-2.36614200
O	5.16826800	-0.06067600	-2.47355600
O	4.73683200	-1.46216000	-0.39891900
C	3.63265500	-2.19131900	-2.69313200
F	4.51067400	-2.40777400	-3.65979500
F	3.48925500	-3.31185800	-1.98939900
F	2.46098600	-1.86999900	-3.23177100
C	4.20642200	2.64256100	-2.22150300
F	4.93872800	2.32247100	-1.17014900
F	4.92119000	2.55807400	-3.32240500

F	3.77118500	3.88982200	-2.07736200
O	2.60438400	1.20142100	-3.77658500
O	1.62189300	2.38092900	-1.78234900
C	3.98980400	1.91360200	1.75507800
C	5.20352200	2.60178600	1.60209100
C	2.80656000	2.64425500	1.56397200
C	5.22668800	3.94328000	1.27420200
H	6.15479700	2.08965300	1.66802300
C	2.85651700	3.97910700	1.20872200
H	1.83237300	2.19070700	1.68033200
C	4.05597200	4.65703900	1.06134300
C	-0.69259600	-3.23153900	-0.97890600
C	0.07974800	-3.43963600	-2.12681700
C	-2.05276100	-2.93770600	-1.11989700
C	-0.49838300	-3.34257000	-3.37897600
H	1.13757600	-3.65909600	-2.06004900
C	-2.60514200	-2.83888900	-2.38422500
H	-2.66582400	-2.72420600	-0.25070800
C	-1.84729800	-3.03684300	-3.52762800
O	0.21559800	0.18802000	-0.77381900
C	2.91174400	0.21140200	-1.30578400
F	6.39069400	4.57964500	1.11580500
F	4.08589800	5.94431600	0.72139900
F	1.71606500	4.65908200	1.01542100
F	-3.88642800	-2.45244100	-2.53540600
F	-2.39478500	-2.91217200	-4.73640900
F	0.22561300	-3.53446900	-4.47938500

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H	0.31482600	-0.22057200	-3.52582900
C	-2.71973100	-4.76476400	-1.42767500
C	-3.16624200	-3.55273800	-1.96859400
C	-2.23253400	-2.67156900	-2.52307700
C	-0.88883600	-3.02601700	-2.49487500
C	-0.47822100	-4.26831900	-1.97152900

C	-1.38936400	-5.16065800	-1.42987300
C	-4.86759800	-4.68861800	-1.09547000
C	-4.59076700	-3.53300900	-1.73802900
H	-2.55459600	-1.72515800	-2.94306300
H	0.57672800	-4.52551300	-1.97912700
H	-1.08257000	-6.10907600	-1.00443200
H	-5.78701500	-5.10696800	-0.71517200
H	-5.30212600	-2.76990100	-2.01561600
O	-3.75828600	-5.45927300	-0.90075000
C	0.15410500	-2.08373500	-3.05049400
O	-0.39387300	-0.76008800	-3.11845700
H	0.42987900	-2.35171900	-4.07628500
C	8.75798200	2.29851200	-1.84039000
C	7.51856600	2.90585500	-1.63500100
C	6.38820000	2.13391600	-1.35961200
C	6.51877100	0.75468300	-1.29159000
C	7.76529900	0.14389200	-1.50014100
C	8.89208900	0.91300200	-1.77398700
H	9.62715300	2.91245900	-2.05534200
H	7.43352300	3.98666400	-1.68999800
H	5.42482800	2.61099700	-1.19720100
H	9.85932400	0.44538100	-1.93410100
C	5.45319000	-0.29506900	-1.03920200
H	4.96883300	-0.15397200	-0.06300000
C	6.25183100	-1.58394000	-1.08127500
C	5.82033400	-2.88970400	-0.89251000
C	6.75311800	-3.92295500	-1.00105300
C	8.09109100	-3.65252200	-1.29215100
C	8.52692200	-2.34220000	-1.47641100
C	7.59932700	-1.31091800	-1.36826500
H	4.78313500	-3.09942400	-0.65597000
H	6.43357200	-4.94978100	-0.85305200
H	8.80005400	-4.47090100	-1.37116600
H	9.56991000	-2.13305400	-1.69723900

C	4.38292600	-0.21728800	-2.12076400
H	3.92799400	0.77830000	-2.15751900
H	4.80516700	-0.43873500	-3.10539700
O	3.37012200	-1.17978400	-1.80435700
C	2.33332300	-1.20769000	-2.64871700
O	2.25330200	-0.50708000	-3.64976500
N	1.36941400	-2.08761900	-2.26421700
H	1.31375700	-2.34724700	-1.28086700
H	-1.02835500	-0.27240600	-1.83496900
C	0.40621800	6.44116700	-2.34794200
C	0.24953300	5.50533400	-1.35310100
C	-0.90316500	4.65612600	-1.32404400
C	-1.87261200	4.77646600	-2.36931100
C	-1.68285200	5.76945500	-3.38560800
C	-0.57571800	6.58337900	-3.37222100
H	1.29262000	7.08256900	-2.36250600
H	1.00752300	5.39116500	-0.57498300
C	-1.09571400	3.65122400	-0.29833900
C	-2.99908200	3.88806000	-2.40923400
H	-2.43590600	5.85727200	-4.17443500
H	-0.43348600	7.33725400	-4.15226200
C	-3.17555700	2.91058700	-1.45103600
C	-2.20093900	2.82599900	-0.40375200
H	-3.72554000	3.97933800	-3.22385000
C	-0.12913000	3.45255800	0.84203400
C	0.20280800	4.53022300	1.74658300
C	0.46046400	2.21194500	1.04348600
C	-0.44876000	5.80398200	1.69193900
C	1.20285200	4.30861900	2.74226600
C	1.45832200	1.95384700	2.04854600
C	-0.10210800	6.80375000	2.56954700
H	-1.23303900	5.96224400	0.94788600
C	1.55386300	5.37840800	3.63035100
C	1.82841300	3.02582600	2.84402400

C	0.91734600	6.59309400	3.54567400
H	-0.61169600	7.77116800	2.52726800
H	2.32818200	5.19947900	4.38237800
H	2.63321900	2.90008300	3.57624500
H	1.17964400	7.40444200	4.23114200
P	-1.38404700	0.56612500	0.27430400
O	0.09632600	1.15916100	0.12712000
O	-2.35545100	1.78345000	0.57434600
S	-2.94977800	-0.45244300	2.66896700
S	-1.06277100	-2.13006500	1.20738800
O	-2.74033000	-1.49539900	3.65916500
O	-3.23973800	0.91802700	3.04286500
C	-4.42753500	-1.01116900	1.65307100
F	-5.45049100	-0.20289100	1.90284500
F	-4.13157100	-0.93440100	0.35458900
F	-4.75726800	-2.24921900	1.95663200
C	-0.16817800	-2.75956300	2.71991200
F	0.27233000	-1.75348400	3.45664800
F	-0.95014600	-3.54132000	3.42937700
F	0.86812000	-3.47108300	2.27744100
O	-2.12611300	-3.09509600	0.99402900
O	-0.00891200	-1.92838000	0.20161700
C	2.08038500	0.62795100	2.26395700
C	2.51974800	0.28752800	3.55243000
C	2.25842500	-0.31089300	1.23968100
C	3.12203600	-0.93165700	3.79555500
H	2.35668400	0.94848200	4.39449000
C	2.81263600	-1.54728600	1.52104400
H	1.93448400	-0.12898000	0.22517100
C	3.27185300	-1.87347600	2.78705400
C	-4.26803400	1.91320600	-1.54983100
C	-5.28413600	1.81407500	-0.59693800
C	-4.24274800	1.01861700	-2.62244500
C	-6.26403100	0.84342800	-0.73690300

H	-5.31843100	2.46685000	0.26837000
C	-5.20928200	0.03650500	-2.72159200
H	-3.43669300	1.04349800	-3.34712800
C	-6.23382900	-0.05810800	-1.79167300
O	-1.71696800	0.05095500	-1.14606200
C	-1.63127000	-0.54369600	1.55978500
F	3.53146100	-1.25103700	5.02496300
F	3.78728200	-3.07289900	3.03968900
F	2.88859900	-2.48434500	0.56810100
F	-5.16362600	-0.86944800	-3.70457000
F	-7.14699500	-1.02490400	-1.89411800
F	-7.25221200	0.73875200	0.15052800

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H	-1.24903200	0.03115900	-2.35283200
C	0.26014500	4.70833200	-0.05926400
C	0.26487300	4.73328900	-1.46442400
C	-0.62166300	3.90805200	-2.14981800
C	-1.48768700	3.10190800	-1.41091100
C	-1.48378200	3.11896800	-0.00077400
C	-0.60146300	3.92315000	0.69892700
C	1.80229400	6.12707100	-0.66239300
C	1.29284100	5.67802600	-1.82867900
H	-0.62308100	3.86227500	-3.23556500
H	-2.15528900	2.47969700	0.56099300
H	-0.56188900	3.91604900	1.78193500
H	2.60018900	6.81431300	-0.43267900
H	1.61128000	5.96380400	-2.81960800
O	1.19861500	5.55589900	0.42362400
C	-2.29020500	2.13552400	-2.16660000
O	-0.89314200	0.90893600	-2.60585200
H	-2.51092200	2.35234700	-3.20705400
C	-4.97306600	3.81069700	0.39385400
C	-5.72419100	3.74899000	-0.77974800

C	-6.41125700	2.58088900	-1.12560900
C	-6.33694200	1.48602800	-0.27776300
C	-5.59320300	1.55451400	0.91334000
C	-4.90412300	2.71393000	1.25468800
H	-4.42814700	4.71775900	0.63695300
H	-5.76809400	4.61258900	-1.43578700
H	-6.96812500	2.52918800	-2.05782300
H	-4.30939200	2.75728400	2.16353300
C	-6.83796200	0.06721600	-0.49432300
H	-7.91937500	0.01425400	-0.67146000
C	-6.43417300	-0.61481400	0.79858300
C	-6.68710500	-1.91323600	1.21080400
C	-6.20222300	-2.32838200	2.45282200
C	-5.45988700	-1.45873900	3.25152800
C	-5.18189000	-0.15982400	2.82917000
C	-5.68279300	0.25706900	1.60045400
H	-7.25884700	-2.59594400	0.58695000
H	-6.40230700	-3.33766600	2.79889000
H	-5.07808700	-1.80242500	4.20748500
H	-4.57667700	0.50119800	3.44286300
C	-6.10897900	-0.56093400	-1.69541500
H	-6.18526100	-1.64923400	-1.69854800
H	-6.45667300	-0.16364200	-2.65210200
O	-4.71755100	-0.25359100	-1.53655000
C	-4.22954000	0.73115100	-2.29653700
O	-4.56988000	1.03717900	-3.40800300
N	-3.22959500	1.38532800	-1.57014900
H	-3.06204100	1.02174700	-0.63372500
H	-0.20654500	1.06798900	-1.87810000
C	6.39513900	-3.50924800	-3.00769700
C	5.31306000	-3.24998800	-2.19972600
C	5.12986100	-1.95600800	-1.61268700
C	6.08020500	-0.93013000	-1.91241700
C	7.20272200	-1.23710000	-2.74954100

C	7.35823600	-2.49420900	-3.28033900
H	6.52191100	-4.50134300	-3.45130800
H	4.57400600	-4.02862500	-1.99880100
C	3.99752900	-1.64214600	-0.76244000
C	5.89136400	0.39259200	-1.39587400
H	7.92598800	-0.44364300	-2.95964100
H	8.21383900	-2.72312500	-3.92228400
C	4.80303500	0.70741600	-0.60679500
C	3.87186900	-0.34312200	-0.30274800
H	6.63524100	1.16453800	-1.62077700
C	2.91400000	-2.65881900	-0.49335300
C	3.15083900	-3.94811000	0.12525700
C	1.62430900	-2.36820800	-0.89999500
C	4.41842500	-4.29558400	0.68881900
C	2.06961300	-4.88143000	0.22068900
C	0.54187700	-3.31538500	-0.89263200
C	4.59991200	-5.51453100	1.30123500
H	5.23170200	-3.56714500	0.63598300
C	2.29897900	-6.14738300	0.85040300
C	0.78636000	-4.55462200	-0.33450200
C	3.53122200	-6.45433600	1.37748300
H	5.56921700	-5.76853600	1.74057200
H	1.46895600	-6.85742700	0.91060000
H	-0.00224200	-5.31604900	-0.33382500
H	3.69837200	-7.41895900	1.86555500
P	1.29507000	0.02792400	-0.10580000
O	1.33874100	-1.03809700	-1.32818200
O	2.76649800	-0.01507500	0.53758100
S	1.18778400	-1.15308900	2.70188900
S	-1.25400000	-0.26153700	1.35241000
O	0.12673900	-1.47177700	3.65054700
O	2.25298500	-2.10117200	2.42519000
C	2.05612500	0.32433900	3.46413200
F	3.37091300	0.12144500	3.45032300

F	1.78312700	1.44127200	2.79819700
F	1.65746100	0.46163600	4.71742600
C	-2.12002300	-1.80576900	1.96842500
F	-3.20333800	-1.95693200	1.21366500
F	-1.34709000	-2.87853600	1.82977100
F	-2.48497500	-1.67728700	3.22556800
O	-1.71088800	0.77809100	2.27020700
O	-1.67452800	-0.15669200	-0.06407300
C	-0.74518600	-2.98919900	-1.54484600
C	-1.96560900	-3.40099700	-0.99977900
C	-0.76817200	-2.27987700	-2.75688400
C	-3.15867900	-3.07413900	-1.62194200
H	-2.00631800	-3.93328600	-0.05959200
C	-1.97164800	-1.99175100	-3.37828400
H	0.14447700	-1.93910200	-3.23129000
C	-3.18115400	-2.39221300	-2.82814100
C	4.59710200	2.08755900	-0.12068700
C	4.26500200	2.34685500	1.21165200
C	4.74772200	3.16200600	-1.00354100
C	4.07074500	3.64656100	1.63814800
H	4.15076200	1.54572000	1.92744800
C	4.56205000	4.45686600	-0.55231000
H	4.97379500	2.99575300	-2.05039000
C	4.22575500	4.71604100	0.76811600
O	0.88387500	1.32261500	-0.72081300
C	0.41619900	-0.57894800	1.28061000
F	-4.32993400	-3.39861300	-1.06635900
F	-4.33228000	-2.11019500	-3.44058100
F	-1.99721200	-1.30673700	-4.52554400
F	4.68718800	5.49783300	-1.38648000
F	4.04183800	5.97012900	1.19070800
F	3.75170500	3.90606400	2.90719100

C	5.50369600	3.90080300	-3.09538200
C	5.07846600	2.77245800	-2.44043500
C	4.26974800	2.86572000	-1.27480200
C	3.86173100	4.15842900	-0.84194000
C	4.33097900	5.30669200	-1.53290400
C	5.14157600	5.18601000	-2.63057500
H	6.12235600	3.80551600	-3.98211500
H	5.36058000	1.79684000	-2.81723400
C	3.80840000	1.71724900	-0.54641200
C	2.93352200	4.28485800	0.22040300
H	4.02901000	6.28552100	-1.17185400
H	5.49561000	6.06999200	-3.15130400
C	2.45853400	3.19155900	0.90200200
C	2.96706200	1.91788400	0.52403900
H	2.51841700	5.26270100	0.44070900
C	4.05772600	0.33669500	-1.04774800
C	5.36399300	-0.20235300	-1.26703000
C	2.96964900	-0.44562300	-1.36740300
C	6.53891600	0.45912100	-0.82569200
C	5.48791100	-1.46272900	-1.91374900
C	3.06220500	-1.68336600	-2.06027300
C	7.77467500	-0.09628600	-1.04019600
H	6.44469000	1.40456500	-0.30096500
C	6.78183500	-2.00254800	-2.13586800
C	4.32423500	-2.15631600	-2.33094900
C	7.90082100	-1.33600700	-1.71027400
H	8.66417900	0.41453400	-0.68560700
H	6.86536200	-2.96281200	-2.63746700
H	4.44174500	-3.08737300	-2.87988500
H	8.88540300	-1.76207400	-1.87378100
P	1.41286400	-0.14962600	0.61428000
O	1.69791500	-0.02575900	-0.97416400
O	2.53643000	0.80667900	1.24671700
S	3.22556500	-1.90836300	2.29098200

S	0.67946300	-2.92016100	1.15548900
O	3.12669700	-3.25884200	2.82986800
O	4.44802300	-1.41075100	1.68906200
C	2.93748800	-0.79406900	3.77198700
F	3.74266600	0.25866500	3.71715500
F	1.67461100	-0.37265900	3.80189800
F	3.19305600	-1.47923200	4.87267300
C	1.52332300	-4.57750500	0.92242100
F	2.73690200	-4.42551500	0.41622900
F	1.56286500	-5.24491000	2.05000900
F	0.76976200	-5.24149900	0.05264800
O	-0.13568000	-3.11063400	2.36732100
O	-0.06463900	-2.67744400	-0.08579100
C	1.84003100	-2.41322100	-2.47898200
C	1.80298400	-3.80705100	-2.39806200
C	0.71604100	-1.72467000	-2.95731200
C	0.65149300	-4.48928500	-2.75374600
H	2.64140100	-4.37661400	-2.01514900
C	-0.41637900	-2.43349300	-3.31079000
H	0.68920500	-0.64488600	-3.03941700
C	-0.47420600	-3.81728200	-3.20152500
C	1.36099400	3.33211100	1.89099800
C	1.40964500	2.67782400	3.12394600
C	0.25742900	4.12667000	1.55372700
C	0.34543300	2.80332100	3.99743900
H	2.25760400	2.07158000	3.41398100
C	-0.79289200	4.22882600	2.45071300
H	0.18425500	4.61161800	0.59004900
C	-0.76384200	3.57396400	3.67446700
O	0.01633500	0.30634400	0.88257100
C	1.85957500	-1.69551700	1.26748100
H	-1.46031400	-2.06688700	1.91467600
C	-3.70427800	-5.52004300	-0.20628900
C	-3.59962400	-5.01229400	1.09550400

C	-3.26916300	-3.66208300	1.27655200
C	-3.03635000	-2.87748900	0.15527300
C	-3.14940900	-3.41136200	-1.16089800
C	-3.49810300	-4.74626900	-1.34992600
C	-4.15428100	-7.17655300	1.14862300
C	-3.90059200	-6.12104000	1.96567200
H	-3.22349700	-3.24957100	2.28480300
H	-2.99609600	-2.75106100	-2.02203800
H	-3.60652100	-5.17565400	-2.35147900
H	-4.42060500	-8.22059500	1.34196700
H	-3.91810400	-6.12035200	3.05518700
O	-4.03769500	-6.82382100	-0.20825400
C	-2.71397800	-1.39303100	0.33523300
O	-1.85968600	-1.22030200	1.55694400
H	-3.61730400	-0.79140800	0.55460500
C	-0.14342800	7.07048900	-0.32094000
C	0.88123800	6.45436800	-1.05864700
C	0.64813500	5.24784000	-1.75480400
C	-0.64352700	4.71099900	-1.73284800
C	-1.69172700	5.36226900	-1.03304600
C	-1.44109600	6.53423800	-0.30561000
H	0.06736200	7.99402800	0.22694900
H	1.86830500	6.92702900	-1.11076500
H	1.45462900	4.76574000	-2.31886300
H	-2.24465500	7.02921400	0.24971900
C	-1.15933900	3.39592900	-2.33297800
H	-0.92698300	3.26608800	-3.40185200
C	-2.66386700	3.49820200	-2.06563000
C	-3.69322900	2.66247500	-2.52710400
C	-5.01682000	3.00846600	-2.23251400
C	-5.30060300	4.15203700	-1.44679700
C	-4.26880300	4.95410500	-0.96664700
C	-2.94787600	4.62904600	-1.28957500
H	-3.46552600	1.78889500	-3.14659500

H	-5.83990400	2.41556300	-2.64018900
H	-6.34243600	4.43565800	-1.26397000
H	-4.48758400	5.83811500	-0.37415200
C	-0.51512400	2.27825300	-1.49480100
H	0.55028700	2.17776700	-1.72842600
H	-0.62582700	2.50472200	-0.43295000
O	-1.08228900	0.98132400	-1.73660700
C	-1.95740600	0.57758800	-0.79915400
O	-2.54931100	1.29361000	-0.02832400
N	-2.07207500	-0.79993500	-0.81040800
H	-1.27485100	-1.30685700	-1.18385400
H	-1.11659400	-0.51673600	1.38820400
F	0.59559500	-5.81752400	-2.65157400
F	-1.56888900	-4.48169700	-3.56537300
F	-1.50321500	-1.79514200	-3.75908200
F	-1.87410900	4.95530100	2.16078400
F	-1.78322300	3.68125300	4.52420000
F	0.36269000	2.18797000	5.18176700
C	-5.75130200	-1.77957400	-0.78952000
C	-5.70059500	-0.48201900	-1.09525400
H	-5.77943700	-2.11577600	0.24563200
H	-5.73473100	-2.55755200	-1.54490800
H	-5.66757100	-0.19645100	-2.14863500
C	-5.69647700	0.65348800	-0.11983400
H	-5.35844000	0.32362000	0.87225900
H	-5.01234200	1.43328600	-0.46358700
Si	-7.42380100	1.39044000	0.15403600
C	-8.47927600	0.05692900	0.96636300
H	-8.06196200	-0.23905000	1.93515400
H	-9.50435100	0.40383400	1.13451100
H	-8.52066100	-0.83611000	0.33385900
C	-7.26853400	2.87378100	1.30370500
H	-6.92887500	2.55907000	2.29623200
H	-6.53899100	3.59078900	0.91637700

H	-8.22764300	3.38835500	1.42690600
C	-8.27373000	1.88855800	-1.45752900
H	-8.17119600	1.10575900	-2.21731700
H	-9.34514900	2.02954900	-1.27632700
H	-7.88691700	2.82262900	-1.87418600

TSIII-3S

H	-1.89140000	1.45533500	-2.52108000
C	-2.02170700	1.95187600	4.62762400
C	-1.33879300	2.70103000	3.64703500
C	-1.58299300	2.42774700	2.29951400
C	-2.48180200	1.40193100	1.97492600
C	-3.15186400	0.67574100	2.99274900
C	-2.93242600	0.94209000	4.33528500
C	-0.74127200	3.37320800	5.68795400
C	-0.50509400	3.62392300	4.37910300
H	-1.06560800	2.96787800	1.51284800
H	-3.85953700	-0.10051900	2.71652000
H	-3.43287200	0.38807600	5.12158900
H	-0.34981400	3.79966700	6.59914200
H	0.17779700	4.35466500	3.97236400
O	-1.66256400	2.36431400	5.87160400
C	-2.74680900	1.11844600	0.55760800
O	-1.24009200	2.13495500	-2.27676500
H	-2.23120800	1.71846200	-0.18777800
C	-8.10356900	-1.72127500	-1.21202400
C	-7.44573200	-1.16072200	-2.31272100
C	-6.22135500	-1.68333600	-2.74976200
C	-5.66947300	-2.76535600	-2.07303800
C	-6.33109300	-3.33014400	-0.96326200
C	-7.55252800	-2.80890900	-0.53049100
H	-9.05567600	-1.30961900	-0.88726800
H	-7.89388100	-0.32258700	-2.84032900
H	-5.71445300	-1.24342500	-3.60506700

H	-8.07065200	-3.24060500	0.32191500
C	-4.37324100	-3.51581200	-2.34702300
H	-4.42234500	-4.00498300	-3.33306500
C	-4.36548300	-4.56489200	-1.24351300
C	-3.41178000	-5.53640200	-0.96451300
C	-3.62075800	-6.39483600	0.12048100
C	-4.77376100	-6.28444600	0.90513900
C	-5.73464400	-5.30994200	0.62598600
C	-5.52290100	-4.44518900	-0.44974400
H	-2.50906500	-5.62838900	-1.55983000
H	-2.87153500	-7.14530400	0.35534100
H	-4.92093600	-6.95978900	1.74367200
H	-6.62652300	-5.22660700	1.24208300
C	-3.12130200	-2.63318800	-2.39006000
H	-2.22596200	-3.23684700	-2.54535600
H	-3.19280500	-1.87569000	-3.17247300
O	-2.93364800	-1.97702300	-1.11554800
C	-3.04152500	-0.64958800	-1.06518900
O	-3.27980400	0.09583300	-2.00957400
N	-2.89587700	-0.21516700	0.23335100
H	-2.51615500	-0.89656600	0.89513700
C	-4.51136900	2.09448500	0.31679200
C	-4.78489800	2.13869900	-1.04736400
H	-4.13389900	3.00107400	0.77969100
H	-5.14133900	1.47738500	0.95079800
H	-5.44540300	1.37700000	-1.45735000
C	-4.25457500	3.13183600	-1.97144100
H	-3.22846600	3.42623900	-1.71444600
H	-4.25800000	2.75880000	-3.00066400
Si	-5.21837800	4.82827700	-1.99025700
C	-4.39817800	5.82993000	-3.36315500
H	-4.48803900	5.33850500	-4.33875600
H	-4.85576700	6.82324200	-3.44701700
H	-3.33210200	5.96902500	-3.15074500

C	-7.04718800	4.51917900	-2.35314800
H	-7.59163800	5.46828200	-2.42894000
H	-7.18659000	3.98484300	-3.30045700
H	-7.52453200	3.92961700	-1.56142200
C	-4.98430700	5.68491000	-0.32460200
H	-5.45552700	6.67559500	-0.33961700
H	-5.43269400	5.12485200	0.50373800
H	-3.92010400	5.83103000	-0.10544900
H	-0.59348800	1.62782200	-1.74175500
C	5.44531800	1.21643600	-5.46819500
C	5.08439200	0.70842200	-4.23984200
C	4.32041500	1.48017000	-3.32023000
C	3.90321700	2.78755800	-3.73028700
C	4.30569400	3.28906000	-4.99769100
C	5.06549000	2.52417200	-5.85088200
H	6.02481500	0.60285600	-6.15258800
H	5.37881600	-0.29847200	-3.97096600
C	3.91319000	0.98947300	-2.02906000
C	3.07458300	3.55217600	-2.87462500
H	3.98841800	4.28899900	-5.28374900
H	5.36356300	2.91420600	-6.82009600
C	2.62915300	3.06943100	-1.66140800
C	3.05457100	1.76635100	-1.26841600
H	2.77530000	4.54812500	-3.19035400
C	4.32718600	-0.36579900	-1.56075100
C	5.70762800	-0.73225900	-1.41578900
C	3.35794800	-1.31168200	-1.26946600
C	6.77105300	0.20467100	-1.51902800
C	6.03277000	-2.09299200	-1.11221200
C	3.65869800	-2.68739500	-1.04129400
C	8.08102400	-0.18862600	-1.35541200
H	6.54059400	1.24676300	-1.70898200
C	7.39501800	-2.47020400	-0.96864900
C	4.99173000	-3.04290500	-0.97858900

C	8.40125800	-1.54032900	-1.08777400
H	8.87619500	0.54860300	-1.42520700
H	7.62518100	-3.50945300	-0.74677900
H	5.25824600	-4.08626400	-0.83296500
H	9.43914500	-1.83699100	-0.96494100
P	1.46228200	0.07097600	-0.04682600
O	2.02295100	-0.92261300	-1.24134700
O	2.58057100	1.27154600	-0.05632100
S	3.12495800	-0.27548800	2.51141300
S	0.33848000	-1.26527700	2.43286500
O	3.00427800	-1.03692800	3.76032200
O	4.33620100	-0.36168200	1.69167900
C	3.07291300	1.54476300	3.08263300
F	3.95548300	2.27554100	2.38528900
F	1.85238100	2.07107600	2.91122500
F	3.39642500	1.60773400	4.37343600
C	0.89749700	-2.99229900	3.04372500
F	-0.06441200	-3.86222300	2.71031700
F	2.03734600	-3.37844200	2.46541400
F	1.03748600	-2.99211500	4.36182100
O	-0.02512000	-0.54929600	3.65988000
O	-0.71471800	-1.58781700	1.44437200
C	2.60119500	-3.72801800	-0.94962200
C	2.71933200	-4.77417500	-0.02131700
C	1.51141200	-3.72909100	-1.83760300
C	1.76528500	-5.78088900	0.02266700
H	3.52357000	-4.79239100	0.70451600
C	0.58411000	-4.75470800	-1.78075500
H	1.38062300	-2.94549100	-2.57291500
C	0.68651200	-5.78930700	-0.85663800
C	1.72001200	3.90775400	-0.82999000
C	2.05861000	4.27655200	0.48101300
C	0.52453800	4.38025300	-1.39364800
C	1.21201200	5.11124900	1.19354800

H	2.96419200	3.92147800	0.95539000
C	-0.31215200	5.19340500	-0.64459200
H	0.19966400	4.05783300	-2.37499200
C	0.01537000	5.57754400	0.65170400
O	0.09378700	0.49421300	-0.45979900
C	1.68215500	-0.55226900	1.57812000
F	1.86263200	-6.77154500	0.92330300
F	-0.23696400	-6.76393300	-0.81184000
F	-0.45908000	-4.77517600	-2.64527100
F	-1.49082900	5.61956000	-1.15599800
F	-0.80337500	6.36514200	1.36525200
F	1.52691000	5.49134400	2.44949600

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H	-0.88058900	-1.04717100	1.05008900
C	-7.40096200	-0.62286900	3.15348400
C	-7.79090000	-1.76524800	2.44119500
C	-7.12169500	-2.07844200	1.25178100
C	-6.09684500	-1.24570300	0.82181700
C	-5.73446300	-0.10462400	1.56836500
C	-6.38016500	0.22749600	2.74859100
C	-9.03029900	-1.53083500	4.27713800
C	-8.86869000	-2.34258900	3.20823700
H	-7.40066900	-2.95244400	0.66943900
H	-4.92716500	0.53360800	1.21727600
H	-6.08799600	1.09168300	3.33271100
H	-9.70781800	-1.55831600	5.11699100
H	-9.43684500	-3.23312800	2.98540000
O	-8.15753900	-0.48398000	4.27314800
C	-5.35822400	-1.55537800	-0.46099700
O	-1.45204400	-1.62393900	1.60196100
H	-5.70526300	-2.51931100	-0.85260000
C	-2.01677200	1.28043300	-0.80952600
C	-1.57211600	0.60729100	-1.95107900

C	-2.26135700	0.73009200	-3.15924100
C	-3.36336000	1.57163000	-3.21944300
C	-3.79303300	2.27051500	-2.08102800
C	-3.13661400	2.11121400	-0.86247400
H	-1.46611500	1.15247400	0.11838500
H	-0.67511600	0.00086700	-1.87956500
H	-1.92990800	0.18393900	-4.03919400
H	-3.48564600	2.62780700	0.02861800
C	-4.29920900	1.83790500	-4.38291200
H	-3.77039800	2.16179500	-5.28809600
C	-5.21178100	2.91079500	-3.82006000
C	-6.23784200	3.60102700	-4.44465300
C	-6.99498700	4.50609200	-3.69693500
C	-6.72944000	4.70289900	-2.34170000
C	-5.69976300	4.00661600	-1.70927000
C	-4.94082600	3.11151500	-2.45703400
H	-6.45307300	3.44570100	-5.49899700
H	-7.79799400	5.05910400	-4.17405400
H	-7.32934600	5.40732800	-1.77382100
H	-5.49337900	4.16640300	-0.65441800
C	-5.10815600	0.57202700	-4.70882700
H	-5.85034300	0.76746300	-5.48658400
H	-4.46601000	-0.25819200	-5.01470100
O	-5.83480300	0.21100000	-3.53660700
C	-5.30561700	-0.75847000	-2.75963800
O	-4.64725900	-1.70063900	-3.16040300
N	-5.65339300	-0.55802400	-1.46473100
H	-6.10824900	0.30870800	-1.21211600
H	-0.76674500	-2.11393200	2.08498600
C	3.22535800	6.73774200	-0.76970700
C	3.46251700	5.40035200	-0.55645900
C	2.59542800	4.62974500	0.28366500
C	1.45999200	5.27058100	0.86967900
C	1.25027100	6.67028400	0.63937200

C	2.11133800	7.38467700	-0.15700100
H	3.89131000	7.31698600	-1.41624400
H	4.31320100	4.90254200	-1.02806000
C	2.81950400	3.22476000	0.54769600
C	0.53028800	4.50363100	1.64148200
H	0.38338500	7.14995700	1.10306000
H	1.94439000	8.45072300	-0.33627900
C	0.68758400	3.14170700	1.82999300
C	1.87864300	2.53676700	1.29481400
H	-0.32667000	5.01779800	2.09021500
C	4.01171900	2.48086100	0.00592400
C	5.37655700	2.86580500	0.30319300
C	3.80396900	1.33741500	-0.74740100
C	5.69071800	3.96935100	1.15966900
C	6.44998500	2.07234600	-0.21235900
C	4.86553900	0.56808600	-1.33796200
C	6.99733200	4.27656700	1.45844100
H	4.87272000	4.55449400	1.58534400
C	7.80079300	2.42749700	0.10912900
C	6.16698900	0.94364000	-1.05032700
C	8.06719400	3.50277200	0.92195400
H	7.22433300	5.11739600	2.12050700
H	8.60980500	1.81487300	-0.29941400
H	6.99883200	0.38790200	-1.49830900
H	9.09916300	3.76549200	1.17180700
P	1.91646400	0.08420300	0.43637100
O	2.47202500	0.84090000	-0.88605500
O	2.13806900	1.17227800	1.60137300
S	4.56340300	-1.02412900	1.62080800
S	2.38370600	-2.82705700	0.96606600
O	5.51618400	-1.91449100	0.97212500
O	4.86812900	0.38850000	1.77440600
C	4.46005700	-1.61793900	3.40248600
F	5.11076000	-0.73038400	4.14890100

F	3.19807100	-1.66710800	3.81803400
F	5.03565200	-2.79377300	3.55218900
C	2.68242600	-3.53303300	-0.71326000
F	2.36461600	-2.64015500	-1.64942000
F	3.93702900	-3.90934600	-0.85904300
F	1.89167100	-4.60644800	-0.87789800
O	3.18878200	-3.65832900	1.84680700
O	0.92394200	-2.88777500	1.05404500
C	4.58933400	-0.52090900	-2.29778600
C	5.31502400	-1.71358900	-2.24135300
C	3.63927700	-0.34734000	-3.31306000
C	5.09369600	-2.69779100	-3.18970300
H	5.99887000	-1.90978300	-1.42253600
C	3.43889600	-1.34514900	-4.24759000
H	3.04979900	0.55932400	-3.38192900
C	4.16404200	-2.52867700	-4.20502200
C	-0.38866000	2.34761500	2.46200900
C	-0.16910400	1.18964200	3.22346000
C	-1.71426100	2.74499000	2.23546200
C	-1.24108100	0.45732800	3.69845400
H	0.82782000	0.82467200	3.43408000
C	-2.76644200	2.00287400	2.73710500
H	-1.93497700	3.60331300	1.61245200
C	-2.55371100	0.84236500	3.46100600
O	0.50116100	-0.27626600	0.16114200
C	2.95997300	-1.22663800	0.96365300
F	5.75150600	-3.85864900	-3.12961700
F	3.95300900	-3.48941500	-5.10796600
F	2.53841200	-1.19290800	-5.22627600
F	-4.03642400	2.37604600	2.48325300
F	-3.57677800	0.11171200	3.90469900
F	-1.03553200	-0.66340100	4.39216900
C	-3.81621300	-1.67466000	-0.23262600
C	-3.56415900	-2.96660700	0.44369200

H	-3.35051300	-1.66418600	-1.22330800
H	-3.43410500	-0.84061100	0.35695100
H	-3.37593700	-2.95380600	1.51447400
C	-3.61558600	-4.15903800	-0.23799800
H	-3.95266000	-4.13940900	-1.27666800
H	-3.75706800	-5.08768900	0.31358900
Si	-1.50994600	-4.40802600	-0.51552100
C	-1.64270100	-5.85189100	-1.70573400
H	-2.18408400	-6.70290300	-1.28272600
H	-0.62197200	-6.18415700	-1.93328200
H	-2.11401300	-5.56176800	-2.64913600
C	-0.97003600	-5.02307400	1.15720800
H	-1.54727400	-5.91790000	1.41510400
H	-1.08298500	-4.27648900	1.94334500
H	0.08969100	-5.28881900	1.11761800
C	-0.88945700	-2.91315400	-1.41262200
H	0.07214600	-3.15981800	-1.87133600
H	-0.73526500	-2.05690800	-0.75624300
H	-1.58758800	-2.65456900	-2.21895900

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C	4.95860700	-2.62034700	-0.02739300
H	5.25403900	-3.38005300	0.70363900
N	6.20029700	-2.02656400	-0.48883000
C	7.26336200	-1.91970600	0.34899800
O	7.32593800	-2.41550800	1.45539500
O	8.25046100	-1.20476800	-0.24027000
C	9.42688300	-1.00305800	0.53780000
H	10.27257100	-1.19886900	-0.12750400
H	9.44246400	-1.72103200	1.36022100
H	6.20865300	-1.47236500	-1.33504200
C	4.13311900	-1.56435500	0.76435100
H	4.77092700	-1.18250200	1.56855700
H	3.25984200	-2.05236000	1.21369000

C	3.68792700	-0.46879500	-0.14037500
C	4.04680100	0.83415500	-0.03349900
H	4.81561400	1.12585100	0.68395600
H	3.88205200	1.49961500	-0.87842700
Si	2.27581300	1.59766600	0.95820600
C	1.21312700	1.34188300	-0.57742900
H	0.17090600	1.60366100	-0.37307100
H	1.21330900	0.32258400	-0.96357600
H	1.58418600	2.00272700	-1.37142400
C	3.07881100	3.30547600	0.99212700
H	4.01024100	3.28168500	1.56359400
H	2.40957200	4.02438000	1.47417500
H	3.29800000	3.67662500	-0.01284000
C	2.57966900	0.63353300	2.53989600
H	2.22418300	-0.39591800	2.48894100
H	2.04884500	1.12926600	3.35575600
H	3.65146000	0.63502300	2.76756300
O	0.53681000	2.40854400	1.96442700
H	-0.20505800	1.74408500	1.97346100
H	0.13009000	3.15166100	1.48357200
C	9.48878300	0.42889000	1.06172900
C	9.58743100	1.48862300	-0.01842200
H	10.37419800	0.48587300	1.71272700
C	8.26234300	0.87369100	1.83773900
C	10.49597600	1.59065600	-1.06102300
C	8.59062200	2.46017500	0.15539000
C	7.64299100	0.26759700	2.92201600
C	7.77489600	2.08480800	1.31980500
C	10.39967200	2.67428800	-1.93534100
H	11.27240500	0.84277500	-1.20078600
C	8.49648700	3.54393700	-0.71245900
C	6.53971600	0.89675800	3.50373600
H	7.99315000	-0.68766100	3.30006700
C	6.68920300	2.72349300	1.91336700

C	9.40900100	3.64205500	-1.76080900
H	11.10213100	2.76635800	-2.75762400
H	7.72729700	4.29964200	-0.58046400
C	6.07799100	2.12108100	3.01355100
H	6.04435000	0.43678500	4.35331700
H	6.32742700	3.67489500	1.53214800
H	9.34955500	4.47924700	-2.44914000
H	5.23470100	2.60713100	3.49715000
C	4.20545700	-3.27444600	-1.17978600
C	4.91423800	-3.75628600	-2.30009400
C	2.82318100	-3.42315200	-1.11706200
C	4.26860800	-4.36239700	-3.37021900
H	5.99460100	-3.65899000	-2.32240300
C	2.14769400	-4.00688600	-2.19213500
H	2.24678300	-3.08386200	-0.26565000
C	2.88650800	-4.46403200	-3.29092500
H	4.81265500	-4.73279200	-4.23187400
C	0.76457100	-4.27202900	-2.51249900
H	-0.10923400	-4.02838100	-1.92375100
O	2.05930600	-4.98697700	-4.23060400
C	0.78982000	-4.85268400	-3.73132500
H	0.00756200	-5.21813500	-4.37890800
H	3.01657000	-0.77065700	-0.94512400
C	-8.43316200	4.16096500	1.16636700
C	-7.64116600	3.11004900	0.76699100
C	-6.27279800	3.32458000	0.40554100
C	-5.73679900	4.64949600	0.48783400
C	-6.59338400	5.72286000	0.89848900
C	-7.90590700	5.48474000	1.22748000
H	-9.47750400	3.98721800	1.44263800
H	-8.03937500	2.09313600	0.72160300
C	-5.40648000	2.23933900	-0.00150900
C	-4.35908600	4.88626600	0.16845500
H	-6.17554800	6.73260600	0.95002100

H	-8.55457900	6.30669900	1.54401800
C	-3.52559400	3.85136400	-0.21007100
C	-4.08410500	2.53074400	-0.28017700
H	-3.97048800	5.90999200	0.20512200
C	-5.85095300	0.80236000	-0.08811800
C	-6.89028000	0.35881500	-0.98871400
C	-5.18354100	-0.14590000	0.66900600
C	-7.57705900	1.25943000	-1.86486900
C	-7.20914300	-1.03388100	-1.04598900
C	-5.51842500	-1.54080400	0.66147700
C	-8.53851000	0.79710400	-2.73181500
H	-7.31519900	2.31978800	-1.83800700
C	-8.22400800	-1.48078800	-1.95464300
C	-6.51861900	-1.95873800	-0.19727500
C	-8.87131600	-0.58909800	-2.77510000
H	-9.05345000	1.49239800	-3.40131500
H	-8.46169600	-2.54830900	-1.98360700
H	-6.80093200	-3.01716000	-0.21711000
H	-9.63994300	-0.93562700	-3.47184100
P	-2.71777900	0.64172900	0.68624400
O	-4.08483600	0.28166400	1.47227300
O	-3.21651600	1.45099600	-0.62175000
S	-2.56491900	-1.47228400	-1.52415300
S	-0.48393400	-1.35713600	0.51033300
O	-2.22424000	-2.88615700	-1.60847900
O	-3.92528800	-1.03304200	-1.78836600
C	-1.55806900	-0.66565800	-2.87559700
F	-2.33090100	-0.53817000	-3.94726700
F	-1.15306400	0.54711500	-2.49501400
F	-0.50539100	-1.39890100	-3.18653200
C	-0.74454600	-2.88759800	1.50064600
F	-1.56163200	-2.62305400	2.51016400
F	-1.22810600	-3.87884000	0.77420100
F	0.44722900	-3.24609500	1.98336200

O	0.35527400	-1.80810100	-0.60173300
O	0.09446800	-0.46166500	1.51241500
C	-4.84918900	-2.51515400	1.54934500
C	-4.33556300	-3.69931400	1.01273400
C	-4.77879900	-2.30597600	2.93146000
C	-3.79817100	-4.66063600	1.85255300
H	-4.31388400	-3.86558500	-0.05911000
C	-4.24544600	-3.28491800	3.74985200
H	-5.14925800	-1.39205800	3.38129700
C	-3.76039600	-4.47663300	3.22642900
C	-2.11134600	4.09042700	-0.55662000
C	-1.56041300	3.55392600	-1.72687600
C	-1.30495800	4.88292600	0.27018900
C	-0.24427000	3.81643300	-2.05267300
H	-2.13954500	2.91061400	-2.37773300
C	0.01546900	5.13199100	-0.07842300
H	-1.69417400	5.29439100	1.19501500
C	0.56098000	4.60510400	-1.24052300
O	-1.87427300	1.44445300	1.60283700
C	-1.98231300	-0.77825900	-0.04887000
F	-3.28004100	-5.78515500	1.35393700
F	-3.23935000	-5.40875700	4.02542000
F	-4.18849600	-3.11043000	5.07374500
F	0.80296900	5.86503200	0.71799800
F	1.84055900	4.81260800	-1.56120000
F	0.30964200	3.28715700	-3.14446500

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C	5.50369600	3.90080300	-3.09538200
C	5.07846600	2.77245800	-2.44043500
C	4.26974800	2.86572000	-1.27480200
C	3.86173100	4.15842900	-0.84194000
C	4.33097900	5.30669200	-1.53290400
C	5.14157600	5.18601000	-2.63057500

H	6.12235600	3.80551600	-3.98211500
H	5.36058000	1.79684000	-2.81723400
C	3.80840000	1.71724900	-0.54641200
C	2.93352200	4.28485800	0.22040300
H	4.02901000	6.28552100	-1.17185400
H	5.49561000	6.06999200	-3.15130400
C	2.45853400	3.19155900	0.90200200
C	2.96706200	1.91788400	0.52403900
H	2.51841700	5.26270100	0.44070900
C	4.05772600	0.33669500	-1.04774800
C	5.36399300	-0.20235300	-1.26703000
C	2.96964900	-0.44562300	-1.36740300
C	6.53891600	0.45912100	-0.82569200
C	5.48791100	-1.46272900	-1.91374900
C	3.06220500	-1.68336600	-2.06027300
C	7.77467500	-0.09628600	-1.04019600
H	6.44469000	1.40456500	-0.30096500
C	6.78183500	-2.00254800	-2.13586800
C	4.32423500	-2.15631600	-2.33094900
C	7.90082100	-1.33600700	-1.71027400
H	8.66417900	0.41453400	-0.68560700
H	6.86536200	-2.96281200	-2.63746700
H	4.44174500	-3.08737300	-2.87988500
H	8.88540300	-1.76207400	-1.87378100
P	1.41286400	-0.14962600	0.61428000
O	1.69791500	-0.02575900	-0.97416400
O	2.53643000	0.80667900	1.24671700
S	3.22556500	-1.90836300	2.29098200
S	0.67946300	-2.92016100	1.15548900
O	3.12669700	-3.25884200	2.82986800
O	4.44802300	-1.41075100	1.68906200
C	2.93748800	-0.79406900	3.77198700
F	3.74266600	0.25866500	3.71715500
F	1.67461100	-0.37265900	3.80189800

F	3.19305600	-1.47923200	4.87267300
C	1.52332300	-4.57750500	0.92242100
F	2.73690200	-4.42551500	0.41622900
F	1.56286500	-5.24491000	2.05000900
F	0.76976200	-5.24149900	0.05264800
O	-0.13568000	-3.11063400	2.36732100
O	-0.06463900	-2.67744400	-0.08579100
C	1.84003100	-2.41322100	-2.47898200
C	1.80298400	-3.80705100	-2.39806200
C	0.71604100	-1.72467000	-2.95731200
C	0.65149300	-4.48928500	-2.75374600
H	2.64140100	-4.37661400	-2.01514900
C	-0.41637900	-2.43349300	-3.31079000
H	0.68920500	-0.64488600	-3.03941700
C	-0.47420600	-3.81728200	-3.20152500
C	1.36099400	3.33211100	1.89099800
C	1.40964500	2.67782400	3.12394600
C	0.25742900	4.12667000	1.55372700
C	0.34543300	2.80332100	3.99743900
H	2.25760400	2.07158000	3.41398100
C	-0.79289200	4.22882600	2.45071300
H	0.18425500	4.61161800	0.59004900
C	-0.76384200	3.57396400	3.67446700
O	0.01633500	0.30634400	0.88257100
C	1.85957500	-1.69551700	1.26748100
H	-1.46031400	-2.06688700	1.91467600
C	-3.70427800	-5.52004300	-0.20628900
C	-3.59962400	-5.01229400	1.09550400
C	-3.26916300	-3.66208300	1.27655200
C	-3.03635000	-2.87748900	0.15527300
C	-3.14940900	-3.41136200	-1.16089800
C	-3.49810300	-4.74626900	-1.34992600
C	-4.15428100	-7.17655300	1.14862300
C	-3.90059200	-6.12104000	1.96567200

H	-3.22349700	-3.24957100	2.28480300
H	-2.99609600	-2.75106100	-2.02203800
H	-3.60652100	-5.17565400	-2.35147900
H	-4.42060500	-8.22059500	1.34196700
H	-3.91810400	-6.12035200	3.05518700
O	-4.03769500	-6.82382100	-0.20825400
C	-2.71397800	-1.39303100	0.33523300
O	-1.85968600	-1.22030200	1.55694400
H	-3.61730400	-0.79140800	0.55460500
C	-0.14342800	7.07048900	-0.32094000
C	0.88123800	6.45436800	-1.05864700
C	0.64813500	5.24784000	-1.75480400
C	-0.64352700	4.71099900	-1.73284800
C	-1.69172700	5.36226900	-1.03304600
C	-1.44109600	6.53423800	-0.30561000
H	0.06736200	7.99402800	0.22694900
H	1.86830500	6.92702900	-1.11076500
H	1.45462900	4.76574000	-2.31886300
H	-2.24465500	7.02921400	0.24971900
C	-1.15933900	3.39592900	-2.33297800
H	-0.92698300	3.26608800	-3.40185200
C	-2.66386700	3.49820200	-2.06563000
C	-3.69322900	2.66247500	-2.52710400
C	-5.01682000	3.00846600	-2.23251400
C	-5.30060300	4.15203700	-1.44679700
C	-4.26880300	4.95410500	-0.96664700
C	-2.94787600	4.62904600	-1.28957500
H	-3.46552600	1.78889500	-3.14659500
H	-5.83990400	2.41556300	-2.64018900
H	-6.34243600	4.43565800	-1.26397000
H	-4.48758400	5.83811500	-0.37415200
C	-0.51512400	2.27825300	-1.49480100
H	0.55028700	2.17776700	-1.72842600
H	-0.62582700	2.50472200	-0.43295000

O	-1.08228900	0.98132400	-1.73660700
C	-1.95740600	0.57758800	-0.79915400
O	-2.54931100	1.29361000	-0.02832400
N	-2.07207500	-0.79993500	-0.81040800
H	-1.27485100	-1.30685700	-1.18385400
H	-1.11659400	-0.51673600	1.38820400
F	0.59559500	-5.81752400	-2.65157400
F	-1.56888900	-4.48169700	-3.56537300
F	-1.50321500	-1.79514200	-3.75908200
F	-1.87410900	4.95530100	2.16078400
F	-1.78322300	3.68125300	4.52420000
F	0.36269000	2.18797000	5.18176700
C	-5.75130200	-1.77957400	-0.78952000
C	-5.70059500	-0.48201900	-1.09525400
H	-5.77943700	-2.11577600	0.24563200
H	-5.73473100	-2.55755200	-1.54490800
H	-5.66757100	-0.19645100	-2.14863500
C	-5.69647700	0.65348800	-0.11983400
H	-5.35844000	0.32362000	0.87225900
H	-5.01234200	1.43328600	-0.46358700
Si	-7.42380100	1.39044000	0.15403600
C	-8.47927600	0.05692900	0.96636300
H	-8.06196200	-0.23905000	1.93515400
H	-9.50435100	0.40383400	1.13451100
H	-8.52066100	-0.83611000	0.33385900
C	-7.26853400	2.87378100	1.30370500
H	-6.92887500	2.55907000	2.29623200
H	-6.53899100	3.59078900	0.91637700
H	-8.22764300	3.38835500	1.42690600
C	-8.27373000	1.88855800	-1.45752900
H	-8.17119600	1.10575900	-2.21731700
H	-9.34514900	2.02954900	-1.27632700
H	-7.88691700	2.82262900	-1.87418600

TSIII-3S'

H	-0.71621600	1.43330000	-1.76525500
C	-1.92867500	4.89189000	1.07584600
C	-2.40578300	4.96792500	-0.23426200
C	-2.68700200	3.79020300	-0.90728800
C	-2.51168100	2.57394700	-0.24281900
C	-2.01119300	2.52571200	1.06119800
C	-1.69324800	3.70359200	1.75133400
C	-2.02356200	7.01421100	0.56856500
C	-2.45585900	6.38581700	-0.54373000
H	-3.01679600	3.80087400	-1.94800800
H	-1.83137300	1.57929700	1.55602100
H	-1.28125700	3.68643000	2.75803700
H	-1.88072700	8.05946400	0.80560400
H	-2.77254900	6.84548300	-1.46921400
O	-1.70180800	6.14475700	1.56239700
C	-2.90859600	1.34738200	-1.00735500
O	-1.53654000	1.66663100	-2.28337600
H	-3.52388400	1.43800600	-1.88363300
C	-7.33715300	-1.92997900	-0.20773800
C	-6.95690700	-1.89007700	-1.54646000
C	-5.81618400	-2.56660500	-1.99009200
C	-5.08664500	-3.30469300	-1.06651500
C	-5.46024400	-3.35394700	0.27940600
C	-6.58546800	-2.65943600	0.72080000
H	-8.21866800	-1.39334900	0.12253900
H	-7.56221100	-1.33602600	-2.26517900
H	-5.51471500	-2.51654500	-3.03593000
H	-6.88399500	-2.69707400	1.76773100
C	-3.82996100	-4.12388200	-1.28757900
H	-4.00069300	-4.92184600	-2.03411900
C	-3.58609100	-4.71981300	0.07950200
C	-2.60320400	-5.61543400	0.47833500
C	-2.55158700	-6.00464400	1.81692700

C	-3.47580600	-5.51344300	2.73314300
C	-4.47324800	-4.61968200	2.33201800
C	-4.52393000	-4.23333400	0.99676100
H	-1.88957500	-6.00885200	-0.23800200
H	-1.78467500	-6.69143200	2.13794800
H	-3.41694100	-5.81986000	3.77210200
H	-5.19500600	-4.24716300	3.04809600
C	-2.66940700	-3.28869600	-1.82505300
H	-1.73341100	-3.85209400	-1.78630300
H	-2.85782100	-2.96059900	-2.85025000
O	-2.46030600	-2.13362600	-1.00369800
C	-2.74594500	-0.94232200	-1.52532400
O	-3.20978700	-0.74648200	-2.64488900
N	-2.46711600	0.08623100	-0.65476400
H	-1.88327700	-0.06869300	0.16816700
H	-1.66351400	0.93990500	-2.92292300
C	6.43458500	2.05230000	-4.60007800
C	5.80709800	1.30467900	-3.62909500
C	4.99734600	1.94453800	-2.63199800
C	4.83660200	3.37254300	-2.68254900
C	5.51648000	4.11376100	-3.70238700
C	6.29007400	3.46994700	-4.64010000
H	7.03811200	1.55240000	-5.35762400
H	5.91054300	0.21801600	-3.59271500
C	4.32236000	1.20013200	-1.58758700
C	4.03227100	4.02277300	-1.69596900
H	5.39896800	5.20000100	-3.72669600
H	6.79651500	4.03629500	-5.41864600
C	3.33407600	3.32027600	-0.72952200
C	3.46579000	1.89130600	-0.74328600
H	4.01482300	5.12757300	-1.68897600
C	4.55744100	-0.27259800	-1.36516900
C	5.87654700	-0.79390600	-1.04066500
C	3.48997700	-1.13459100	-1.33749400

C	7.03504700	0.04323100	-0.96838700
C	6.00724200	-2.18420200	-0.71694500
C	3.60407700	-2.54434000	-1.06655100
C	8.25338900	-0.49062400	-0.60863300
H	6.93062000	1.11053800	-1.17193600
C	7.29037200	-2.69883600	-0.36021000
C	4.86246600	-3.03797200	-0.75978700
C	8.38453900	-1.86896900	-0.31273700
H	9.12891700	0.15985200	-0.54080000
H	7.38105900	-3.76432400	-0.11999800
H	4.98387700	-4.11034100	-0.56605400
H	9.36851700	-2.27627300	-0.02745500
P	1.60201300	0.13418300	-0.15779900
O	2.17533300	-0.60250400	-1.47701200
O	2.77353300	1.15782200	0.25352500
S	3.04215200	-1.41466900	2.09852900
S	0.16034300	-1.26879000	2.08391600
O	2.94509100	-2.83022300	2.44201500
O	4.23799100	-0.90634500	1.43785500
C	3.07604200	-0.48980100	3.74092800
F	4.32646900	-0.08100700	3.92895900
F	2.28697000	0.58040200	3.69490400
F	2.73757600	-1.27495600	4.74523200
C	-0.44865500	-2.89001700	1.45078400
F	0.19633500	-3.91041400	1.98615700
F	-1.73420200	-2.95209800	1.76936000
F	-0.30556300	-2.94484400	0.12489400
O	0.41369500	-1.50335900	3.48779600
O	-0.93548400	-0.37332300	1.69364200
C	2.45466800	-3.45845500	-1.23114700
C	2.19636800	-4.44896000	-0.26472500
C	1.64763800	-3.39075900	-2.37741900
C	1.18311100	-5.35959400	-0.48083300
H	2.73783300	-4.45516000	0.66960200

C	0.65325200	-4.32915700	-2.56498700
H	1.81269600	-2.62324100	-3.12635700
C	0.41973900	-5.33112400	-1.64032400
C	2.55125800	4.04804500	0.30299900
C	2.43937300	3.57068800	1.61800200
C	1.97867600	5.28759100	-0.00806200
C	1.77482800	4.32606400	2.57459100
H	2.85220500	2.62949900	1.93531100
C	1.35801200	6.03511400	0.97784000
H	2.00211200	5.67965900	-1.01377100
C	1.24885100	5.57291400	2.27681400
O	0.29561700	0.71654100	-0.57182800
C	1.60595200	-0.87850500	1.26954700
F	0.87843400	-6.28745100	0.43644900
F	-0.54907900	-6.23271700	-1.85966800
F	-0.12555400	-4.28143800	-3.65535100
F	0.83429100	7.23699900	0.68499100
F	0.62670400	6.28994300	3.21822400
F	1.63814100	3.86976400	3.81906600
C	-4.71955600	0.89984200	-0.18326600
C	-5.25268900	2.13945300	-0.10345100
H	-4.95887500	0.25868200	-1.03105700
H	-4.43566100	0.38866900	0.73712600
H	-5.14889700	2.68993400	0.83167900
C	-5.82719100	2.89252400	-1.23683000
H	-5.65086000	2.37255500	-2.19407800
H	-5.39348000	3.90765300	-1.29380600
Si	-7.71716100	3.15746700	-1.07900000
C	-8.31214700	3.87909500	-2.72057200
H	-8.49454900	3.08946200	-3.45731000
H	-7.58468900	4.57397100	-3.14208700
H	-9.26355600	4.42482100	-2.58618800
C	-8.03052200	4.37216100	0.32364800
H	-7.66930500	3.97287300	1.27870400

H	-9.09293100	4.58078200	0.43063300
H	-7.52013800	5.32281100	0.15002100
C	-8.51977100	1.49500000	-0.72671300
H	-9.56164200	1.45961800	-1.07737300
H	-8.51136500	1.27975800	0.34981300
H	-7.96281400	0.69284800	-1.22433500

Pr2-S

C	-1.88019500	0.57343000	1.02812800
H	-1.98498300	0.83849900	2.08571000
N	-0.84134600	-0.45017700	0.99028900
C	0.25397800	-0.29461300	1.78569600
O	0.31658100	0.44195000	2.74885900
O	1.25637800	-1.10564300	1.36565800
C	2.46478500	-1.05074000	2.11915800
H	2.72909800	-2.08373500	2.36467100
H	2.28281300	-0.49863300	3.04309200
H	-0.66444300	-0.87712900	0.08727400
C	-1.39588000	1.83541700	0.27780000
H	-0.46859200	2.15026900	0.77126100
H	-2.11914600	2.64710200	0.41056700
C	-1.12786500	1.56650600	-1.17786800
C	0.05811900	1.15838100	-1.62509600
H	0.90485800	1.04435800	-0.95046100
H	0.23198200	0.93124400	-2.67304000
C	3.58482700	-0.39861700	1.31252900
C	4.07527900	-1.19279900	0.11699500
H	4.42320900	-0.25833700	2.01224600
C	3.22711700	0.93705900	0.68690600
C	4.49968300	-2.51139400	0.05732600
C	4.09745600	-0.38519700	-1.03008300
C	2.64160200	2.05288800	1.26964600
C	3.57950000	0.94441500	-0.67336100
C	4.94433200	-3.02231400	-1.16333500

H	4.48987100	-3.14220100	0.94283700
C	4.54554300	-0.89143100	-2.24611700
C	2.43038800	3.18713600	0.48120300
H	2.33056100	2.03943300	2.31040500
C	3.38861600	2.08240700	-1.45102600
C	4.96814900	-2.21773500	-2.30344200
H	5.27579100	-4.05417900	-1.22641900
H	4.56338300	-0.26872900	-3.13622300
C	2.81026300	3.20485200	-0.86175800
H	1.96652400	4.06532500	0.91991200
H	3.66629200	2.09225600	-2.50155300
H	5.31956300	-2.63034900	-3.24420000
H	2.63936100	4.09736900	-1.45583600
C	-3.19926100	-0.00651300	0.53388200
C	-3.51297000	-1.34905100	0.84013500
C	-4.11778900	0.77409600	-0.15893500
C	-4.71455300	-1.93144100	0.46695700
H	-2.78160500	-1.93667200	1.38532100
C	-5.33865800	0.21066000	-0.54854300
H	-3.90312900	1.81000600	-0.40086700
C	-5.60549700	-1.12497200	-0.22804600
H	-4.95242900	-2.96288000	0.70200200
C	-6.50528800	0.66942200	-1.26601700
H	-6.68258200	1.64960000	-1.68332200
O	-6.83013500	-1.49032900	-0.69534700
C	-7.34403600	-0.38845200	-1.31458000
H	-8.32575000	-0.52123100	-1.74380100
H	-1.95966900	1.66361600	-1.87389300

TSIII-1R

C	5.82510200	0.71319200	-2.74773500
C	5.53291200	-0.64380300	-2.53329100
C	4.23020300	-1.00078000	-2.17747800
C	3.27721100	0.00704200	-2.06247900
C	3.60375300	1.35779000	-2.28389800

C	4.89137300	1.73739900	-2.62650000
C	7.67770900	-0.39213200	-3.08555700
C	6.77612500	-1.34450100	-2.76363000
H	3.96247500	-2.03847200	-1.99270400
H	2.81533600	2.09553500	-2.21112000
H	5.15645800	2.77389700	-2.79843200
H	8.72814600	-0.43418900	-3.32982700
H	6.95940900	-2.40671600	-2.69764100
O	7.13227300	0.86147000	-3.08799000
C	1.88259500	-0.35624100	-1.70670500
O	0.96423200	0.50372800	-1.78758400
H	1.64320900	-1.41851200	-1.83328800
C	10.50645700	0.65371600	1.27844100
C	9.69712300	1.15066300	0.25585200
C	8.41002300	0.64646200	0.05995800
C	7.95469200	-0.36084900	0.89798300
C	8.76244700	-0.85344300	1.93390700
C	10.04584500	-0.35081700	2.12796100
H	11.50394600	1.05915800	1.41719000
H	10.06917700	1.93945300	-0.39049900
H	7.77992000	1.04437200	-0.73159700
H	10.67742200	-0.72762900	2.92749200
C	6.61308500	-1.06438300	0.89266200
H	6.47271100	-1.61641000	-0.04726500
C	6.74052400	-2.01517000	2.06659800
C	5.81676000	-2.92101700	2.56941800
C	6.16912900	-3.69630900	3.67598400
C	7.42726000	-3.56603400	4.26582600
C	8.35710900	-2.65771900	3.76367300
C	8.00607800	-1.88301800	2.66252800
H	4.83738800	-3.02194200	2.11236300
H	5.45697500	-4.40802400	4.08168800
H	7.68361200	-4.17779100	5.12518100
H	9.33507600	-2.55689500	4.22584600

C	5.47708300	-0.06148700	1.01399100
H	5.53336500	0.69701900	0.22473500
H	5.48930200	0.44288700	1.98466200
O	4.23989100	-0.77577100	0.85930800
C	3.16506400	0.01830800	0.76268100
O	3.16215200	1.20632700	0.95169600
N	2.06406400	-0.70016500	0.28723000
H	2.11134400	-1.70344400	0.45520100
H	1.16107100	-0.31596800	0.61260900
H	-0.26871000	-0.02944300	-1.66747900
C	-5.76546400	3.66072800	4.25232000
C	-5.43675800	2.90179900	3.15354700
C	-4.17300500	3.06887600	2.50189000
C	-3.24773700	4.02058000	3.03403200
C	-3.62705900	4.80443700	4.17237700
C	-4.85475700	4.63079800	4.76434500
H	-6.73214800	3.52034800	4.74524200
H	-6.13430400	2.15429100	2.76951700
C	-3.77963600	2.28078700	1.34920200
C	-1.95396400	4.17274900	2.43556600
H	-2.91233900	5.53535900	4.56214800
H	-5.13807200	5.22691800	5.63685000
C	-1.55803300	3.40208400	1.36025900
C	-2.50688800	2.45568400	0.84386800
H	-1.26845300	4.92798000	2.83515700
C	-4.70282100	1.25075200	0.75335100
C	-6.02566900	1.61671100	0.28852500
C	-4.34086700	-0.08603000	0.71244200
C	-6.42301300	2.98321600	0.13990100
C	-6.94986600	0.58824600	-0.06479300
C	-5.30099400	-1.14432900	0.51272000
C	-7.67414000	3.29920100	-0.33700000
H	-5.70785900	3.76907200	0.39580800
C	-8.25158100	0.94983200	-0.54011600

C	-6.57868100	-0.78165200	0.13049400
C	-8.60195200	2.27204500	-0.67742800
H	-7.96471000	4.34657600	-0.46155600
H	-8.95338700	0.15108200	-0.79760900
H	-7.34649100	-1.55545800	0.02068400
H	-9.59315300	2.54599900	-1.05026400
P	-1.71972700	0.15171700	0.22596700
O	-2.98674900	-0.46492800	1.00256000
O	-2.13318700	1.61738600	-0.26196100
S	-2.56086100	-0.20203800	-2.75740100
S	-0.90500300	-2.30004500	-1.43141900
O	-2.66747000	-1.35252200	-3.63799900
O	-3.74258200	0.47706800	-2.25747800
C	-1.57982100	1.03747800	-3.71590100
F	-2.35597400	1.52251500	-4.67183100
F	-1.18137900	2.01916300	-2.92114400
F	-0.52952700	0.43862200	-4.24566200
C	-2.49533000	-3.29139500	-1.42132800
F	-3.52178800	-2.45024700	-1.36638300
F	-2.56681300	-4.02574700	-2.50721800
F	-2.50181100	-4.06272400	-0.34932200
O	-0.23117500	-2.59701000	-2.68062500
O	-0.24228300	-2.56338200	-0.16143900
C	-5.02603000	-2.55322500	0.87088700
C	-5.62522300	-3.59229300	0.14586400
C	-4.23869600	-2.88276800	1.97973400
C	-5.43672600	-4.90836700	0.52221900
H	-6.20778400	-3.38497800	-0.74434400
C	-4.06277900	-4.20868300	2.33835100
H	-3.74823100	-2.12249800	2.57524200
C	-4.65599400	-5.23818200	1.62282900
C	-0.21419900	3.56259200	0.77341000
C	-0.03392000	3.64493200	-0.60869600
C	0.89849600	3.66458300	1.61432200

C	1.23770800	3.81875700	-1.12157700
H	-0.86926100	3.57882100	-1.29251300
C	2.15957300	3.84169300	1.07745500
H	0.79584400	3.56173300	2.68822700
C	2.34517400	3.92054000	-0.29481300
O	-0.52840000	0.05334900	1.08964500
C	-1.41888800	-0.58482800	-1.41933800
F	-5.99299500	-5.90095000	-0.17720300
F	-4.47860100	-6.51025000	1.97657700
F	-3.32019900	-4.52810400	3.40055000
F	3.23051800	3.91629800	1.86474300
F	3.56847400	4.06178800	-0.81225900
F	1.43494300	3.88803400	-2.44511300

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C	6.14603600	3.10724500	-1.29205900
C	5.99411700	1.83488800	-1.86269800
C	4.70655800	1.30053200	-1.97965800
C	3.63191300	2.05637700	-1.52949500
C	3.81577800	3.33970600	-0.97628600
C	5.08359100	3.88674700	-0.84658800
C	8.14809500	2.39676400	-1.78666000
C	7.33264800	1.39343000	-2.17825000
H	4.54937100	0.31144100	-2.40261400
H	2.94382500	3.89709600	-0.65040400
H	5.24474800	4.87069500	-0.42189700
H	9.22035300	2.51699600	-1.81285900
H	7.63361400	0.45983800	-2.62998000
O	7.46042400	3.44726600	-1.24779600
C	2.25136500	1.46547100	-1.57999700
O	1.29569500	2.40055400	-1.79804700
H	2.19267200	0.61634600	-2.26602800
C	9.97333300	0.26841100	2.82620600
C	9.40802300	1.35119500	2.15073800

C	8.18075300	1.21688000	1.49852300
C	7.53996800	-0.01268600	1.53571400
C	8.10125300	-1.10079700	2.22167600
C	9.32594700	-0.96532500	2.86907400
H	10.92946200	0.39004000	3.32581700
H	9.92627500	2.30482700	2.13352300
H	7.74065100	2.06285100	0.97395400
H	9.77168100	-1.80194700	3.39949100
C	6.21356200	-0.40834200	0.92058900
H	6.24114200	-0.29892200	-0.17136000
C	6.08225900	-1.86195500	1.32628500
C	5.06575800	-2.76123300	1.04148100
C	5.15876800	-4.05922000	1.54612200
C	6.25931100	-4.44690800	2.31193500
C	7.28751100	-3.54760000	2.59071300
C	7.19217100	-2.25142200	2.09445900
H	4.20805900	-2.47245700	0.44492300
H	4.36407100	-4.76605900	1.33157600
H	6.31699100	-5.46162700	2.69357300
H	8.14405800	-3.85518200	3.18391500
C	5.10489500	0.48471000	1.45207900
H	5.31168300	1.54230000	1.25355500
H	4.94865300	0.34157900	2.52477500
O	3.88939200	0.14076600	0.74858300
C	2.90762700	1.01330800	0.87696300
O	2.81389900	1.91881400	1.64833700
N	1.92230000	0.76148100	-0.16210200
H	1.79593300	-0.24385700	-0.34998100
H	0.96386300	1.10008800	0.11893800
H	0.51999700	1.96203100	-2.20729000
C	-6.17419400	-0.49880800	5.29704100
C	-5.59692700	-0.74783800	4.07454500
C	-5.08273000	0.32464200	3.27616300
C	-5.15092900	1.65597400	3.79332700

C	-5.76864100	1.88226700	5.06724900
C	-6.27044000	0.83303700	5.79793600
H	-6.56206900	-1.32615100	5.89866700
H	-5.51838300	-1.76939200	3.69614600
C	-4.46319600	0.10270000	1.98614400
C	-4.58363300	2.73897500	3.04802900
H	-5.82246800	2.90792200	5.44397800
H	-6.73745300	1.00845900	6.77147200
C	-3.96225700	2.53329500	1.83099300
C	-3.92810700	1.19181600	1.31908700
H	-4.65479300	3.75570800	3.44905000
C	-4.29035300	-1.27939600	1.41182000
C	-5.38818400	-2.18358600	1.14132600
C	-3.00821400	-1.71092200	1.12220600
C	-6.75453700	-1.79398300	1.31067800
C	-5.09874200	-3.49335700	0.64246900
C	-2.68798700	-3.02676400	0.64575500
C	-7.77305500	-2.67042800	1.01622000
H	-6.97035000	-0.78372100	1.66740700
C	-6.18420600	-4.38545100	0.36017600
C	-3.73894600	-3.89678800	0.42752900
C	-7.48599800	-3.98387000	0.54227500
H	-8.81523200	-2.36148100	1.13999500
H	-5.95140700	-5.38674500	-0.01390500
H	-3.53666100	-4.91991300	0.09055200
H	-8.31128400	-4.66554000	0.31684800
P	-1.87980300	0.25362600	0.00581900
O	-1.93698500	-0.77034200	1.25224200
O	-3.31466900	0.97747300	0.04313900
S	-3.47386800	-0.62132300	-2.43536700
S	-0.52291700	-0.70789100	-2.37773200
O	-3.15026300	-1.14810500	-3.75638900
O	-4.56664400	-1.16528600	-1.64837700
C	-3.97605900	1.14621400	-2.80101000

F	-4.99395000	1.51556300	-2.03076400
F	-2.95095200	1.96983300	-2.60414800
F	-4.35425200	1.22384100	-4.06662200
C	-0.54982000	-2.11446800	-3.62906700
F	-1.40214000	-3.07047700	-3.31611600
F	-0.78276600	-1.65240900	-4.83506800
F	0.68342500	-2.61294200	-3.58757200
O	-0.14776100	0.45500300	-3.20028500
O	0.48429000	-1.15022600	-1.39432600
C	-1.28685600	-3.40463800	0.37222600
C	-0.98692700	-4.16754300	-0.76005600
C	-0.23376000	-2.99798100	1.20204700
C	0.32578200	-4.47120700	-1.07753600
H	-1.77051500	-4.47941700	-1.43859200
C	1.06703400	-3.32180000	0.87178600
H	-0.40887700	-2.41035000	2.09409400
C	1.37023000	-4.05193500	-0.26747600
C	-3.33136700	3.66456200	1.11930800
C	-3.52491400	3.87939700	-0.24773600
C	-2.53592200	4.56200100	1.83949500
C	-2.92341200	4.95829100	-0.86997700
H	-4.14237500	3.21738300	-0.83834800
C	-1.95244800	5.64040500	1.19898900
H	-2.34025600	4.41023300	2.89457200
C	-2.13498200	5.85394500	-0.15988600
O	-0.70165800	1.14566300	0.17589600
C	-2.00795100	-0.55817000	-1.54705400
F	0.61418200	-5.15363300	-2.18810900
F	2.64310900	-4.32180700	-0.57793900
F	2.08629500	-2.91117900	1.64179100
F	-1.18566500	6.50100700	1.87558900
F	-1.56512400	6.89483600	-0.76687900
F	-3.10024900	5.17230000	-2.17590400

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H	-0.83873200	0.04210800	-2.53360600
C	-5.14579100	-3.37629800	-1.27295400
C	-4.66352500	-3.20470500	-2.58021000
C	-4.01498000	-2.01439500	-2.90348200
C	-3.87710800	-1.04044800	-1.91413900
C	-4.38624500	-1.23921900	-0.61571000
C	-5.03171300	-2.41575400	-0.27540200
C	-5.63030300	-5.19539500	-2.36583500
C	-5.00332200	-4.42124500	-3.27687900
H	-3.60752300	-1.84884000	-3.89744300
H	-4.26313900	-0.46555000	0.13445900
H	-5.41050600	-2.59362300	0.72430500
H	-6.06080700	-6.18360800	-2.42040400
H	-4.79962300	-4.67159600	-4.30683400
O	-5.73044400	-4.58903700	-1.14547400
C	-3.20367000	0.21905200	-2.28449600
O	-1.57041600	-0.47499500	-2.99162100
H	-3.44856500	0.65705000	-3.24760100
C	-6.09979300	1.46277900	0.58094600
C	-6.20884500	2.35332300	-0.48724700
C	-5.35148800	3.45364300	-0.58348300
C	-4.39452700	3.64383000	0.40265000
C	-4.27727500	2.74051700	1.47156200
C	-5.12518700	1.64182900	1.56394600
H	-6.77289500	0.61213900	0.63967800
H	-6.96347100	2.18989600	-1.24996800
H	-5.42697900	4.13581900	-1.42636000
H	-5.02299300	0.93346300	2.38160200
C	-3.30521100	4.69846700	0.49375100
H	-3.70884500	5.71651300	0.42997300
C	-2.67106200	4.38539000	1.83606300
C	-1.63134600	5.04098600	2.47911100
C	-1.12896800	4.49773300	3.66140500

C	-1.64621600	3.30562300	4.17385200
C	-2.67817200	2.63711400	3.52177900
C	-3.19630500	3.19530700	2.35740100
H	-1.22237900	5.96524200	2.08028100
H	-0.31095100	4.99294000	4.17623400
H	-1.22634800	2.88409200	5.08088400
H	-3.05229300	1.69285100	3.90571500
C	-2.27071200	4.51101100	-0.63430000
H	-1.31416900	4.95667300	-0.36331600
H	-2.61238900	4.91156500	-1.59100000
O	-2.02842100	3.10067300	-0.75061000
C	-2.64133600	2.46637500	-1.74111600
O	-2.99250500	2.91990400	-2.79918700
N	-2.83779900	1.12300600	-1.37079500
H	-2.68089100	0.88362800	-0.38489400
C	7.61358100	-1.40520700	-2.40181300
C	6.48142000	-1.44640200	-1.62314100
C	5.61219300	-0.31155100	-1.53423000
C	5.93088200	0.85549000	-2.29708600
C	7.12315300	0.86782900	-3.09383200
C	7.94479600	-0.23165700	-3.14153800
H	8.26836200	-2.27958400	-2.46276500
H	6.22658300	-2.34963600	-1.06459900
C	4.41276500	-0.31725500	-0.72200200
C	5.04857900	1.98322000	-2.27554200
H	7.35699000	1.77055900	-3.66585900
H	8.85294200	-0.21880800	-3.75126500
C	3.88672700	1.97709000	-1.52718500
C	3.60535800	0.80706200	-0.74040300
H	5.30515800	2.86948300	-2.86612000
C	3.96102400	-1.55656200	0.01060600
C	4.74345200	-2.23530500	1.02128400
C	2.72953100	-2.09234700	-0.32460300
C	5.97415500	-1.70301900	1.52131300

C	4.24938700	-3.46383100	1.56451100
C	2.21742700	-3.33377500	0.18730600
C	6.67396100	-2.36496600	2.50343100
H	6.33837000	-0.75547200	1.11600700
C	5.01227400	-4.13398300	2.57563400
C	3.00444700	-4.00577400	1.10381800
C	6.19039400	-3.59673000	3.03512600
H	7.60959000	-1.94698500	2.88702700
H	4.62751300	-5.07493100	2.97993600
H	2.67935200	-4.97742100	1.49296600
H	6.76044600	-4.10357800	3.81917000
P	1.17916200	-0.08370300	-0.49358800
O	1.89224800	-1.34606400	-1.20521700
O	2.41035500	0.79999400	0.04501400
S	1.18417800	-0.14975100	2.55666300
S	-1.22374700	-0.79464200	0.98844500
O	0.19124000	-0.44886600	3.58411600
O	2.54081600	-0.66482400	2.63746000
C	1.37542300	1.70670300	2.67896200
F	2.63394600	2.06811600	2.44005500
F	0.57232000	2.31933500	1.81965400
F	1.07286600	2.07533300	3.91493800
C	-1.69666700	-2.08313700	2.27430900
F	-2.55628200	-2.89997800	1.66655400
F	-0.66793000	-2.78791900	2.70726400
F	-2.31220900	-1.50463300	3.28604200
O	-2.10016000	0.33228000	1.34831100
O	-1.48250300	-1.43576300	-0.30795000
C	0.89726300	-3.85129500	-0.23253400
C	0.12337000	-4.57135000	0.68539300
C	0.36293100	-3.63472000	-1.51158900
C	-1.14001100	-5.01933700	0.34874600
H	0.47083900	-4.73727000	1.69690800
C	-0.91022800	-4.07586900	-1.81767700

H	0.90620200	-3.09135400	-2.27270500
C	-1.68517300	-4.76783600	-0.90106000
C	2.94511800	3.11389900	-1.58790900
C	2.32559400	3.62057500	-0.44161000
C	2.67099300	3.71138000	-2.82357400
C	1.45718700	4.68854200	-0.54758100
H	2.50392900	3.19018700	0.53275900
C	1.79597200	4.78039400	-2.90463500
H	3.10201000	3.32174000	-3.73843600
C	1.17682400	5.28271100	-1.76947100
O	0.32333000	0.56519300	-1.52193200
C	0.45264100	-0.49855300	1.04594100
H	-1.51659700	-1.36136600	-2.58518300
F	-1.89281800	-5.65609000	1.24917300
F	-2.91817400	-5.17854000	-1.20376700
F	-1.44080800	-3.80672000	-3.02375600
F	1.51851300	5.34699800	-4.08173100
F	0.31124400	6.29782900	-1.84473500
F	0.84954600	5.18524700	0.53890300

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H	0.27271700	1.56455800	-3.07099000
C	3.28007900	5.29407500	-0.11991400
C	3.60892400	4.87064100	-1.42145000
C	3.47504100	3.52429700	-1.73477700
C	2.99430700	2.65374800	-0.74791500
C	2.64232700	3.12055600	0.54279100
C	2.80470300	4.44786000	0.88146300
C	3.93716500	7.05804700	-1.21110100
C	4.03724500	6.06171500	-2.11468200
H	3.71296800	3.14384100	-2.72346900
H	2.27872100	2.42243800	1.28965000
H	2.55792900	4.83197200	1.86340700
H	4.13588700	8.11721100	-1.26465600

H	4.35922200	6.14930600	-3.14095900
O	3.48908900	6.61685200	0.00440700
C	2.95779000	1.25934200	-1.07270700
O	0.69827900	2.00836600	-2.31950900
H	3.46444000	0.89317200	-1.96388600
C	7.03975200	-3.61700500	0.27466100
C	6.27022500	-3.90360700	-0.85559900
C	4.88352700	-4.03007300	-0.75848100
C	4.28127000	-3.86232300	0.48070200
C	5.05281100	-3.55042100	1.61013300
C	6.43633000	-3.43098100	1.51739900
H	8.11957000	-3.53631200	0.18155600
H	6.75523700	-4.03397400	-1.81801900
H	4.29062500	-4.24701100	-1.64225800
H	7.03411300	-3.20020200	2.39480700
C	2.81884800	-3.99665900	0.86550400
H	2.49313900	-5.03895600	0.73332100
C	2.83942300	-3.64567000	2.34269800
C	1.78585200	-3.55164700	3.24020000
C	2.05846000	-3.19666200	4.56243400
C	3.36617700	-2.94464900	4.97940700
C	4.42744200	-3.04474900	4.08238000
C	4.15423000	-3.39588200	2.76338300
H	0.76868300	-3.76042600	2.92523400
H	1.24361400	-3.11617300	5.27516300
H	3.55826700	-2.67078900	6.01225600
H	5.44608600	-2.84898200	4.40693800
C	1.85385300	-3.15652300	0.04034300
H	0.82285100	-3.35270000	0.33495000
H	1.96211500	-3.33970200	-1.03149800
O	2.03668200	-1.75472000	0.29196100
C	2.66835000	-1.05472500	-0.62385700
O	3.35185400	-1.41673100	-1.53652500
N	2.45576800	0.32983100	-0.31718900

H	1.73150600	0.52051500	0.38543700
C	4.84412400	1.23194600	2.09177900
C	5.18234600	0.05436000	1.55877600
H	5.00446400	2.16524200	1.55510200
H	4.40692300	1.30289200	3.08320700
H	5.01628100	-0.85020800	2.14425400
C	5.83486400	-0.13217900	0.22358900
H	5.45807300	0.60832800	-0.49861400
H	5.62980700	-1.12724000	-0.18761800
Si	7.71364100	0.17484400	0.29819300
C	7.96506800	2.03762400	0.45370700
H	7.47841900	2.57814100	-0.36586800
H	9.03021000	2.29239800	0.43790500
H	7.54705900	2.40736600	1.39594200
C	8.48258800	-0.44396700	-1.30712200
H	8.26987100	-1.50814900	-1.45363200
H	9.56937700	-0.30903200	-1.31052100
H	8.07588100	0.09615000	-2.16889900
C	8.52478400	-0.64653600	1.78919900
H	7.90502100	-0.52512800	2.68456300
H	9.49495500	-0.17855400	1.98932900
H	8.69609700	-1.71445300	1.63151000
C	-5.36053500	1.41034500	5.44514300
C	-5.01599200	0.89426100	4.21856100
C	-4.23116800	1.66268000	3.30003300
C	-3.79414500	2.96529500	3.68796200
C	-4.18374500	3.48028200	4.96819300
C	-4.94651600	2.72245100	5.82303500
H	-5.95636800	0.81513500	6.14344700
H	-5.33044900	-0.11077200	3.92683700
C	-3.85785800	1.16237500	1.99669300
C	-2.97555100	3.72881900	2.79629800
H	-3.85202300	4.48401100	5.24962500
H	-5.23712900	3.11532900	6.80168500

C	-2.54044600	3.22835500	1.58049300
C	-3.01411700	1.92124900	1.20483400
H	-2.70410400	4.74876200	3.08853800
C	-4.38047800	-0.14555300	1.46968000
C	-5.80187700	-0.37510600	1.31643500
C	-3.49304300	-1.12453500	1.05495200
C	-6.78093200	0.62739800	1.61285300
C	-6.24552500	-1.63150000	0.80142600
C	-3.92020000	-2.40146800	0.55026200
C	-8.12021500	0.37394600	1.43192200
H	-6.44558300	1.60303700	1.97084200
C	-7.64969200	-1.87067900	0.64052700
C	-5.28286000	-2.62969300	0.45253100
C	-8.56345400	-0.89291600	0.94953600
H	-8.85876900	1.15049600	1.65225500
H	-7.97172000	-2.84266300	0.25535600
H	-5.63847600	-3.60989900	0.11683500
H	-9.63421300	-1.07303000	0.81730400
P	-1.60133600	0.17355600	-0.08853600
O	-2.09431600	-0.81858100	1.09673100
O	-2.66561900	1.38797900	-0.07252200
S	-3.49979100	-0.24165400	-2.43740900
S	-0.68733000	-0.98567900	-2.70493000
O	-3.59068300	-1.07282700	-3.62545500
O	-4.59238100	-0.21524700	-1.47989700
C	-3.41626100	1.51411100	-3.09104200
F	-4.18181100	2.30998100	-2.35022800
F	-2.16979500	1.98278800	-3.05546200
F	-3.85261700	1.53698800	-4.33868500
C	-0.82320200	-2.80667100	-3.00809000
F	-0.51459100	-3.42583200	-1.86508500
F	-2.00912100	-3.21569900	-3.40920500
F	0.08710400	-3.12653700	-3.91938900
O	-0.76028800	-0.35556800	-4.01712900

O	0.57555200	-0.93854400	-1.97124900
C	-3.00210900	-3.49602600	0.17954200
C	-3.31671700	-4.28671400	-0.93337800
C	-1.88818200	-3.84217400	0.95435300
C	-2.56977100	-5.41115100	-1.23060600
H	-4.12902800	-4.00901700	-1.59504800
C	-1.15846300	-4.97346200	0.63358600
H	-1.59898500	-3.25210500	1.81694400
C	-1.48664800	-5.78003300	-0.44546200
C	-1.63278300	4.03658400	0.73775700
C	-1.63981700	3.98824500	-0.66148600
C	-0.74239600	4.92119100	1.36424600
C	-0.77061700	4.77768800	-1.39648500
H	-2.32150800	3.34967200	-1.20275700
C	0.07595900	5.73805300	0.61040600
H	-0.66717500	4.97357100	2.44360500
C	0.09371100	5.66709300	-0.77417600
O	-0.20957200	0.61000200	0.20559400
C	-1.96167900	-0.49737400	-1.67277400
H	0.30965300	1.58252500	-1.53371500
F	-2.85766000	-6.15743300	-2.29795600
F	-0.75810500	-6.85743500	-0.73780200
F	-0.08407000	-5.31908500	1.36713400
F	0.91807800	6.59047200	1.21354700
F	0.93828200	6.42490800	-1.48126900
F	-0.77056900	4.72543700	-2.72557500

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H	1.87855200	1.96202800	1.72209500
C	0.37738600	-3.94237900	4.39655300
C	0.11070000	-2.57629600	4.62240700
C	0.83796100	-1.62051000	3.90743100
C	1.78345500	-2.06117600	2.97147100
C	2.03068800	-3.44264800	2.78106400

C	1.33124000	-4.40606000	3.49515200
C	-1.22886700	-3.84508700	5.88014400
C	-0.94932600	-2.54981500	5.60142900
H	0.65007200	-0.55791400	4.02765600
H	2.77678900	-3.75876200	2.05749500
H	1.50353100	-5.46704200	3.35127100
H	-1.94830500	-4.31670000	6.53217500
H	-1.44061100	-1.68257000	6.01861700
O	-0.43447400	-4.71587400	5.16870900
C	2.45273600	-1.03255800	2.15229600
O	1.29087700	1.85571200	2.48911700
H	2.15839800	-0.00859200	2.36911300
C	8.01361200	-1.15458100	-1.30170600
C	7.47146600	0.13437700	-1.24156600
C	6.24289800	0.41901300	-1.85329700
C	5.57130600	-0.60247100	-2.51640800
C	6.11261100	-1.90300300	-2.57370900
C	7.33986600	-2.18154700	-1.96751100
H	8.97165100	-1.35828600	-0.82997500
H	8.01350800	0.92443700	-0.72797800
H	5.82704800	1.42231500	-1.80629900
H	7.76781900	-3.17994600	-2.00985700
C	4.24642100	-0.55510800	-3.26438400
H	4.34348500	0.09705100	-4.14729600
C	4.06566500	-2.00156200	-3.70231000
C	3.00181300	-2.58889400	-4.37670600
C	3.06767100	-3.95412900	-4.67677800
C	4.18423100	-4.71322300	-4.31023500
C	5.24907100	-4.12792300	-3.62189700
C	5.18156800	-2.76847000	-3.31152300
H	2.11793600	-2.01738300	-4.64606700
H	2.23674800	-4.42855200	-5.19052500
H	4.21831100	-5.77167400	-4.55443200
H	6.10868800	-4.72563800	-3.32875000

C	3.08190600	0.02658200	-2.46364900
H	2.17004800	0.06538000	-3.06119000
H	3.31867600	1.02512500	-2.10171800
O	2.77926900	-0.82865600	-1.33873500
C	2.91146700	-0.35054200	-0.10374400
O	3.30056100	0.76675700	0.21858500
N	2.58968100	-1.32997800	0.81106500
H	2.05905900	-2.11754200	0.43431100
C	4.24847600	-0.87545800	2.96748100
C	4.81993400	0.25351900	2.37697800
H	3.90621400	-0.77904800	3.99526700
H	4.64804300	-1.85050500	2.70195600
H	5.40433200	0.11737400	1.46893400
C	4.69062800	1.61270800	2.87345100
H	3.84780500	1.72641600	3.56533200
H	4.58216500	2.32472200	2.04733100
Si	6.28165100	2.24167000	3.81368300
C	5.91299300	4.04634000	4.22332500
H	5.66988000	4.61524700	3.31850600
H	6.77776500	4.52447800	4.69907800
H	5.06407000	4.13522300	4.91109100
C	7.76899000	2.09394800	2.65990800
H	7.61076900	2.65597600	1.73182800
H	7.97900800	1.05245000	2.38953300
H	8.66967500	2.49700100	3.13866000
C	6.52872500	1.21670400	5.37973200
H	7.39507900	1.58164000	5.94477200
H	6.70548700	0.15879900	5.15372200
H	5.65655300	1.27811700	6.04120000
C	-5.08753600	5.57293200	2.33667800
C	-4.80243000	4.45492700	1.58410700
C	-3.52305500	4.27685800	0.98770600
C	-2.53019900	5.27977600	1.22510700
C	-2.86062000	6.43123500	1.98980300

C	-4.11440500	6.58045400	2.53400700
H	-6.07070900	5.67940000	2.78688000
H	-5.55923100	3.69148900	1.45229300
C	-3.17793400	3.12096500	0.20016400
C	-1.22922300	5.09984700	0.70076500
H	-2.09483800	7.18724000	2.14642400
H	-4.35625200	7.46068800	3.12312400
C	-0.86371600	3.96155500	0.01024800
C	-1.86031300	2.95813500	-0.19709100
H	-0.49603300	5.88832800	0.84773100
C	-4.21266400	2.09746300	-0.12376300
C	-5.40363900	2.44044200	-0.84936200
C	-4.03924500	0.78623100	0.28371100
C	-5.59745800	3.70506200	-1.46851000
C	-6.42942700	1.45324300	-0.99655000
C	-5.08044400	-0.18736000	0.22375800
C	-6.74956000	3.98227000	-2.17082900
H	-4.81507600	4.45239400	-1.40275100
C	-7.61461500	1.77702900	-1.71013600
C	-6.25255100	0.17778500	-0.40953200
C	-7.77563200	3.01530700	-2.28638000
H	-6.86810400	4.95161500	-2.64737900
H	-8.38719000	1.01775900	-1.80442400
H	-7.07574200	-0.53023000	-0.45084700
H	-8.68084400	3.24917600	-2.83978000
P	-1.43150200	0.35929600	-0.07190800
O	-2.81674300	0.40561500	0.82510300
O	-1.47809400	1.79628600	-0.86212200
S	-2.32279000	-0.50422700	-2.89720400
S	-0.67251900	-2.36130700	-1.27592800
O	-2.80031000	-1.73625400	-3.52592700
O	-3.22615700	0.63749800	-2.72414300
C	-1.01208900	0.14911600	-4.09820200
F	-1.62526100	0.86256800	-5.04540800

F	-0.13633300	0.95229900	-3.45875200
F	-0.32750100	-0.83886900	-4.67451500
C	-1.94947800	-3.63766500	-0.74174300
F	-2.29948600	-3.38269000	0.52712700
F	-3.03949200	-3.63559200	-1.50266900
F	-1.37579200	-4.84448800	-0.79704400
O	-0.20048700	-2.79417700	-2.59286100
O	0.24156500	-2.40466700	-0.11998200
C	-4.97513300	-1.51769400	0.87823200
C	-5.49828200	-2.65524200	0.24353700
C	-4.44259900	-1.64423500	2.17257000
C	-5.48955000	-3.87911700	0.89697100
H	-5.88098100	-2.60927900	-0.76959900
C	-4.44589700	-2.87871600	2.80170600
H	-4.02594500	-0.79404300	2.69766400
C	-4.97177300	-4.00947600	2.18217800
C	0.52825800	3.83938600	-0.49637100
C	0.79546300	3.46472400	-1.82181900
C	1.59984800	4.15998300	0.35569100
C	2.10767800	3.41011400	-2.26504300
H	0.00233300	3.19670300	-2.50690800
C	2.90145800	4.08801500	-0.11596200
H	1.42929500	4.39920200	1.39856900
C	3.17519100	3.71752200	-1.42646900
O	-0.31139700	0.23354600	0.90293400
C	-1.48049100	-0.81920000	-1.38972000
H	0.51999900	1.40651400	2.07592900
F	-5.97853600	-4.97498000	0.29273600
F	-4.96624400	-5.19695800	2.80406200
F	-3.94544400	-3.00863100	4.04574400
F	3.94272000	4.33275500	0.71174000
F	4.44185700	3.59903900	-1.86155700
F	2.38833600	3.01779000	-3.52209100

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H	-0.71046900	-0.54911900	-0.10546500
C	-2.97153700	1.52938800	-2.09892100
C	-2.94067200	0.36292300	-2.88238200
C	-3.98420500	-0.56349700	-2.74944300
C	-4.99701000	-0.30627800	-1.83365500
C	-4.98658600	0.87299600	-1.05642600
C	-3.97428800	1.81328500	-1.18079000
C	-1.16537700	1.64361600	-3.30058400
C	-1.73030000	0.46528800	-3.65718500
H	-3.98810300	-1.48231900	-3.33053100
H	-5.78590200	1.04099900	-0.33621800
H	-3.94957700	2.72294500	-0.59137500
H	-0.24974900	2.13601600	-3.58659600
H	-1.33277100	-0.24664900	-4.36448500
O	-1.90333900	2.30675900	-2.36785900
C	-6.04852100	-1.34964200	-1.52630800
O	-0.70345800	-1.34049000	0.46077900
H	-6.01947100	-2.14509800	-2.28284700
C	-6.88656300	-0.41811300	3.08932600
C	-7.91963200	-1.35813900	3.05048000
C	-9.05492400	-1.13484100	2.27089500
C	-9.14629100	0.04310300	1.54431800
C	-8.09971800	0.97811100	1.56568700
C	-6.96209500	0.75556500	2.33956600
H	-6.01726600	-0.60141700	3.71611700
H	-7.84401400	-2.26629700	3.64132100
H	-9.85163700	-1.87291500	2.23788400
H	-6.15949400	1.48862500	2.37892900
C	-10.28580400	0.53861700	0.67117100
H	-11.19862500	0.65782600	1.27163200
C	-9.75973200	1.88221900	0.19718100
C	-10.35255000	2.80759300	-0.64868900
C	-9.64788400	3.96668200	-0.98019900

C	-8.36708100	4.19292500	-0.47364100
C	-7.76823000	3.26651000	0.37729700
C	-8.47255000	2.11209200	0.70753400
H	-11.34670800	2.63830300	-1.05416500
H	-10.09900600	4.69868700	-1.64249500
H	-7.83360900	5.09831100	-0.74443200
H	-6.77321100	3.44662100	0.77634700
C	-10.61130400	-0.39978600	-0.49755700
H	-11.47648400	-0.03492700	-1.05583900
H	-10.80562900	-1.42045500	-0.15460300
O	-9.52580600	-0.39476600	-1.41498800
C	-8.52018500	-1.27378300	-1.16107600
O	-8.67436900	-2.37915200	-0.68610600
N	-7.34848700	-0.70450100	-1.53275800
H	-7.40444800	0.24025000	-1.88919000
C	-5.77060100	-1.98332200	-0.12338400
C	-4.46673500	-2.72458600	-0.15230100
H	-5.74637000	-1.15645600	0.59790500
H	-6.59678400	-2.64502800	0.14127200
H	-4.50132800	-3.81128500	-0.25408700
C	-3.24196500	-2.13055300	-0.20491200
H	-3.14056100	-1.04823100	-0.19541400
H	-2.34164500	-2.69127600	-0.43119500
Si	-3.33864000	-2.48830300	1.97758800
C	-3.21502100	-0.68645400	2.43050300
H	-2.26916100	-0.29289500	2.04534600
H	-3.24137900	-0.57539200	3.52075300
H	-4.04706100	-0.11083500	2.00823800
C	-1.87226300	-3.59215400	2.24180900
H	-2.04062200	-4.58902900	1.82430600
H	-1.73213100	-3.70415100	3.32430700
H	-0.97113700	-3.15715100	1.80757000
C	-4.86510600	-3.33407100	2.66952600
H	-5.80158500	-2.82653900	2.43118700

H	-4.75350500	-3.33606700	3.76195700
H	-4.92875000	-4.37777200	2.34707100
C	8.47975100	-3.91772200	1.68880500
C	7.69945900	-2.87886200	1.23903300
C	6.35630500	-3.11120200	0.80003600
C	5.83436300	-4.43980900	0.86223200
C	6.67946400	-5.50340200	1.32080700
C	7.96777300	-5.24873400	1.72271600
H	9.50298700	-3.72902100	2.02692400
H	8.08824200	-1.85787800	1.21262700
C	5.50812600	-2.04438900	0.31341700
C	4.47563300	-4.68450400	0.48635600
H	6.27031600	-6.51740700	1.35301000
H	8.60791900	-6.06104500	2.07854300
C	3.63159800	-3.66012700	0.09384900
C	4.19037000	-2.33624900	0.00332200
H	4.10654100	-5.71565000	0.50215800
C	6.00959700	-0.63310500	0.16065800
C	7.12613000	-0.28895200	-0.69627500
C	5.33049500	0.39231200	0.79405800
C	7.82701900	-1.26641200	-1.47290100
C	7.49468200	1.08685200	-0.83418500
C	5.72815300	1.77204800	0.73036900
C	8.85026600	-0.89412300	-2.31291200
H	7.52415400	-2.31300700	-1.39877900
C	8.57416200	1.43856400	-1.70853900
C	6.79400500	2.09460200	-0.09222100
C	9.23573000	0.47305200	-2.42812800
H	9.37292700	-1.64955700	-2.90686800
H	8.84818100	2.49400700	-1.79608600
H	7.13090200	3.13566900	-0.15384000
H	10.05388700	0.74634900	-3.10040800
P	2.84359700	-0.15789100	0.52228400
O	4.12570600	0.08260300	1.48706300

O	3.36644200	-1.29663700	-0.49971200
S	3.60658800	1.62845400	-1.88585500
S	1.09056300	2.06893500	-0.49628700
O	3.89524900	3.05455600	-1.91275800
O	4.69036000	0.66683900	-2.00064500
C	2.63095300	1.30015000	-3.46002700
F	3.45038100	0.71243300	-4.32551900
F	1.60928000	0.47119200	-3.23076900
F	2.17522700	2.41257300	-4.01416600
C	1.27095000	3.31271500	0.85888600
F	1.94037900	2.78441600	1.87836200
F	1.91337100	4.37635800	0.40462100
F	0.06478900	3.68100500	1.27700000
O	0.96577000	2.86757200	-1.71020200
O	-0.05121600	1.27119600	-0.04970400
C	5.08578100	2.80041600	1.57610200
C	4.76176500	4.04783800	1.03871300
C	4.84546100	2.55777700	2.93461900
C	4.22041100	5.02711900	1.85350200
H	4.86467900	4.23716200	-0.02416500
C	4.30694300	3.55370800	3.72668800
H	5.06841800	1.59703800	3.38333900
C	3.99161600	4.80018100	3.20205300
C	2.20620400	-3.94622600	-0.17694900
C	1.44835800	-3.27230800	-1.14590000
C	1.57618800	-4.94323800	0.58611100
C	0.11250800	-3.58605000	-1.31687900
H	1.86559500	-2.47446900	-1.74661900
C	0.25090100	-5.26086200	0.37019200
H	2.10578400	-5.45052700	1.38277600
C	-0.49788700	-4.58690400	-0.58015200
O	1.71343400	-0.54469600	1.39763600
C	2.55159600	1.18412200	-0.57602600
H	0.15032500	-1.19168800	0.92600700

F	3.87477500	6.21438300	1.34915700
F	3.46554100	5.75175400	3.97670600
F	4.08286000	3.34467800	5.02923000
F	-0.36598100	-6.18856200	1.11585500
F	-1.81361000	-4.84195000	-0.71616800
F	-0.64606000	-2.91088700	-2.18790800

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C	5.15567800	0.63288200	-0.07303300
H	4.91049300	0.97389300	0.94325800
N	6.22618200	-0.34960900	0.02017500
C	7.10392900	-0.29500200	1.06761000
O	7.36869500	0.68883600	1.71615900
O	7.63634800	-1.53877800	1.27436200
C	7.73769400	-1.91671200	2.63987400
H	8.41027200	-2.78257100	2.65371400
H	8.19096300	-1.10322700	3.22579100
H	5.98388200	-1.30494600	-0.22870800
C	3.91901200	-0.11662300	-0.60760800
H	3.65236700	-0.90035400	0.11120700
H	3.08038400	0.59485700	-0.66463600
C	4.19230700	-0.69727300	-1.95453400
C	4.02124900	-1.99240300	-2.29102300
H	3.78524100	-2.74176200	-1.52957000
H	4.38208600	-2.35662500	-3.24517500
Si	1.78270300	-1.67622800	-2.91289300
C	1.95949600	-0.06229000	-3.85329400
H	0.96666700	0.26095400	-4.22387300
H	2.33071100	0.75334400	-3.20596900
H	2.65211200	-0.19599200	-4.71396200
C	2.08394600	-3.23611500	-3.93108600
H	1.13960600	-3.62238300	-4.32203300
H	2.75144400	-3.03217700	-4.77753000
H	2.53168400	-4.02998600	-3.32011400

C	1.23338600	-1.88734500	-1.14463900
H	0.15966300	-1.70243300	-1.06794100
H	1.44008900	-2.91534200	-0.84262300
H	1.72536600	-1.21806400	-0.43312400
O	-0.34893700	-1.89702300	-3.39056900
H	-0.91516000	-1.21177800	-2.91238000
H	-0.59104000	-1.86479600	-4.32825600
C	6.36696500	-2.29370000	3.20839300
C	5.55198300	-3.21903300	2.30682100
H	6.54661400	-2.79379000	4.17095700
C	5.40174400	-1.13025700	3.42037700
C	5.91196200	-4.40677300	1.68817900
C	4.25779100	-2.69919300	2.12881600
C	5.59712300	0.06496700	4.09723200
C	4.17047900	-1.40211500	2.80547900
C	4.96641200	-5.08362300	0.91347800
H	6.91414100	-4.81479200	1.80458700
C	3.30286300	-3.38894900	1.38835500
C	4.55515400	0.99278500	4.13293600
H	6.55290600	0.30359000	4.55150300
C	3.12526000	-0.48434500	2.85519100
C	3.66738700	-4.58482000	0.77177000
H	5.23643800	-6.01117700	0.41812600
H	2.28852200	-3.00659900	1.30310100
C	3.32898700	0.72514300	3.51803200
H	4.70350700	1.94603400	4.64053900
H	2.16867200	-0.68154500	2.38595600
H	2.92469300	-5.12845200	0.18608200
H	2.52317800	1.45219300	3.54332400
C	5.48358100	1.84198500	-0.92897000
C	6.67890900	1.93302600	-1.65437000
C	4.53655200	2.86165200	-0.98981100
C	6.96381100	3.03389200	-2.46024500
H	7.39880300	1.13116300	-1.57024000

C	4.79204200	3.97593200	-1.79687600
H	3.61250300	2.79666300	-0.41632400
C	5.99551100	4.03266500	-2.50755300
H	7.88772400	3.11582300	-3.01408000
C	4.09576500	5.19567500	-2.12225600
H	3.12898600	5.52052700	-1.77549900
O	6.07099900	5.18776900	-3.22594600
C	4.91398400	5.86269400	-2.97270100
H	4.81901800	6.81200300	-3.47849800
C	-8.89443200	-1.73020900	-1.02789100
C	-7.75985100	-1.15110100	-0.50362100
C	-6.48380000	-1.77580200	-0.66355600
C	-6.40161200	-3.00389100	-1.38773200
C	-7.59859300	-3.58506800	-1.91250900
C	-8.81551400	-2.96478800	-1.73302200
H	-9.86459200	-1.24489400	-0.90270000
H	-7.81830300	-0.20480700	0.03549200
C	-5.26788400	-1.18547100	-0.13879400
C	-5.12477700	-3.63386400	-1.58284500
H	-7.52832800	-4.52707500	-2.45945700
H	-9.72445300	-3.40927500	-2.14086200
C	-3.96338600	-3.06291800	-1.10782100
C	-4.06850300	-1.81763300	-0.39648000
H	-5.08534000	-4.59764800	-2.10293700
C	-5.25969400	0.10593900	0.63607400
C	-5.96897900	0.26150300	1.88754400
C	-4.50035500	1.16605200	0.17143900
C	-6.69898100	-0.81134200	2.49362300
C	-5.88851200	1.51454000	2.57186900
C	-4.46074900	2.45145500	0.80973500
C	-7.32284500	-0.63419600	3.70266700
H	-6.73553800	-1.77647400	1.98324000
C	-6.56763600	1.66883500	3.83141300
C	-5.15310100	2.59968500	1.99404300

C	-7.26540300	0.62150600	4.38216600
H	-7.87111300	-1.46243300	4.16146400
H	-6.50648700	2.63517300	4.34061400
H	-5.16608200	3.57514700	2.49925700
H	-7.77484900	0.73975200	5.34289800
P	-2.36952700	0.06857700	-0.78472600
O	-3.69984500	0.95754600	-0.98939900
O	-2.86363600	-1.20928900	0.06977800
S	-1.44717600	0.59295200	2.06967800
S	0.29316400	1.34619900	-0.15981900
O	-0.58799700	1.52383200	2.78147200
O	-2.85345600	0.47896100	2.42753800
C	-0.75343400	-1.10324000	2.47795800
F	-1.74264100	-1.98042400	2.62073500
F	0.05881800	-1.54785400	1.51382300
F	-0.07261300	-1.03359800	3.60343100
C	0.14215700	3.18014900	-0.20592200
F	-0.82688600	3.50275200	-1.04848200
F	-0.11052800	3.67596900	0.98676400
F	1.29430300	3.68850100	-0.65975300
O	1.35091200	1.07243500	0.81256900
O	0.54847500	1.01090500	-1.56098400
C	-3.75641000	3.60977700	0.21633200
C	-3.00063800	4.45227400	1.03590900
C	-3.90537300	3.92932300	-1.13528100
C	-2.42753100	5.59592600	0.50691400
H	-2.82593000	4.21098500	2.08113600
C	-3.32135100	5.07977400	-1.63979700
H	-4.47251000	3.29706100	-1.80741800
C	-2.59066700	5.93506000	-0.82616000
C	-2.65537100	-3.71835100	-1.32015900
C	-1.72625400	-3.84168700	-0.27469000
C	-2.33519500	-4.24374400	-2.57145900
C	-0.51973700	-4.47285200	-0.50668300

H	-1.91670300	-3.43319600	0.70952200
C	-1.11407500	-4.84749600	-2.79001600
H	-3.02346000	-4.13229200	-3.41048500
C	-0.18988500	-4.96995000	-1.76168800
O	-1.86464300	-0.24306500	-2.14711700
C	-1.22905500	0.75456300	0.35927600
F	-1.68782800	6.40381000	1.27660100
F	-2.02649600	7.03758900	-1.32858100
F	-3.47044400	5.41297900	-2.92368000
F	-0.76974900	-5.28932100	-4.00701100
F	1.01440800	-5.52346700	-1.97249200
F	0.39956300	-4.57872200	0.46684600
H	4.55143700	-0.00073000	-2.71396000

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H	-1.30717900	0.50263200	2.32948600
C	1.63286600	5.51021400	1.96267600
C	0.65502200	5.43127700	2.96416000
C	-0.28689500	4.39854700	2.90450500
C	-0.20840900	3.48665700	1.86184100
C	0.79672700	3.58842400	0.87748200
C	1.72646200	4.61560800	0.90389600
C	1.99176200	7.17689500	3.31540300
C	0.91857700	6.54599800	3.84209500
H	-1.06750500	4.30859100	3.65473400
H	0.84282200	2.86022700	0.07205100
H	2.48730800	4.72421400	0.14032800
H	2.54648600	8.05087300	3.62138300
H	0.38000000	6.82751800	4.73437000
O	2.44448100	6.57540800	2.17918300
C	-1.20103200	2.35996900	1.80871500
O	-0.57009900	1.15736600	2.32778300
H	-2.05215200	2.55346100	2.46897600
C	-7.65269400	-2.50370800	-3.35266900

C	-6.34453700	-2.77933100	-3.75404200
C	-5.31836500	-1.86394100	-3.51536700
C	-5.62624800	-0.67175100	-2.87630800
C	-6.93888500	-0.39798200	-2.46302900
C	-7.96164300	-1.31140700	-2.70164100
H	-8.43704600	-3.22889800	-3.54603100
H	-6.12285700	-3.71631500	-4.25501200
H	-4.29902200	-2.09074400	-3.81590900
H	-8.98036100	-1.10318500	-2.38569000
C	-4.69932400	0.45287800	-2.46089400
H	-4.15660300	0.88482500	-3.31075200
C	-5.65278800	1.44483600	-1.82680700
C	-5.38255200	2.68599500	-1.26485800
C	-6.42607800	3.38945300	-0.65885000
C	-7.71493800	2.85484600	-0.61476500
C	-7.99134000	1.61367200	-1.18804300
C	-6.95368800	0.91426000	-1.79869900
H	-4.37719100	3.09508600	-1.28351800
H	-6.23225800	4.35992900	-0.21232400
H	-8.51235000	3.41314100	-0.13315900
H	-8.99742600	1.20313900	-1.15416400
C	-3.68933200	-0.07740100	-1.44606700
H	-3.05979900	-0.85312000	-1.89451100
H	-4.20916300	-0.48357400	-0.57546000
O	-2.85140700	1.00837900	-1.04414600
C	-2.44775300	1.03957100	0.22328300
O	-2.71521800	0.20006800	1.07484500
N	-1.69840300	2.14936700	0.47340300
H	-1.21309600	2.54888900	-0.32312200
C	-4.41271700	1.90791700	3.55242900
C	-5.35168200	1.88985500	2.60202200
H	-3.81653100	1.02234800	3.76591100
H	-4.22083200	2.79223800	4.15368400
H	-5.93332300	2.79590500	2.42259600

C	-5.72405600	0.70068400	1.78178200
H	-4.90429200	-0.02563700	1.77045100
H	-5.92238100	0.99590600	0.74439100
Si	-7.24926700	-0.22270500	2.41882200
C	-6.79725500	-1.04648500	4.05209900
H	-6.01556800	-1.79771400	3.89823400
H	-7.65956500	-1.54187000	4.51038900
H	-6.41578400	-0.30376000	4.76123900
C	-7.70287400	-1.51432900	1.12541800
H	-8.08473300	-1.03256000	0.21840500
H	-8.46747900	-2.20936000	1.48837100
H	-6.82127600	-2.09759100	0.83720600
C	-8.68255000	0.97369100	2.68497300
H	-8.43244700	1.72279300	3.44410300
H	-9.58414900	0.44798000	3.01720300
H	-8.92112700	1.50152200	1.75538700
C	4.21309600	-3.98183600	5.17779000
C	4.19053100	-3.40302100	3.93081900
C	2.98080800	-3.37235000	3.16507600
C	1.79112400	-3.92961300	3.73031200
C	1.85273400	-4.53415800	5.02880400
C	3.03301700	-4.56137500	5.73165600
H	5.14074100	-3.99921600	5.75793100
H	5.09207000	-2.95458300	3.50632900
C	2.91380800	-2.77700500	1.84894500
C	0.55762400	-3.86151300	3.00510200
H	0.93810100	-4.96497400	5.44689700
H	3.07588400	-5.01968700	6.72415700
C	0.47167700	-3.25439200	1.76507800
C	1.68829000	-2.73218200	1.20879700
H	-0.33806100	-4.31487800	3.44351800
C	4.11247800	-2.16968100	1.16975000
C	5.29050600	-2.94101100	0.84055700
C	4.07101100	-0.83827700	0.78903900

C	5.38315900	-4.34459500	1.10927000
C	6.37655900	-2.29427000	0.17126200
C	5.16495700	-0.15510500	0.16263200
C	6.50423300	-5.05295400	0.74710400
H	4.54157200	-4.84471800	1.59406300
C	7.53616600	-3.06037200	-0.18088300
C	6.29507800	-0.89647500	-0.13161900
C	7.59762300	-4.40385000	0.10024300
H	6.56255000	-6.12686100	0.94827700
H	8.36202400	-2.55144400	-0.68689200
H	7.15482200	-0.39963600	-0.59497800
H	8.48017300	-4.98777600	-0.17737200
P	1.71900100	-0.54402600	-0.12070300
O	2.82459800	-0.12477900	0.96335200
O	1.64696000	-2.13501300	-0.09955500
S	2.97767100	-1.27375400	-2.72476400
S	1.15371300	1.05263500	-2.62455400
O	3.43389400	-0.63153100	-3.94092300
O	3.91317500	-2.00082500	-1.88085900
C	1.72039000	-2.56470000	-3.25469500
F	1.91088300	-3.67637300	-2.55054900
F	0.47850000	-2.14389700	-3.04199800
F	1.88300700	-2.82823900	-4.53881400
C	2.32930200	2.46516400	-2.76812900
F	2.66351600	2.84779200	-1.52945900
F	3.42069900	2.14505400	-3.43616500
F	1.71395900	3.46990000	-3.37351100
O	0.86098400	0.61811900	-3.97524500
O	0.10613100	1.62709500	-1.78572800
C	5.13662500	1.29069600	-0.13542400
C	5.54791200	1.73951000	-1.39343700
C	4.78043600	2.22723900	0.84161200
C	5.61386900	3.09711600	-1.65559200
H	5.77364000	1.03777400	-2.18945100

C	4.88047200	3.57843000	0.56441700
H	4.45216600	1.91991300	1.82793600
C	5.29155700	4.03167800	-0.68253400
C	-0.83459700	-3.13280300	1.08501200
C	-0.98576300	-3.31559500	-0.29512200
C	-1.96549900	-2.83721100	1.85613600
C	-2.24242900	-3.21181000	-0.86376400
H	-0.14374100	-3.53458900	-0.93967500
C	-3.21026700	-2.74635900	1.26252800
H	-1.88011600	-2.64063600	2.91857500
C	-3.36977800	-2.94844200	-0.09803800
O	0.40593100	0.05009800	0.39069600
C	2.03695300	-0.16348500	-1.76769100
H	0.19439000	0.57076200	1.28637400
F	5.96157700	3.53862200	-2.86475700
F	5.33977400	5.33814300	-0.94260900
F	4.58251300	4.49121700	1.49461300
F	-4.28939800	-2.42928900	1.98536900
F	-4.56952600	-2.83433500	-0.67024200
F	-2.40528200	-3.34777400	-2.18436400

TSIII-3R'

H	-1.59808700	1.50158300	1.28291100
C	-0.21189800	2.03756900	-3.86986600
C	-0.62471800	3.20916900	-3.21513500
C	-1.49158700	3.10350300	-2.12687400
C	-1.90147900	1.83443400	-1.73063100
C	-1.46989600	0.67874600	-2.41156300
C	-0.61151300	0.76153000	-3.49682100
C	0.72948700	3.70201500	-4.91235100
C	0.01614500	4.28936000	-3.92724900
H	-1.81540700	3.98139400	-1.57466900
H	-1.81686800	-0.29912300	-2.08828500
H	-0.27440500	-0.12041800	-4.02860400

H	1.36684700	4.10021900	-5.68717300
H	-0.04589600	5.34695800	-3.72001900
O	0.61024600	2.34297400	-4.90528900
C	-2.85713500	1.72434400	-0.59930400
O	-1.38268900	2.10194900	0.55494500
H	-3.23377800	2.62259000	-0.12423400
C	-8.88572000	0.25818400	0.53415700
C	-8.38873000	0.83926100	1.70378900
C	-7.35295600	0.22952700	2.41209500
C	-6.82513200	-0.96132300	1.93549100
C	-7.31302800	-1.54020300	0.75392100
C	-8.34930400	-0.93352900	0.04568600
H	-9.70897000	0.73259600	0.00649300
H	-8.81997200	1.76634600	2.07091500
H	-6.96229200	0.68843500	3.31603400
H	-8.74323400	-1.38322500	-0.86201100
C	-5.74487800	-1.83506800	2.54371300
H	-6.09839300	-2.22224300	3.51092400
C	-5.63867900	-2.96656200	1.53784500
C	-4.79058800	-4.06418000	1.53774100
C	-4.88326700	-4.98269700	0.49100500
C	-5.81373600	-4.80497800	-0.53440800
C	-6.66487800	-3.70239200	-0.53751700
C	-6.56647000	-2.78248100	0.50154200
H	-4.06377800	-4.21169100	2.33106700
H	-4.22398400	-5.84452600	0.47455600
H	-5.87250300	-5.53257800	-1.33772900
H	-7.38789300	-3.56536400	-1.33663900
C	-4.41782300	-1.13562900	2.83334700
H	-3.75448800	-1.79418000	3.39846700
H	-4.57842000	-0.21259200	3.39794200
O	-3.69522600	-0.84780800	1.63559000
C	-3.82012600	0.36900200	1.11115100
O	-4.64570200	1.20966100	1.41000600

N	-2.90150100	0.55357000	0.11191200
H	-2.04541100	-0.01016700	0.09610000
C	-4.57685900	1.57464900	-1.80091600
C	-5.62997200	1.65164700	-0.92841700
H	-4.30514400	2.44963900	-2.38545000
H	-4.32447300	0.62061100	-2.24941900
H	-6.06945800	0.73315000	-0.53915200
C	-6.27443600	2.90087900	-0.51021500
H	-5.58222700	3.75076600	-0.56173700
H	-6.67813700	2.80876900	0.50165100
Si	-7.72048400	3.30877800	-1.73133500
C	-7.08304300	4.62713400	-2.91327400
H	-6.80536800	5.54302100	-2.38159600
H	-7.84582000	4.88703100	-3.65509900
H	-6.20163400	4.27096900	-3.45845700
C	-9.15800600	3.96213400	-0.71146100
H	-9.52230200	3.20121300	-0.01369100
H	-9.99424100	4.26016400	-1.35259200
H	-8.85633000	4.83680300	-0.12598100
C	-8.20644900	1.78688600	-2.72494400
H	-7.39670200	1.49560200	-3.40243500
H	-9.09192900	1.99991100	-3.33382200
H	-8.43226600	0.92977500	-2.08449600
C	7.34696200	2.66788900	-3.19856000
C	6.61091300	1.72161600	-2.52589300
C	5.82694200	2.08426200	-1.38330200
C	5.80393100	3.45184900	-0.96971100
C	6.59213300	4.41118200	-1.68668200
C	7.34423800	4.02869400	-2.77033100
H	7.94057600	2.38288300	-4.07224700
H	6.60782500	0.67885200	-2.85307300
C	5.03619000	1.11988900	-0.65239500
C	4.99022300	3.84299500	0.14184600
H	6.57314500	5.45319600	-1.35398000

H	7.94015700	4.76444400	-3.31789700
C	4.19467000	2.93643000	0.81900900
C	4.24571000	1.56392000	0.39295600
H	5.02107600	4.88564000	0.47595600
C	5.01390000	-0.34248400	-1.00373600
C	6.19987000	-1.16975300	-0.97445300
C	3.80022400	-0.93302300	-1.31175000
C	7.47674900	-0.66104600	-0.57104300
C	6.08763900	-2.55495000	-1.31058500
C	3.67779500	-2.30878800	-1.69733700
C	8.57663400	-1.48437700	-0.52703300
H	7.55697500	0.39056000	-0.28600800
C	7.25724100	-3.38291900	-1.26563200
C	4.81702700	-3.09103000	-1.69813900
C	8.46917100	-2.86078200	-0.88421300
H	9.54565800	-1.08821800	-0.20943000
H	7.15733800	-4.43936300	-1.53124000
H	4.74964600	-4.13783300	-2.01401600
H	9.35788900	-3.49709300	-0.84362100
P	2.10242200	0.16318300	0.28149400
O	2.61645400	-0.13630200	-1.22729100
O	3.44365400	0.59582900	1.07373700
S	2.96662500	-2.20011300	1.97522500
S	0.12774800	-1.66672100	1.67093300
O	2.41810900	-3.45611500	2.46040800
O	4.22978400	-2.18369100	1.25839100
C	3.29229200	-1.19601600	3.52964900
F	4.48034700	-0.60246300	3.44380100
F	2.36563500	-0.26198000	3.70422400
F	3.29603300	-2.00914800	4.57378800
C	-0.47534700	-3.32770700	1.07484200
F	-0.65187200	-3.24789700	-0.24192400
F	0.27881600	-4.36830900	1.34913100
F	-1.66953200	-3.49114600	1.64751500

O	0.02097000	-1.71831300	3.11984400
O	-0.83557900	-0.84417100	0.92469300
C	2.39572600	-2.86638000	-2.16848400
C	1.87111800	-4.02714900	-1.59631600
C	1.72843700	-2.27324000	-3.24522100
C	0.71581000	-4.58753200	-2.11408200
H	2.33432100	-4.48106100	-0.72586800
C	0.57317000	-2.84797400	-3.73718100
H	2.10528000	-1.36453800	-3.70197200
C	0.05194200	-4.01129500	-3.18750100
C	3.33217600	3.39154000	1.92799000
C	3.14855900	2.63267300	3.08813800
C	2.70437200	4.63956400	1.83545700
C	2.35153700	3.11332000	4.11138500
H	3.62811900	1.67263400	3.21742500
C	1.92870100	5.10902700	2.87901700
H	2.78672400	5.24026700	0.93750000
C	1.73536300	4.35495400	4.02709100
O	1.09480400	1.24835800	0.21760400
C	1.71981600	-1.33176200	1.13370500
H	-0.44994900	1.85791300	0.28328100
F	0.18095800	-5.67606200	-1.55667900
F	-1.07105600	-4.54841800	-3.66740300
F	-0.08295500	-2.28441200	-4.76473700
F	1.33035700	6.30287000	2.79721600
F	0.97617600	4.81309200	5.02327600
F	2.17482500	2.39830300	5.22428500

Pr2-R

C	5.51162200	-1.03334100	-0.61855800
C	5.37507600	-0.11564500	0.42979200
C	4.13893000	0.51506700	0.61984300
C	3.08872100	0.21594600	-0.23739400
C	3.27208000	-0.71158600	-1.28505100

C	4.48191200	-1.35623800	-1.49300300
C	7.44032200	-0.95249900	0.38950500
C	6.66589000	-0.08437700	1.07672400
H	3.99696400	1.22693900	1.42824400
H	2.44390900	-0.93064300	-1.95553400
H	4.62677400	-2.07338000	-2.29301600
H	8.46910200	-1.25953400	0.50305000
H	6.96244400	0.50367500	1.93242000
O	6.77223600	-1.54322100	-0.64293400
C	1.74232800	0.88893300	-0.05183400
H	1.78552700	1.54496900	0.82222500
C	-3.46570100	2.86440700	-0.88985300
C	-3.11568300	3.06043700	0.44777700
C	-3.03611400	1.98108000	1.32873400
C	-3.32320200	0.70974500	0.85351600
C	-3.66061000	0.50998700	-0.49442300
C	-3.73411200	1.58603100	-1.37475300
H	-3.51889800	3.71614900	-1.56173300
H	-2.89417000	4.06131500	0.80569600
H	-2.73806700	2.13605200	2.36137100
H	-3.99785800	1.43596200	-2.41797900
C	-3.34836400	-0.60882900	1.60501800
H	-4.12632700	-0.58631000	2.38237800
C	-3.72552600	-1.59224300	0.51374900
C	-3.89432500	-2.96573400	0.59792600
C	-4.24559000	-3.67405700	-0.55256000
C	-4.42430700	-3.01051400	-1.76702100
C	-4.25451500	-1.63018600	-1.85504000
C	-3.90252400	-0.92549700	-0.70785400
H	-3.75735400	-3.48735900	1.54212900
H	-4.38200200	-4.74997000	-0.50247000
H	-4.69882700	-3.57628800	-2.65210100
H	-4.39518500	-1.11800000	-2.80286400
C	-2.03144700	-0.95226800	2.30044500

H	-2.09328500	-1.94450800	2.75668800
H	-1.78773000	-0.21501800	3.06908900
O	-0.97519500	-1.01618000	1.35001300
C	-0.14638000	0.05895200	1.29342400
O	-0.17146700	0.99648300	2.06280100
N	0.71137500	-0.09172400	0.25606000
H	0.62690700	-0.93265800	-0.29789700
C	1.34643300	1.73661300	-1.27662700
C	0.08261800	2.51412400	-1.04904200
H	2.17333300	2.41448400	-1.51802900
H	1.22294900	1.06205800	-2.13642400
H	-0.79891100	1.94065300	-0.76017400
C	-0.00657300	3.83486800	-1.17165700
H	0.85135100	4.44020200	-1.45597500
H	-0.94063000	4.35756700	-0.99124100