

**Electronic Supplementary Information For**  
**DFT study on isothiourea-catalyzed C-C bond activation of**  
**cyclobutenone: role of catalyst and origin of stereoselectivity**

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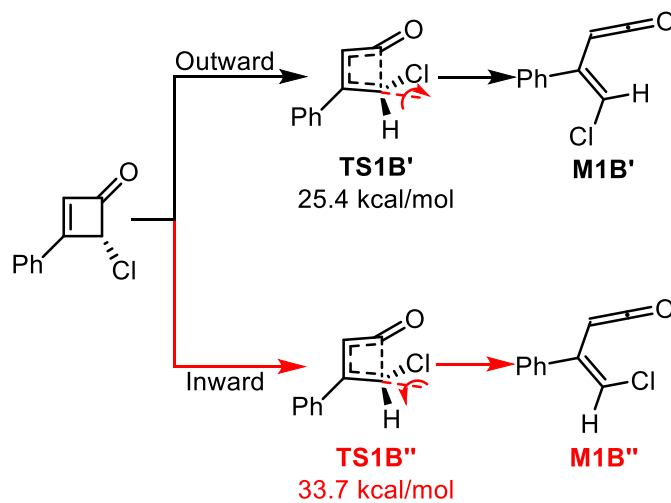
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## Part 1: Benchmark study for C-C bond cleavage process

**Table S1.** Gibbs free energy barriers for C-C bond cleavage process in different methods

	B3LYP	B3PW91	CamB3LYP	M06-2X-D3	$\omega$ B97X-D
<b>TS1A</b>	-	28.2	25.9	19.5	20.7
<b>TS2A</b>	47.1	46.5	43.4	36.0	42.4
<b>TS1B</b>	24.2	25.0	27.4	26.2	27.8

## Part 2: Possible electrocyclic ring-open modes



**Scheme S1.** The possible electrocyclic ring-open modes for the ring-open process of cyclobutenone

### Part 3: Energy profile involved in R-configured cyclobutenone R-R1

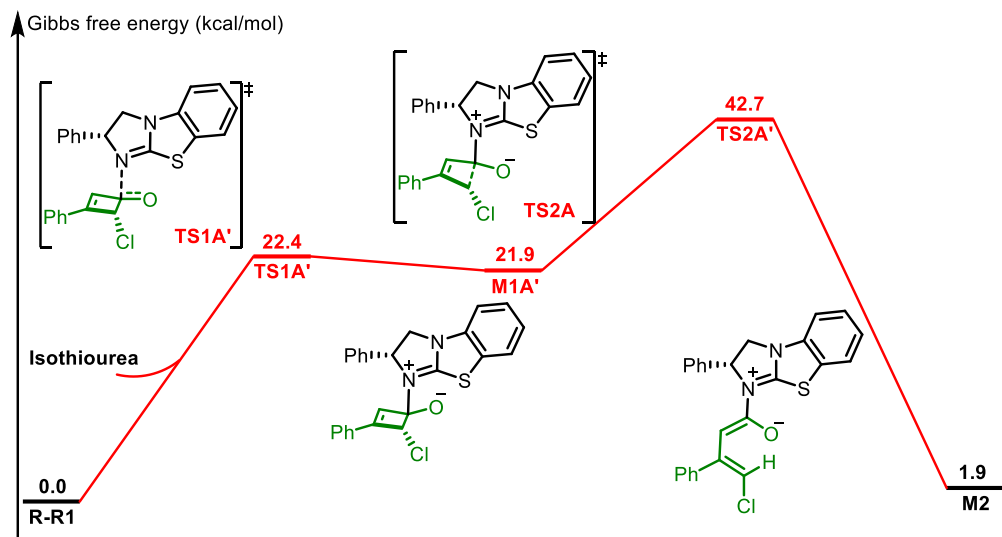
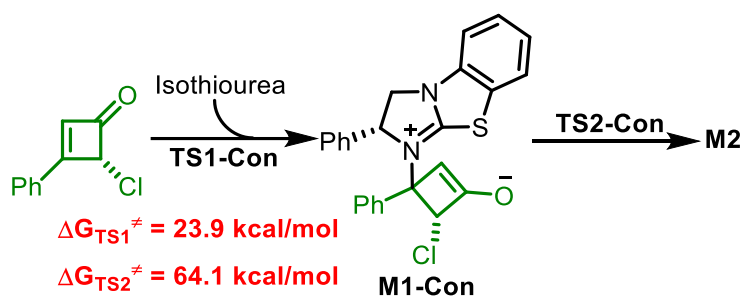


Fig. S1 Energy profile involved in R-configured cyclobutenone R-R1

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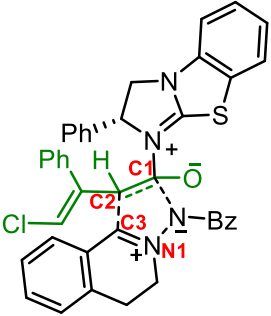
## Part 4: The alternative conjugate-addition mechanism



**Scheme S2.** The alternative conjugate-addition mechanism

## Part 5: Configurational search for stereoselective transition states

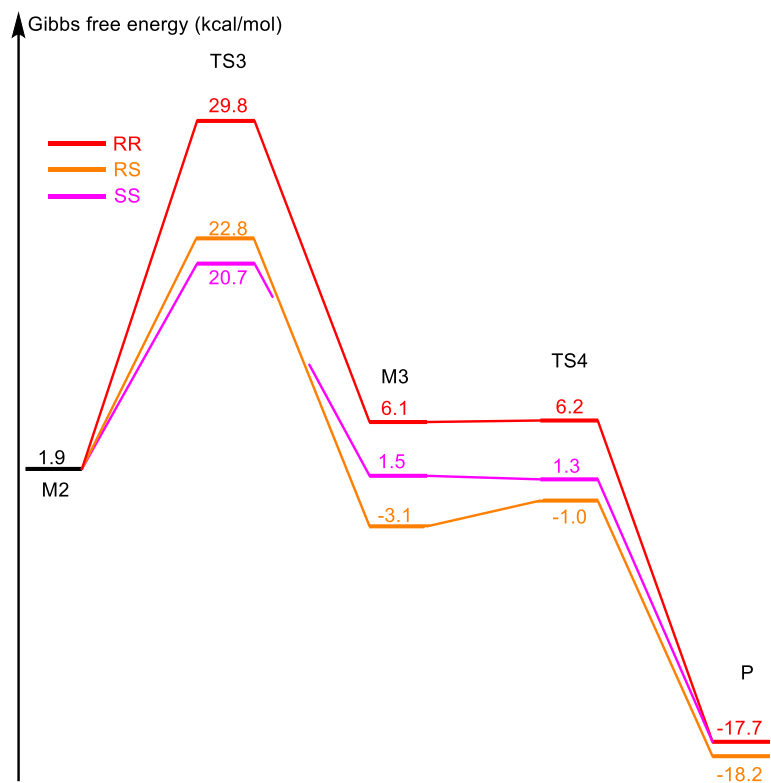
**Table S2.** Different conformations of the transition states involved in the [3 + 2] cycloaddition step



	TS3	TS3-90	TS3-180	TS3-270
RR	29.8	29.9	34.5	38.4
RS	22.8	35.33	33.9	25.0
SR	17.7	20.6	27.9	30.3
SS	20.7	20.9	25.5	20.7

We have additionally considered and investigated the different conformations of TS3s involved in the [3 + 2] cycloaddition step. By rotating dihedral angle  $\Phi_1(\text{C1-C2-C3-N1})$  from 0~360° at intervals of 90° based on the original transition states TS3RR, TS3RS, TS3SR, and TS3SS, we have constructed sixteen ( $4 \times 4 = 16$ ) initial structures of TS3s and located sixteen conformations after the optimization, which are summarized in Table S2. As an important note, the initial structures by rotating the dihedral  $\Phi_1$  with 90° would lead to the same conformations of those with  $\Phi_1 = 0^\circ/360^\circ$  after the structural optimizations. Moreover, the TS3RR-90, TS3SS-90 and TS3SS-270 have the same structure with the corresponding original transition states after optimizations. The relative Gibbs free energies depicted in Table S2 show that the one-step transition state indeed have the lowest energies among their stepwise conformers.

## Part 6: Energy profile of the other three pathways

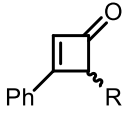


**Fig. S2** Energy profiles for the reaction between ammonium-bound enolate and azomethine imine involved in RR, RS, and SS pathways

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## Part 7: Substituent effects on the ring-open process

**Table S3.** The energy barriers for different types of cyclobutenones (values in parentheses represent the energy barriers of *S*-configured cyclobutenone)

	$\Delta G^{\ddagger}_{\text{TS1B}}$	$\Delta G^{\ddagger}_{\text{TS2A}}$
R=Cl	25.4(25.4)	42.7 (29.6)
R=H	28.3	49.0
R=Me	29.2(29.3)	48.3(37.6)



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## Part 8: Derivation of the calculated ee value

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

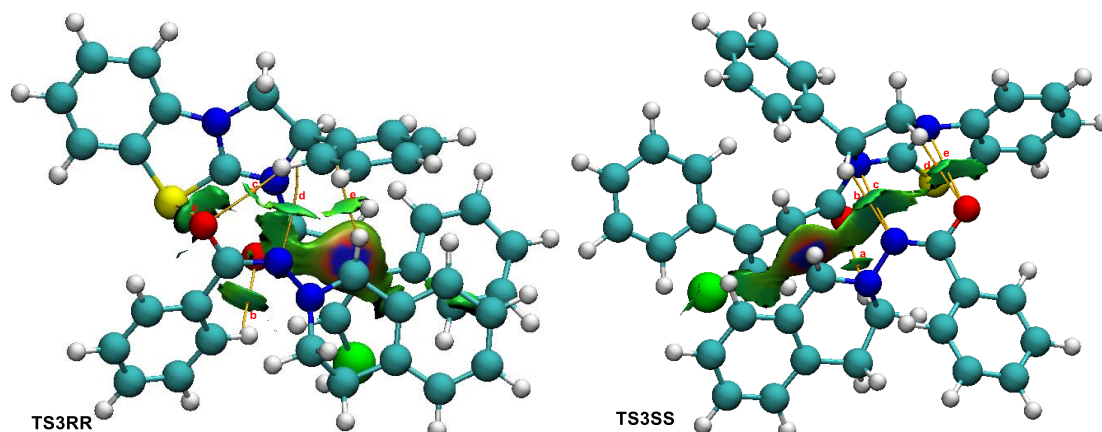
$$\frac{[R]}{[S]} = \frac{e^{-G_R^\ddagger/RT}}{e^{-G_S^\ddagger/RT}} = e^{\Delta G^\ddagger/RT} \quad (1)$$

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

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

For the present study, the computational results show that the reaction between ammonium-bound enolate **M2** and azomethine imine **R2** determines the stereoselectivity associated with transition state **TS3**. The calculated results also indicate that the *SR*-configured pathway has the lowest energy barrier and the energy difference between **TS3SR** and **TS3RS** is 5.2 kcal/mol. That is, the value of  $\Delta G^\ddagger$  in equation (1) is 5.2 kcal/mol. Thus, we can obtain the value of  $[R]/[S]$ , which is calculated to be 6735.1. Then, the value of  $[R]/[S]$  is substituted into equation, the calculated ee value can be obtained by 99.9%, which is very closed to the experimental observed ee value (92%).

## Part 9: NCI and AIM analyses for TS3RR and TS3SS



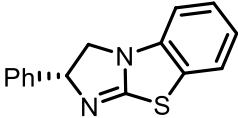
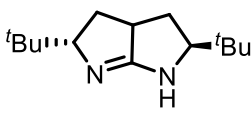
**Fig. S3** Qualitative analysis for the stereoselective transition states TS3RR and TS3SS using NCI and AIM

**Table S4.** Quantitative verifications of the weak interactions involved in the stereoselective transition states TS3RS and TS3SR

TS3RS				TS3SR			
BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)	BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)
a	O...S	3.22	0.3417	a	C-H...O	2.37	0.4118
b	C-H...O	2.35	0.5227	b	C-H...N	2.46	0.4264
c	C-H...O	2.57	0.2700	c	LP... $\pi$	2.79	0.6107
d	C-H...N	2.53	0.3679	d	C-H...O	2.49	0.3950
e	C-H... $\pi$	2.53	0.3747	e	LP... $\pi$	2.89	0.4306

## Part 10: Catalyst effect

Table S5. Energy barriers associated with stereoselectivity-determining step using guanidine as

	catalyst	
	$\Delta G^\ddagger$	
		
TS3RR	29.8	14.4
TS3RS	22.8	13.0
TS3SR	17.7	12.7
TS3SS	20.7	15.7

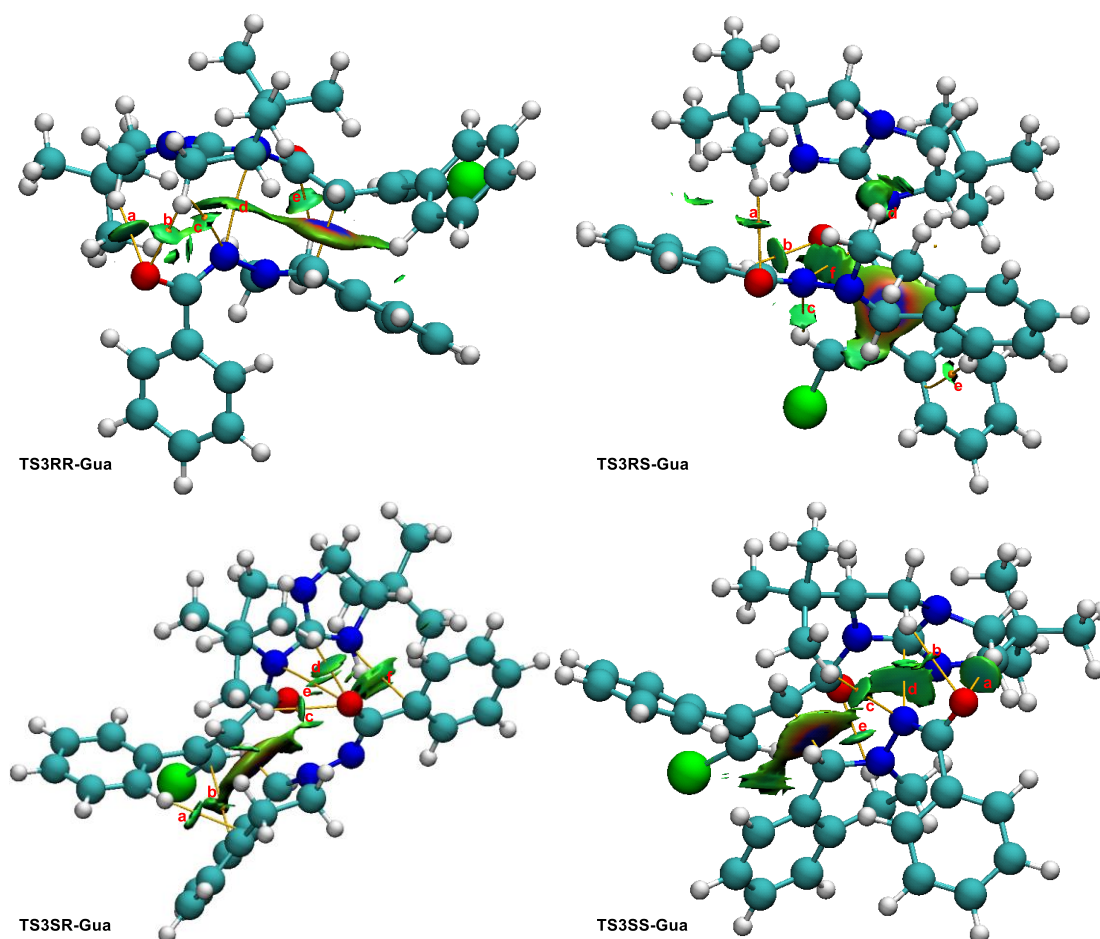


Fig. S4 NCI and AIM analysis for the stereoselective transition states involved in guanidine catalysis

**Table S6.** Quantitative verifications of the weak interactions involved in the stereoselective transition states **TS3RS-Gua** and **TS3SR-Gua**

<b>TS3RS-Gua</b>				<b>TS3SR-Gua</b>			
BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)	BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)
a	C-H... $\pi$	2.45	0.3913	a	C-H... $\pi$	2.57	0.4103
b	C-H...O	2.26	0.4532	b	C-H... $\pi$	2.66	0.3512
c	C-H...N	2.52	0.3278	c	C-H...O	2.42	0.3640
d	C-H... $\pi$	2.60	0.3646	d	C-H...O	2.20	0.5155
e	C-H... $\pi$	2.76	0.2223	e	LP... $\pi$	3.15	0.3358
f	LP... $\pi$	2.86	0.5198	f	LP... $\pi$	3.07	0.4622

**Table S7.** Quantitative verifications of the weak interactions involved in the stereoselective transition states **TS3RR-Gua** and **TS3SS-Gua**

<b>TS3RR-Gua</b>				<b>TS3SS-Gua</b>			
BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)	BCP index	Type of interaction	Distance (Å)	$\rho_{\text{bcp}} \times 10^{-1}$ (a.u.)
a	C-H...O	2.23	0.4793	a	C-H...O	2.20	0.4926
b	C-H...O	2.39	0.3749	b	C-H...O	2.55	0.2963
c	C-H...N	2.62	0.3468	c	C-H...N	2.46	0.3322
d	LP... $\pi$	2.88	0.5093	d	LP... $\pi$	2.96	0.4835
e	C-H...O	2.32	0.4662	e	C-H...O	2.30	0.4428

## Part 11: IRC plots of TS3SR

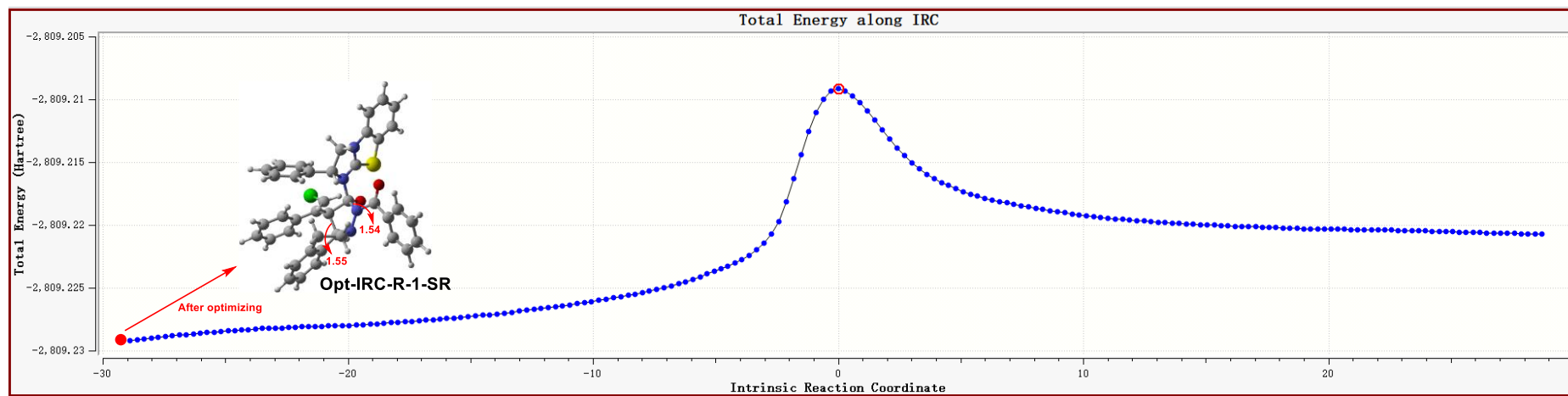


Fig. S5 IRC calculations for TS3SR

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## Part 12: Cartesian coordinates of all the stationary points involved in the calculations

### R-R1

C	-0.45338400	-0.59226900	0.16684300
C	-1.60023400	0.33089900	0.53143800
C	-2.46827300	-0.91853500	0.22134400
C	-1.23433300	-1.68894700	-0.01579500
H	-1.62826500	0.69957200	1.55790300
H	-1.03107400	-2.72951400	-0.23706900
O	-3.65454400	-1.09805800	0.16692700
C	0.96998100	-0.31492300	0.09208900
C	1.45817900	0.94075300	0.47538600
C	1.86334600	-1.29996800	-0.35385300
C	2.82228900	1.20398900	0.42147000
H	0.76708600	1.70727700	0.81338500
C	3.22364100	-1.03246700	-0.40772300
H	1.48353900	-2.26996600	-0.66083300
C	3.70383800	0.21943200	-0.01928500
H	3.19726600	2.17650900	0.72149500
H	3.91231600	-1.79550000	-0.75427500
H	4.76801400	0.42698700	-0.06357000
Cl	-1.87899000	1.73419500	-0.55199600

### S-R1

C	0.45327200	-0.59242900	0.16680300
C	1.60018600	0.33055500	0.53167400
C	2.46824200	-0.91872400	0.22171400

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C	1.23432700	-1.68894700	-0.01652200
H	1.62886800	0.69967300	1.55804300
H	1.03113700	-2.72918700	-0.23934800
O	3.65460200	-1.09802100	0.16668700
C	-0.97008000	-0.31502500	0.09229700
C	-1.45812300	0.94090900	0.47498100
C	-1.86356300	-1.30013200	-0.35328800
C	-2.82219100	1.20427200	0.42091300
H	-0.76708900	1.70752700	0.81280900
C	-3.22384100	-1.03252500	-0.40723300
H	-1.48384000	-2.27031200	-0.65979100
C	-3.70387800	0.21959400	-0.01937800
H	-3.19701800	2.17698400	0.72045400
H	-3.91261900	-1.79559300	-0.75349300
H	-4.76802100	0.42727000	-0.06386200
Cl	1.87915700	1.73426600	-0.55176900

**R2**

N	-0.78915000	0.57057300	0.30826200
N	0.52709000	0.18587500	0.28013400
C	1.42526300	0.95717800	-0.23477600
H	1.05939300	1.86266000	-0.70905100
C	0.95528300	-1.01041100	1.05497700
H	0.09927200	-1.67426000	1.11189700
C	2.13928400	-1.67387300	0.37582200
H	1.80111300	-2.08865400	-0.58235200
C	3.23593700	-0.66853300	0.13765800
C	4.58990100	-0.97908200	0.16431000
H	4.90187000	-1.99164400	0.40264800

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C	5.54191600	0.00157100	-0.11398300
H	6.59677000	-0.25140000	-0.08586500
C	5.14915300	1.30138800	-0.43143000
H	5.89459700	2.05835600	-0.64870900
C	3.79828900	1.62418800	-0.46924600
H	3.47737000	2.63164700	-0.71748100
C	2.84479100	0.64494000	-0.17470600
C	-1.60262800	-0.39187400	-0.17923400
O	-1.25215800	-1.47261700	-0.68136400
C	-3.06430200	-0.03870500	-0.09245700
C	-3.51664000	1.14556600	0.49499600
C	-3.98800400	-0.94192100	-0.61997200
C	-4.87973000	1.41891100	0.55362100
H	-2.79203200	1.84280700	0.90061300
C	-5.35103500	-0.66853300	-0.56177900
H	-3.61163300	-1.85428000	-1.07006800
C	-5.79910200	0.51291900	0.02583800
H	-5.22744900	2.34013200	1.01085500
H	-6.06443600	-1.37565000	-0.97342700
H	-6.86211900	0.72853700	0.07225000
H	1.21505100	-0.64015300	2.05259800
H	2.49367100	-2.50467400	0.99039500

**Isothiourea**

C	4.74373600	0.84880900	-0.73132600
C	4.20546200	-0.42905400	-0.56037600
C	2.89439200	-0.54256700	-0.12900700
C	2.12395500	0.60087100	0.14700100
C	2.65730300	1.87275000	-0.02745700



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C	3.97485800	1.98172700	-0.47238200
C	0.54006000	-1.07324100	0.52957800
C	-1.37823400	-0.14655100	1.02200400
C	-0.39542200	1.00628300	0.62574700
H	5.76693200	0.95441500	-1.07400300
H	4.79665000	-1.31363300	-0.77213700
H	2.05787300	2.75186800	0.18409900
H	4.40485500	2.96735500	-0.61540000
H	-1.53955400	-0.11173600	2.10779300
H	-0.38776700	1.82056800	1.35235700
N	0.86236800	0.27127800	0.60941700
S	1.96754300	-2.03621300	0.14372900
N	-0.67547000	-1.41065200	0.70787800
C	-2.71389300	-0.01396800	0.33002100
C	-3.70222200	0.80114300	0.88467100
C	-2.95518300	-0.64362700	-0.89153600
C	-4.91404900	0.99078800	0.22605600
H	-3.52240500	1.28679800	1.84101200
C	-4.16941700	-0.46009300	-1.54801500
H	-2.18933700	-1.28764700	-1.31244400
C	-5.15030000	0.35908900	-0.99300200
H	-5.67563400	1.62590400	0.66742100
H	-4.35101300	-0.95970900	-2.49450200
H	-6.09674800	0.50076300	-1.50485700
H	-0.61910000	1.40593400	-0.37194400
<b>TS1A</b>			
C	-6.55111500	-0.38015300	-0.32526600
C	-5.62480000	-0.93469500	0.55947300

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C	-4.27911500	-0.66368900	0.36374000
C	-3.86626500	0.15836000	-0.69578200
C	-4.78254200	0.71263000	-1.58128300
C	-6.13249100	0.42959900	-1.38134000
C	-1.82394500	-0.38755600	0.26264200
C	-0.17943100	0.62840000	-0.89010500
C	-1.53104300	0.86905600	-1.64424200
H	-7.60689700	-0.58473000	-0.18740300
H	-5.94853100	-1.56672700	1.37961600
H	-4.45065900	1.34413500	-2.39842000
H	-6.86665900	0.84872600	-2.06079900
H	0.54421800	0.14109600	-1.54866000
H	-1.58196900	0.31942800	-2.58896900
N	-2.48953600	0.31669800	-0.69089400
S	-2.90303200	-1.24522300	1.33554100
N	-0.53943700	-0.31026200	0.19622700
C	0.42954800	1.89567200	-0.32820600
C	1.69679000	2.30797500	-0.73507500
C	-0.26781200	2.65303200	0.61661900
C	2.26484100	3.46609700	-0.20613600
H	2.25137900	1.70848200	-1.45297800
C	0.29761100	3.80773000	1.14630900
H	-1.25187000	2.33006300	0.94988600
C	1.56676700	4.21658500	0.73560500
H	3.25564100	3.77437000	-0.52561900
H	-0.24840300	4.38726600	1.88359900
H	2.00862300	5.11613900	1.15162900
H	-1.71834800	1.92969500	-1.82475000
C	2.41558500	-0.96420800	0.72545000

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C	1.41256900	-2.07929400	0.57321300
C	0.45661500	-1.16547000	1.45971500
C	1.65440800	-0.23554200	1.56448000
H	1.65981600	-3.00568000	1.09512400
H	1.83970400	0.65261100	2.16102700
O	-0.33663800	-1.55238700	2.32869600
C	3.76051700	-0.81705000	0.17610800
C	4.37392800	-1.87623900	-0.50319200
C	4.45241000	0.39358200	0.32339800
C	5.65843300	-1.72920800	-1.01878900
H	3.84088200	-2.81477800	-0.62419100
C	5.73389500	0.53762800	-0.19282800
H	3.97202200	1.22101500	0.83845900
C	6.33997800	-0.52434200	-0.86522200
H	6.12779500	-2.55649000	-1.54114700
H	6.26146800	1.47860800	-0.07379700
H	7.34009900	-0.41052200	-1.27083100
Cl	0.94494700	-2.58403000	-1.10194300

**TS1A'**

C	6.68271600	-0.21920200	0.15038700
C	5.71136000	-0.95623400	-0.52720300
C	4.37547200	-0.67863400	-0.27555900
C	4.02116800	0.32468100	0.63723800
C	4.98170100	1.06328800	1.31713300
C	6.32045200	0.77504500	1.06031100
C	1.93628300	-0.43131700	-0.03092900
C	0.34002200	0.79663800	1.01155800
C	1.73970300	1.20304900	1.58506900

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H	7.73119900	-0.42477700	-0.03392100
H	5.99280000	-1.73127300	-1.23234800
H	4.69377500	1.83670200	2.02100000
H	7.09127000	1.33541500	1.57799400
H	-0.31075400	0.43928500	1.81523100
H	1.86831900	0.89832200	2.62727100
N	2.64065000	0.44229500	0.72316000
S	2.94889700	-1.47009500	-0.99313600
N	0.65003900	-0.33684000	0.10320100
C	-0.35635900	1.92037100	0.27301200
C	-1.64385400	2.30954000	0.63506000
C	0.27717200	2.55019300	-0.80151700
C	-2.29906300	3.31722300	-0.06990300
H	-2.14839600	1.80414400	1.45480300
C	-0.37585200	3.55482400	-1.50737300
H	1.27801300	2.24181900	-1.09777200
C	-1.66663200	3.93928400	-1.14272500
H	-3.30779800	3.60214300	0.21204900
H	0.11874500	4.03610000	-2.34468200
H	-2.17665900	4.72110600	-1.69599000
H	1.92083500	2.27623000	1.49240300
C	-2.37151400	-0.91113100	-0.36766700
C	-1.40811100	-1.88680800	0.25680100
C	-0.35741300	-1.34467400	-0.82080600
C	-1.49915300	-0.43270600	-1.27248600
H	-1.17777600	-1.76471200	1.31865900
H	-1.55877300	0.35084000	-2.02312700
O	0.38179800	-2.06171600	-1.53792200
C	-3.74085000	-0.56931300	0.01222100

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C	-4.39284800	-1.26866500	1.03416500
C	-4.40417800	0.49391300	-0.61750900
C	-5.68299400	-0.91271600	1.41843100
H	-3.88698200	-2.09737300	1.52155400
C	-5.69110700	0.84664100	-0.23324200
H	-3.89631600	1.04771300	-1.40232800
C	-6.33436400	0.14376500	0.78670400
H	-6.18060000	-1.46178900	2.21130700
H	-6.19541000	1.67119400	-0.72709300
H	-7.34016300	0.42004900	1.08630500
Cl	-1.80926100	-3.62861100	0.03298000

**M1A**

C	-6.50323900	-0.52475400	-0.34520300
C	-5.58415300	-1.00613900	0.58689000
C	-4.23976400	-0.71796300	0.39920100
C	-3.82852200	0.04701300	-0.70197700
C	-4.73623300	0.52952900	-1.63648500
C	-6.08260500	0.23039200	-1.44167800
C	-1.81104700	-0.38723100	0.32965900
C	-0.14298000	0.63451400	-0.83899900
C	-1.48140200	0.76827100	-1.63698900
H	-7.55728200	-0.74235400	-0.21402700
H	-5.91030400	-1.59496700	1.43767500
H	-4.40270500	1.11733400	-2.48487800
H	-6.81356200	0.59404900	-2.15550600
H	0.61467500	0.13297100	-1.44502400
H	-1.48185700	0.16391100	-2.54819400
N	-2.45055300	0.22834100	-0.68342500

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S	-2.86628400	-1.20792700	1.42772700
N	-0.51709200	-0.25430200	0.28640600
C	0.39914300	1.95586800	-0.33787100
C	1.65362200	2.39840300	-0.75377800
C	-0.34648700	2.73425000	0.55024500
C	2.16089000	3.61025800	-0.28899500
H	2.24444100	1.78119900	-1.42630000
C	0.15956700	3.94314900	1.01625000
H	-1.31974400	2.38790400	0.89156700
C	1.41487400	4.38298700	0.59704200
H	3.14084200	3.94485700	-0.61437900
H	-0.42267500	4.54051900	1.71011800
H	1.81038200	5.32429600	0.96435000
H	-1.70814900	1.80780200	-1.88073100
C	2.40934400	-0.90210000	0.69962400
C	1.35457000	-1.96225600	0.57083000
C	0.38284500	-0.94851600	1.36897300
C	1.66545700	-0.10437800	1.48668300
H	1.51858600	-2.86785700	1.15621300
H	1.89622100	0.77877100	2.07654600
O	-0.34256500	-1.33451100	2.34348500
C	3.77744000	-0.84513200	0.18742400
C	4.37705200	-1.97770500	-0.37506400
C	4.50258200	0.35320800	0.24761100
C	5.68164400	-1.91667500	-0.85614500
H	3.81669800	-2.90658000	-0.42988400
C	5.80523300	0.41125800	-0.23225100
H	4.03087200	1.23874800	0.66621000
C	6.39816400	-0.72426000	-0.78489200

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H	6.13903700	-2.80134400	-1.28734000
H	6.35972700	1.34288800	-0.18029900
H	7.41453400	-0.67697400	-1.16245100
Cl	0.92287400	-2.54543800	-1.10274600

**M1A'**

C	-6.63292500	-0.41093600	-0.37465400
C	-5.67426000	-1.07274500	0.39233100
C	-4.34022600	-0.73164400	0.22158000
C	-3.97816800	0.26056900	-0.70006900
C	-4.92547700	0.92570900	-1.46816800
C	-6.26149800	0.57346000	-1.29202500
C	-1.91246200	-0.36781600	0.12300200
C	-0.29711400	0.86789200	-0.90067300
C	-1.68498500	1.22099200	-1.53657100
H	-7.67951600	-0.66766200	-0.25512100
H	-5.96364600	-1.83981900	1.10282600
H	-4.62818200	1.69070200	-2.17742800
H	-7.02313400	1.07499500	-1.87897800
H	0.38275400	0.47536200	-1.66308200
H	-1.76031100	0.89943800	-2.57854500
N	-2.60129500	0.44480000	-0.70357600
S	-2.92318500	-1.42519900	1.05547400
N	-0.62321300	-0.21950100	0.05425800
C	0.36503800	2.03518900	-0.20098200
C	1.64175100	2.44703100	-0.57662800
C	-0.28699600	2.68161000	0.85185700
C	2.26695500	3.49664200	0.09336600
H	2.16044300	1.92794700	-1.37880100

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C	0.33700500	3.72747600	1.52343900
H	-1.27785200	2.35289600	1.15923200
C	1.61625200	4.13583400	1.14540500
H	3.26580200	3.80375100	-0.20008000
H	-0.17068800	4.22094900	2.34562400
H	2.10426400	4.94870900	1.67309700
H	-1.90338700	2.28886500	-1.46654800
C	2.37493800	-0.88327000	0.37658900
C	1.32886600	-1.84015200	-0.13279300
C	0.35187300	-1.15821900	0.94874800
C	1.57833700	-0.29708500	1.28738200
H	1.06248300	-1.78297800	-1.19227000
H	1.72616900	0.51828900	1.99100700
O	-0.35794000	-1.80913300	1.77078900
C	3.74182800	-0.65638000	-0.09184000
C	4.31860400	-1.52030400	-1.03000400
C	4.47872100	0.44689400	0.36228300
C	5.60867400	-1.29087500	-1.49952500
H	3.75380900	-2.37966700	-1.38002100
C	5.76585100	0.67422700	-0.10847000
H	4.02896500	1.12975200	1.07816700
C	6.33479900	-0.19495900	-1.04056200
H	6.04717500	-1.97010500	-2.22352700
H	6.32783500	1.53190900	0.24783000
H	7.34044600	-0.01613300	-1.40740100
Cl	1.63060600	-3.58369800	0.20336600

**TS2A**

C	-6.36052800	-0.28955100	-0.75919400
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C	-5.59942900	-0.69399000	0.33640000
C	-4.22665300	-0.49519200	0.29240500
C	-3.63109000	0.10680400	-0.82491500
C	-4.38287800	0.51078600	-1.92147000
C	-5.75826100	0.30117600	-1.87233800
C	-1.79210100	-0.30654700	0.49734400
C	0.06963300	0.47326500	-0.56081500
C	-1.14151400	0.52938200	-1.54332500
H	-7.43402200	-0.44011000	-0.74500800
H	-6.06675100	-1.15724000	1.19855900
H	-3.90808100	0.97073700	-2.78111800
H	-6.36932800	0.60339600	-2.71560800
H	0.88044800	-0.10869000	-1.00439400
H	-1.07270600	-0.24221400	-2.31617200
N	-2.25754500	0.22482700	-0.64746300
S	-3.02547600	-0.92466200	1.53714200
N	-0.48651200	-0.26639100	0.58968000
C	0.58121700	1.84214900	-0.15937200
C	1.49749700	2.47970400	-0.99813300
C	0.13891200	2.48883600	0.99428100
C	1.96389100	3.75425000	-0.69018500
H	1.85820900	1.96762300	-1.88715300
C	0.60919300	3.76286200	1.30354400
H	-0.55651200	1.99070500	1.66500100
C	1.51941300	4.39855900	0.46262500
H	2.68099900	4.23875600	-1.34500100
H	0.26682100	4.25645600	2.20730000
H	1.88632100	5.38980300	0.70816600
H	-1.25457000	1.51376700	-1.99920800

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C	2.24902500	-1.22148900	0.82456100
C	1.27053000	-2.24116200	0.58040300
C	0.22872600	-0.84510600	1.76471000
C	1.65078600	-0.48438900	1.81260200
H	1.14072300	-3.05961300	1.27589100
H	2.10184000	0.09182200	2.61749900
O	-0.53341200	-1.12234400	2.70414800
C	3.53865400	-0.96610700	0.16575500
C	4.25718700	-1.99675600	-0.45287400
C	4.06865900	0.33070200	0.16204700
C	5.48253200	-1.73550400	-1.05572200
H	3.84980600	-3.00336700	-0.44594200
C	5.29918800	0.58919600	-0.43356300
H	3.49503900	1.13449800	0.61700400
C	6.00743600	-0.44333300	-1.04571800
H	6.03281600	-2.54126800	-1.53125000
H	5.70078900	1.59777900	-0.42918500
H	6.96423200	-0.24262900	-1.51742000
Cl	0.96747600	-2.82277500	-1.09819100

**TS2A'**

C	-6.52450200	-1.42738100	0.01152000
C	-5.43529900	-1.80017300	0.79568900
C	-4.20722900	-1.20448900	0.53829400
C	-4.08063300	-0.25665100	-0.48654400
C	-5.16235200	0.12084000	-1.27373800
C	-6.38811400	-0.48088200	-1.00813400
C	-1.93183400	-0.33716500	0.32440900
C	-0.60707500	1.08776600	-0.89682100

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C	-2.06934600	1.12468400	-1.46020400
H	-7.49176600	-1.88088900	0.19614500
H	-5.54212100	-2.53665300	1.58444300
H	-5.04799200	0.85646400	-2.06228500
H	-7.25165000	-0.20833000	-1.60451000
H	0.08743200	0.69137700	-1.64319400
H	-2.13469400	0.77060300	-2.49083200
N	-2.77026800	0.20144500	-0.56661700
S	-2.65934100	-1.50141500	1.36364700
N	-0.69677000	0.11121100	0.21539000
C	-0.12572100	2.44035800	-0.42409900
C	0.91066300	3.08803300	-1.09330000
C	-0.72679700	3.05184200	0.67813100
C	1.34211900	4.34255900	-0.66779800
H	1.38980400	2.60385400	-1.93987200
C	-0.29335200	4.30219600	1.10541600
H	-1.52597500	2.54338900	1.21305100
C	0.74184800	4.94967600	0.43178200
H	2.15293100	4.83963600	-1.18983900
H	-0.75904600	4.76967600	1.96662000
H	1.08277900	5.92307400	0.76851300
H	-2.50037100	2.12538800	-1.38617400
C	2.55088800	-0.77354200	0.07641200
C	1.65046800	-1.64389700	-0.61217600
C	0.43152400	-0.55370400	0.91765800
C	1.73935600	0.10613300	0.74383100
H	1.12033100	-1.29419500	-1.48935500
H	1.93147800	1.15189000	0.98020500
O	0.04674900	-1.32036300	1.80856200

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C	4.02563400	-0.74696500	0.05715300
C	4.74329100	-1.26495200	-1.02804100
C	4.72996300	-0.15752200	1.11360000
C	6.13131000	-1.18851300	-1.05744200
H	4.19880000	-1.72124700	-1.84931100
C	6.11814900	-0.07055700	1.07987700
H	4.17410700	0.21474700	1.96972200
C	6.82253200	-0.58813300	-0.00529600
H	6.67678300	-1.59412200	-1.90401000
H	6.65166100	0.39090500	1.90511600
H	7.90619600	-0.52941100	-0.02942100
Cl	2.05959300	-3.37862300	-0.82260900

**M2**

C	-6.91981700	-0.78569600	0.30710000
C	-5.81101000	-1.60476700	0.50732300
C	-4.55644000	-1.10132300	0.19066300
C	-4.42166700	0.19808100	-0.31729900
C	-5.52225400	1.02192500	-0.52037400
C	-6.77529800	0.50887200	-0.19918100
C	-2.23009500	-0.50179100	-0.27483100
C	-0.88360200	1.19850200	-1.02787700
C	-2.38138200	1.65333000	-1.09660100
H	-7.90800900	-1.16072900	0.54833900
H	-5.92319400	-2.60927500	0.90044300
H	-5.40286700	2.02483200	-0.91536000
H	-7.65357500	1.12756800	-0.34700600
H	-0.45172500	1.16784400	-2.03220100
H	-2.70674800	1.85648600	-2.11885200

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N	-3.08451900	0.48752600	-0.56424700
S	-2.98397900	-1.91977400	0.35355100
N	-0.97498600	-0.19493600	-0.52374600
C	-0.03324400	2.08288300	-0.13998700
C	0.84729000	2.99427200	-0.71921000
C	-0.13128400	2.00312900	1.25024200
C	1.62962100	3.82225500	0.08407800
H	0.93644300	3.04490500	-1.80134500
C	0.65259100	2.82648600	2.05194700
H	-0.80239800	1.27932900	1.70657800
C	1.53458500	3.73781700	1.47008400
H	2.32074200	4.52217100	-0.37410600
H	0.58196100	2.75130400	3.13203600
H	2.14985800	4.37416100	2.09779900
H	-2.56696900	2.52812300	-0.46938700
C	2.60163400	-1.38901300	-0.26387800
C	2.62565300	-2.68899300	0.09280400
C	0.11323800	-1.15880100	-0.26517200
C	1.36613400	-0.69986000	-0.59158100
H	1.73562300	-3.29890400	0.11897500
H	1.47124200	0.28428500	-1.02330200
O	-0.29515800	-2.23277700	0.23002900
C	3.81363400	-0.51723900	-0.29636600
C	4.99989300	-0.90819200	-0.92536400
C	3.74673600	0.76063700	0.27459500
C	6.09598800	-0.05084400	-0.96746100
H	5.05595900	-1.88511500	-1.39447600
C	4.84405900	1.61521900	0.23842000
H	2.82228100	1.08050400	0.75084400

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C	6.02445400	1.21153800	-0.38201900
H	7.00724900	-0.36819100	-1.46514100
H	4.77135900	2.59911400	0.69300400
H	6.88128800	1.87720500	-0.41485700
Cl	4.04861400	-3.53151300	0.68509300

**TS1B**

C	0.60671100	-0.38957800	0.47980100
C	1.61166400	0.59580400	0.50139400
C	2.50997100	-1.24158200	0.07866100
C	1.30274300	-1.61316700	0.61989700
H	2.25675100	0.71607800	1.35946400
H	1.02855000	-2.55579300	1.07704200
O	3.50112600	-1.35371000	-0.53947500
C	-0.82618200	-0.26146600	0.20134700
C	-1.51246700	0.92055100	0.51238800
C	-1.53253100	-1.35083200	-0.32397100
C	-2.88204500	1.00709100	0.29820600
H	-0.97001200	1.75787800	0.93891600
C	-2.90367100	-1.26170800	-0.53421000
H	-0.99388200	-2.25708000	-0.58432500
C	-3.57810600	-0.08191900	-0.22619200
H	-3.41013600	1.92209900	0.54440400
H	-3.44440700	-2.10738800	-0.94576500
H	-4.64758300	-0.00946600	-0.39566800
Cl	1.49383500	2.08377600	-0.43071800

**TS1B'**

C	-0.60772600	-0.38972500	0.47918400
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C	-1.60774900	0.59965300	0.50076100
C	-2.51474900	-1.23001200	0.07749100
C	-1.30729600	-1.60978300	0.61598700
H	-2.26090600	0.71868200	1.35279300
H	-1.03523700	-2.55923100	1.06035600
O	-3.51326100	-1.34929400	-0.52797400
C	0.82531600	-0.26375400	0.20220500
C	1.51308500	0.91599800	0.51829800
C	1.52939500	-1.35171700	-0.32859100
C	2.88285000	1.00118400	0.30515300
H	0.97078100	1.75292500	0.94618200
C	2.90075700	-1.26383400	-0.53819600
H	0.98894700	-2.25538400	-0.59427900
C	3.57720800	-0.08687000	-0.22367600
H	3.41244200	1.91430000	0.55510000
H	3.43985500	-2.10826400	-0.95446100
H	4.64694800	-0.01560100	-0.39192800
Cl	-1.48254600	2.08353500	-0.43539200

**M1B**

C	-0.79677000	-0.03035300	0.32428600
C	-1.41869200	1.14793100	0.16681100
C	-2.80703900	-1.41291400	0.16945800
C	-1.60061200	-1.21916500	0.67317200
H	-2.47316900	1.28110100	0.37372200
H	-1.21097200	-1.99122300	1.32657700
O	-3.86510400	-1.58233900	-0.28177100
C	0.66119200	-0.26261100	0.15376400
C	1.60563700	0.61245400	0.70205800

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C	1.10483100	-1.40160700	-0.52691500
C	2.96552800	0.36142200	0.55317400
H	1.27136500	1.48119200	1.25925300
C	2.46537100	-1.64609800	-0.68338300
H	0.37416600	-2.09046600	-0.94036600
C	3.39921400	-0.76437400	-0.14395800
H	3.68816100	1.04452800	0.98763500
H	2.79541700	-2.52726900	-1.22404500
H	4.46081300	-0.95708900	-0.26055200
Cl	-0.67393500	2.59469600	-0.44699100

**TS2B**

C	-7.11846500	-0.81680700	0.20127100
C	-6.00660300	-1.65510900	0.30051800
C	-4.75443000	-1.12342800	0.03797500
C	-4.60719500	0.22402600	-0.32944600
C	-5.71201000	1.06211200	-0.42529000
C	-6.96857000	0.52366800	-0.15233700
C	-2.38050900	-0.46314800	-0.32001200
C	-1.08594800	1.25794200	-0.84927100
C	-2.55135700	1.79131900	-0.70002200
H	-8.10577700	-1.21579200	0.40507000
H	-6.11815700	-2.69652900	0.58288000
H	-5.59144600	2.10282200	-0.70625500
H	-7.84283700	1.16224500	-0.21861400
H	-0.80098200	1.27712500	-1.90882300
H	-2.87456400	2.37037100	-1.56633800
N	-3.28256700	0.53484300	-0.58291500
S	-3.18707300	-1.96084700	0.11954300



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N	-1.14002700	-0.15627400	-0.41669700
C	-0.08100000	2.06602200	-0.05950200
C	0.73984500	2.99021100	-0.70364500
C	0.01551200	1.91200100	1.32626700
C	1.63658500	3.76831300	0.02743900
H	0.67975300	3.10094600	-1.78332500
C	0.91142600	2.68595800	2.05707200
H	-0.60455300	1.17061700	1.82356400
C	1.72046600	3.62021000	1.40890600
H	2.27268700	4.48353100	-0.48437100
H	0.98396100	2.55735400	3.13229000
H	2.41904100	4.22315500	1.98067000
H	-2.67599500	2.39042100	0.20993800
C	2.82973000	-1.49023800	-0.19963300
C	3.04978300	-2.78223500	0.09635800
C	0.40790100	-1.63548300	0.08912900
C	1.46532100	-0.98334600	-0.40472300
H	2.25336800	-3.51453500	0.13655700
H	1.31383400	-0.03788400	-0.89859300
O	-0.21987400	-2.47715500	0.61612900
C	3.89384700	-0.45519700	-0.31825300
C	5.08272500	-0.70693000	-1.01206300
C	3.68382400	0.81791300	0.22521200
C	6.05224900	0.28328700	-1.13365300
H	5.23799300	-1.67753200	-1.47082100
C	4.65896800	1.80425600	0.11039500
H	2.75221300	1.03340800	0.74367400
C	5.84723800	1.53951900	-0.56618900
H	6.96697400	0.07464800	-1.67932600

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H	4.48072900	2.78270900	0.54638000
H	6.60568400	2.31013400	-0.66136500
Cl	4.58720000	-3.45679100	0.57255000

**TS3RR**

C	7.19878400	-0.77862000	-1.28577200
C	6.13096200	0.09478100	-1.46710800
C	4.84767500	-0.37618200	-1.21431100
C	4.65129700	-1.69523000	-0.78649800
C	5.71197300	-2.57571500	-0.60509700
C	6.99095400	-2.09561200	-0.86178200
C	2.49966500	-0.90315100	-0.81864900
C	1.06355900	-2.63685600	-0.27377900
C	2.54429800	-3.13625300	-0.22215300
H	8.20775200	-0.42964000	-1.47472400
H	6.29318200	1.11601000	-1.79399500
H	5.54257900	-3.59333900	-0.27058800
H	7.84078300	-2.75529200	-0.72622200
H	0.52455700	-3.12206000	-1.09342400
H	2.73637500	-3.94418600	-0.93045400
N	3.29760300	-1.94582400	-0.60052700
S	3.31848500	0.49899900	-1.38051200
N	1.21143400	-1.19345400	-0.62879500
C	0.34278000	-2.87878500	1.02979600
C	-0.82105900	-3.64765500	1.05126500
C	0.85497700	-2.34493300	2.21476600
C	-1.48246800	-3.88187500	2.25532700
H	-1.21690100	-4.05629200	0.12388100
C	0.19177400	-2.58290000	3.41496700

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H	1.71681400	-1.68011500	2.18770400
C	-0.97347100	-3.34811500	3.43769500
H	-2.38950300	-4.47740700	2.26777600
H	0.57605700	-2.14983800	4.33239800
H	-1.48801500	-3.52397600	4.37694800
H	2.82178300	-3.45310800	0.78525600
C	-2.19960900	0.16484800	-1.53401900
C	-2.06436700	1.45857200	-1.87702100
C	0.20651900	-0.21806100	-0.96061100
C	-1.16895500	-0.54230300	-0.75117700
H	-1.18133100	2.03744600	-1.65816100
H	-1.39159000	-1.58731800	-0.56435300
O	0.64859200	0.84915700	-1.38403300
C	-3.40784800	-0.63880000	-1.87943300
C	-4.69566500	-0.18535100	-1.57976600
C	-3.25960800	-1.89037500	-2.48775700
C	-5.80831400	-0.96003600	-1.88999100
H	-4.81658500	0.76439600	-1.06706000
C	-4.37291300	-2.66215200	-2.80900700
H	-2.26178500	-2.25304600	-2.72096500
C	-5.65184200	-2.19773000	-2.51103100
H	-6.80017700	-0.59903000	-1.63557200
H	-4.24091600	-3.62596500	-3.29064300
H	-6.52131100	-2.79958700	-2.75587800
Cl	-3.22585100	2.35549500	-2.83283500
N	0.67115000	0.61156400	1.92788100
N	-0.57905300	1.12304200	1.55409400
C	-1.43321900	0.12264500	1.26552100
H	-1.08288100	-0.85411700	1.57944200

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C	-1.10715100	2.35639900	2.15747800
H	-0.34170500	3.12782500	2.10360900
C	-2.37689500	2.79187200	1.43627700
H	-2.13317600	3.05642300	0.39886100
C	-3.37869400	1.66587300	1.46068900
C	-4.74809500	1.86188000	1.62908900
H	-5.13669300	2.87414700	1.70039800
C	-5.61147400	0.77238600	1.73340400
H	-6.67490700	0.93930600	1.87331500
C	-5.11090300	-0.52773100	1.67465500
H	-5.78247700	-1.37554500	1.76056600
C	-3.74839700	-0.73352500	1.49601400
H	-3.34013400	-1.74085900	1.44145800
C	-2.88241900	0.35696500	1.38598400
C	1.81398100	1.20646500	1.59348100
O	2.88549900	0.58027900	1.80704200
C	1.98039300	2.61062100	1.02179400
C	1.07837100	3.26851600	0.17852900
C	3.17557600	3.26261600	1.34862600
C	1.36254700	4.53922400	-0.31705900
H	0.16433100	2.77022300	-0.11454000
C	3.45413500	4.53871400	0.87084800
H	3.88352900	2.73358400	1.97664100
C	2.54694600	5.18269100	0.03122500
H	0.65366900	5.02402200	-0.98179700
H	4.38243600	5.02961500	1.14771000
H	2.76294500	6.17564800	-0.35138900
H	-1.31857100	2.15585700	3.21699900
H	-2.78791400	3.68329800	1.91808600

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**TS3RS**

C	-6.90280800	2.09031000	-1.10656400
C	-5.76670800	1.80545900	-1.85909400
C	-4.53038800	1.85641900	-1.22757600
C	-4.44437800	2.18649800	0.13176000
C	-5.57294400	2.47881600	0.88843300
C	-6.80566300	2.42410300	0.24787000
C	-2.24130400	1.85059700	-0.39617300
C	-0.98541000	2.04324900	1.52837000
C	-2.43710200	2.56108600	1.78393900
H	-7.87691100	2.05061900	-1.58099400
H	-5.84346800	1.54725200	-2.90943600
H	-5.48858800	2.73424800	1.93902200
H	-7.70563100	2.64391900	0.81128900
H	-0.25369300	2.82746800	1.73627400
H	-2.48055200	3.64679700	1.90183500
N	-3.12033100	2.17732800	0.54956900
S	-2.93333400	1.58581600	-1.94107100
N	-0.99585500	1.81395400	0.05507500
C	-0.67163200	0.82282900	2.37040000
C	0.47180800	0.81203000	3.16856000
C	-1.55966700	-0.25571200	2.41519100
C	0.73402200	-0.26974500	4.00858900
H	1.16538000	1.64920100	3.12949800
C	-1.30507700	-1.32548600	3.26705700
H	-2.43100000	-0.27549100	1.76107800
C	-0.15973600	-1.33555500	4.06454100
H	1.62901200	-0.27116100	4.62216600

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H	-1.99535600	-2.16324800	3.29651000
H	0.03593800	-2.17433100	4.72508000
H	-2.89091300	2.07496000	2.64805400
C	2.58531400	1.66753600	-0.73574900
C	2.74427000	2.14841400	-1.98179600
C	0.09145000	1.52363700	-0.84917200
C	1.32387300	1.04121200	-0.29511700
H	1.96107300	2.11828100	-2.72524400
H	1.29717700	0.82821100	0.76695200
O	-0.13868400	1.75755100	-2.03401100
C	3.64875800	1.74622700	0.30904800
C	3.97300700	0.63160900	1.09143300
C	4.28484200	2.96292100	0.58215100
C	4.93120500	0.72429700	2.09715800
H	3.48275000	-0.31827100	0.90200300
C	5.23596200	3.05757800	1.59323100
H	4.01978600	3.84216600	0.00411400
C	5.56763500	1.93663200	2.35128500
H	5.18009200	-0.15571200	2.68230000
H	5.71510000	4.01122000	1.79162700
H	6.31220400	2.01035300	3.13763300
Cl	4.24523200	2.79293200	-2.60938400
N	-0.94363000	-0.90731100	-0.62317400
N	0.27867900	-1.57713700	-0.60636800
C	1.25148500	-0.91967100	-1.25826300
H	0.93301300	-0.40115600	-2.16120200
C	0.67305600	-2.20145300	0.66511800
H	-0.19596200	-2.71271500	1.07607400
C	1.81469800	-3.17552600	0.43862600

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H	1.43276100	-4.04085200	-0.12020200
C	2.92738300	-2.53378700	-0.34895700
C	4.23797500	-2.99993200	-0.27833800
H	4.47342800	-3.81383100	0.40246600
C	5.23745100	-2.43898900	-1.06956400
H	6.25664600	-2.80430500	-0.99448500
C	4.91983200	-1.42757800	-1.97317300
H	5.68532900	-1.00539700	-2.61570700
C	3.61395200	-0.95873200	-2.05733800
H	3.36161800	-0.18401600	-2.77144000
C	2.61802900	-1.47395200	-1.21893000
C	-2.05518100	-1.61995000	-0.44694100
O	-3.15002900	-1.04766900	-0.22255700
C	-2.07411800	-3.13571900	-0.50075200
C	-1.30224200	-3.87837100	-1.39985500
C	-2.95135200	-3.80565300	0.35541500
C	-1.39536700	-5.26803100	-1.42506200
H	-0.63314500	-3.36655200	-2.08323400
C	-3.03162600	-5.19515700	0.34403300
H	-3.57375500	-3.21243600	1.01813400
C	-2.25107500	-5.92993900	-0.54677300
H	-0.80105600	-5.83529700	-2.13492800
H	-3.70890200	-5.70525800	1.02230400
H	-2.31619800	-7.01343700	-0.56303700
H	0.95969200	-1.40036700	1.36680900
H	2.18282300	-3.54578100	1.40002900
<b>TS3SR</b>			
C	7.00040600	-1.32570400	1.56132900

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C	5.84605200	-1.14773200	2.31794900
C	4.61917300	-1.30657900	1.68493700
C	4.55785200	-1.64274400	0.32731600
C	5.70636600	-1.82151600	-0.43497100
C	6.92949700	-1.65448300	0.20326400
C	2.33600200	-1.50363200	0.84653300
C	1.12068700	-1.62736800	-1.09246900
C	2.62343100	-1.91621300	-1.40037800
H	7.96876300	-1.20242900	2.03306900
H	5.90061800	-0.88604700	3.36887500
H	5.64249900	-2.07569100	-1.48714300
H	7.84498100	-1.78168800	-0.36381200
H	0.87268600	-0.62492100	-1.45686300
H	3.04233800	-1.16567100	-2.07119900
N	3.24027300	-1.76820700	-0.08569900
S	3.00059100	-1.12254000	2.38387800
N	1.08650800	-1.54183300	0.38827700
C	0.17428900	-2.66274300	-1.64796300
C	-0.50121400	-2.39678700	-2.83899100
C	-0.02211600	-3.88550500	-1.00258800
C	-1.36196100	-3.34564100	-3.38667700
H	-0.36157600	-1.43777200	-3.33199500
C	-0.89080200	-4.82893000	-1.54365400
H	0.49127200	-4.08810900	-0.06631200
C	-1.56057500	-4.56160000	-2.73773700
H	-1.88775400	-3.12767200	-4.31065400
H	-1.04954200	-5.77215100	-1.03136800
H	-2.24040400	-5.29706200	-3.15559600
H	2.78254100	-2.92820300	-1.78129100



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C	-2.49579700	-0.87789700	1.16139900
C	-2.67492400	-0.88972900	2.49296400
C	0.01621800	-1.01258800	1.19479300
C	-1.18934400	-0.61377100	0.54003800
H	-1.87388900	-0.73133800	3.19953300
H	-1.19303200	-0.71849200	-0.53889500
O	0.25046700	-0.95015900	2.40412900
C	-3.60136400	-1.08295100	0.17949600
C	-3.45949800	-2.05669200	-0.81668100
C	-4.74852600	-0.28496500	0.18804200
C	-4.45009900	-2.23657300	-1.77723700
H	-2.56918000	-2.68090400	-0.83237700
C	-5.73193900	-0.45495700	-0.78307200
H	-4.85516600	0.48373900	0.94715100
C	-5.58818100	-1.43232500	-1.76572300
H	-4.32480500	-3.00250700	-2.53690000
H	-6.61024500	0.18343700	-0.77351200
H	-6.35732100	-1.56445600	-2.52032800
Cl	-4.20899600	-1.23468200	3.26556200
N	1.07105700	1.20515200	-0.11025800
N	-0.11677800	1.92723200	-0.12181100
C	-0.97763500	1.53366300	0.82615700
H	-0.53455600	1.29628200	1.79242400
C	-0.62582000	2.46703900	-1.39999400
H	0.01099800	2.05513600	-2.18674400
C	-2.09143400	2.11033500	-1.63724300
H	-2.19197300	1.03409800	-1.83828900
C	-2.90296700	2.45202700	-0.41740000
C	-4.16194500	3.03932700	-0.45230900

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H	-4.60686600	3.29778900	-1.40929500
C	-4.85289700	3.28793800	0.73419900
H	-5.83494300	3.74907900	0.69951200
C	-4.28740300	2.94452100	1.96079200
H	-4.82643600	3.13449000	2.88292600
C	-3.02496900	2.35737900	2.00300200
H	-2.57336000	2.08885400	2.95331100
C	-2.32855900	2.11960000	0.81692700
C	2.18362500	1.74431300	-0.61043500
O	3.17983900	1.01870600	-0.83996500
C	2.31857600	3.22460000	-0.89821100
C	1.73740000	4.20731900	-0.09147200
C	3.12229700	3.61338300	-1.97200100
C	1.94099800	5.55633900	-0.37096000
H	1.12778800	3.91308100	0.75727000
C	3.31162600	4.96047200	-2.26381400
H	3.59817600	2.83850600	-2.56417900
C	2.71956400	5.93562400	-1.46299000
H	1.49393500	6.31276500	0.26662200
H	3.92607300	5.25138200	-3.11025900
H	2.87079400	6.98769100	-1.68385500
H	-0.49757000	3.55500800	-1.39919400
H	-2.45578100	2.64372400	-2.51911800
<b>TS3SS</b>			
C	6.36289100	-2.32465600	1.52403100
C	5.29403400	-1.74663800	2.20186000
C	4.03812700	-1.80404400	1.60961200
C	3.86243200	-2.43660200	0.37433700

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C	4.92503400	-3.01451400	-0.30941700
C	6.17960500	-2.94576700	0.28332100
C	1.73335800	-1.73783700	0.81593700
C	0.42971200	-2.10862600	-1.03874900
C	1.88605900	-2.60311500	-1.30851100
H	7.35291500	-2.28839300	1.96460500
H	5.43674500	-1.26103400	3.16091500
H	4.77465600	-3.49056800	-1.27196900
H	7.03103300	-3.38303600	-0.22629500
H	0.23987500	-1.23963900	-1.67192600
H	2.40032800	-1.96505000	-2.03027200
N	2.53009800	-2.39663200	-0.01280200
S	2.51591600	-1.13154900	2.21715500
N	0.48662800	-1.61822000	0.35990500
C	-0.63741700	-3.16246700	-1.21388100
C	-1.47860800	-3.12046400	-2.32508600
C	-0.79827200	-4.17538500	-0.26540800
C	-2.47408000	-4.08117300	-2.48963100
H	-1.36312700	-2.32466800	-3.05663600
C	-1.79564200	-5.13224000	-0.42648100
H	-0.15591700	-4.20033000	0.61124900
C	-2.63412200	-5.08698700	-1.54014200
H	-3.13103400	-4.03586400	-3.35202500
H	-1.92242800	-5.91042100	0.31886800
H	-3.41392500	-5.83175700	-1.66324000
H	1.91952700	-3.65497200	-1.59790500
C	-2.75992600	0.12033800	0.87210400
C	-2.75170100	0.93381500	1.93916100
C	-0.38489200	-0.63723500	0.94887200

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C	-1.49763000	-0.17745700	0.15178900
H	-1.85253500	1.41808800	2.29216900
H	-1.67518200	-0.78326600	-0.73089200
O	-0.08982000	-0.29987100	2.09237800
C	-3.99131800	-0.53153500	0.33666200
C	-3.96596700	-1.88778900	-0.01494100
C	-5.17763100	0.18700200	0.14079100
C	-5.09972500	-2.51088600	-0.52896900
H	-3.05356100	-2.46400800	0.12247100
C	-6.30740700	-0.43415500	-0.38206300
H	-5.20275700	1.24286900	0.38823900
C	-6.27415900	-1.78674700	-0.71544500
H	-5.05749500	-3.56460000	-0.78740800
H	-7.21554300	0.14123900	-0.53333900
H	-7.15653800	-2.27039100	-1.12257900
Cl	-4.12552700	1.26993300	2.96497000
N	1.37777400	0.75684500	-0.79298300
N	0.51699400	1.83112500	-0.52650600
C	-0.75462400	1.58163000	-0.88495900
H	-0.84235300	1.04182800	-1.82203100
C	0.70530000	2.57917700	0.73048100
H	1.77517000	2.73554300	0.86699500
C	-0.02546700	3.91017400	0.64054200
H	0.50552500	4.55644300	-0.07117500
C	-1.44753800	3.72909400	0.17115000
C	-2.43460900	4.67970300	0.43258800
H	-2.18592500	5.54670200	1.03866600
C	-3.72011200	4.53142400	-0.07785300
H	-4.47737500	5.27900500	0.13532900

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C	-4.03302900	3.42435200	-0.86756900
H	-5.03275500	3.30479600	-1.27300000
C	-3.06198800	2.46620600	-1.12378900
H	-3.30615000	1.58165600	-1.70798000
C	-1.77236600	2.60783000	-0.60494800
C	2.66320100	1.02029300	-1.03129000
O	3.48981600	0.08458300	-1.13996600
C	3.20856300	2.42833500	-1.17650300
C	2.54431600	3.44842200	-1.86484600
C	4.47340300	2.68358400	-0.64028000
C	3.13174800	4.70564900	-1.99566100
H	1.56904400	3.25814600	-2.30045100
C	5.05141100	3.94421700	-0.75249500
H	4.99205200	1.87191500	-0.14005400
C	4.37982000	4.95990900	-1.43107000
H	2.61324500	5.48823600	-2.54126700
H	6.02850700	4.13295400	-0.31829000
H	4.83042900	5.94288300	-1.52709700
H	0.33391700	1.97042800	1.56308300
H	-0.00419000	4.41266500	1.61216800

**M4RR**

C	-7.62494200	0.66843400	-1.09551700
C	-6.36237200	1.15417900	-1.44335800
C	-5.25976300	0.69828900	-0.73967300
C	-5.40587000	-0.24633700	0.29134500
C	-6.66137200	-0.73044000	0.64027700
C	-7.76844500	-0.25849900	-0.06446700
C	-3.10630400	0.15084900	0.39824200

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C	-2.25627100	-1.01467500	2.05328100
C	-3.81274500	-1.20509000	2.10446100
H	-8.49846800	1.01949200	-1.63354400
H	-6.24701700	1.88028000	-2.24111400
H	-6.76776900	-1.45873000	1.43718200
H	-8.75597700	-0.62401100	0.19634800
H	-1.89112700	-0.66605500	3.02408900
H	-4.27163700	-0.66488400	2.94064800
N	-4.18440600	-0.59069100	0.83935800
S	-3.55724300	1.15193100	-0.97938700
N	-2.00341400	0.02683300	1.03243900
C	-1.54107500	-2.30682800	1.70272000
C	-1.06276200	-3.13435600	2.72106500
C	-1.38435400	-2.70302000	0.37251800
C	-0.43898800	-4.34316600	2.41885600
H	-1.17310000	-2.82566000	3.75794500
C	-0.76793800	-3.91531600	0.07035700
H	-1.71378100	-2.05323600	-0.43454800
C	-0.29283400	-4.73753200	1.09043400
H	-0.06506300	-4.97343400	3.21962200
H	-0.65715300	-4.20967200	-0.96893900
H	0.19357400	-5.67821300	0.85211200
H	-4.10220900	-2.25727800	2.14509700
C	1.63546800	2.34667500	-0.41402500
C	2.88689000	2.02248300	-0.74971700
C	0.15792900	0.37049000	-0.93547300
C	0.72872700	1.26889900	0.17130200
H	3.29231200	1.03141600	-0.58359200
H	-0.12201800	1.73138700	0.67338000

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O	-0.67292900	0.66264800	-1.76101400
C	1.04147700	3.70286400	-0.54151200
C	1.70982700	4.82481800	-0.03934100
C	-0.23104600	3.86102900	-1.10422600
C	1.12518200	6.08507400	-0.11657200
H	2.68265300	4.70229400	0.42647900
C	-0.80812400	5.12437400	-1.18815400
H	-0.75668400	2.98841800	-1.48359800
C	-0.13230100	6.23895500	-0.69624500
H	1.65079600	6.94719200	0.28154100
H	-1.79058100	5.23689700	-1.63567900
H	-0.58644200	7.22275500	-0.75857400
Cl	4.03019100	3.10206500	-1.49554800
N	0.85865500	-0.84046900	-0.88237200
N	1.90308900	-0.78543200	0.10092600
C	1.36896700	0.20697700	1.05919900
H	0.52151700	-0.26075800	1.59140900
C	2.12819000	-2.03306300	0.84387600
H	2.30244100	-2.86050900	0.15485500
C	3.38309200	-1.77808000	1.67889600
H	4.25416200	-1.81801000	1.01328200
C	3.37640400	-0.43427800	2.38461200
C	4.34103400	-0.15019900	3.35395200
H	5.07451600	-0.91171400	3.60763100
C	4.37384100	1.08468800	3.99208700
H	5.13103800	1.28563900	4.74318500
C	3.43488600	2.06126000	3.66460200
H	3.45730400	3.02872800	4.15544200
C	2.47019700	1.79326000	2.69960100

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H	1.74107000	2.55482000	2.43206100
C	2.43839500	0.55420800	2.05889400
C	0.84653800	-1.77206600	-1.93448700
O	-0.18551400	-2.00086000	-2.52856700
C	2.12764000	-2.45596200	-2.28984800
C	3.36448500	-1.80640000	-2.24454900
C	2.04167600	-3.76947600	-2.75675800
C	4.51099100	-2.48068500	-2.65093700
H	3.42110600	-0.78045600	-1.89982900
C	3.19336300	-4.44614900	-3.14258600
H	1.06792400	-4.24504600	-2.81554100
C	4.42791800	-3.80222000	-3.08771100
H	5.47000600	-1.97399900	-2.62750800
H	3.12801900	-5.47098300	-3.49227700
H	5.32679800	-4.32845400	-3.39258300
H	1.25891200	-2.28161600	1.47005600
H	3.50392500	-2.58239700	2.41114200

**M4RS**

C	-6.81116100	-0.12306100	0.46606900
C	-5.76373000	0.73527900	0.12286500
C	-4.48867400	0.44533000	0.57993500
C	-4.25625200	-0.68641000	1.38109400
C	-5.29487400	-1.54615200	1.72052700
C	-6.57490600	-1.25195800	1.24952800
C	-2.07149700	0.08520300	1.08256400
C	-0.72531200	-1.18965600	2.25151200
C	-2.11519300	-1.88336300	2.24947000
H	-7.81389500	0.09001500	0.11221300



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H	-5.93999800	1.60032300	-0.50839300
H	-5.10487400	-2.42176300	2.33251400
H	-7.39686600	-1.91377000	1.50119100
H	-0.61144400	-0.68776200	3.22385000
H	-2.42746000	-2.19277300	3.24810800
N	-2.92545800	-0.78634200	1.73779200
S	-2.98389600	1.29726100	0.18734600
N	-0.81671900	-0.10711700	1.23347400
C	0.48683800	-2.06635100	2.04534700
C	1.67268900	-1.72871000	2.70458300
C	0.48944800	-3.15385600	1.17370200
C	2.83898000	-2.45809000	2.49515200
H	1.67879900	-0.87964500	3.38515100
C	1.65333400	-3.88946500	0.96519300
H	-0.40554300	-3.41986500	0.62214900
C	2.83069600	-3.54416800	1.62259500
H	3.75448600	-2.17627800	3.00477300
H	1.63790600	-4.72848800	0.27611100
H	3.74244400	-4.10763000	1.44989000
H	-2.16862700	-2.74547300	1.57136000
C	2.01612200	2.40181300	-0.28169500
C	3.15901500	2.88606000	-0.77163300
C	0.45755100	0.64688500	-1.21999000
C	1.71780000	0.92868400	-0.40911000
H	3.90191100	2.27491000	-1.26883300
H	1.48500200	0.49768500	0.57729200
O	-0.46837400	1.38555900	-1.42733000
C	0.98912100	3.20972500	0.43090000
C	0.44066900	4.35644300	-0.15121300

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C	0.52401600	2.79420300	1.68202500
C	-0.54813800	5.07770200	0.50897400
H	0.77837400	4.66723500	-1.13471500
C	-0.46243700	3.51885600	2.34412300
H	0.92348000	1.89305500	2.13723200
C	-1.00188100	4.66143200	1.75931600
H	-0.97224100	5.96083700	0.04203200
H	-0.81458000	3.18458900	3.31490500
H	-1.77843600	5.22067100	2.27131500
Cl	3.66976700	4.54433800	-0.63390300
N	0.60462600	-0.66536300	-1.73553400
N	1.86898300	-1.19733600	-1.31500700
C	2.70471600	0.00181600	-1.09336100
H	2.99706600	0.44149700	-2.06847400
C	2.45830500	-2.12230600	-2.29495600
H	2.13002900	-1.86022000	-3.31118100
C	4.00184500	-2.08217500	-2.22456300
H	4.37378200	-1.40717300	-3.00546100
C	4.53908300	-1.59031300	-0.90379900
C	5.62966700	-2.16253100	-0.25749400
H	6.10370000	-3.04416600	-0.68071300
C	6.11782300	-1.60237000	0.92323100
H	6.97399600	-2.04915300	1.41885700
C	5.51205200	-0.47181100	1.46365700
H	5.89274200	-0.03665200	2.38222800
C	4.40211100	0.09414700	0.83500300
H	3.91241000	0.96385400	1.26551000
C	3.92287000	-0.46298900	-0.34459300
C	-0.43678700	-1.59657000	-1.85452700

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O	-0.21372100	-2.78316300	-1.70559500
C	-1.80210500	-1.11594600	-2.21274900
C	-2.03488300	-0.13936400	-3.17964300
C	-2.87564300	-1.77918800	-1.61071200
C	-3.34241200	0.18209100	-3.53051900
H	-1.19833700	0.36476300	-3.65014100
C	-4.18035500	-1.43907300	-1.94541200
H	-2.67254200	-2.55578800	-0.87789300
C	-4.41257500	-0.45669200	-2.90702500
H	-3.52535400	0.93668500	-4.28837700
H	-5.01406500	-1.92197700	-1.44341000
H	-5.43178400	-0.18909400	-3.16876900
H	2.08785600	-3.12002800	-2.06306200
H	4.39946600	-3.07302700	-2.45633000

**M4SR**

C	-7.41324900	-1.69171400	-0.26022400
C	-6.45321300	-0.74149500	-0.61446100
C	-5.14670500	-0.92995700	-0.19405500
C	-4.79154400	-2.06249000	0.55915600
C	-5.74494100	-3.00966300	0.91391500
C	-7.06049500	-2.80796900	0.49682200
C	-2.74922800	-0.93093800	0.49039500
C	-1.27465400	-2.05829000	1.65922200
C	-2.65992500	-2.76117600	1.86276100
H	-8.44103900	-1.55523800	-0.57765500
H	-6.72475600	0.13091200	-1.19935800
H	-5.46449900	-3.88137200	1.49559700
H	-7.81820000	-3.53615100	0.76637900

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H	-0.82853500	-1.82955500	2.63295000
H	-3.08249700	-2.57274300	2.85685400
N	-3.43846500	-2.07444300	0.84470100
S	-3.74825200	0.12253600	-0.50650800
N	-1.55800300	-0.79668900	0.93831900
C	-0.31079000	-2.94049200	0.88283400
C	0.42581100	-3.91421400	1.56574800
C	-0.17270000	-2.82956600	-0.50206400
C	1.28268200	-4.76706300	0.87647900
H	0.32862300	-4.00000600	2.64593500
C	0.69103800	-3.68056900	-1.19083700
H	-0.71161200	-2.05162900	-1.03725800
C	1.41670200	-4.65126900	-0.50660700
H	1.85329300	-5.51455400	1.41884100
H	0.80874500	-3.56799400	-2.26477000
H	2.09572200	-5.30444200	-1.04515700
H	-2.61034000	-3.83698900	1.68277000
C	2.08740500	-0.55322500	-1.58199900
C	1.75345900	-0.68428600	-2.86807000
C	-0.09452900	0.78810800	-1.17910500
C	1.22532600	0.24994500	-0.63028900
H	0.86410100	-0.25282700	-3.30275300
H	0.93730000	-0.40426800	0.20375400
O	-0.85032000	0.26089700	-1.95958500
C	3.31116600	-1.14731000	-0.97572000
C	3.22983700	-1.87686800	0.21504000
C	4.56778400	-0.92343400	-1.54803400
C	4.37905500	-2.38467900	0.81062700
H	2.26289500	-2.05881800	0.67660600

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C	5.71848100	-1.42233000	-0.94543400
H	4.64030000	-0.33872300	-2.46008300
C	5.62715800	-2.15611700	0.23476100
H	4.29741200	-2.95540000	1.73056600
H	6.68735000	-1.23441700	-1.39734900
H	6.52484000	-2.54522300	0.70490600
Cl	2.63769300	-1.66086800	-4.01155500
N	-0.25194600	2.06694700	-0.63008400
N	0.75800500	2.40952700	0.29780200
C	1.89672000	1.53788900	-0.07156500
H	2.42703300	2.02353100	-0.90164800
C	0.27875100	2.32780800	1.70042100
H	-0.81357400	2.32816000	1.67321500
C	0.79663700	1.11773100	2.48281800
H	0.30819900	0.21253100	2.10569500
C	2.29307100	1.04708100	2.34390800
C	3.14781700	0.78263600	3.41274600
H	2.72576100	0.58025700	4.39373000
C	4.52830300	0.78589400	3.23127400
H	5.18443900	0.57085400	4.06882600
C	5.06574600	1.08211600	1.98032100
H	6.14105000	1.09579000	1.83539900
C	4.21906100	1.36149200	0.91230400
H	4.63207500	1.58772800	-0.06675700
C	2.83700000	1.32414000	1.08417600
C	-1.23429400	2.99629800	-0.99450000
O	-2.21341800	2.65580500	-1.62483800
C	-1.04924600	4.42145800	-0.56176800
C	0.18028800	5.08677800	-0.58429900

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C	-2.21361700	5.12107400	-0.23572200
C	0.23724500	6.44034500	-0.27020600
H	1.08157500	4.54665900	-0.84682400
C	-2.14794600	6.46847700	0.10300600
H	-3.16304000	4.59594100	-0.25447100
C	-0.92186300	7.12878700	0.08493700
H	1.18981200	6.95896300	-0.29980800
H	-3.05236900	7.00377600	0.37222900
H	-0.86923500	8.18191200	0.34232100
H	0.60424400	3.24554200	2.20116100
H	0.51331200	1.22330300	3.53466100

**M4SS**

C	-7.30289300	-1.70572200	-1.69738500
C	-6.24478200	-0.88412700	-2.09139800
C	-5.07349200	-0.91196500	-1.35174900
C	-4.95716600	-1.73798500	-0.22079000
C	-6.00736000	-2.56016600	0.17109700
C	-7.18015700	-2.53503300	-0.58384300
C	-2.82111700	-0.79566200	-0.29108400
C	-1.62698600	-1.61797500	1.35860700
C	-2.96828400	-2.41753000	1.31308500
H	-8.22433200	-1.69866400	-2.26876900
H	-6.33171600	-0.24442900	-2.96331300
H	-5.91151400	-3.19896200	1.04274300
H	-8.00928200	-3.17161500	-0.29398300
H	-1.64942200	-0.94859500	2.23145000
H	-3.44495700	-2.49551000	2.29138400
N	-3.72764200	-1.57920400	0.39512700

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S	-3.58107100	0.00106100	-1.66431500
N	-1.61501400	-0.77878600	0.13733100
C	-0.41075800	-2.50801500	1.46974000
C	0.19657300	-2.72486500	2.70746700
C	0.09296700	-3.16109900	0.34050000
C	1.28631300	-3.58655400	2.82121500
H	-0.18319500	-2.21171500	3.58730600
C	1.18541100	-4.01748000	0.45157200
H	-0.37940800	-2.99041300	-0.62416700
C	1.78444900	-4.23323400	1.69302500
H	1.75168700	-3.74221300	3.78925000
H	1.56799100	-4.52169000	-0.43100400
H	2.63792600	-4.89855500	1.77656500
H	-2.83020300	-3.42112300	0.89017200
C	2.47307100	0.26374400	-1.83042000
C	2.50931700	1.12018600	-2.85379500
C	0.02885900	0.91237500	-1.53315500
C	1.21515600	0.12312400	-0.98540400
H	1.68124700	1.76031500	-3.13201100
H	0.91157400	-0.92914000	-0.98733700
O	-0.61440500	0.66894900	-2.52504800
C	3.60649100	-0.63335600	-1.47728500
C	3.41496500	-2.01658700	-1.43780600
C	4.85373000	-0.10609300	-1.13147500
C	4.45245200	-2.86089200	-1.05265000
H	2.44843100	-2.43476000	-1.70615000
C	5.88708300	-0.94890300	-0.74006400
H	4.99487700	0.97079800	-1.13766700
C	5.68951800	-2.32832600	-0.69909200

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H	4.29193600	-3.93452500	-1.02622500
H	6.84566300	-0.52759200	-0.45397900
H	6.49674700	-2.98440800	-0.38926900
Cl	3.86473500	1.30106200	-3.93125700
N	-0.20286000	1.96397600	-0.64169800
N	0.71449300	2.00751300	0.43546100
C	1.25133300	0.63250500	0.48592600
H	0.49967200	0.03435000	1.01279000
C	1.74744200	3.02480900	0.16625600
H	1.23738000	3.98786200	0.07333900
C	2.72105400	3.04339100	1.33367700
H	2.20042100	3.41491600	2.22452500
C	3.27192300	1.66592400	1.61641500
C	4.48240900	1.49677200	2.29828500
H	5.05214500	2.37670100	2.58654700
C	4.95505700	0.22913600	2.61213100
H	5.89939600	0.11756600	3.13586000
C	4.21182300	-0.89852400	2.25529500
H	4.56937300	-1.89484000	2.49671900
C	3.01321900	-0.74151300	1.57712300
H	2.43196900	-1.61204100	1.28220100
C	2.54974200	0.53297000	1.23817300
C	-1.37332900	2.74087700	-0.62912100
O	-1.93575800	3.02254400	-1.66485700
C	-1.90022000	3.16735800	0.70240100
C	-2.57091200	4.38885800	0.77075100
C	-1.85110300	2.32734700	1.81805900
C	-3.16358000	4.78943600	1.96370100
H	-2.62138700	5.01111700	-0.11697700



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C	-2.46521800	2.72064800	3.00138900
H	-1.34724400	1.36935700	1.73969800
C	-3.11140200	3.95454100	3.07791100
H	-3.67236000	5.74588800	2.02258800
H	-2.44020100	2.06653400	3.86685800
H	-3.58023100	4.26270300	4.00716700
H	2.27794100	2.82368100	-0.77439200
H	3.53457500	3.74320500	1.12050000

**TS4RR**

C	-7.36246800	0.95167200	-0.85130900
C	-6.15313000	1.01309500	-1.54298100
C	-4.97923300	0.76121300	-0.84699500
C	-5.01949100	0.44553700	0.51822000
C	-6.21982000	0.38408500	1.21570300
C	-7.39265500	0.64425200	0.51010500
C	-2.73639100	0.39635100	0.11119200
C	-1.68075200	-0.18369700	2.01683700
C	-3.18679800	0.08235300	2.34572400
H	-8.28876000	1.14765900	-1.37970500
H	-6.12891600	1.25598000	-2.60007300
H	-6.23664400	0.13883000	2.27214300
H	-8.34322700	0.60346400	1.03075300
H	-1.04841700	0.44210400	2.65454600
H	-3.33508000	1.01369900	2.90180000
N	-3.74060700	0.21129800	1.00312900
S	-3.31731400	0.79883300	-1.47800100
N	-1.54412800	0.25372500	0.60779000
C	-1.30720300	-1.64055200	2.21308200

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C	-0.70624000	-2.03972100	3.40732800
C	-1.59718600	-2.59193700	1.23401500
C	-0.38840600	-3.37945100	3.62198200
H	-0.47242700	-1.29743000	4.16721300
C	-1.27594500	-3.92934800	1.44796700
H	-2.02831000	-2.27869300	0.28644400
C	-0.67126300	-4.32603200	2.64038200
H	0.08701600	-3.68009700	4.55012800
H	-1.49022700	-4.66309900	0.67700400
H	-0.41780900	-5.36883900	2.80204200
H	-3.63980900	-0.74886700	2.88878000
C	1.74112500	2.10745100	-0.49861900
C	2.76429100	1.61211700	-1.19542300
C	-0.17818200	0.43826100	-0.50835200
C	0.89749500	1.17699400	0.35990900
H	3.04013400	0.56495900	-1.16060000
H	0.38036400	1.78373600	1.10695100
O	-0.65635600	0.96118300	-1.52994200
C	1.36847100	3.54622300	-0.45860000
C	2.31436900	4.51349500	-0.10288500
C	0.04610000	3.93770000	-0.69878100
C	1.94927300	5.85295800	-0.00411000
H	3.33480100	4.20744300	0.10915100
C	-0.31265300	5.27940000	-0.60684000
H	-0.67876400	3.17628000	-0.97664000
C	0.63557100	6.23961200	-0.25962600
H	2.69107000	6.59417900	0.27658200
H	-1.33746800	5.57605300	-0.80806300
H	0.35152000	7.28461500	-0.18522200

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Cl	3.78012200	2.54697000	-2.25968700
N	0.35469900	-0.95378500	-0.59325800
N	1.66933200	-1.02926800	-0.02343700
C	1.62113300	0.00995500	1.02124500
H	0.95524900	-0.34914100	1.82627600
C	1.97572500	-2.30255700	0.64328800
H	1.80519600	-3.13604900	-0.03838500
C	3.45707200	-2.23092300	1.01022700
H	4.04516900	-2.35811800	0.09250000
C	3.84840300	-0.91773000	1.65976000
C	5.09487600	-0.78331300	2.27687700
H	5.76587800	-1.63847700	2.30156900
C	5.48299400	0.42020300	2.85441700
H	6.45535400	0.50588300	3.32894500
C	4.62177700	1.51598600	2.82012900
H	4.91967100	2.46041600	3.26394500
C	3.37988800	1.39661800	2.20664200
H	2.70977600	2.25237500	2.16450600
C	2.99019300	0.18870800	1.62616400
C	-0.09293100	-1.78999400	-1.58190500
O	-1.28139200	-1.80403700	-1.88400600
C	0.87388500	-2.70234800	-2.27666500
C	2.14970500	-2.27923100	-2.65862400
C	0.42888100	-3.97814300	-2.62566700
C	2.97831500	-3.13912200	-3.37254800
H	2.48005600	-1.27938000	-2.40003300
C	1.26672900	-4.84270500	-3.32278800
H	-0.57679700	-4.27548300	-2.34592200
C	2.54250600	-4.42332000	-3.69572100

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H	3.96377200	-2.80564700	-3.68102200
H	0.92355300	-5.83878800	-3.58279000
H	3.19473900	-5.09428000	-4.24582400
H	1.33900600	-2.44576300	1.53034900
H	3.71399000	-3.06499800	1.67083700

**TS4RS**

C	-6.89485800	-1.84913400	-0.87186300
C	-5.75387500	-1.67010400	-1.65452700
C	-4.57353700	-1.29563100	-1.02928400
C	-4.53959000	-1.09520500	0.35881600
C	-5.67180700	-1.27165900	1.14551700
C	-6.85135900	-1.65300500	0.50922800
C	-2.33080800	-0.64941100	-0.20752500
C	-1.21094600	-0.07962600	1.65283800
C	-2.66040100	-0.50076600	2.06986200
H	-7.82410100	-2.14590800	-1.34539400
H	-5.78608400	-1.82485000	-2.72784000
H	-5.63044300	-1.11658000	2.21836700
H	-7.74880800	-1.79947800	1.10063700
H	-1.09617900	0.99849600	1.81674400
H	-3.17109600	0.28827200	2.62703000
N	-3.27598000	-0.70715500	0.76714200
S	-2.99072700	-1.00263600	-1.78356000
N	-1.14321900	-0.34090000	0.19865400
C	-0.13397900	-0.81772300	2.40974700
C	0.54534300	-0.18540800	3.45000700
C	0.18416600	-2.13701400	2.07435000
C	1.54598600	-0.86070100	4.14779600

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H	0.30404800	0.84572800	3.69868700
C	1.18010300	-2.81129700	2.77369300
H	-0.32673600	-2.61266500	1.23916300
C	1.86639800	-2.17245600	3.80738500
H	2.07835500	-0.35965700	4.94986200
H	1.43697200	-3.83013200	2.49939900
H	2.65085500	-2.69663600	4.34372400
H	-2.66802800	-1.43035300	2.64888600
C	0.04837900	2.57095500	-0.93121700
C	0.19113800	3.12706300	-2.13084200
C	0.10541200	0.07279900	-1.11877200
C	0.80498600	1.33392400	-0.53161400
H	0.89656500	2.78501400	-2.87777000
H	0.82104100	1.27110300	0.56284100
O	-0.54472400	0.10745400	-2.16673100
C	-1.00798800	2.96139100	0.04260800
C	-0.67766900	3.56178400	1.25991700
C	-2.32950000	2.57722300	-0.20227200
C	-1.66099400	3.77478200	2.22480200
H	0.35342400	3.84845300	1.45176300
C	-3.30799600	2.77482600	0.76890400
H	-2.56540200	2.08858900	-1.14468500
C	-2.97402500	3.37253900	1.98458200
H	-1.40013800	4.24733600	3.16648500
H	-4.32880800	2.45594400	0.57871300
H	-3.73628700	3.52729600	2.74160300
Cl	-0.74199300	4.49573800	-2.66658800
N	1.15114800	-0.94764100	-0.94920000
N	2.43473600	-0.37899900	-0.72854300

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C	2.24615700	1.06254000	-1.01880700
H	2.27710900	1.16929200	-2.11148800
C	2.91406400	-0.63843100	0.63882500
H	2.90919100	-1.72078000	0.78394200
C	4.32118400	-0.08458900	0.74092600
H	4.96881100	-0.62461600	0.03875900
C	4.32287200	1.38870900	0.42146100
C	5.30685800	2.22982300	0.94802300
H	6.06834400	1.80233900	1.59542400
C	5.32072300	3.58857000	0.66150800
H	6.09181000	4.22691300	1.08075900
C	4.33743400	4.12403500	-0.16825000
H	4.33747800	5.18259300	-0.40685500
C	3.35485700	3.29716500	-0.69849700
H	2.59868900	3.71950000	-1.35104300
C	3.32971800	1.92809000	-0.40658900
C	0.94833900	-2.27296700	-1.19586700
O	-0.18557500	-2.73371500	-1.27949900
C	2.14096700	-3.18721600	-1.27137300
C	3.32575900	-2.87003900	-1.94181200
C	1.98904900	-4.45025200	-0.69376600
C	4.34959700	-3.80976400	-2.01803300
H	3.44165000	-1.89242600	-2.39360700
C	3.02362900	-5.37832300	-0.75118800
H	1.04776800	-4.69161900	-0.20953000
C	4.20602200	-5.05825900	-1.41492800
H	5.26302900	-3.56599400	-2.55091200
H	2.90370300	-6.35283200	-0.28889400
H	5.01219300	-5.78304800	-1.46964000

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H	2.26761000	-0.19229500	1.40708100
H	4.71571700	-0.25284700	1.74759300
<b>TS4SR</b>			
C	7.06097500	-2.39008600	0.51387800
C	6.05834900	-1.90239200	1.35270200
C	4.83731900	-1.55641300	0.79341100
C	4.62274800	-1.69645400	-0.58624900
C	5.61807300	-2.17820500	-1.42820700
C	6.84164200	-2.52294900	-0.85766600
C	2.57473400	-0.84242200	0.09850100
C	1.21117600	-0.70700300	-1.67702300
C	2.64180300	-1.10173700	-2.18936600
H	8.02071000	-2.66649600	0.93607500
H	6.22975900	-1.79315900	2.41840300
H	5.44126000	-2.28078100	-2.49344700
H	7.63416300	-2.90044800	-1.49467800
H	0.88472900	0.22371600	-2.15741300
H	3.12157000	-0.29872200	-2.75651200
N	3.33709800	-1.30856400	-0.92471400
S	3.41327400	-0.89271900	1.62667700
N	1.38412100	-0.46852100	-0.23394700
C	0.18948100	-1.79921600	-1.94196000
C	-0.57953500	-1.77444000	-3.10788900
C	0.04492400	-2.86515600	-1.05033900
C	-1.47955700	-2.80384800	-3.38130000
H	-0.47333700	-0.94671200	-3.80574100
C	-0.85596200	-3.89067500	-1.32180400
H	0.62116000	-2.87768400	-0.12994700

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C	-1.61810800	-3.86386900	-2.48840500
H	-2.07529100	-2.77307900	-4.28797900
H	-0.97105500	-4.70464100	-0.61338000
H	-2.32649400	-4.65980300	-2.69376500
H	2.62265200	-2.01478800	-2.78798300
C	-1.59743100	-1.13441500	1.39671200
C	-0.84592000	-1.82354400	2.26115100
C	0.40122000	0.51988900	1.01747200
C	-1.03604300	0.07308000	0.67715300
H	0.14035200	-1.50657100	2.56513100
H	-1.05319800	-0.17364900	-0.38940100
O	0.97813300	0.32283800	2.09339200
C	-2.96605600	-1.56750500	0.99416000
C	-3.30708500	-1.69778800	-0.35571300
C	-3.94145800	-1.82413900	1.96336000
C	-4.58994200	-2.08763900	-0.72616900
H	-2.56570500	-1.50446300	-1.12727100
C	-5.22563900	-2.20958600	1.59327100
H	-3.69061900	-1.70458500	3.01297400
C	-5.55358300	-2.34470800	0.24636400
H	-4.83455300	-2.18697900	-1.77952600
H	-5.97245300	-2.39798800	2.35819100
H	-6.55591900	-2.64348000	-0.04414000
Cl	-1.32003000	-3.35170100	2.96632500
N	0.44784100	1.86528500	0.42618800
N	-0.84172000	2.39407900	0.17421500
C	-1.77629600	1.43351300	0.81191200
H	-1.84045100	1.68466300	1.87845500
C	-1.06834600	2.71315900	-1.25276400



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H	-0.08800700	2.77080100	-1.73242400
C	-1.99722300	1.75107300	-1.99720000
H	-1.50841200	0.78023900	-2.15798200
C	-3.26279800	1.58651900	-1.20052000
C	-4.52740200	1.57854600	-1.78591000
H	-4.61482300	1.67367400	-2.86518700
C	-5.66862300	1.45070500	-0.99978200
H	-6.64910600	1.43699900	-1.46542000
C	-5.55082000	1.35110700	0.38489400
H	-6.43729000	1.25467700	1.00341500
C	-4.29226600	1.37964200	0.97643900
H	-4.19394900	1.29952100	2.05594700
C	-3.14644200	1.48479400	0.19055700
C	1.57610600	2.64315800	0.44503700
O	2.68616300	2.13337000	0.53652200
C	1.44921600	4.13414800	0.26847800
C	0.42435100	4.90975900	0.81960000
C	2.49919600	4.76042600	-0.40857900
C	0.45161100	6.29429900	0.67862800
H	-0.38743300	4.42658600	1.34935100
C	2.51161100	6.14179600	-0.56705800
H	3.30510100	4.14644700	-0.79678600
C	1.48589700	6.91129500	-0.02260300
H	-0.33941800	6.89339300	1.11820100
H	3.32442300	6.61873100	-1.10513600
H	1.49513900	7.99050500	-0.13860700
H	-1.50735100	3.71648500	-1.29328600
H	-2.21716900	2.15808100	-2.98902400

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**TS4SS**

C	7.22483800	-2.30805800	1.01576500
C	6.08362000	-2.07723700	1.78263000
C	4.91844400	-1.69124800	1.13446100
C	4.90509400	-1.53028200	-0.25764700
C	6.03777800	-1.75645200	-1.03015800
C	7.20013500	-2.14957900	-0.37152000
C	2.71132600	-1.01298300	0.27116400
C	1.60918400	-0.47511300	-1.62356900
C	3.06934100	-0.89485000	-2.00311100
H	8.14192100	-2.61537800	1.50600900
H	6.10328500	-2.19962400	2.86034100
H	6.01060500	-1.62837300	-2.10689700
H	8.09947800	-2.33510300	-0.94858000
H	1.47613500	0.60174800	-1.79539600
H	3.60899900	-0.10797300	-2.53342000
N	3.64908900	-1.13145500	-0.68884900
S	3.33802600	-1.32562100	1.86013400
N	1.51534000	-0.72274900	-0.16671000
C	0.57424200	-1.24114000	-2.42199300
C	-0.01606600	-0.65807100	-3.54396700
C	0.21698200	-2.54216100	-2.05914500
C	-0.96257600	-1.35932200	-4.28820100
H	0.25349900	0.35722900	-3.82561100
C	-0.73645700	-3.23992300	-2.79567800
H	0.67301700	-2.99500500	-1.18176600
C	-1.32899200	-2.64917000	-3.91124900
H	-1.42205200	-0.89244300	-5.15315800
H	-1.01854400	-4.24490200	-2.49740900

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H	-2.07560100	-3.19181700	-4.48172200
H	3.08274000	-1.81375400	-2.59677000
C	-1.96333100	-0.88720600	1.62210800
C	-1.75932600	-0.61428700	2.91309300
C	0.43633100	0.00083300	1.00856800
C	-0.97678300	-0.48493700	0.53297000
H	-0.88827300	-0.08960100	3.27599200
H	-0.82723500	-1.38001900	-0.07435300
O	0.90655400	-0.28446500	2.12825000
C	-3.14860000	-1.65684700	1.14419900
C	-2.98187300	-2.80166700	0.35880000
C	-4.44537400	-1.21873400	1.43072200
C	-4.08693300	-3.49052700	-0.13334700
H	-1.98213200	-3.16058800	0.12824700
C	-5.54891800	-1.90448300	0.93755600
H	-4.58052800	-0.30970900	2.00932200
C	-5.37378900	-3.04209900	0.15192900
H	-3.94003800	-4.37859900	-0.74071600
H	-6.54828400	-1.53916600	1.15276200
H	-6.23593200	-3.57374800	-0.23848500
Cl	-2.80972700	-1.14808100	4.20470600
N	0.45841500	1.43404200	0.54245500
N	-0.80047000	1.89136000	0.10622000
C	-1.41717700	0.66807400	-0.42187200
H	-0.92155100	0.47578700	-1.37961800
C	-1.57068700	2.49922000	1.20582400
H	-0.98863600	3.34995100	1.57110400
C	-2.90744500	2.96805800	0.64740100
H	-2.73051800	3.83041100	-0.00778400

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C	-3.60990600	1.89224100	-0.15089300
C	-4.98208700	1.97461200	-0.41441300
H	-5.55373800	2.79150600	0.01957200
C	-5.61235300	1.03937300	-1.22515200
H	-6.67851400	1.11748500	-1.41417500
C	-4.87127300	0.00664400	-1.80354700
H	-5.35494300	-0.72350000	-2.44453800
C	-3.51246200	-0.08846600	-1.54396100
H	-2.92319400	-0.89663000	-1.97562100
C	-2.88448600	0.83404900	-0.70130700
C	1.58730200	2.18930800	0.44635700
O	2.68493600	1.73689400	0.76029600
C	1.48488300	3.61897800	-0.02573500
C	2.33533300	4.52790800	0.61020900
C	0.69555300	4.05079200	-1.09662600
C	2.37074500	5.85965800	0.21137600
H	2.96895500	4.17231700	1.41589000
C	0.75270100	5.37937700	-1.50968100
H	0.03809400	3.35136800	-1.59720800
C	1.57837500	6.28780600	-0.85161400
H	3.02201800	6.56030800	0.72386200
H	0.14620100	5.70505700	-2.34878200
H	1.60873500	7.32503900	-1.17022700
H	-1.71994700	1.80084100	2.03742500
H	-3.54751000	3.31383800	1.46490100
<b>PRR</b>			
N	1.28835900	-0.94303700	1.22313500
N	1.19406000	0.42651500	0.80110000

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C	-0.09176800	0.84618100	1.39373500
H	0.04642800	0.91698300	2.48871800
C	2.23662700	1.30910900	1.33534100
H	3.22449500	0.91647800	1.09284700
C	2.03333500	2.65617400	0.63777400
H	2.42785100	2.57476300	-0.38226700
C	0.58100100	3.09119200	0.55915900
C	0.25912500	4.37981600	0.12742000
H	1.06144800	5.06914900	-0.12343800
C	-1.06578000	4.78674300	0.01562400
H	-1.29630100	5.79240100	-0.32080600
C	-2.09525900	3.90271100	0.33495900
H	-3.13098400	4.21318700	0.24609900
C	-1.78973600	2.61625300	0.76355900
H	-2.58893300	1.91828300	1.00278200
C	-0.46011400	2.20901800	0.87434300
C	2.42216500	-1.74953600	0.97299300
O	2.56851000	-2.77940700	1.59003000
C	3.40329700	-1.29703900	-0.05948600
C	3.01581500	-0.67309500	-1.24867000
C	4.74689000	-1.60535300	0.16656000
C	3.97778900	-0.34735400	-2.19874400
H	1.96922300	-0.45846200	-1.42958600
C	5.70676800	-1.25930200	-0.77734700
H	5.02188200	-2.11419100	1.08468700
C	5.32203700	-0.62918200	-1.95946800
H	3.67738700	0.12458800	-3.12825400
H	6.75176900	-1.48610900	-0.59497200
H	6.06996000	-0.36381700	-2.69981700

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H	2.15299900	1.39372400	2.43011200
H	2.62538400	3.42226200	1.14737400
C	-1.68833700	-0.49770100	-0.17702200
C	-1.03978900	-0.08695700	-1.27011600
C	0.01183400	-1.49562400	1.39640900
C	-1.00225000	-0.35970900	1.17971300
H	-0.06290500	0.37917400	-1.22320000
H	-1.75883900	-0.42931000	1.96368400
O	-0.23024100	-2.65555400	1.61593400
C	-3.06165700	-1.06487700	-0.16570300
C	-4.11114600	-0.39376400	-0.80337000
C	-3.33104900	-2.24393300	0.53902600
C	-5.40395600	-0.90573000	-0.75645400
H	-3.91151000	0.53829400	-1.32308800
C	-4.62381500	-2.75790900	0.57462000
H	-2.52018200	-2.75748200	1.04884000
C	-5.66210700	-2.09215000	-0.07349400
H	-6.21105800	-0.37466200	-1.25070100
H	-4.82090900	-3.67941600	1.11287600
H	-6.67036600	-2.49219600	-0.03942000
Cl	-1.63996700	-0.23742200	-2.89458800

**PRS**

C	-1.39174400	-1.18078700	0.51441600
C	-1.30901300	-1.30286400	1.84105900
C	0.95285000	-0.48441100	-0.18482500
C	-0.53642400	-0.13623900	-0.18190400
H	-0.67032800	-0.68113800	2.45673000
H	-0.83167800	-0.07022300	-1.23751400

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O	1.43537800	-1.58105000	-0.31831800
C	-2.23444400	-2.03732400	-0.35815900
C	-3.60206400	-2.20259300	-0.11825900
C	-1.65244400	-2.66179700	-1.46717000
C	-4.37356800	-2.98550900	-0.97200200
H	-4.06087300	-1.70810700	0.73261700
C	-2.42410800	-3.45293200	-2.31199100
H	-0.58688200	-2.54087400	-1.64651200
C	-3.78642700	-3.61455400	-2.06729000
H	-5.43556700	-3.10195900	-0.78186100
H	-1.96060800	-3.94292600	-3.16197100
H	-4.38958000	-4.22709900	-2.72949700
Cl	-2.14871300	-2.49951800	2.77799100
N	1.65836600	0.72730500	-0.03566600
N	0.73034500	1.81587900	-0.18594100
C	-0.50335700	1.27128700	0.39766300
H	-0.37110800	1.18680900	1.49286800
C	1.09968800	3.02003500	0.56199600
H	2.10060100	3.33590900	0.27227700
C	0.08287800	4.09488100	0.17032000
H	0.36815400	4.49856800	-0.80745800
C	-1.34389000	3.58917900	0.07007600
C	-2.38793100	4.49198000	-0.13633400
H	-2.16521800	5.55512300	-0.18175100
C	-3.69805400	4.05056700	-0.29061300
H	-4.49578500	4.76912800	-0.44851000
C	-3.98090300	2.68728800	-0.24887800
H	-4.99834800	2.33366600	-0.37847700
C	-2.95041700	1.77524100	-0.04304900

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H	-3.16738100	0.71043600	-0.01608900
C	-1.63871500	2.21974400	0.11855200
C	2.95420700	0.93252300	-0.57119400
O	3.19707000	1.93620000	-1.20695500
C	3.99341700	-0.08101200	-0.24810100
C	3.95439100	-0.85723100	0.91232000
C	5.08600100	-0.16629100	-1.11433400
C	5.00354200	-1.72363900	1.19623300
H	3.11263700	-0.77402000	1.59139800
C	6.12440700	-1.04639400	-0.83606100
H	5.10421600	0.46060200	-1.99951300
C	6.08322700	-1.82404500	0.32001900
H	4.97966800	-2.32188400	2.10066900
H	6.96633700	-1.12311200	-1.51569600
H	6.89682700	-2.50731800	0.54168800
H	1.08814800	2.82269400	1.64611600
H	0.13769500	4.92342200	0.88313500

**PSR**

C	-1.39174400	-1.18078700	0.51441600
C	-1.30901300	-1.30286400	1.84105900
C	0.95285000	-0.48441100	-0.18482500
C	-0.53642400	-0.13623900	-0.18190400
H	-0.67032800	-0.68113800	2.45673000
H	-0.83167800	-0.07022300	-1.23751400
O	1.43537800	-1.58105000	-0.31831800
C	-2.23444400	-2.03732400	-0.35815900
C	-3.60206400	-2.20259300	-0.11825900
C	-1.65244400	-2.66179700	-1.46717000



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C	-4.37356800	-2.98550900	-0.97200200
H	-4.06087300	-1.70810700	0.73261700
C	-2.42410800	-3.45293200	-2.31199100
H	-0.58688200	-2.54087400	-1.64651200
C	-3.78642700	-3.61455400	-2.06729000
H	-5.43556700	-3.10195900	-0.78186100
H	-1.96060800	-3.94292600	-3.16197100
H	-4.38958000	-4.22709900	-2.72949700
Cl	-2.14871300	-2.49951800	2.77799100
N	1.65836600	0.72730500	-0.03566600
N	0.73034500	1.81587900	-0.18594100
C	-0.50335700	1.27128700	0.39766300
H	-0.37110800	1.18680900	1.49286800
C	1.09968800	3.02003500	0.56199600
H	2.10060100	3.33590900	0.27227700
C	0.08287800	4.09488100	0.17032000
H	0.36815400	4.49856800	-0.80745800
C	-1.34389000	3.58917900	0.07007600
C	-2.38793100	4.49198000	-0.13633400
H	-2.16521800	5.55512300	-0.18175100
C	-3.69805400	4.05056700	-0.29061300
H	-4.49578500	4.76912800	-0.44851000
C	-3.98090300	2.68728800	-0.24887800
H	-4.99834800	2.33366600	-0.37847700
C	-2.95041700	1.77524100	-0.04304900
H	-3.16738100	0.71043600	-0.01608900
C	-1.63871500	2.21974400	0.11855200
C	2.95420700	0.93252300	-0.57119400
O	3.19707000	1.93620000	-1.20695500

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C	3.99341700	-0.08101200	-0.24810100
C	3.95439100	-0.85723100	0.91232000
C	5.08600100	-0.16629100	-1.11433400
C	5.00354200	-1.72363900	1.19623300
H	3.11263700	-0.77402000	1.59139800
C	6.12440700	-1.04639400	-0.83606100
H	5.10421600	0.46060200	-1.99951300
C	6.08322700	-1.82404500	0.32001900
H	4.97966800	-2.32188400	2.10066900
H	6.96633700	-1.12311200	-1.51569600
H	6.89682700	-2.50731800	0.54168800
H	1.08814800	2.82269400	1.64611600
H	0.13769500	4.92342200	0.88313500

**PSS**

N	1.89368800	0.76419000	-0.08813200
N	0.89846700	1.73361800	-0.37670600
C	-0.21713700	0.94574500	-0.97283200
H	-0.06080900	0.94743800	-2.05591200
C	0.55629300	2.54759700	0.81448800
H	0.36427700	3.56230800	0.45357900
C	-0.67030900	2.05362600	1.58093100
H	-0.88322900	2.73057100	2.41348700
C	-1.82910600	2.00704900	0.62085000
C	-3.10271500	2.48365100	0.92763700
H	-3.30193300	2.86535500	1.92561500
C	-4.10909800	2.47799300	-0.03478900
H	-5.09968200	2.84369900	0.21677300
C	-3.84142700	2.01751500	-1.32252800

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H	-4.62238000	2.01694200	-2.07601600
C	-2.56861000	1.55570700	-1.64084800
H	-2.35453900	1.18538100	-2.64007500
C	-1.56867600	1.53638300	-0.67083800
C	3.22810200	1.19955900	-0.00534400
O	3.46828600	2.37283100	0.18832900
C	4.31281900	0.19846300	-0.22286400
C	4.21882300	-0.79035100	-1.20446100
C	5.49904500	0.36438900	0.49300700
C	5.30435200	-1.62049300	-1.45486000
H	3.30614300	-0.89995100	-1.78210000
C	6.57653900	-0.48217900	0.25521500
H	5.56431700	1.15776700	1.23045700
C	6.47933600	-1.47323000	-0.71919400
H	5.23439600	-2.38194000	-2.22426800
H	7.49372500	-0.36377500	0.82233800
H	7.32273700	-2.12855000	-0.91161300
H	1.44449500	2.58713800	1.44319100
H	-0.47554800	1.06435800	2.01274400
C	-1.08616200	-1.16937200	0.39980600
C	-0.79505600	-1.53786100	1.64994800
C	1.39352300	-0.52411100	0.09003300
C	-0.01964400	-0.53349200	-0.47795300
H	0.17867900	-1.39882500	2.09975000
H	0.05743600	-1.16747200	-1.36957700
O	1.99877600	-1.45941200	0.55815600
C	-2.40904500	-1.39643500	-0.24558800
C	-3.58666200	-0.97132500	0.37741500
C	-2.48961400	-1.99631600	-1.50649300

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C	-4.81625200	-1.13837900	-0.24864600
H	-3.52686300	-0.47360300	1.33985000
C	-3.72228300	-2.17086300	-2.12918500
H	-1.59004200	-2.34553900	-2.00524800
C	-4.88859700	-1.73849200	-1.50382700
H	-5.71896600	-0.78576900	0.24030200
H	-3.76997700	-2.64556400	-3.10401700
H	-5.84899700	-1.86661700	-1.99274900
Cl	-1.88737900	-2.37435300	2.71476400

**TS3SR<sup>D</sup>**

C	-0.48214900	1.85973500	0.58660800
C	0.15293400	2.32521400	-0.50344000
C	1.44835600	0.66598000	1.77702500
C	0.33325400	1.42208800	1.72335000
H	1.22514600	2.44943500	-0.53233800
H	0.03595900	1.74142400	2.71990800
O	2.35646900	0.21462600	2.37854500
C	-1.95935100	1.74125900	0.74111100
C	-2.85431300	2.63355900	0.13560000
C	-2.48572700	0.71146400	1.53260900
C	-4.22838500	2.46476700	0.27528700
H	-2.47470000	3.47438400	-0.43281200
C	-3.85813600	0.53647200	1.66632700
H	-1.80296000	0.03562700	2.03805000
C	-4.73646500	1.40931500	1.02914100
H	-4.90449400	3.16876600	-0.19943400
H	-4.24022600	-0.28325900	2.26663400
H	-5.80902200	1.27654600	1.13020400

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Cl	-0.56884000	2.63914700	-2.06587400
N	1.49426000	-0.35381900	-0.08753100
N	0.32053900	-1.08696000	-0.12405800
C	-0.61155800	-0.76981000	-0.95662500
H	-0.37001000	0.00450900	-1.67848300
C	0.08662200	-2.09797000	0.93568200
H	-0.30022300	-1.54913900	1.80100100
C	-0.88223100	-3.16551800	0.45019200
H	-1.13917400	-3.82353700	1.28314900
C	-2.11519300	-2.53587100	-0.14696300
C	-3.39615700	-3.05984100	-0.03234300
H	-3.55767500	-3.96792000	0.54092800
C	-4.47256300	-2.41993900	-0.64998600
H	-5.47007100	-2.83429800	-0.54463500
C	-4.28183300	-1.25849100	-1.39768700
H	-5.12613900	-0.76575700	-1.86671900
C	-3.00472400	-0.72865700	-1.53054300
H	-2.83337100	0.19054800	-2.08454400
C	-1.93279200	-1.36422400	-0.89842700
C	2.57503600	-1.14925700	-0.34158200
O	2.50497400	-2.34551500	-0.64051000
C	3.90471100	-0.45820900	-0.26768600
C	4.03941400	0.92671000	-0.15083000
C	5.04828900	-1.25582900	-0.34201400
C	5.30305000	1.50570400	-0.10379200
H	3.15391000	1.55043400	-0.10191400
C	6.31220900	-0.67825700	-0.29047600
H	4.92159500	-2.32851500	-0.44141000
C	6.44115100	0.70403900	-0.17084200

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H	5.40044400	2.58289000	-0.01502000
H	7.19695200	-1.30464600	-0.34238500
H	7.42690400	1.15688700	-0.13043600
H	-0.37689900	-3.77334700	-0.31057500
H	1.05849100	-2.52058200	1.17934900

**M3SR<sup>D</sup>**

C	0.42378700	-1.84697000	0.48415200
C	-0.15035500	-2.20383400	-0.68392800
C	-1.42419600	-0.40776700	1.49423300
C	-0.41655900	-1.35396600	1.57002400
H	-1.22190000	-2.23644800	-0.82187200
H	-0.20962800	-1.71081600	2.57406100
O	-2.21996200	0.01283800	2.33475900
C	1.89906400	-1.88188600	0.70656800
C	2.70689600	-2.91540800	0.21643700
C	2.50602300	-0.84833700	1.42960400
C	4.08399100	-2.89195700	0.41185100
H	2.24828000	-3.74690000	-0.30808900
C	3.88438300	-0.81400100	1.61380300
H	1.87867400	-0.06355400	1.84223600
C	4.67915600	-1.83514400	1.09910200
H	4.69454300	-3.70438000	0.03059200
H	4.33645500	0.00924700	2.15822400
H	5.75470000	-1.81603500	1.24359200
Cl	0.69530500	-2.46743700	-2.20405700
N	-1.44387400	0.36605500	0.14772500
N	-0.28078900	1.13230100	0.06681600
C	0.59080800	0.87172300	-0.84965700

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H	0.32557500	0.11234100	-1.57850600
C	-0.04145500	2.13760900	1.13015200
H	0.39068700	1.60217900	1.98167600
C	0.86819800	3.24154100	0.61233400
H	1.15964400	3.88211300	1.44706900
C	2.07883700	2.66329600	-0.07623700
C	3.34822200	3.22141500	-0.02404900
H	3.52092800	4.11586800	0.56653900
C	4.40206100	2.62924800	-0.72409900
H	5.39240400	3.06897600	-0.66423000
C	4.20235600	1.48333400	-1.49375400
H	5.03169700	1.02977000	-2.02417300
C	2.93503300	0.92182600	-1.57060000
H	2.75448900	0.01519800	-2.14194400
C	1.88591900	1.51067800	-0.85733600
C	-2.57359400	1.09443800	-0.24123400
O	-2.46396800	2.23267400	-0.66701100
C	-3.88147200	0.38015900	-0.19286400
C	-4.00145200	-0.99588300	0.02004300
C	-5.02345300	1.15040400	-0.42308200
C	-5.25770200	-1.59065400	0.00437800
H	-3.12207800	-1.60466500	0.20301600
C	-6.27873700	0.55405600	-0.43015700
H	-4.90573200	2.21478000	-0.59501400
C	-6.39623900	-0.81772600	-0.21661200
H	-5.34840200	-2.65906200	0.16861600
H	-7.16401900	1.15690900	-0.60334100
H	-7.37544200	-1.28598900	-0.22298500
H	0.30658800	3.85824300	-0.09985400

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H	-1.02068400	2.51889700	1.41516800
<b>TS4SR<sup>D</sup></b>			
C	0.59177200	1.56431900	-0.01887500
C	-0.06162800	1.70678400	1.16016000
C	-0.97143800	-0.14350900	-1.17861300
C	0.25794500	0.56686300	-1.02824900
H	-0.94027200	1.13724600	1.42863300
H	0.72078600	0.74226800	-1.99388000
O	-1.63489400	-0.33423800	-2.17859800
C	1.78389000	2.39624200	-0.36626200
C	1.76874600	3.78728600	-0.21949000
C	2.92501100	1.78970300	-0.90382500
C	2.87731500	4.54852800	-0.57625400
H	0.87755600	4.27274100	0.16405600
C	4.03896900	2.54960700	-1.24913400
H	2.93305100	0.71366700	-1.05374000
C	4.01918200	3.93205300	-1.08358600
H	2.84627100	5.62739700	-0.46224500
H	4.91924000	2.06115700	-1.65487600
H	4.88436500	4.52696500	-1.35789800
Cl	0.44162400	2.76003500	2.46459200
N	-1.37460200	-0.92443700	0.04956600
N	-0.40250600	-1.89203200	0.29811700
C	0.78094000	-1.33075500	0.54133400
H	0.77243000	-0.42010800	1.13089300
C	-0.44511700	-3.07758000	-0.58553200
H	-0.23117300	-2.73717300	-1.60754500
C	0.58785400	-4.08960100	-0.11621400



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H	0.62605200	-4.92111800	-0.82383300
C	1.94353300	-3.45046900	0.03344400
C	3.13245200	-4.16031100	-0.09773400
H	3.10107000	-5.20913400	-0.37756600
C	4.35579100	-3.53497700	0.13538400
H	5.27573800	-4.09973700	0.02397700
C	4.40999000	-2.19444800	0.52340300
H	5.36559300	-1.72034900	0.71716500
C	3.23338500	-1.47495800	0.66509000
H	3.25096600	-0.43294100	0.97344600
C	2.00344000	-2.09375900	0.39821400
C	-2.69283200	-1.28614500	0.34164100
O	-2.94546900	-2.35153400	0.87259800
C	-3.75021000	-0.27282000	0.04645900
C	-3.49557400	1.09197800	-0.11830000
C	-5.06413600	-0.74492600	-0.00238600
C	-4.55033900	1.97051400	-0.33929700
H	-2.48507800	1.48578400	-0.06454200
C	-6.11468500	0.13439700	-0.23469900
H	-5.24221700	-1.80468400	0.14429300
C	-5.85791300	1.49361400	-0.40334100
H	-4.34964400	3.02945800	-0.46091500
H	-7.13211600	-0.23895500	-0.28206600
H	-6.67676000	2.18318100	-0.58159200
H	0.27458600	-4.49788000	0.85246300
H	-1.45344300	-3.48270600	-0.53809700

**R1-H**

C	0.88196600	-0.07021600	0.00022400
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C	1.86809400	1.09360000	0.00047000
C	2.90979200	-0.05536100	-0.00007400
C	1.81900300	-1.05150800	-0.00003400
H	1.86960100	1.72195900	-0.89503800
H	1.78317600	-2.13422300	0.00007200
O	4.11503600	-0.07878200	-0.00050000
C	-0.57267100	-0.04574000	0.00013000
C	-1.24408200	1.18266400	-0.00005800
C	-1.31452700	-1.23637500	0.00016500
C	-2.63450600	1.22237800	-0.00022700
H	-0.66994500	2.10477300	-0.00003800
C	-2.70158100	-1.19430500	0.00002400
H	-0.79553900	-2.19055600	0.00033700
C	-3.36294100	0.03523000	-0.00019800
H	-3.14948000	2.17722600	-0.00038100
H	-3.27157800	-2.11735900	0.00008600
H	-4.44769600	0.06536100	-0.00033100
H	1.86990500	1.72087400	0.89676500

**R-R1-Me**

C	0.66845400	-0.33634500	-0.12967800
C	1.75423600	0.72826200	-0.30644900
C	2.68743300	-0.50532500	-0.19456000
C	1.51637100	-1.39229600	-0.04454900
H	1.76754400	1.18874800	-1.30161800
H	1.38525900	-2.46049500	0.08353700
O	3.88795200	-0.62660400	-0.18943500
C	-0.77878500	-0.18856000	-0.07141500
C	-1.36701900	1.04802300	-0.36449800

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C	-1.59827800	-1.27619400	0.26503000
C	-2.74985600	1.19426100	-0.32731500
H	-0.73712500	1.89129000	-0.63224900
C	-2.97746700	-1.12729400	0.30493600
H	-1.14466000	-2.23507400	0.49847400
C	-3.55512000	0.10836500	0.00817500
H	-3.19915400	2.15445800	-0.55799700
H	-3.60536700	-1.97195200	0.56810800
H	-4.63369300	0.22346800	0.04067800
C	1.92371500	1.76879400	0.79312800
H	2.89446800	2.26085100	0.69263600
H	1.14723600	2.53674800	0.74880600
H	1.87977000	1.29465100	1.77826500

**S-R1-Me**

C	-0.66843500	-0.33629700	-0.12950500
C	-1.75430500	0.72831200	-0.30637300
C	-2.68743600	-0.50539900	-0.19456900
C	-1.51632300	-1.39226200	-0.04462900
H	-1.76750700	1.18879800	-1.30155700
H	-1.38508200	-2.46044000	0.08352400
O	-3.88792600	-0.62686500	-0.18955000
C	0.77880100	-0.18844800	-0.07127900
C	1.36708200	1.04808500	-0.36442000
C	1.59826700	-1.27612000	0.26514000
C	2.74993300	1.19420600	-0.32737500
H	0.73726600	1.89142300	-0.63213000
C	2.97747600	-1.12733400	0.30492200
H	1.14461000	-2.23497200	0.49862100

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C	3.55517600	0.10828000	0.00808300
H	3.19927900	2.15436100	-0.55814400
H	3.60531900	-1.97205100	0.56803100
H	4.63375600	0.22335100	0.04045100
C	-1.92391200	1.76890700	0.79304900
H	-1.14724600	2.53668200	0.74889700
H	-2.89448600	2.26121200	0.69214100
H	-1.88043200	1.29498200	1.77830600

**TS1B-H**

C	-0.91977200	0.25741500	0.35917000
C	-1.68038600	1.40166600	0.04351200
C	-2.89411800	-0.27765700	-0.04856900
C	-1.83547100	-0.76820900	0.68078000
H	-2.37184800	1.79142700	0.77938500
H	-1.77590900	-1.66470200	1.28394500
O	-3.86466500	-0.36496800	-0.71050100
C	0.52178000	0.08635200	0.14874200
C	1.35615700	1.20978300	0.08803600
C	1.08109300	-1.19206000	0.02147100
C	2.72445000	1.05787600	-0.10330700
H	0.92355500	2.19799100	0.21229100
C	2.45064800	-1.34277700	-0.15767000
H	0.43142700	-2.06211000	0.03988800
C	3.27285100	-0.21814600	-0.22362200
H	3.36522900	1.93220800	-0.14813400
H	2.87795600	-2.33495500	-0.25839300
H	4.34174900	-0.33718500	-0.36928700
H	-1.33823000	2.11161300	-0.70693800

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**R-TS1B-Me**

C	0.77609800	-0.10234400	-0.49859800
C	1.66198300	0.99136900	-0.37318700
C	2.68341200	-0.76841400	-0.05154900
C	1.57579000	-1.25406300	-0.70098800
H	2.36403900	1.14321600	-1.18592100
H	1.40674600	-2.20575300	-1.18827800
O	3.64463400	-0.83752900	0.63406600
C	-0.66472500	-0.11616300	-0.21194300
C	-1.43213400	1.04150000	-0.39817300
C	-1.29551700	-1.29439800	0.20721400
C	-2.80247100	1.01999600	-0.16761200
H	-0.94845800	1.94997700	-0.74525200
C	-2.66735000	-1.31608600	0.43155100
H	-0.69695400	-2.18498500	0.37530200
C	-3.42165900	-0.15872500	0.24676300
H	-3.39000500	1.91982100	-0.31772200
H	-3.14776000	-2.23243600	0.75861900
H	-4.49180800	-0.17446600	0.42639600
C	1.48375900	2.14679100	0.57155400
H	2.41777900	2.31459800	1.11992200
H	1.24909600	3.08135100	0.04980600
H	0.69713500	1.95214500	1.30439800

**S-TS1B-Me**

C	-0.77570300	-0.10581500	-0.49512200
C	-1.66282700	0.98784200	-0.37867500
C	-2.68408500	-0.77126700	-0.04802800

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C	-1.57403100	-1.25987300	-0.69107300
H	-2.36270000	1.13376900	-1.19436400
H	-1.40421300	-2.21319400	-1.17496700
O	-3.64628500	-0.83485100	0.63694200
C	0.66509000	-0.11678500	-0.20876100
C	1.42928300	1.04425300	-0.38730200
C	1.29976800	-1.29648000	0.20050700
C	2.79998200	1.02467400	-0.15879700
H	0.94270600	1.95417500	-0.72634400
C	2.67203900	-1.31643600	0.42195000
H	0.70398000	-2.18999700	0.36290500
C	3.42301000	-0.15563700	0.24507500
H	3.38481900	1.92729600	-0.30250600
H	3.15546200	-2.23403200	0.74098200
H	4.49347100	-0.16993600	0.42295000
C	-1.48708100	2.14998400	0.55827100
H	-1.24311700	3.07925900	0.03116500
H	-2.42495500	2.32719300	1.09689300
H	-0.70784300	1.95751300	1.29948500

**TS1-Con**

C	6.07907000	-0.30704300	0.12046700
C	5.10022900	0.59663700	0.53179800
C	3.78097500	0.33155600	0.19690000
C	3.44059600	-0.82197500	-0.52353900
C	4.41237200	-1.72656700	-0.93495700
C	5.73691700	-1.45075800	-0.60361000
C	1.35751500	0.16892700	-0.27596600
C	-0.19557000	-1.18194300	-1.16533300

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C	1.21277400	-1.72880700	-1.55980200
H	7.11738900	-0.11433100	0.36556500
H	5.36232700	1.48682100	1.09303400
H	4.14122100	-2.61527900	-1.49418500
H	6.51370200	-2.14014200	-0.91588000
H	-0.81918800	-1.06205700	-2.05340700
H	1.44258700	-1.56096700	-2.61667200
N	2.07041200	-0.89335500	-0.72507900
S	2.34951400	1.30561500	0.60428100
N	0.09502900	0.15296900	-0.57584500
C	-0.91386600	-2.06897800	-0.16865600
C	-1.99403900	-2.84300600	-0.58542300
C	-0.50676400	-2.11854800	1.16743700
C	-2.66704600	-3.65789700	0.32192400
H	-2.32829600	-2.78638300	-1.61808800
C	-1.17778500	-2.93235300	2.07336400
H	0.32031300	-1.50028900	1.50910800
C	-2.26149000	-3.70271700	1.65228100
H	-3.51793700	-4.24527600	-0.00845800
H	-0.86080700	-2.96003000	3.11099800
H	-2.79053900	-4.33043800	2.36207600
H	1.32776900	-2.78648500	-1.31628500
C	-1.08942100	1.31281200	0.25615900
C	-0.67894800	2.68531400	-0.30993300
C	-0.23237800	2.99240700	1.14388000
C	-0.61153600	1.68550900	1.54599000
H	0.08291600	2.67400900	-1.09173400
H	-0.56880500	1.14367200	2.48311000
O	0.22328000	4.01652900	1.63210900

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C	-2.37263000	0.62678600	-0.06439600
C	-2.82677000	0.54697000	-1.38364800
C	-3.13474800	0.06339300	0.95883600
C	-4.01954800	-0.10538300	-1.67786600
H	-2.23860900	1.00214200	-2.17714000
C	-4.32345700	-0.59732300	0.66529400
H	-2.78530000	0.13780900	1.98412700
C	-4.76685100	-0.68347200	-0.65250100
H	-4.36869800	-0.15925600	-2.70414400
H	-4.90221700	-1.04749700	1.46542900
H	-5.69584800	-1.19637300	-0.88086900
Cl	-2.00318400	3.74822000	-0.91104100

**M1-Con**

C	6.06919700	-0.36118800	0.08194600
C	5.11279600	0.50386700	0.61023500
C	3.78180500	0.28663900	0.28233300
C	3.41843000	-0.78083600	-0.54702500
C	4.36497500	-1.64986200	-1.07603200
C	5.69855300	-1.42153700	-0.74917100
C	1.36240600	0.18414800	-0.13916800
C	-0.24442800	-1.09350900	-1.12973500
C	1.15656500	-1.58760400	-1.59670000
H	7.11542600	-0.20468900	0.31909800
H	5.39947200	1.32909700	1.25283900
H	4.06976500	-2.47227800	-1.71829400
H	6.46058100	-2.08123800	-1.14893900
H	-0.87247300	-0.87564700	-1.99343500
H	1.35732600	-1.34592900	-2.64412200



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N	2.04045900	-0.80990400	-0.73263900
S	2.36164000	1.21925400	0.82726500
N	0.07484100	0.17518900	-0.41012000
C	-0.95556000	-2.06788400	-0.21430900
C	-2.08379400	-2.74531600	-0.66948300
C	-0.49817400	-2.28285800	1.08822900
C	-2.75511100	-3.63065300	0.17006400
H	-2.45671500	-2.55633600	-1.67248600
C	-1.16856300	-3.16705400	1.92598500
H	0.36811100	-1.74040700	1.46146800
C	-2.30019500	-3.84110800	1.46832400
H	-3.64313500	-4.14267500	-0.18650600
H	-0.81332300	-3.32365500	2.93925700
H	-2.82909900	-4.52295500	2.12632000
H	1.28646700	-2.65795800	-1.42925600
C	-0.90865900	1.19339200	0.18541700
C	-0.56977300	2.63804200	-0.32593600
C	-0.27989900	2.99475200	1.15317300
C	-0.49215000	1.66706200	1.53305800
H	0.27707000	2.67763900	-1.01599000
H	-0.43190700	1.12737200	2.47177100
O	0.02617800	4.08230200	1.64794600
C	-2.30367900	0.64658500	-0.04759700
C	-2.85556700	0.59413900	-1.33068300
C	-3.03708300	0.14336000	1.02551800
C	-4.11026500	0.02866200	-1.53951400
H	-2.30278400	1.00795700	-2.17053500
C	-4.28751800	-0.43252600	0.81940700
H	-2.61470900	0.19684900	2.02415500

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C	-4.82530200	-0.49395200	-0.46376000
H	-4.53028700	-0.00068300	-2.54008200
H	-4.84092700	-0.83528300	1.66188300
H	-5.80182700	-0.94008000	-0.62428300
Cl	-1.86669600	3.62875700	-1.09534100

**TS2-Con**

C	6.01343300	-0.59537100	0.22827100
C	5.09301900	0.23363200	0.86677600
C	3.75770700	0.12815800	0.50411600
C	3.35357000	-0.78643200	-0.47499500
C	4.26602200	-1.61397800	-1.11832700
C	5.60400100	-1.50309200	-0.75156300
C	1.32858800	0.19150400	0.06618800
C	-0.30376400	-0.86063300	-1.13658400
C	1.08706000	-1.30006700	-1.67901800
H	7.06173500	-0.53109700	0.49695400
H	5.41141200	0.94202800	1.62373000
H	3.94035700	-2.31640800	-1.87771000
H	6.33922100	-2.13528000	-1.23694900
H	-0.90552800	-0.39388300	-1.91960700
H	1.31743200	-0.87434400	-2.65950500
N	1.98030600	-0.72253700	-0.67406400
S	2.38281300	1.07209700	1.12929100
N	0.03309100	0.20150100	-0.14932100
C	-1.04034400	-2.00487100	-0.47161400
C	-2.19984100	-2.52699800	-1.03837300
C	-0.52951800	-2.57497200	0.69801600
C	-2.84775400	-3.60678000	-0.44001700

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H	-2.60890900	-2.07577300	-1.93809400
C	-1.17260100	-3.65362300	1.29285500
H	0.36955500	-2.16705500	1.15500300
C	-2.33536200	-4.17220400	0.72352500
H	-3.75786300	-3.99978500	-0.88172200
H	-0.77049400	-4.08765300	2.20255100
H	-2.84175100	-5.01075000	1.19037000
H	1.18296400	-2.38620100	-1.70826800
C	-0.90551100	1.37699900	0.12641500
C	-0.69897900	2.27153700	-1.08286200
C	0.02982200	3.28914000	0.91335500
C	-0.42369600	2.09934200	1.33940900
H	0.32417300	2.56993300	-1.29450800
H	-0.49595900	1.84643800	2.39617300
O	0.46109900	4.37988500	0.86451900
C	-2.29919300	0.76565600	0.26831700
C	-3.18686100	0.73442700	-0.80705900
C	-2.66735500	0.14929100	1.46698100
C	-4.42718400	0.11088200	-0.68123200
H	-2.89307600	1.19963900	-1.74162500
C	-3.89799800	-0.48672700	1.59015500
H	-1.97823800	0.14503800	2.30702200
C	-4.78527900	-0.50233800	0.51510400
H	-5.11166700	0.10283500	-1.52401100
H	-4.16412100	-0.97182500	2.52405500
H	-5.74928400	-0.99216500	0.61186900
Cl	-1.84996500	3.62447200	-1.32081700

**TS3RR-90**

S91/S147

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C	7.15864300	-0.86318400	-1.31604700
C	6.09188900	0.00484700	-1.52683000
C	4.80840900	-0.45490100	-1.25547300
C	4.60978100	-1.75806700	-0.78203100
C	5.66960500	-2.63283900	-0.57062200
C	6.94903300	-2.16385300	-0.84516700
C	2.46116000	-0.96105800	-0.83404200
C	1.02049900	-2.66590200	-0.21554900
C	2.49999100	-3.16609700	-0.14342100
H	8.16797700	-0.52279800	-1.51829000
H	6.25484200	1.01376200	-1.88957700
H	5.49962500	-3.63748000	-0.19936800
H	7.79809000	-2.81925700	-0.68602300
H	0.48322100	-3.17736000	-1.02051000
H	2.68579100	-4.01242600	-0.80705500
N	3.25556800	-1.99996600	-0.58777800
S	3.28157900	0.41838000	-1.44717100
N	1.17336700	-1.23631600	-0.62201900
C	0.29282600	-2.86389800	1.09229300
C	-0.88855100	-3.60507300	1.12564500
C	0.81375800	-2.31956100	2.26877300
C	-1.55959800	-3.79976100	2.33125200
H	-1.29083700	-4.02315800	0.20522100
C	0.14181000	-2.51908200	3.47136300
H	1.69262000	-1.67820600	2.23176400
C	-1.04149800	-3.25555700	3.50483300
H	-2.47972300	-4.37455400	2.35201200
H	0.53464100	-2.07968600	4.38214900
H	-1.56196900	-3.40198000	4.44587800

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H	2.78175200	-3.42904000	0.87828000
C	-2.23663800	0.10542000	-1.54283200
C	-2.08685700	1.36834900	-1.98173700
C	0.17278300	-0.26482700	-0.97087800
C	-1.20339300	-0.56470900	-0.72934900
H	-1.19294500	1.94872600	-1.81776700
H	-1.43138600	-1.59799100	-0.49247300
O	0.61538100	0.78517100	-1.43548200
C	-3.46450500	-0.69994400	-1.80589800
C	-4.73920800	-0.19114200	-1.53969400
C	-3.35122200	-2.00661800	-2.29462400
C	-5.87185900	-0.96577400	-1.76436000
H	-4.83413400	0.80483700	-1.11760200
C	-4.48453300	-2.78010300	-2.52901800
H	-2.36485500	-2.41293600	-2.50352000
C	-5.74952600	-2.26086400	-2.26415200
H	-6.85275000	-0.55939400	-1.53709700
H	-4.37898200	-3.78751100	-2.91922100
H	-6.63454800	-2.86375400	-2.44190000
Cl	-3.24752400	2.21151000	-2.98760400
N	0.70523700	0.62677600	1.84718500
N	-0.52826000	1.17685600	1.47724100
C	-1.42613300	0.19784100	1.24311500
H	-1.11324300	-0.77530100	1.60656800
C	-1.00337200	2.46030700	2.01545000
H	-0.20912900	3.19732600	1.92479500
C	-2.25145000	2.90673500	1.26430300
H	-1.99263900	3.09177300	0.21363800
C	-3.30184400	1.83049100	1.35878000

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C	-4.66012200	2.09784900	1.51748300
H	-5.00309400	3.12890700	1.52242600
C	-5.56964400	1.05663100	1.69639300
H	-6.62412600	1.27809800	1.82814700
C	-5.12623000	-0.26489600	1.72414200
H	-5.83374000	-1.07447000	1.86960500
C	-3.77497200	-0.54255500	1.55435800
H	-3.41211800	-1.56842300	1.56428900
C	-2.86350900	0.49911200	1.36653500
C	1.86888500	1.18860200	1.53430600
O	2.92001500	0.52831100	1.75130300
C	2.08744300	2.59507900	0.99118700
C	1.27494400	3.25279900	0.06097200
C	3.24335700	3.24372200	1.44109900
C	1.60975400	4.52599100	-0.39728500
H	0.39353700	2.75420100	-0.32323400
C	3.56710700	4.52295100	1.00216500
H	3.88582500	2.71141600	2.13375500
C	2.75009600	5.16936200	0.07633500
H	0.97404800	5.01473400	-1.12966900
H	4.46110100	5.01318900	1.37603400
H	3.00274600	6.16475800	-0.27614900
H	-1.22754000	2.32526200	3.08299700
H	-2.62264700	3.84472900	1.68628700

**TS3RR-180**

C	-8.04959300	0.71325700	0.27907000
C	-7.02742200	1.18936900	-0.53494500
C	-5.71609000	0.92621300	-0.15449100

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C	-5.44658300	0.21059200	1.01815100
C	-6.46340900	-0.26674200	1.83852900
C	-7.77057500	-0.00350200	1.44865000
C	-3.32539600	0.62216100	0.24681800
C	-1.80194200	-0.23431300	1.75890800
C	-3.25622600	-0.57455800	2.22053600
H	-9.08005900	0.90359700	0.00149400
H	-7.24615800	1.74635000	-1.43898300
H	-6.23995300	-0.81988600	2.74396400
H	-8.58837300	-0.36023700	2.06446500
H	-1.36278900	0.51490100	2.42462600
H	-3.48275500	-0.17229200	3.20897400
N	-4.07295600	0.08113800	1.20168400
S	-4.22644200	1.43707500	-0.96771800
N	-2.01286800	0.42244300	0.43043800
C	-0.94223100	-1.47310500	1.73467700
C	0.04416000	-1.64407100	2.70610300
C	-1.20645600	-2.49408500	0.82164400
C	0.75338900	-2.84112000	2.77571500
H	0.24935800	-0.84904100	3.41824700
C	-0.49077700	-3.68486300	0.88886600
H	-1.95899300	-2.35365700	0.04734300
C	0.48644800	-3.86242200	1.86774500
H	1.50907100	-2.97507700	3.54274500
H	-0.69002000	-4.47145800	0.16777100
H	1.04181100	-4.79309400	1.91815600
H	-3.43791200	-1.65154700	2.20547700
C	1.22886300	2.13780500	-0.01938600
C	1.04117800	3.21986800	-0.78969200

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C	-1.06796000	1.23643100	-0.29522100
C	0.33442200	0.94586300	-0.15418000
H	0.28291100	3.27713700	-1.55561000
H	0.56166600	0.15292500	0.55302200
O	-1.56090300	2.06714300	-1.05237400
C	2.27786900	2.05015400	1.03363000
C	3.61143200	2.36928700	0.76089500
C	1.94493600	1.58516200	2.31119000
C	4.58697700	2.20120700	1.73913500
H	3.89858600	2.68567800	-0.23533500
C	2.91778000	1.42931100	3.29310200
H	0.90752600	1.35159000	2.53732100
C	4.24723700	1.73192100	3.00533700
H	5.62245200	2.41757300	1.49654900
H	2.63845800	1.07097900	4.27957900
H	5.01338500	1.59587400	3.76211200
Cl	1.91778700	4.71989200	-0.61668400
N	3.00349700	0.69644900	-2.16755700
N	2.04085800	-0.29922600	-1.93432400
C	0.75623600	0.14221400	-1.91517500
H	0.62708400	1.12309500	-2.38271600
C	2.33530800	-1.66717600	-2.37444700
H	3.35538900	-1.91077300	-2.08661900
C	1.35468800	-2.63344200	-1.73511600
H	1.46909200	-2.58231300	-0.64320900
C	-0.03363700	-2.23108200	-2.14135900
C	-1.02135100	-3.15933800	-2.46673100
H	-0.79146100	-4.22001100	-2.40169900
C	-2.28242200	-2.74173100	-2.88239300



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H	-3.04533900	-3.47400500	-3.12730900
C	-2.54460500	-1.37937600	-3.02045800
H	-3.50991600	-1.04097700	-3.38411600
C	-1.55337100	-0.44707100	-2.72991400
H	-1.74280500	0.61008500	-2.88198400
C	-0.30195100	-0.85894100	-2.25448800
C	4.18926000	0.54830300	-1.57335300
O	5.13303100	1.33371700	-1.82021300
C	4.51441900	-0.54453100	-0.55735300
C	3.64382600	-0.99556800	0.44015400
C	5.81211500	-1.06219500	-0.59286200
C	4.06162000	-1.94640500	1.36801600
H	2.63945400	-0.59014200	0.50290900
C	6.22525300	-2.03028300	0.31746700
H	6.49178000	-0.67705700	-1.34574700
C	5.34913900	-2.47542900	1.30519100
H	3.37564900	-2.26915700	2.14520100
H	7.23372300	-2.42977600	0.26329300
H	5.67019000	-3.22222300	2.02528100
H	2.26866400	-1.71679700	-3.47156400
H	1.56689600	-3.66074400	-2.04529000

**TS3RR-270**

C	-6.58533700	-1.78441400	-1.72064200
C	-5.39739400	-2.42836200	-1.39184000
C	-4.22124500	-1.68767300	-1.44107100
C	-4.24339200	-0.33971700	-1.82101000
C	-5.42811900	0.31083800	-2.14886200
C	-6.59932500	-0.43424500	-2.09099200

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C	-2.01206800	-0.64300800	-1.37774000
C	-0.90209500	1.24348600	-2.02932600
C	-2.41318600	1.54513600	-1.92813300
H	-7.51601800	-2.33894200	-1.68439000
H	-5.38783700	-3.47250100	-1.09981400
H	-5.43184000	1.35798500	-2.42980000
H	-7.54163000	0.04278500	-2.33562300
H	-0.65795000	0.98360900	-3.06557300
H	-2.79095300	2.04627900	-2.81888200
N	-2.95797300	0.19212100	-1.79821800
S	-2.57659100	-2.23766300	-1.07520900
N	-0.81187000	-0.05666700	-1.25245300
C	-0.05670300	2.41062200	-1.60049600
C	0.66877600	3.11396600	-2.56261700
C	-0.05077400	2.84545400	-0.27575300
C	1.40217600	4.24084100	-2.19165400
H	0.66766000	2.78033900	-3.59686600
C	0.71424000	3.94090700	0.10733000
H	-0.61924400	2.29875100	0.46644900
C	1.43619300	4.64453000	-0.85812400
H	1.96251700	4.78776700	-2.94300200
H	0.73103300	4.21331600	1.15914200
H	2.02845000	5.50744800	-0.57038000
H	-2.65707100	2.11890800	-1.02690800
C	2.86045700	-0.59379000	-1.02526700
C	3.06135900	-1.78277000	-1.61825400
C	0.35367600	-0.88997700	-0.98033300
C	1.52481100	-0.21523700	-0.51412800
H	2.27815100	-2.51933200	-1.72495200

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H	1.39872200	0.84876100	-0.36558800
O	0.17113400	-2.09914400	-1.08507600
C	3.93400000	0.41500900	-0.78020800
C	5.19032700	0.04985900	-0.27867400
C	3.67746300	1.77426900	-0.99895300
C	6.15874600	1.01358600	-0.01388600
H	5.41589700	-0.99432000	-0.09120600
C	4.64796400	2.73646200	-0.74389100
H	2.71437300	2.08700500	-1.38807700
C	5.89371200	2.36037300	-0.24859800
H	7.12229800	0.70799600	0.38114500
H	4.42128900	3.78216400	-0.92915700
H	6.65039900	3.11045100	-0.04234200
Cl	4.56515200	-2.30638100	-2.33352100
N	0.78553900	1.21808500	2.60287500
N	0.56043300	-0.11951100	2.21334300
C	1.60309300	-0.64911500	1.51976500
H	2.49400600	-0.02378000	1.55000000
C	-0.18858600	-1.02537800	3.09657600
H	-1.08763700	-0.52232500	3.44199100
C	-0.53407700	-2.29934500	2.33807300
H	-1.15311300	-2.04358800	1.46686200
C	0.74452700	-2.95563800	1.89765300
C	0.93147900	-4.33338700	1.89474000
H	0.10374100	-4.98321500	2.16552600
C	2.17340500	-4.87736900	1.57175700
H	2.30927700	-5.95422900	1.57205700
C	3.24792700	-4.03895900	1.28637400
H	4.22602900	-4.45617900	1.07017500

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C	3.06859300	-2.65911200	1.28758300
H	3.90721000	-1.99881000	1.09754200
C	1.81308200	-2.10835000	1.56188400
C	-0.24982900	2.03081600	2.80268100
O	-0.05526100	3.21696600	3.16691400
C	-1.73212600	1.67757200	2.61205800
C	-2.23513700	0.74510200	1.69690600
C	-2.65026300	2.42532500	3.35596500
C	-3.60738700	0.55577600	1.54122400
H	-1.53740400	0.15423900	1.11521100
C	-4.02119900	2.23370800	3.21286900
H	-2.25569200	3.16921600	4.03831800
C	-4.50746200	1.29867300	2.30094300
H	-3.98019700	-0.18865900	0.84154100
H	-4.71271700	2.81940600	3.81089100
H	-5.57609500	1.14642400	2.18548900
H	0.42915700	-1.26301300	3.97490800
H	-1.11865800	-2.97243200	2.97138700

**TS3RS-90**

C	-6.06206700	-4.22753800	-1.32585700
C	-4.77074100	-3.98672500	-1.78420100
C	-4.09673300	-2.87959500	-1.28221000
C	-4.71341100	-2.03599800	-0.34961100
C	-6.00505200	-2.26789800	0.11036600
C	-6.66985400	-3.37925000	-0.39354800
C	-2.66872400	-1.02453100	-0.58737700
C	-2.59278200	0.84898100	0.75672600
C	-3.98524300	0.14803000	0.90542700

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H	-6.60488600	-5.08823500	-1.69978800
H	-4.30314500	-4.64372800	-2.50874100
H	-6.46838500	-1.60431900	0.83217200
H	-7.67843300	-3.59047900	-0.05652700
H	-2.69985600	1.81716500	0.25833200
H	-4.81332100	0.78590400	0.59183700
N	-3.85971300	-0.99549400	0.00295500
S	-2.47331000	-2.30763600	-1.71418200
N	-1.85328800	-0.05228500	-0.17700200
C	-1.92744700	1.03512900	2.09838300
C	-1.81446700	2.31586800	2.63511100
C	-1.52502900	-0.07320300	2.84748500
C	-1.33062200	2.48875700	3.93122700
H	-2.10726600	3.17764900	2.04012600
C	-1.05038200	0.10079600	4.14111800
H	-1.58684700	-1.07130100	2.41769400
C	-0.96242000	1.38152500	4.68738500
H	-1.24600500	3.48744400	4.34707000
H	-0.73549900	-0.76024400	4.72073700
H	-0.58547900	1.51336400	5.69662600
H	-4.15014800	-0.19872900	1.92765500
C	0.55475600	2.41127100	-1.46112400
C	1.31550600	2.07710600	-2.51267500
C	-0.71120600	0.32645700	-1.00680400
C	0.12540200	1.36261000	-0.49234300
H	1.67719200	1.06287300	-2.68394300
H	-0.20566000	1.76795700	0.45869300
O	-0.56033900	-0.33051300	-2.02462600
C	0.02123300	3.77897100	-1.19283400

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C	0.12109600	4.34703200	0.08377200
C	-0.65794000	4.49321900	-2.18662600
C	-0.42118600	5.59978600	0.35414400
H	0.63178600	3.80652200	0.87631500
C	-1.20594200	5.74378600	-1.91614600
H	-0.76521800	4.05679300	-3.17402200
C	-1.08754600	6.30401600	-0.64652200
H	-0.32082500	6.02599800	1.34762100
H	-1.73170100	6.27899700	-2.70057100
H	-1.51383300	7.27999700	-0.43778300
Cl	1.86060200	3.21533800	-3.72480800
N	2.39267400	-0.88250300	-2.09486000
N	1.94353300	-0.90688900	-0.75673400
C	1.84472500	0.22126200	-0.05555700
H	2.44877900	1.03043500	-0.46022100
C	1.30231900	-2.10419700	-0.21627100
H	1.49121200	-2.91647100	-0.91806000
C	1.83487800	-2.41876600	1.17804400
H	2.83851800	-2.85543900	1.10951000
C	1.89553400	-1.17231500	2.02715300
C	2.09098500	-1.25620500	3.40797600
H	2.15606400	-2.23812100	3.87063600
C	2.22594200	-0.11176300	4.18367500
H	2.38530900	-0.19728800	5.25431200
C	2.15066700	1.14666200	3.58509800
H	2.24809800	2.04607900	4.18451000
C	1.94932300	1.24311700	2.21646200
H	1.92173600	2.21689900	1.73345100
C	1.83187500	0.09336100	1.42769300

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C	3.54360600	-1.54998700	-2.27163200
O	4.03384700	-1.74986500	-3.39633600
C	4.30112400	-2.12170800	-1.08119100
C	4.77876200	-1.31866800	-0.04153500
C	4.56524500	-3.49194800	-1.05208500
C	5.48251800	-1.87941500	1.02090200
H	4.59485500	-0.24796800	-0.06250500
C	5.24736300	-4.06107000	0.02123000
H	4.22405700	-4.10715000	-1.87985900
C	5.70442400	-3.25530600	1.06312300
H	5.84802600	-1.24385300	1.82193800
H	5.43027900	-5.13130600	0.04172400
H	6.23926900	-3.69644000	1.89861800
H	0.21462700	-1.94431600	-0.16389400
H	1.18797000	-3.16397700	1.65407100

**TS3RS-180**

C	-7.28761700	-1.86532900	-1.54957100
C	-5.95924200	-2.20642000	-1.78181500
C	-4.97546000	-1.32002200	-1.35796400
C	-5.32576900	-0.12139900	-0.72335200
C	-6.65163600	0.22702800	-0.49005900
C	-7.62805900	-0.66557900	-0.91418600
C	-3.03754300	0.03016300	-0.74643100
C	-2.42789100	1.92877600	0.41920000
C	-3.95574400	1.95631200	0.12412500
H	-8.07142300	-2.54243500	-1.86935500
H	-5.69848600	-3.13364000	-2.27932100
H	-6.90560400	1.15868000	0.00339400

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H	-8.67223800	-0.42593300	-0.74840200
H	-1.93854800	2.81820200	0.01831700
H	-4.22718500	2.68175300	-0.64640600
N	-4.18466600	0.60192500	-0.38911100
S	-3.21940700	-1.47167400	-1.55344000
N	-1.96959900	0.74830000	-0.38859200
C	-2.12263200	1.77362000	1.89314700
C	-1.13601900	2.55190300	2.49714700
C	-2.82427600	0.83734100	2.65895500
C	-0.83007900	2.37534100	3.84588700
H	-0.59191700	3.29179900	1.91395900
C	-2.52410400	0.66547700	4.00497600
H	-3.59591600	0.22121000	2.20174500
C	-1.51995800	1.42992400	4.59887400
H	-0.05328600	2.97817400	4.30374100
H	-3.06968700	-0.06788200	4.58987500
H	-1.28100100	1.29065400	5.64782200
H	-4.53714400	2.13613500	1.02859200
C	1.38314200	1.93019000	-1.23624500
C	1.61605400	1.60265000	-2.51147900
C	-0.68264000	0.50997900	-0.99860400
C	0.44757700	1.15617100	-0.38167700
H	1.14258900	0.77037500	-3.01208000
H	0.18187500	1.70454700	0.51715000
O	-0.67925900	-0.27769000	-1.93491000
C	2.01550800	3.11076300	-0.57456300
C	3.38888200	3.15892200	-0.32019700
C	1.20893300	4.18859800	-0.19165400
C	3.93709600	4.27437200	0.30973400



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H	3.99099000	2.29566500	-0.58957900
C	1.76061200	5.30206900	0.43609600
H	0.14343800	4.16408800	-0.41223800
C	3.13011300	5.34474300	0.68938100
H	5.00379100	4.30340300	0.50932800
H	1.12567700	6.13608300	0.71878500
H	3.56613400	6.20976900	1.17935900
Cl	2.68799200	2.50137200	-3.55166400
N	3.69962300	0.02358900	-0.51245900
N	2.51377300	-0.74084600	-0.49029000
C	1.52055800	-0.37723000	0.33594500
H	1.88105300	0.19825900	1.18739100
C	2.23501800	-1.66523400	-1.59089000
H	3.19073100	-1.87705800	-2.07148700
C	1.60220600	-2.94304900	-1.05074000
H	2.37526300	-3.54942300	-0.55987500
C	0.51904600	-2.64909100	-0.04168900
C	-0.44622500	-3.60836000	0.27165300
H	-0.44213200	-4.55225000	-0.26766400
C	-1.39579400	-3.37733800	1.26119100
H	-2.13711500	-4.13682700	1.48986500
C	-1.38098200	-2.17460900	1.96832600
H	-2.09848400	-1.99426800	2.76280200
C	-0.42829600	-1.20970000	1.66255600
H	-0.40257200	-0.27295900	2.21579700
C	0.51080600	-1.43037600	0.65124400
C	4.77608200	-0.67105400	-0.12393100
O	5.92959300	-0.20311700	-0.17470000
C	4.63755600	-2.10179100	0.38061400

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C	3.87563400	-2.43002300	1.50604400
C	5.33369100	-3.11524400	-0.28030900
C	3.79384700	-3.74741600	1.94853800
H	3.34136500	-1.64713100	2.03739800
C	5.23548900	-4.43897500	0.14394500
H	5.94866800	-2.85297200	-1.13648400
C	4.46325500	-4.75854600	1.25957800
H	3.19988600	-3.98796400	2.82529000
H	5.76770100	-5.22088700	-0.38967600
H	4.38965700	-5.78830400	1.59566100
H	1.56957100	-1.19908300	-2.32476600
H	1.19556400	-3.53596300	-1.87635900

**TS3RS-270**

C	8.07149700	-0.64288900	0.35257600
C	7.09264200	0.10031000	1.00516200
C	5.78957600	0.02472900	0.52742400
C	5.48394300	-0.78007800	-0.57729700
C	6.45704200	-1.52200500	-1.23728300
C	7.75754500	-1.43986000	-0.75390200
C	3.42413800	0.10294900	-0.08122000
C	1.86891400	-0.88475400	-1.45385500
C	3.30088800	-1.19311900	-1.98146100
H	9.09435500	-0.60065700	0.70908300
H	7.33848900	0.71977100	1.86035200
H	6.20346500	-2.13654200	-2.09376300
H	8.54157400	-2.00466600	-1.24548800
H	1.24723400	-0.46121100	-2.24367800
H	3.55413100	-0.63425200	-2.88593800

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N	4.12556100	-0.71084100	-0.86971200
S	4.35424500	0.86872900	1.14518000
N	2.13547700	0.15477500	-0.41249900
C	1.21304600	-2.11258400	-0.85886600
C	0.16023400	-2.72967300	-1.53183300
C	1.67015000	-2.64402700	0.35265500
C	-0.43646800	-3.86921800	-0.99402600
H	-0.25504900	-2.29968500	-2.43874000
C	1.07220300	-3.77995200	0.88706400
H	2.47922300	-2.16358600	0.89834500
C	0.01636000	-4.39429000	0.21249100
H	-1.28393500	-4.30663900	-1.51234700
H	1.42472900	-4.18075500	1.83166600
H	-0.46118200	-5.27150400	0.63740100
H	3.44553100	-2.26159200	-2.14212500
C	-0.73953300	2.55983900	-0.22957300
C	-0.84635700	3.14866000	0.97238700
C	1.26199800	1.14779700	0.19139900
C	-0.05155400	1.24505300	-0.34686000
H	-0.41585900	2.73231000	1.87161800
H	-0.19563600	0.76036700	-1.30885600
O	1.77327600	1.77863800	1.11564100
C	-1.23948000	3.16358200	-1.50164500
C	-1.89067200	2.38525900	-2.46873300
C	-0.99002400	4.51302400	-1.78505400
C	-2.31946100	2.95941700	-3.66303900
H	-2.05969400	1.32370400	-2.29250800
C	-1.41252300	5.08033700	-2.98276400
H	-0.44308200	5.11659100	-1.06886000

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C	-2.08914400	4.30766100	-3.92355800
H	-2.83243500	2.34345300	-4.39514400
H	-1.20477000	6.12688800	-3.18303300
H	-2.42313600	4.75000400	-4.85695200
Cl	-1.74130200	4.61471700	1.29773000
N	-2.12436700	-0.76701300	-1.40374900
N	-2.32493800	-0.31066900	-0.08749600
C	-1.20955000	-0.19450300	0.64678400
H	-0.49296100	-0.98867900	0.46428500
C	-3.44577000	0.60235900	0.14580000
H	-4.29376800	0.20333900	-0.41503500
C	-3.77407800	0.67024600	1.63216800
H	-4.28577600	-0.25784900	1.91995600
C	-2.54217200	0.80786900	2.49232000
C	-2.60433800	1.34147500	3.77880500
H	-3.54543200	1.74790300	4.13931500
C	-1.48061500	1.35270600	4.60040500
H	-1.54449700	1.78082100	5.59567900
C	-0.28069800	0.79836400	4.15396200
H	0.59027400	0.78493000	4.80036200
C	-0.20447700	0.26894300	2.87175700
H	0.72806600	-0.15275100	2.50763200
C	-1.32084800	0.29777100	2.02963300
C	-2.82046900	-1.85947600	-1.73411200
O	-2.72182000	-2.37362200	-2.86725500
C	-3.77492600	-2.53342200	-0.76148400
C	-3.42863600	-2.89525400	0.54516100
C	-5.04189000	-2.87452800	-1.24128800
C	-4.34136400	-3.56697700	1.35606100

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H	-2.43710000	-2.66903500	0.92393800
C	-5.96304100	-3.52479700	-0.42531000
H	-5.28897400	-2.62681100	-2.26900900
C	-5.61414100	-3.87220300	0.87857900
H	-4.05676900	-3.85238200	2.36441600
H	-6.94896900	-3.76956300	-0.80881200
H	-6.32702700	-4.38588700	1.51619300
H	-3.21110900	1.59663200	-0.25421500
H	-4.46717900	1.49513100	1.82050000

**TS3SR-90**

C	7.57693800	0.85888900	1.35532400
C	6.55655900	0.16120300	1.99440800
C	5.31835700	0.09625900	1.36641600
C	5.11667900	0.71553000	0.12633000
C	6.13152400	1.41426700	-0.51832100
C	7.36575100	1.47603700	0.11728300
C	3.04444400	-0.18146700	0.52070700
C	1.68451600	0.25459000	-1.29870900
C	3.04191400	1.00626600	-1.46175300
H	8.55079800	0.92478200	1.82698300
H	6.72057700	-0.31593900	2.95416200
H	5.96067700	1.88864200	-1.47826200
H	8.17871600	2.01299100	-0.35821300
H	0.83394500	0.94709100	-1.31856000
H	2.93106100	2.09060200	-1.39081000
N	3.81082300	0.51739500	-0.31181000
S	3.84839400	-0.71576900	1.94382000
N	1.79905700	-0.32666800	0.07490400

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C	1.45916900	-0.81506400	-2.34247200
C	0.55180900	-0.55569700	-3.37147800
C	2.15123000	-2.02753900	-2.30132700
C	0.34663200	-1.51576900	-4.36157000
H	-0.00062800	0.38390400	-3.37285300
C	1.93732500	-2.98346200	-3.28979900
H	2.84527500	-2.23747300	-1.49000500
C	1.03559800	-2.72596900	-4.32256200
H	-0.36498900	-1.32153800	-5.15762800
H	2.46946300	-3.92835600	-3.25240300
H	0.86770500	-3.47311600	-5.09206600
H	3.54241200	0.74307900	-2.39487400
C	-1.45528300	-2.11368000	0.65576700
C	-1.55756100	-2.49577300	1.94004000
C	0.82034900	-1.07973900	0.82157200
C	-0.50324900	-1.04078400	0.28411300
H	-0.99030300	-2.02882300	2.73264700
H	-0.56903900	-0.73862100	-0.75834900
O	1.22384400	-1.56065500	1.87878500
C	-2.21281300	-2.73381300	-0.47173400
C	-1.55045000	-3.00586400	-1.67617800
C	-3.57719000	-3.03878100	-0.38011700
C	-2.22758100	-3.57544700	-2.74973300
H	-0.49147700	-2.77906700	-1.77111800
C	-4.25613900	-3.60010900	-1.45699300
H	-4.11459200	-2.82727100	0.53819100
C	-3.58370100	-3.87365600	-2.64554100
H	-1.68874400	-3.77940400	-3.67000600
H	-5.31521400	-3.82000800	-1.36660400

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H	-4.11384400	-4.31238500	-3.48493300
Cl	-2.51611000	-3.83466400	2.52373700
N	-1.24155600	1.46310600	-1.28693700
N	-1.82143700	1.39169700	-0.00958100
C	-1.02665200	0.84744600	0.93073900
H	-0.00432700	1.22205100	0.88634200
C	-3.28255400	1.35829500	0.11224200
H	-3.67751400	1.12307500	-0.87931700
C	-3.76552600	0.33401600	1.13743300
H	-3.67954300	-0.66737000	0.70334600
C	-2.94804600	0.36931100	2.40169900
C	-3.47407200	0.10504900	3.66310400
H	-4.53757000	-0.09131500	3.76824500
C	-2.64437800	0.07941100	4.78276900
H	-3.06531600	-0.13174100	5.76060600
C	-1.27832100	0.32505800	4.65115500
H	-0.63417800	0.30540400	5.52379000
C	-0.74348000	0.60050600	3.39638500
H	0.32080100	0.78565500	3.27822000
C	-1.57612100	0.62382100	2.27596700
C	-1.38369000	2.60936000	-1.96101400
O	-0.98533800	2.71163500	-3.13956600
C	-2.01583200	3.84018000	-1.33722600
C	-1.67572400	4.29629400	-0.06024900
C	-2.90857800	4.58733900	-2.10803200
C	-2.23297700	5.46980700	0.44116900
H	-0.97087200	3.73141500	0.54178400
C	-3.48331600	5.74927600	-1.60058400
H	-3.13931800	4.24531200	-3.11209900

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C	-3.14573600	6.19364900	-0.32372800
H	-1.95397700	5.82012400	1.43023300
H	-4.18714900	6.31429800	-2.20410500
H	-3.58592200	7.10385700	0.07151700
H	-3.62876700	2.36286300	0.38635200
H	-4.82379200	0.50686000	1.35235700

**TS3SR-180**

C	-7.06690200	-2.33739400	0.84192400
C	-5.95713900	-2.09061700	1.64332600
C	-4.91575400	-1.34601200	1.10163800
C	-4.99393900	-0.86315900	-0.21127700
C	-6.10220000	-1.10220000	-1.01639200
C	-7.13736000	-1.84971600	-0.46813000
C	-2.92997300	-0.10735400	0.42819800
C	-1.98938600	1.08444800	-1.31569200
C	-3.36377200	0.48939200	-1.76209400
H	-7.89084300	-2.91739200	1.24178300
H	-5.90409900	-2.46714900	2.65874500
H	-6.15063000	-0.71812300	-2.02925100
H	-8.01538300	-2.05854900	-1.06876800
H	-1.20198700	0.68135500	-1.95440000
H	-3.24790000	-0.26417900	-2.54409200
N	-3.84245100	-0.15213000	-0.53588900
S	-3.39934000	-0.87205800	1.88934100
N	-1.82216600	0.53366700	0.05506100
C	-1.91874100	2.59477400	-1.31591200
C	-1.21321300	3.24334400	-2.32877900
C	-2.54508200	3.34339600	-0.31671900



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C	-1.13654000	4.63383300	-2.34848900
H	-0.70899100	2.66052700	-3.09526900
C	-2.46157100	4.73220700	-0.33365900
H	-3.08267300	2.84360500	0.48575300
C	-1.75762500	5.37869900	-1.34983100
H	-0.57791600	5.13142400	-3.13415900
H	-2.94073900	5.30960700	0.44976300
H	-1.68856000	6.46149600	-1.35706700
H	-4.06027100	1.26505500	-2.08489900
C	1.58901000	1.67798600	1.09246800
C	1.86828300	1.27038900	2.33277900
C	-0.68442800	0.62304600	0.92269500
C	0.57296900	0.95811000	0.27536800
H	1.36967700	0.44174400	2.81449300
H	0.40348400	1.47909600	-0.66447000
O	-0.88477600	0.30595200	2.08647200
C	2.26642300	2.81593600	0.41192300
C	1.49880600	3.89782800	-0.03383400
C	3.64390400	2.80043300	0.17288300
C	2.10251500	4.96729700	-0.68869700
H	0.42379300	3.90357200	0.13960300
C	4.24234300	3.87276100	-0.48471500
H	4.20607600	1.91796300	0.46487600
C	3.47813000	4.95768500	-0.91146800
H	1.49639300	5.80438100	-1.02296700
H	5.31107600	3.85523900	-0.67442900
H	3.95262100	5.78927000	-1.42347500
Cl	3.06821900	2.01686100	3.35197500
N	3.64079600	-0.43691800	0.32577500

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N	2.39614000	-1.09812600	0.42578700
C	1.36662000	-0.64996300	-0.33918100
H	1.73383400	-0.22023300	-1.27151800
C	2.22430500	-2.08393800	1.48220000
H	2.76924800	-1.72695900	2.36267100
C	0.75385800	-2.33574700	1.82576100
H	0.36881400	-1.52057800	2.44796600
C	-0.09430600	-2.43475500	0.58245500
C	-1.20294000	-3.27376600	0.47936100
H	-1.48015100	-3.89325700	1.32832500
C	-1.95604900	-3.32303800	-0.69380900
H	-2.82255000	-3.97412100	-0.75410700
C	-1.56682100	-2.56944400	-1.80059800
H	-2.11077100	-2.65122800	-2.73708600
C	-0.45410000	-1.73370500	-1.71037200
H	-0.12581600	-1.16335100	-2.57717000
C	0.25047700	-1.62840400	-0.51105500
C	4.61518900	-1.16340200	-0.23498500
O	5.78857600	-0.74573900	-0.30746800
C	4.36848200	-2.56334200	-0.78675300
C	3.35735200	-2.87188500	-1.70090300
C	5.24555200	-3.57757700	-0.39432800
C	3.20597000	-4.16976600	-2.18350800
H	2.68915000	-2.09292500	-2.05368400
C	5.08918600	-4.87965400	-0.86146100
H	6.05564200	-3.32434500	0.28278100
C	4.06333500	-5.18109000	-1.75566800
H	2.41519700	-4.39019000	-2.89486500
H	5.77146600	-5.65849900	-0.53372700

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H	3.93936900	-6.19459700	-2.12469500
H	2.69297100	-3.02694100	1.16435900
H	0.67434000	-3.25639200	2.41075300

**TS3SR-270**

C	6.68177100	-3.16551200	-1.48487500
C	5.52317000	-2.83080800	-2.17886400
C	4.57290200	-2.05509000	-1.52463500
C	4.78788600	-1.63017800	-0.20777800
C	5.94241100	-1.96150300	0.49266000
C	6.88676400	-2.73730300	-0.16849700
C	2.73158900	-0.71642900	-0.64503300
C	2.07601400	0.54330000	1.17520100
C	3.37937600	-0.24511900	1.52157600
H	7.43720400	-3.76887800	-1.97511700
H	5.36542700	-3.16422600	-3.19842200
H	6.09309300	-1.62496400	1.51243700
H	7.79878900	-3.01403500	0.34817200
H	1.28909600	0.26867900	1.87976600
H	3.20168600	-1.01908000	2.27209900
N	3.71277500	-0.86832200	0.23918500
S	3.01618800	-1.48390100	-2.15670200
N	1.72198400	0.01706700	-0.17423700
C	2.27158000	2.04213400	1.16940500
C	1.79174600	2.79079100	2.24312000
C	2.95615400	2.67576600	0.12982000
C	2.00242000	4.16720200	2.28478800
H	1.24253800	2.29489000	3.04014500
C	3.15934400	4.05181900	0.16938900

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H	3.31530300	2.10081200	-0.72083400
C	2.68616800	4.79820100	1.24854900
H	1.62094000	4.74627700	3.11937200
H	3.68204800	4.54316200	-0.64427400
H	2.84374600	5.87144400	1.27557500
H	4.18375500	0.41808700	1.84411800
C	-1.31139500	1.96571800	-1.20242800
C	-1.72382500	1.62367500	-2.42672300
C	0.57041000	0.30501100	-0.99649500
C	-0.49256300	1.03610900	-0.37296500
H	-1.55444200	0.64837000	-2.85782000
H	-0.21345900	1.49254600	0.57270000
O	0.57531000	-0.21018400	-2.10835900
C	-1.66834900	3.24881900	-0.53375500
C	-0.66633500	4.07296300	-0.00986600
C	-3.00673000	3.62024600	-0.36884900
C	-0.99468500	5.25598800	0.64521700
H	0.37708400	3.78877200	-0.12696000
C	-3.33500800	4.79937600	0.29455400
H	-3.78589000	2.97273500	-0.75999400
C	-2.33026900	5.62197900	0.79972200
H	-0.20308400	5.88796500	1.03719400
H	-4.37770200	5.07338900	0.42029100
H	-2.58746200	6.54141700	1.31613300
Cl	-2.62403900	2.68819800	-3.47636000
N	-3.02303400	-1.05898600	-1.62805900
N	-2.06563800	-1.33280000	-0.62211600
C	-1.70951800	-0.38003800	0.25907200
H	-2.49832200	0.35334600	0.42314100

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C	-1.43185900	-2.64581300	-0.68093000
H	-1.27214200	-2.88146500	-1.73657500
C	-0.11523100	-2.72349600	0.08801900
H	0.68115600	-2.29978500	-0.53204000
C	-0.19181000	-1.99109800	1.40459200
C	0.52756000	-2.38830700	2.53246300
H	1.15580500	-3.27409100	2.47843200
C	0.43818700	-1.67010500	3.72436200
H	1.00065300	-1.99274100	4.59464200
C	-0.39148200	-0.55102100	3.80316500
H	-0.47963900	-0.00079700	4.73427700
C	-1.11069900	-0.14458900	2.68211700
H	-1.74934500	0.73467200	2.72704100
C	-1.00246300	-0.85187000	1.48264200
C	-4.20327500	-1.66885300	-1.44220400
O	-5.10677500	-1.63000400	-2.29902600
C	-4.51626800	-2.47804100	-0.18664400
C	-4.37642000	-1.99004100	1.11506400
C	-5.03312200	-3.76474600	-0.36526100
C	-4.71678800	-2.78005400	2.21158200
H	-4.01918200	-0.97853500	1.27954500
C	-5.35813000	-4.56391600	0.72672300
H	-5.17792300	-4.12572400	-1.37892800
C	-5.19679600	-4.07370400	2.02179800
H	-4.60678400	-2.38175000	3.21599800
H	-5.74728200	-5.56548000	0.56912400
H	-5.45439500	-4.69136900	2.87666500
H	-2.13901100	-3.38322300	-0.27767900
H	0.14190700	-3.77336900	0.25402700

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**TS3SS-90**

C	7.45890300	0.08535000	1.21765200
C	6.35737500	-0.34136600	1.95317500
C	5.12110600	-0.37189800	1.31910800
C	5.00059600	0.01477800	-0.02156000
C	6.09624700	0.44345700	-0.76282000
C	7.32849100	0.47232300	-0.12062000
C	2.82974300	-0.52541800	0.48492900
C	1.52871900	-0.24236000	-1.40510700
C	2.98655200	0.23461000	-1.69243900
H	8.43309000	0.11855200	1.69214000
H	6.45870800	-0.64064400	2.99047100
H	5.98635100	0.74214000	-1.79946500
H	8.20356200	0.80090100	-0.67002800
H	0.80462200	0.57396700	-1.52849600
H	3.04483000	1.31117400	-1.86776500
N	3.68062200	-0.09735400	-0.44500200
S	3.55891900	-0.86212500	2.00634100
N	1.57756200	-0.60087400	0.04567900
C	1.09054900	-1.39214700	-2.28118600
C	0.24002900	-1.11001600	-3.35230000
C	1.53986200	-2.69594300	-2.06294200
C	-0.14289500	-2.13719100	-4.21402900
H	-0.13006900	-0.09324500	-3.48587300
C	1.14561100	-3.71838700	-2.92071400
H	2.18425800	-2.91747000	-1.21480100
C	0.30716200	-3.43811700	-4.00047800
H	-0.80642500	-1.92075600	-5.04530300

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H	1.48837700	-4.73304700	-2.74600600
H	-0.00036400	-4.23708900	-4.66783900
H	3.43472800	-0.30254400	-2.53042500
C	-1.73487300	-2.12566000	0.79387200
C	-1.68797300	-2.66310400	2.02475300
C	0.51132300	-1.03669500	0.92372900
C	-0.79562100	-1.07997100	0.35147600
H	-0.97144100	-2.36096000	2.77313700
H	-0.83360800	-0.87512900	-0.71345500
O	0.87138300	-1.33990400	2.06176500
C	-2.74748000	-2.51515900	-0.23156900
C	-2.31820300	-2.89307900	-1.50916500
C	-4.12015900	-2.46959500	0.03258900
C	-3.23908900	-3.23369500	-2.49379300
H	-1.25400700	-2.92890700	-1.72700800
C	-5.04243400	-2.80031000	-0.95659600
H	-4.46992300	-2.17473900	1.01749200
C	-4.60468900	-3.18609400	-2.22129200
H	-2.88439500	-3.53063600	-3.47631100
H	-6.10465100	-2.75364500	-0.73859400
H	-5.32474300	-3.44376600	-2.99153700
Cl	-2.74508100	-3.94434800	2.57340700
N	-1.05718000	1.41893800	-1.36476500
N	-1.21442700	1.70435500	0.00033900
C	-1.84993400	0.75161200	0.70291000
H	-2.68461700	0.29706900	0.17509200
C	-0.08169000	2.36188700	0.65760700
H	0.27365300	3.15090300	-0.00671500
C	-0.49672300	2.93323200	2.00228700

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H	-1.14904700	3.79893100	1.82677500
C	-1.25129700	1.91963900	2.82445900
C	-1.35402600	2.03556800	4.20779600
H	-0.80381500	2.82350700	4.71519300
C	-2.16646700	1.17073800	4.93767700
H	-2.23313700	1.27188800	6.01623500
C	-2.91537400	0.19952100	4.27847300
H	-3.57767900	-0.45445200	4.83594700
C	-2.81896300	0.07246600	2.89720600
H	-3.42035700	-0.66372600	2.37780100
C	-1.96000100	0.90081100	2.16502900
C	-1.08783900	2.46761700	-2.19924600
O	-0.73255900	2.34354200	-3.38788700
C	-1.53785800	3.84725100	-1.75031300
C	-2.61031500	4.06207000	-0.87863600
C	-0.87437300	4.95008300	-2.29312900
C	-2.99676100	5.35849400	-0.54574900
H	-3.14876700	3.21465300	-0.46884400
C	-1.24613600	6.24536900	-1.94567200
H	-0.07073700	4.76911700	-2.99974900
C	-2.30889700	6.45193200	-1.06822000
H	-3.83844300	5.51492600	0.12202400
H	-0.71501000	7.09376500	-2.36637900
H	-2.60631300	7.46097600	-0.80007500
H	0.72481700	1.62240100	0.78442500
H	0.38443200	3.29361700	2.54088400

**TS3SS-180**

C	-7.60223000	-1.34445300	0.55729300
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C	-6.65449100	-0.85356100	1.45053800
C	-5.40225100	-0.51388000	0.95231700
C	-5.11647300	-0.66336100	-0.41086900
C	-6.05826100	-1.15165400	-1.30970100
C	-7.30663000	-1.49193900	-0.80227900
C	-3.12041000	0.13213700	0.38429800
C	-1.65196800	0.37283100	-1.37792700
C	-2.97711400	-0.28169500	-1.88374000
H	-8.58506600	-1.61742400	0.92422600
H	-6.88433000	-0.74017300	2.50418300
H	-5.82223000	-1.25909000	-2.36262200
H	-8.06352800	-1.87784300	-1.47567800
H	-0.81639600	-0.30364600	-1.57577300
H	-2.82653500	-1.31636400	-2.20253700
N	-3.81246600	-0.26086200	-0.68143100
S	-4.01079400	0.12439800	1.85243900
N	-1.86347300	0.45014700	0.08996900
C	-1.36342000	1.73906700	-1.95898500
C	-0.33976700	1.89136600	-2.89249800
C	-2.11263800	2.84968100	-1.56313200
C	-0.06303200	3.14663000	-3.42902300
H	0.25153700	1.02956400	-3.19251800
C	-1.83545000	4.10289900	-2.09907200
H	-2.89961100	2.74180300	-0.82037400
C	-0.81006600	4.25224600	-3.03268800
H	0.74415600	3.26100800	-4.14452000
H	-2.41459900	4.96449400	-1.78414800
H	-0.59096400	5.23199800	-3.44477000
H	-3.44012300	0.29969600	-2.68277500

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C	1.38158700	1.71206500	1.47964900
C	1.39364900	1.67549900	2.81816000
C	-0.92003900	0.80581500	1.11981400
C	0.44586900	0.85865900	0.70895200
H	0.75924300	1.02147900	3.40000700
H	0.59063000	0.95789500	-0.36236600
O	-1.39986000	0.91652500	2.24675000
C	2.20815600	2.65427800	0.67060100
C	1.56264900	3.54825000	-0.18903200
C	3.60537900	2.64814700	0.72671400
C	2.29758700	4.44519100	-0.96150200
H	0.47592400	3.54164900	-0.25667700
C	4.33641300	3.54170200	-0.04918200
H	4.11144100	1.89622300	1.32117500
C	3.68758000	4.44723100	-0.88838500
H	1.77915600	5.13395400	-1.62226300
H	5.42106200	3.51604200	-0.01110600
H	4.26511700	5.14019700	-1.49292400
Cl	2.37327600	2.72345200	3.81471500
N	3.20951100	-0.38766900	0.48091200
N	2.15233200	-1.24433200	0.14799300
C	1.07344100	-1.12155000	0.94194800
H	1.31744800	-0.94067500	1.98683000
C	1.89959200	-1.43417400	-1.28051400
H	2.86018800	-1.58380700	-1.77227800
C	0.98702800	-2.62779800	-1.52179800
H	1.56841100	-3.54429500	-1.35626400
C	-0.19366600	-2.64575200	-0.58314500
C	-1.34782600	-3.37368300	-0.87632600

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H	-1.42553400	-3.87712300	-1.83699200
C	-2.38156200	-3.48046600	0.05231300
H	-3.27344000	-4.04931100	-0.19090800
C	-2.24813800	-2.88562500	1.30684700
H	-3.03046500	-2.99686100	2.05108600
C	-1.11067600	-2.14084400	1.60314500
H	-1.01528900	-1.65026500	2.56767600
C	-0.09643500	-1.98407000	0.65107900
C	4.44052000	-0.86535200	0.26272800
O	5.44875700	-0.14714200	0.40762400
C	4.69579300	-2.30234000	-0.17921000
C	4.03132900	-3.41366000	0.34992900
C	5.70812600	-2.50942100	-1.12059200
C	4.36259100	-4.70088400	-0.07054300
H	3.26067000	-3.27285500	1.09997400
C	6.02567300	-3.79161400	-1.55779500
H	6.24513600	-1.64280700	-1.49302600
C	5.35126900	-4.89286400	-1.03345900
H	3.85030800	-5.55622400	0.36003200
H	6.80540400	-3.93404500	-2.29989600
H	5.60194900	-5.89583300	-1.36500100
H	1.46870200	-0.49963500	-1.68041100
H	0.65600700	-2.64113100	-2.56519000

**TS3SS-270**

C	6.36474500	-2.32637300	1.52371100
C	5.29542200	-1.75131600	2.20326600
C	4.03994000	-1.80617600	1.60982100
C	3.86529400	-2.43318900	0.37155400

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C	4.92844500	-3.00791200	-0.31406500
C	6.18247700	-2.94189700	0.28002200
C	1.73566800	-1.73751000	0.81506700
C	0.43191800	-2.10540300	-1.04048300
C	1.88900000	-2.59659300	-1.31201800
H	7.35443900	-2.29211800	1.96519100
H	5.43740900	-1.26977600	3.16447300
H	4.77881500	-3.47964000	-1.27885700
H	7.03434400	-3.37685800	-0.23082500
H	0.24057000	-1.23524800	-1.67151400
H	2.40177500	-1.95603400	-2.03265400
N	2.53323300	-2.39169300	-0.01618800
S	2.51729800	-1.13607500	2.21885100
N	0.48841900	-1.61829900	0.35943400
C	-0.63357800	-3.16059700	-1.21717100
C	-1.47475100	-3.11876800	-2.32842900
C	-0.79305100	-4.17457200	-0.26961500
C	-2.46908600	-4.08055900	-2.49363500
H	-1.36039200	-2.32217000	-3.05928300
C	-1.78914000	-5.13260300	-0.43145500
H	-0.15064900	-4.19942600	0.60700800
C	-2.62782000	-5.08737400	-1.54495100
H	-3.12619900	-4.03533000	-3.35591700
H	-1.91480700	-5.91160700	0.31321900
H	-3.40667500	-5.83303300	-1.66863800
H	1.92436100	-3.64785500	-1.60336300
C	-2.75836300	0.11867200	0.87400000
C	-2.74978400	0.92940500	1.94303200
C	-0.38311000	-0.63871400	0.94974300

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C	-1.49572000	-0.17656900	0.15218900
H	-1.85023300	1.41200500	2.29750000
H	-1.67435000	-0.78275200	-0.73007900
O	-0.08910000	-0.30268600	2.09360300
C	-3.98933700	-0.53382000	0.33842200
C	-3.96217100	-1.88906200	-0.01699700
C	-5.17727700	0.18310700	0.14638800
C	-5.09553200	-2.51269100	-0.53127800
H	-3.04874900	-2.46433400	0.11763800
C	-6.30664100	-0.43855700	-0.37675100
H	-5.20395800	1.23825500	0.39662700
C	-6.27146200	-1.79009900	-0.71416000
H	-5.05175300	-3.56559200	-0.79276500
H	-7.21601200	0.13567200	-0.52503100
H	-7.15354500	-2.27411300	-1.12148400
Cl	-4.12300300	1.26233300	2.97047800
N	1.37903800	0.75809900	-0.78991000
N	0.51531400	1.83048100	-0.52307300
C	-0.75636700	1.57645900	-0.88143300
H	-0.84139300	1.03872800	-1.82006700
C	0.70048500	2.57763000	0.73454700
H	1.76993300	2.73537500	0.87308100
C	-0.03191400	3.90772400	0.64347600
H	0.49927700	4.55433300	-0.06776000
C	-1.45293600	3.72476000	0.17155600
C	-2.44106600	4.67520700	0.42994200
H	-2.19410100	5.54280700	1.03588200
C	-3.72527200	4.52617500	-0.08345200
H	-4.48325400	5.27374300	0.12720300

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C	-4.03581200	3.41843600	-0.87316200
H	-5.03448200	3.29816400	-1.28099500
C	-3.06387700	2.46024800	-1.12593700
H	-3.30642000	1.57510800	-1.70993200
C	-1.77556800	2.60263500	-0.60413900
C	2.66290200	1.02570000	-1.03107500
O	3.49251000	0.09285900	-1.14298500
C	3.20384500	2.43560200	-1.17555100
C	2.53622500	3.45436100	-1.86260400
C	4.46831400	2.69419300	-0.64000200
C	3.11994700	4.71339700	-1.99281100
H	1.56111500	3.26164300	-2.29745400
C	5.04259600	3.95658400	-0.75152200
H	4.98972600	1.88363200	-0.14084800
C	4.36763300	4.97088100	-1.42883900
H	2.59880700	5.49490500	-2.53746400
H	6.01944900	4.14777000	-0.31782300
H	4.81533700	5.95522900	-1.52440800
H	0.32811700	1.96885500	1.56672800
H	-0.01285500	4.41077500	1.61487000

**Guanidine**

C	2.10404300	-0.04864200	0.76996300
C	1.21512700	1.21928100	0.61773300
C	-0.01065900	-0.60846700	-0.02638400
C	-1.20931100	1.28364300	-0.23851300
C	-2.02202000	0.00624300	-0.60360600
H	2.40666900	-0.16577000	1.81801400
H	0.80989900	1.53067700	1.59299700

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H	-1.46134300	1.65359000	0.76891700
H	-1.35136900	2.09670800	-0.95369400
H	-2.14639700	-0.01807800	-1.69903800
H	1.75950500	2.06287400	0.18746000
N	0.15035900	0.75809800	-0.26208600
N	-1.16694200	-1.12739600	-0.19856200
N	1.17983300	-1.13197600	0.39610300
H	1.16487900	-1.99579200	0.91567900
C	-3.43443900	-0.07378900	0.00584200
C	-4.13364200	-1.30848300	-0.57312900
C	-3.37748600	-0.20515800	1.53065400
C	-4.21682700	1.18523500	-0.38232300
H	-4.22474300	-1.22933600	-1.66224400
H	-3.56302000	-2.21193000	-0.34266200
H	-5.14043700	-1.41230600	-0.15501300
H	-2.92470700	0.67284600	2.00305400
H	-4.38965000	-0.31075700	1.93487400
H	-2.79517600	-1.08542900	1.81500700
H	-5.25132200	1.11566000	-0.03036900
H	-3.77590900	2.08565800	0.05949800
H	-4.23845700	1.31469700	-1.47039000
C	3.38681800	-0.05592000	-0.09131000
C	4.05797500	-1.42601100	0.05636900
C	3.05586600	0.18998100	-1.56569800
C	4.34451800	1.02294700	0.42599500
H	4.28843000	-1.64124800	1.10629100
H	3.41019000	-2.21980200	-0.32608900
H	4.99624000	-1.45182000	-0.50624200
H	2.60596000	1.17564700	-1.72069700

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H	3.96889600	0.13750500	-2.16742800
H	2.35599900	-0.56532100	-1.93475100
H	5.28356800	0.99118000	-0.13505500
H	3.92969800	2.02960000	0.31578500
H	4.58007400	0.86471200	1.48435400

**M2-Gua**

C	4.18348900	-0.55469400	0.21019600
C	4.15783800	0.68678800	-0.72343300
C	2.09221600	0.37528700	0.18135600
C	2.05530300	2.19742500	-1.16042200
C	0.67425200	2.04392600	-0.46026600
H	4.71706700	-0.29563000	1.13509900
H	5.01010500	1.34482400	-0.55286200
H	2.42143700	3.22397400	-1.15074400
H	2.02284200	1.83698400	-2.19679500
H	-0.12317800	2.00275800	-1.20738300
H	4.13284500	0.39705600	-1.78283100
N	2.89858100	1.32630500	-0.34553100
N	0.80532100	0.69792800	0.16725100
N	2.75244800	-0.71802700	0.51551000
H	2.26977300	-1.45609800	1.01563600
C	0.36102300	3.17476900	0.55405400
C	-0.95614500	2.88915800	1.28449200
C	1.48026300	3.32081000	1.59129200
C	0.19553000	4.48664400	-0.22606300
H	-1.79501000	2.83483100	0.58289900
H	-0.91893900	1.94837800	1.83839300
H	-1.15869600	3.70051200	1.99083500



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H	2.44081100	3.57246100	1.13156200
H	1.22415600	4.12156500	2.29150700
H	1.60384500	2.39920300	2.16900500
H	-0.11659600	5.28087400	0.45840200
H	1.12288400	4.81512600	-0.70392700
H	-0.57387700	4.38941000	-0.99943700
C	4.82878600	-1.82386700	-0.37509100
C	4.83830400	-2.90624400	0.71165000
C	4.06422300	-2.34436500	-1.59639000
C	6.27204400	-1.48041300	-0.76160900
H	5.36467200	-2.56225900	1.60792900
H	3.82362100	-3.20030100	0.99936000
H	5.34555100	-3.80252900	0.34304200
H	4.07319400	-1.63252600	-2.42725400
H	4.53284600	-3.26661400	-1.95221600
H	3.02253700	-2.56771300	-1.34882100
H	6.78785300	-2.37859500	-1.11294400
H	6.30822600	-0.73967900	-1.56750200
H	6.82778900	-1.08500500	0.09553000
C	-2.59468000	-1.01004400	0.19450500
C	-2.47511800	-2.22482200	0.77013700
C	-0.20971900	-0.33481800	0.47839200
C	-1.48141300	-0.09533800	0.01068500
H	-1.53791300	-2.61463000	1.13292500
H	-1.69125600	0.81363300	-0.53421000
O	0.25373800	-1.31725300	1.10483200
C	-3.90751100	-0.49622700	-0.30129500
C	-4.65996600	-1.20669800	-1.24095700
C	-4.38070300	0.74428900	0.13953700

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C	-5.86063000	-0.69354900	-1.72314800
H	-4.29161000	-2.16352100	-1.59772600
C	-5.58606000	1.25528900	-0.33466900
H	-3.79735200	1.30073200	0.86855700
C	-6.32908800	0.53797000	-1.26941100
H	-6.43009000	-1.25496900	-2.45742900
H	-5.94517300	2.21426800	0.02607900
H	-7.26658600	0.93670100	-1.64408100
Cl	-3.83550200	-3.29213500	1.09581700

**TS3RR-Gua**

C	-3.57748500	-2.23101900	1.43489900
C	-3.61843700	-2.61036500	-0.06764400
C	-1.47337900	-2.20345600	0.55312400
C	-1.50998500	-2.85342400	-1.62244900
C	-0.03508600	-2.63557100	-1.18144300
H	-3.68022000	-3.13988000	2.04535300
H	-4.22878900	-3.49538200	-0.24999900
H	-1.64864000	-3.79844700	-2.14908600
H	-1.89154900	-2.01662000	-2.21498900
H	0.41097400	-1.87165200	-1.82186400
H	-3.93149100	-1.77455100	-0.70496600
N	-2.20268200	-2.87543700	-0.33657900
N	-0.18224100	-2.07573800	0.19630300
N	-2.18260100	-1.75281400	1.57188000
H	-1.72775600	-1.41038800	2.40672100
C	0.83112300	-3.91934500	-1.19576400
C	2.23346100	-3.63570300	-0.63953800
C	0.17958700	-5.02077400	-0.35101400

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C	0.98090900	-4.38739700	-2.64931500
H	2.77794400	-2.90995700	-1.25366500
H	2.19853800	-3.25534200	0.38635900
H	2.81290700	-4.56411400	-0.63168200
H	-0.81042800	-5.29773900	-0.72643300
H	0.80592100	-5.91759400	-0.36902000
H	0.07651300	-4.70376800	0.69178700
H	1.64646500	-5.25474200	-2.68931600
H	0.02745400	-4.68537400	-3.09478500
H	1.41861400	-3.59961800	-3.27178100
C	-4.64164500	-1.22319800	1.90245500
C	-4.31879500	-0.80355800	3.34197200
C	-4.70256500	0.01733800	1.00544700
C	-5.99568300	-1.94274500	1.87377000
H	-4.18084500	-1.67522800	3.99156400
H	-3.41295100	-0.18872100	3.38680700
H	-5.13796600	-0.20473500	3.75027400
H	-5.10130600	-0.21285400	0.01372600
H	-5.35131700	0.76948500	1.46559300
H	-3.71153200	0.45482500	0.85826800
H	-6.78602400	-1.26111500	2.20143800
H	-6.24503500	-2.27917800	0.86189800
H	-6.00050800	-2.81319600	2.53831100
C	2.94293200	-0.10946900	0.70937800
C	2.98780900	0.45151600	1.92882500
C	0.62098300	-1.08640300	0.84523600
C	1.66075000	-0.47228400	0.06822900
H	2.10292500	0.62811200	2.52060300
H	1.82449900	-0.95548800	-0.88413700

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O	0.29773300	-0.79248900	1.99689800
C	4.15495400	-0.40483200	-0.10851800
C	5.26152200	-1.05610000	0.44910100
C	4.17416400	-0.12293700	-1.48021100
C	6.36251400	-1.38756500	-0.33480700
H	5.24899800	-1.32035000	1.50097100
C	5.27750300	-0.44609900	-2.26437100
H	3.31262500	0.35046800	-1.94194700
C	6.37889100	-1.07816500	-1.69275600
H	7.20696100	-1.89794700	0.11749200
H	5.27292000	-0.20844500	-3.32343200
H	7.23835100	-1.33749000	-2.30238800
Cl	4.43813100	1.03283800	2.71250800
N	-1.48199500	0.23311500	-0.93364800
N	-0.70994600	1.22495400	-0.29187000
C	0.59405300	1.26982700	-0.59546400
H	0.80273900	0.98707700	-1.62391500
C	-1.25480600	1.81467600	0.93457200
H	-1.84624100	1.03478400	1.42164500
C	-0.18410600	2.31763400	1.90244100
H	0.16953800	1.46719600	2.49334000
C	0.99000900	2.93695100	1.19295500
C	1.72281400	3.99134300	1.72979300
H	1.41871700	4.41960800	2.68115300
C	2.83755900	4.49271400	1.06113600
H	3.40400700	5.31159800	1.49283800
C	3.21997500	3.94639000	-0.16180800
H	4.08200500	4.33902800	-0.69066500
C	2.48848900	2.89707200	-0.70887400

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H	2.77535700	2.47997200	-1.66972700
C	1.38041500	2.38535600	-0.03340700
C	-2.55282200	0.66884300	-1.60115200
O	-3.37122800	-0.13672500	-2.10466700
C	-2.86072800	2.14440900	-1.77560300
C	-1.90913400	3.08720800	-2.17593600
C	-4.18058900	2.55692000	-1.57895400
C	-2.27039600	4.42048400	-2.35347200
H	-0.88528200	2.77889500	-2.36069600
C	-4.53906600	3.89256200	-1.73560200
H	-4.92128900	1.81071100	-1.30812800
C	-3.58248300	4.82880400	-2.12225300
H	-1.52533200	5.14197300	-2.67459300
H	-5.56590300	4.20203100	-1.56590300
H	-3.85916500	5.87045500	-2.25208100
H	-1.93315800	2.62777200	0.64468300
H	-0.63560400	3.03500200	2.59343600

**TS3RS-Gua**

C	3.59770700	-1.65379900	-1.22163200
C	3.00517900	-2.97455500	-0.66408900
C	1.32415600	-1.50443600	-1.12165700
C	0.41548600	-3.48623300	-0.44677600
C	-0.72652700	-2.50977400	-0.85768100
H	3.86483000	-1.80699400	-2.27677300
H	3.43373500	-3.85235000	-1.14781900
H	0.29018000	-4.47531100	-0.88691600
H	0.49598800	-3.59412600	0.64198200
H	-1.43735900	-2.38516900	-0.03302800

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H	3.13461100	-3.05675800	0.42330200
N	1.59062900	-2.81669900	-0.99397600
N	0.02054100	-1.22954700	-1.04936100
N	2.41317600	-0.76431700	-1.17834200
H	2.37285700	0.22659300	-1.39443100
C	-1.48219900	-2.97432600	-2.13120300
C	-2.49187700	-1.91423300	-2.58131000
C	-0.51059200	-3.24126000	-3.28684600
C	-2.26046700	-4.25067300	-1.78064100
H	-3.23453200	-1.70680300	-1.80395600
H	-1.99809000	-0.97641900	-2.85426200
H	-3.02610200	-2.27688200	-3.46491800
H	0.21022100	-4.03006400	-3.05284500
H	-1.07454900	-3.55737400	-4.16916700
H	0.04257300	-2.33467300	-3.55345900
H	-2.85777900	-4.56132900	-2.64243500
H	-1.60647800	-5.08708100	-1.51900900
H	-2.94382300	-4.07463400	-0.94288800
C	4.83477100	-1.10716800	-0.49155400
C	5.25677300	0.20120000	-1.17141400
C	4.56313000	-0.84788300	0.99182400
C	5.95186100	-2.14654900	-0.64816900
H	5.41826800	0.05345800	-2.24507000
H	4.51131500	0.99068400	-1.03142800
H	6.19164600	0.56381800	-0.73394600
H	4.40968200	-1.77552700	1.55267900
H	5.42320700	-0.33770000	1.43613400
H	3.69180500	-0.20621400	1.13744400
H	6.86997600	-1.77478100	-0.18462100

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H	5.69421500	-3.09297700	-0.16042200
H	6.16378000	-2.34817600	-1.70377100
C	-2.27310700	1.74063600	-0.51026300
C	-1.53622600	2.85003600	-0.34576000
C	-0.43638800	0.15344800	-1.11390800
C	-1.62140100	0.42413500	-0.34522600
H	-0.48481600	2.81006100	-0.08309700
H	-2.31362300	-0.40843200	-0.30504900
O	0.25540800	0.90028500	-1.79338700
C	-3.74440100	1.76500600	-0.74395500
C	-4.29999600	1.09944400	-1.84099400
C	-4.59921200	2.41153000	0.15622200
C	-5.67765700	1.08724200	-2.04058000
H	-3.64174000	0.60598900	-2.54950500
C	-5.97764700	2.39077700	-0.03631900
H	-4.17248600	2.92159900	1.01547400
C	-6.52029300	1.72990300	-1.13633700
H	-6.09332300	0.57693300	-2.90382500
H	-6.62840400	2.89037800	0.67435900
H	-7.59483300	1.71580500	-1.28794600
Cl	-2.14122300	4.47283900	-0.57664000
N	0.97570000	1.17268000	1.16508100
N	0.22334500	0.27369700	1.92014800
C	-1.09985100	0.36223900	1.71782000
H	-1.47468700	1.38276800	1.73143400
C	0.84709000	-1.00565200	2.25981500
H	1.86051700	-0.77956300	2.58830000
C	0.06375900	-1.69208100	3.36495200
H	0.20604900	-1.12486300	4.29325000

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C	-1.40614400	-1.74248500	3.04160500
C	-2.23481000	-2.75413900	3.52990300
H	-1.79668900	-3.55826000	4.11536400
C	-3.60330100	-2.73520800	3.28442200
H	-4.23472700	-3.53059200	3.66701600
C	-4.16280800	-1.68667800	2.55308400
H	-5.23147800	-1.65705900	2.36853800
C	-3.34715400	-0.67939300	2.05573600
H	-3.77933500	0.13421300	1.47724300
C	-1.96508500	-0.70577500	2.27997500
C	2.10971500	1.56712600	1.74743300
O	2.53988900	1.28583400	2.88679200
C	2.96172100	2.41036200	0.82201800
C	2.54430500	2.77476800	-0.46421700
C	4.22657500	2.79948600	1.26493900
C	3.38558600	3.52192600	-1.28667300
H	1.56720000	2.45524400	-0.81679400
C	5.06716800	3.54369100	0.44126700
H	4.52881000	2.49814700	2.26260700
C	4.64835500	3.90751600	-0.83744900
H	3.05433500	3.80361100	-2.28175100
H	6.04996900	3.84081700	0.79511600
H	5.30133700	4.48992400	-1.48033800
H	0.89659400	-1.63877200	1.36532400
H	0.45867400	-2.69810700	3.53653400

**TS3SR-Gua**

C	-4.09514200	-1.35754200	-0.27958200
C	-3.78507500	-2.54134600	0.68536900



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C	-1.94506100	-1.21428700	0.48196400
C	-1.42014700	-2.98877000	1.78377400
C	-0.25467700	-1.96288700	1.82604600
H	-4.77673100	-0.64619300	0.20543300
H	-4.55339400	-2.65608300	1.44993800
H	-1.66026400	-3.39007200	2.76808400
H	-1.21970500	-3.81700600	1.09188000
H	0.69729100	-2.43385500	1.56409200
H	-3.67113700	-3.49067600	0.14662100
N	-2.50132700	-2.14885600	1.26857200
N	-0.62482000	-1.04420500	0.69293600
N	-2.77261800	-0.72011300	-0.40140100
H	-2.50419100	0.02190300	-1.03700200
C	-0.11872700	-1.27549200	3.21049200
C	0.80695500	-0.06252600	3.10773300
C	-1.46721500	-0.79172600	3.76235000
C	0.50027700	-2.30281700	4.16888400
H	1.82654200	-0.35441400	2.82871400
H	0.39845500	0.65301600	2.38567100
H	0.86643500	0.43181700	4.08335700
H	-2.17817400	-1.61110500	3.90485200
H	-1.29740900	-0.33145400	4.74117500
H	-1.90397300	-0.03551100	3.10467900
H	0.64052400	-1.84559300	5.15263100
H	-0.13549500	-3.18368000	4.30541800
H	1.47890900	-2.64018200	3.81099300
C	-4.68044100	-1.74580400	-1.64930200
C	-4.95608600	-0.45539000	-2.43100600
C	-3.71352000	-2.62890600	-2.44498300

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C	-6.00203300	-2.48203100	-1.40474300
H	-5.59603800	0.22439000	-1.85903400
H	-4.03255300	0.08138700	-2.67435000
H	-5.45510400	-0.68995900	-3.37605600
H	-3.56616400	-3.60764500	-1.97768300
H	-4.12107900	-2.80476700	-3.44478900
H	-2.73525000	-2.14976200	-2.55238800
H	-6.47734400	-2.72090700	-2.36043500
H	-5.84838800	-3.42346900	-0.86644700
H	-6.69633900	-1.86317800	-0.82638200
C	2.60295200	-0.91807500	-1.13952100
C	2.37843800	-0.96714700	-2.46434700
C	0.20188400	-0.74799400	-0.46016500
C	1.57449700	-0.41299500	-0.20507600
H	1.43729700	-0.68960900	-2.91458800
H	1.87640800	-0.44877300	0.83374300
O	-0.33434900	-0.74417800	-1.56398800
C	3.88363000	-1.36683700	-0.51690400
C	4.38431100	-2.64384200	-0.79590200
C	4.57014100	-0.56294400	0.40004200
C	5.55178100	-3.09861400	-0.19142300
H	3.84464600	-3.28496300	-1.48575900
C	5.74383100	-1.01509600	0.99751100
H	4.19404300	0.42754500	0.63792200
C	6.23985900	-2.28255100	0.70356900
H	5.92224500	-4.09348500	-0.41802100
H	6.27105100	-0.37102500	1.69460500
H	7.15353600	-2.63458900	1.17201100
Cl	3.58247300	-1.42690300	-3.64914100

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N	-0.90812600	2.20968800	-0.35049500
N	0.40515400	2.18594500	0.14603800
C	1.33813500	1.59980100	-0.62409100
H	0.97054300	1.32328700	-1.61394300
C	0.75672700	3.15918000	1.18381300
H	0.01109200	3.07515900	1.97560200
C	2.15470000	2.90256800	1.73291400
H	2.15059100	1.97938700	2.32415800
C	3.14852000	2.77571800	0.61311300
C	4.45514900	3.24993900	0.69902800
H	4.78118700	3.74821800	1.60819100
C	5.33528200	3.09258500	-0.36938300
H	6.35328500	3.46060200	-0.29095700
C	4.90027200	2.48323900	-1.54439300
H	5.57546100	2.37779400	-2.38700900
C	3.59459900	2.01311300	-1.64253300
H	3.25067400	1.54876000	-2.56019800
C	2.72125500	2.13242000	-0.55684100
C	-1.84035300	2.03621700	0.58264200
O	-1.69680600	1.70949300	1.78614100
C	-3.24764800	2.27905700	0.06917200
C	-3.50994900	2.81721700	-1.19492600
C	-4.31936400	1.97340800	0.91185000
C	-4.82122700	3.05020300	-1.60313200
H	-2.67245000	3.06042100	-1.83946600
C	-5.63105900	2.20276700	0.50350100
H	-4.09565800	1.56459700	1.89256600
C	-5.88549700	2.74772300	-0.75455500
H	-5.01261200	3.47601100	-2.58361000

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H	-6.45572900	1.96649200	1.16971200
H	-6.90675700	2.93677000	-1.07125300
H	0.69736200	4.16433900	0.74232900
H	2.43387200	3.71645300	2.40785300

**TS3SS-Gua**

C	3.86055600	-1.08890600	1.18861600
C	3.97841200	-1.54302400	-0.29511400
C	1.84103500	-1.84230900	0.40467000
C	2.02401100	-2.54708200	-1.73784900
C	0.62627100	-2.91661400	-1.19648300
H	4.14692300	-0.03470900	1.28150400
H	4.84373300	-2.18695400	-0.46271800
H	2.47421700	-3.38413200	-2.27193800
H	2.01946700	-1.63765400	-2.35276500
H	0.67788000	-3.94322600	-0.80762300
H	3.99175200	-0.69470600	-0.98946300
N	2.73000000	-2.28704800	-0.48918100
N	0.56137600	-2.05507400	0.05676300
N	2.40703200	-1.20798700	1.41481600
H	1.87647500	-0.93060600	2.22790500
C	-0.48496600	-2.91012000	-2.26081200
C	-0.02863100	-3.91230000	-3.34235900
C	-0.65752800	-1.52614700	-2.93480200
C	-1.78784500	-3.48775700	-1.67453000
H	0.19138200	-4.89624200	-2.91412100
H	0.85482800	-3.55812300	-3.88025600
H	-0.83305600	-4.03461200	-4.07353800
H	-0.16751900	-0.73013600	-2.36570600

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H	-1.71723400	-1.28123600	-3.06004100
H	-0.20483300	-1.52364300	-3.93025700
H	-2.58273400	-3.44257200	-2.42566200
H	-2.14232100	-2.96688300	-0.78468800
H	-1.63740700	-4.53887300	-1.40596300
C	4.68382500	-1.90900700	2.20540600
C	6.17076400	-1.63211700	1.95694300
C	4.39341300	-3.40703500	2.07346900
C	4.32348300	-1.44203100	3.62112700
H	6.39515700	-0.56546700	2.06371200
H	6.48749700	-1.94844300	0.95853500
H	6.77726600	-2.17871500	2.68497300
H	3.32979500	-3.61756400	2.22318800
H	4.95463900	-3.96053000	2.83241100
H	4.68632700	-3.79443300	1.09270300
H	4.97193900	-1.93109900	4.35388700
H	3.29033400	-1.69594600	3.87873300
H	4.45350100	-0.35916000	3.72665300
C	-2.83026300	-0.58420000	0.78929700
C	-2.93080000	-0.19957500	2.07181700
C	-0.43383000	-1.33963000	0.82369000
C	-1.51362400	-0.71527500	0.12653400
H	-2.06601300	0.00223300	2.68600800
H	-1.59984400	-1.03194000	-0.89820000
O	-0.18041100	-1.20753300	2.02281700
C	-4.00226400	-0.89289400	-0.07969000
C	-5.02319900	-1.74082500	0.36435300
C	-4.05687500	-0.42259000	-1.39786600
C	-6.07638500	-2.08840900	-0.47632300

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H	-4.97721000	-2.14469600	1.37007100
C	-5.11325200	-0.76209600	-2.23793200
H	-3.26076200	0.21330900	-1.77624700
C	-6.12938100	-1.59640900	-1.77820500
H	-6.85339500	-2.75410000	-0.11406100
H	-5.13855300	-0.37829100	-3.25291500
H	-6.95131100	-1.86867000	-2.43230900
Cl	-4.43126400	0.11090200	2.90850600
N	1.45415300	0.54889400	-1.02539200
N	0.64266900	1.30846500	-0.16074800
C	-0.68637400	1.22013000	-0.30142000
H	-1.00510400	1.06726200	-1.32974500
C	1.26150700	1.94205000	1.00545700
H	2.16539800	1.37074000	1.23286700
C	0.32217500	1.99119700	2.20620200
H	0.20969200	0.98309700	2.62191400
C	-1.03327700	2.50358800	1.78895400
C	-1.82581300	3.31110400	2.59983800
H	-1.45491100	3.61450900	3.57507500
C	-3.08349500	3.72912900	2.16922800
H	-3.69495900	4.35409600	2.81203300
C	-3.55150500	3.35139900	0.91305200
H	-4.52633100	3.68141600	0.57043900
C	-2.76494000	2.54632600	0.09617400
H	-3.12876700	2.24957600	-0.88316000
C	-1.51247700	2.11335200	0.53216900
C	2.29294500	1.23767700	-1.80456000
O	3.13849300	0.64319300	-2.51205300
C	2.30311800	2.75441700	-1.86264900

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C	1.15002800	3.53503400	-1.98847100
C	3.54860200	3.38642800	-1.84467600
C	1.24428400	4.92224600	-2.07046900
H	0.17452900	3.06185800	-2.03606800
C	3.64403600	4.77309900	-1.90734000
H	4.43983700	2.76913400	-1.78928300
C	2.48947400	5.54541700	-2.01835600
H	0.34221400	5.51723400	-2.17520400
H	4.61824700	5.25164300	-1.87825300
H	2.55968700	6.62730400	-2.07316600
H	1.56708000	2.95918500	0.72439200
H	0.75538300	2.63194100	2.97928200

**TS1B''**

C	0.42214700	0.19733700	-0.17118400
C	1.36195900	-0.62878500	0.48872700
C	2.17810000	1.28988300	0.17645800
C	1.12956700	1.28888900	-0.71468700
H	1.07011200	-1.19763000	1.36677600
H	0.95823900	1.94858100	-1.55527000
O	3.03864800	1.73478200	0.83627500
C	-1.03209100	0.08003100	-0.05820300
C	-1.61515600	-1.16428900	0.21552300
C	-1.85134200	1.20164000	-0.24635800
C	-2.99724600	-1.28286000	0.30156100
H	-0.97935100	-2.03669100	0.33363700
C	-3.23232500	1.07748600	-0.17136600
H	-1.39433000	2.17019600	-0.42743300
C	-3.80522300	-0.16393300	0.10601800

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H	-3.44612500	-2.24828700	0.50957200
H	-3.86362600	1.94785100	-0.31600000
H	-4.88441700	-0.25865400	0.17047100
Cl	2.63999800	-1.50447200	-0.37240500
<b>M1B''</b>			
C	0.40714500	-0.06543400	0.05846600
C	0.99994900	-1.22091700	-0.27798600
C	2.37601100	1.45907700	0.28436900
C	1.09162500	1.16807600	0.44030600
H	0.45468000	-2.09324100	-0.60960000
H	0.52670100	1.96590000	0.91111900
O	3.47841600	1.80579700	0.17533000
C	-1.08135000	-0.00653400	0.03513200
C	-1.84893400	-1.08166100	0.49654000
C	-1.73466300	1.12831600	-0.45884200
C	-3.23837800	-1.03018400	0.44602300
H	-1.35257900	-1.94959900	0.91970500
C	-3.12401000	1.17913700	-0.50627300
H	-1.14866500	1.96624600	-0.82504500
C	-3.88024000	0.09942400	-0.05590800
H	-3.82025200	-1.86999500	0.81194000
H	-3.61587000	2.06283000	-0.89979800
H	-4.96398400	0.14098700	-0.08973800
Cl	2.72292400	-1.43795900	-0.25836400
Opt-IRC-R-1-SR			
C	-6.93158500	-2.48133600	-0.82117400
C	-5.89652200	-2.02320500	-1.63343900



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C	-4.69120000	-1.67946400	-1.03519900
C	-4.53547600	-1.79469800	0.35233800
C	-5.56227700	-2.24805600	1.17147000
C	-6.76629100	-2.58887700	0.56229100
C	-2.46926600	-1.00196300	-0.27055900
C	-1.19114300	-0.68996300	1.59310800
C	-2.62285300	-1.15814500	2.02252300
H	-7.87890200	-2.75619000	-1.27157200
H	-6.02856000	-1.93459500	-2.70652100
H	-5.42433100	-2.33085800	2.24409800
H	-7.58787000	-2.94390700	1.17461000
H	-1.00492300	0.32962700	1.94901100
H	-3.17407400	-0.37993500	2.55518500
N	-3.25438700	-1.40848700	0.73018600
S	-3.22880400	-1.02992800	-1.81467500
N	-1.26289400	-0.64629600	0.11918100
C	-0.11049800	-1.62474200	2.09360400
C	0.59286400	-1.31315300	3.25808200
C	0.15039600	-2.82791200	1.43267700
C	1.54219300	-2.20068400	3.76497400
H	0.39617400	-0.37452200	3.77098500
C	1.09959300	-3.71106600	1.93753200
H	-0.37637400	-3.06061200	0.51115000
C	1.79372100	-3.40160100	3.10658900
H	2.08649400	-1.94930400	4.66947400
H	1.30648100	-4.63680400	1.41075600
H	2.53752500	-4.08958900	3.49491600
H	-2.58643600	-2.07007300	2.62165900
C	1.68423200	-1.18367600	-1.21497400

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C	0.99062500	-1.89351100	-2.11172400
C	-0.45466400	0.26775300	-0.79629500
C	1.05726800	0.03304200	-0.56829500
H	0.01798500	-1.57850800	-2.46486200
H	1.22226000	-0.06163900	0.51083200
O	-0.91394500	0.20957800	-1.99411900
C	3.04858800	-1.56148600	-0.74575400
C	3.35711500	-1.58295200	0.61812200
C	4.05946500	-1.87138500	-1.66356300
C	4.63057200	-1.93685500	1.05453700
H	2.59488000	-1.34165300	1.35333500
C	5.33489900	-2.21408500	-1.22947800
H	3.84451300	-1.82294400	-2.72627800
C	5.62417200	-2.25518300	0.13317600
H	4.84181300	-1.96053700	2.11948000
H	6.10666400	-2.44308300	-1.95777600
H	6.61904800	-2.52582700	0.47251100
Cl	1.51270800	-3.42102200	-2.78454000
N	-0.54650400	1.66954500	-0.15768800
N	0.68110900	2.37695700	-0.30273900
C	1.60103700	1.42372700	-0.97683700
H	1.45818600	1.52098700	-2.05950600
C	1.15032600	2.94073700	0.98121000
H	0.27492700	3.05425000	1.62429800
C	2.25195200	2.14150600	1.68229100
H	1.86147000	1.17884900	2.04084600
C	3.38266100	1.94311600	0.70937500
C	4.72243200	2.09830700	1.05770300
H	4.98060500	2.34029300	2.08550800

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C	5.72353100	1.94567000	0.10120200
H	6.76527000	2.06035700	0.38362100
C	5.38458100	1.65448000	-1.21815300
H	6.15990000	1.53622000	-1.96818700
C	4.04621900	1.52176600	-1.57648700
H	3.77487800	1.29468700	-2.60459800
C	3.04370400	1.65479300	-0.61838300
C	-1.73325100	2.31102000	-0.00463200
O	-2.77410500	1.67770600	0.20695400
C	-1.78213700	3.81635400	0.00421200
C	-1.05974500	4.61920700	-0.88359300
C	-2.68946100	4.40718500	0.88680700
C	-1.24239000	5.99907200	-0.87416000
H	-0.36027100	4.15995000	-1.57134400
C	-2.85062700	5.78852500	0.91163000
H	-3.26978200	3.76609900	1.54233200
C	-2.12665600	6.58685000	0.02867800
H	-0.68937700	6.61807300	-1.57342000
H	-3.54740300	6.24001100	1.61059300
H	-2.25549000	7.66462300	0.03949800
H	1.53106900	3.94703400	0.77280800
H	2.59500700	2.69076300	2.56470300