

**Electronic Supplementary Information For**  
**Mechanisms and stereoselectivities of Rh(I)-catalyzed**  
**carbenoid carbon insertion reaction of**  
**benzocyclobutenol with diazoester**

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## 1. Test Results of Basis Sets

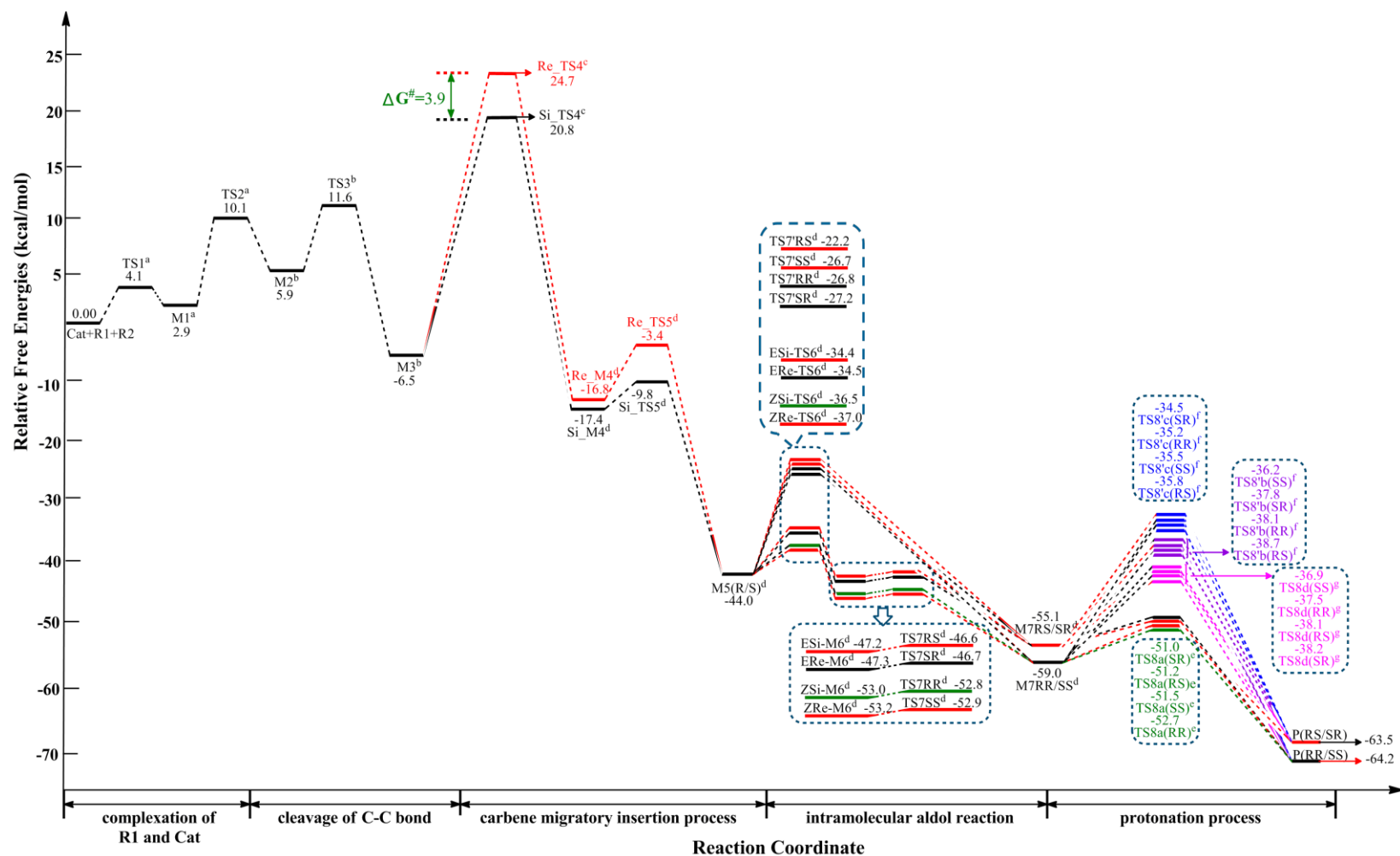
To examine the basis set dependence, single-point energy calculations were also done for selected key structures using different functionals and larger basis set. The results show that both the small and large basis sets give the same conclusion. For example, using the smaller basis set, the difference of free energy barriers between **Re\_TS4** and **Si\_TS4** is 3.9 kcal/mol. As shown in **Table S1**, when the larger basis set is used, the difference of free energy barriers between **Re\_TS4** and **Si\_TS4** are 3.7 kcal/mol, 3.3 kcal/mol, 2.9 kcal/mol, 3.2 kcal/mol, 3.6 kcal/mol, respectively.

**Table S1** Comparisons of relative free energies of B3LYP/6-31G\*\*//Lan12dz optimization with single-point refinement for selected stationary points (Unit: a.u.).

		Optimization	Refinement				
		B3LYP	B3LYP	M06-L	M06	M06	M06-L
C, H, O, N		6-31G*	6-311+G**				6-311++G(2d,2p)
Rh		Lan12DZ	Lan12DZ			SDD	Lan12DZ
<b>Re_ TS4</b>	<i>G</i>	-1683.3626					
	<i>G<sub>TC</sub></i> <sup>a</sup>	0.5049					
	<i>E</i>		-1684.3153	-1684.15822	-1683.1648	-1684.2165	-1684.1948
	<i>E+</i> <i>G<sub>TC</sub></i>		-1683.8104	-1683.6533	-1682.6599	-1683.7116	-1683.6899
<b>Si_ TS4</b>	<i>G</i>	-1683.3689					
	<i>G<sub>TC</sub></i>	0.5027					
	<i>E</i>		-1684.3191	-1684.1614	-1683.1672	-1684.2188	-1684.1980
	<i>E+</i> <i>G<sub>TC</sub></i>		-1683.8163	-1683.6587	-1682.6645	-1683.7161	-1683.6953
$\Delta G$ (kcal/mol)		3.9	3.7	3.3	2.9	3.2	3.6

<sup>a</sup> *G<sub>TC</sub>* represents “Thermal correction to Gibbs Free Energy”. *G* and *E* represent “Gibbs free energy” and “electronic energy”, respectively.

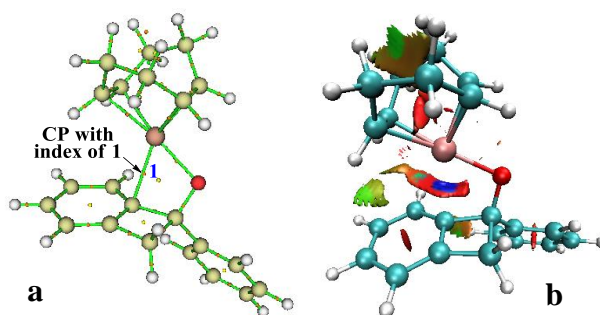
## 2. Free Energy Profiles of the Entire Reaction



**Fig.S1** Free energy profiles of the entire catalytic cycle (unit: kcal/mol, the superscripts “a ~ g” represent adding the energy of **R2**, **H<sub>2</sub>O** plus **R2**, **H<sub>2</sub>O**, **H<sub>2</sub>O** plus **N<sub>2</sub>**, **N<sub>2</sub>**, **N<sub>2</sub>** minus **R1**, **N<sub>2</sub>** minus **R1** plus **H<sub>2</sub>O**, respectively).

### 3. Further AIM and NBO Analyses

Topology analysis of electron density is a main ingredient of Bader's atom in molecules (AIM) theory. Here, to further prove the interaction of Rh and benzene ring of **M2**, the topology analysis of electron density is performed using MULTIWFN program. As can be seen in **Fig.S2a** obviously, the index 1 corresponds to the bond critical point (BCP) of Rh- $\pi$  bond. What's more, **Fig.S2b** shows the strong interaction of Rh- $\pi$  clearly. As summarized in **Table S2**, the value of NBO charge of phenyl group and C5 atom in **R1** is 0.24 e increases to 0.36 e in **M2**, whereas the value of NBO charge of Rh in **Cat** is 0.41 e reduces to 0.27 e in **M2**, indicating that Rh obtains electron from the phenyl group and C5 atom.



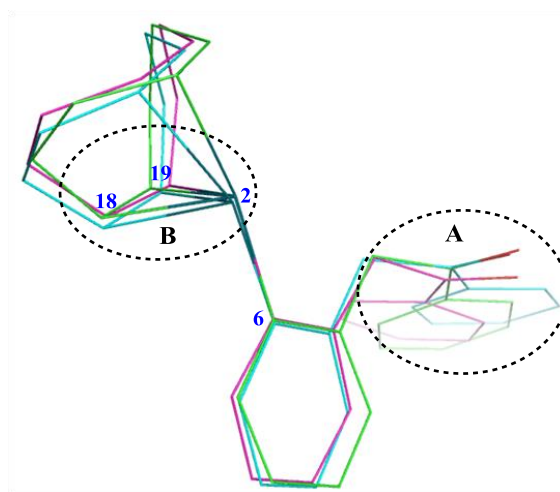
**Fig.S2** (a) AIM analysis for **M2**, orange spheres correspond to (3, -1) critical points, the indices of CPs are labeled by blue number; (b) Interaction analysis (blue, strong attraction; green, weak interaction) for **M2**.

**Table S2** The values of NBO charge on the “phenyl group + C5 atom” and Rh atom in **R1**, **Cat** and **M2** (unit: e)

	Phenyl group + C5 atom	Rh
<b>R1</b>	0.24	
<b>Cat</b>		0.41
<b>M2</b>	0.36	0.27

## 4. Superposition of M3-Part

Further investigation about the distortion of **M3** part has been conducted. As shown in **Fig.S3**, the distortion mainly comes from two parts (i.e. A and B), while of the two parts, part B plays more important role in this step process. The superposition between M3-parts of **M3** and **Si\_TS4** are better than **Re\_TS4**. Which is mainly responsible for the lower distortion energies via **Si\_TS4**.

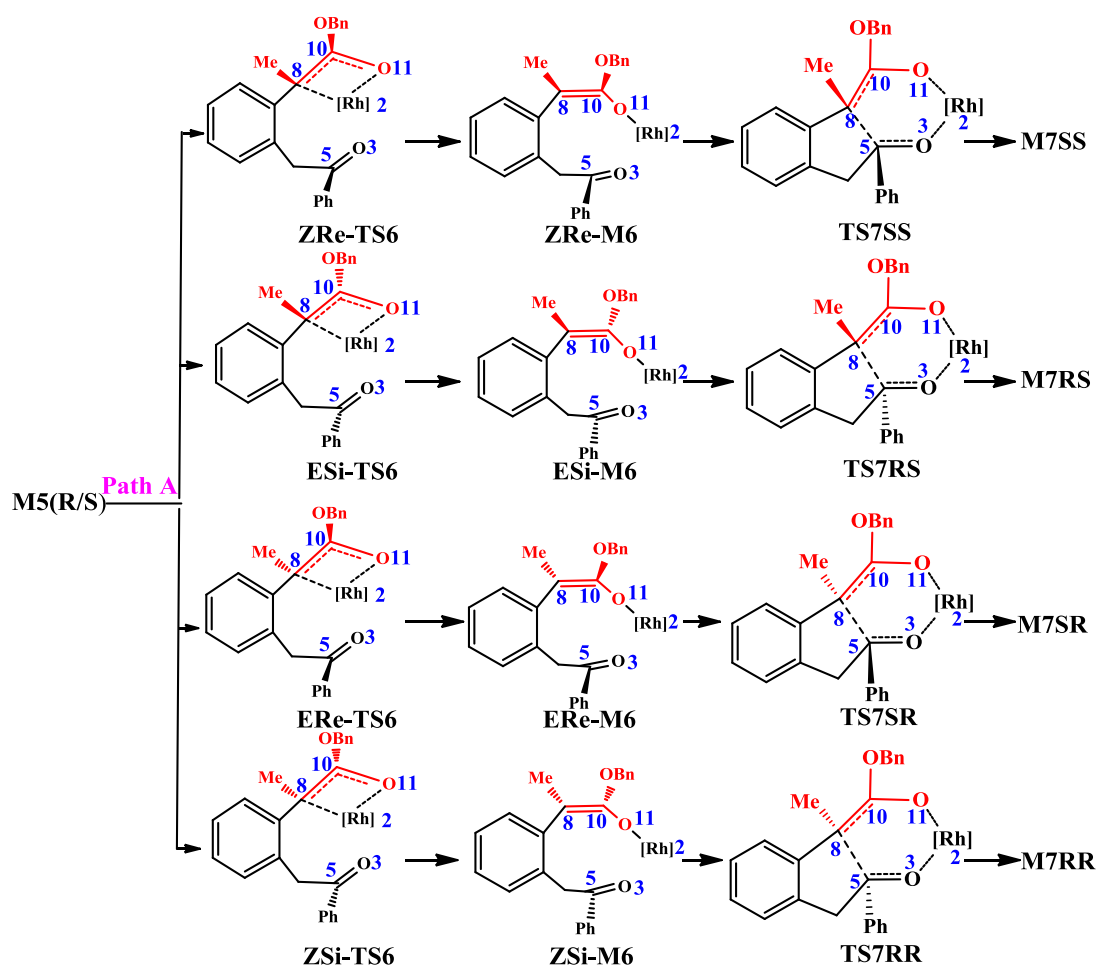


**Fig.S3** Superposition of M3-part from **M3** (green), **Si\_TS4** (pink) and **Re\_TS4** (cyan) (the hydrogen atoms are omitted).

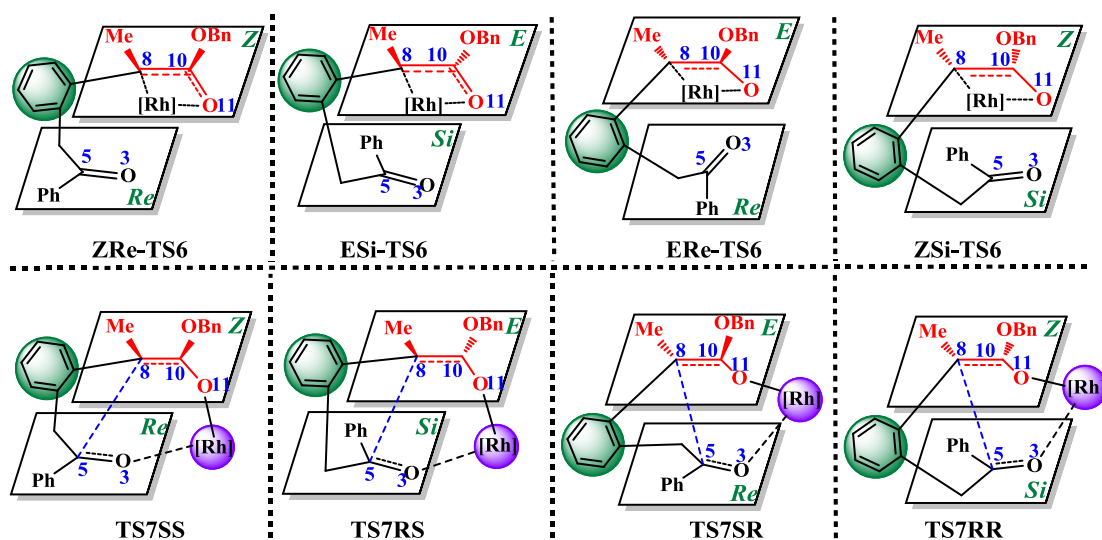
## 5. Additional Description for the Fourth Stage

**Enol-Type mechanism (Path A):** Scheme S1 illustrates the detailed reaction processes of the enol-type aldol reaction pathway, from which we can see the enol-type mechanism includes two steps: tautomerism between **M5** and **M6** (i.e. the first step) and intramolecular aldol-type reaction (i.e. the second step). In the first step, **M5(R/S)** could correspondingly convert to **M6(ZRe-M6/ESi-M6/ERe-M6/ZSi-M6)** via transition states **TS6(ZRe-TS6/ESi-TS6/ERe-TS6/ZSi-TS6)**. The next step is the intramolecular aldol-type reaction of intermediates **M6(ZRe-M6/ESi-M6/ERe-M6/ZSi-M6)** to form intermediates **M7(SS/RS/SR/RR)**

via transition states **TS7(SS/RS/SR/RR)**, respectively. The specific attack modes of the transition states **TS6** and **TS7** are presented in **Scheme S2**. As shown in **Scheme S2**, the intramolecular attack from the C8 atom with *E*- or *Z*-isomerism of C8=C10 double bond to the C5 atom with *Re*- or *Si*- face of the carbonyl group can afford correspondingly four distereoisomers **M7(SR/RS/SS/RR)**, respectively. The distance changes of Rh2–O11, Rh2–C8, C10–C8, C8–C5, C5–O3 and O3–Rh2 summarized in **Table S2** and **Fig.S4** reveal the gradual accomplishment of this stage.



**Scheme S1** Possible reaction modes in Path A in the fourth stage

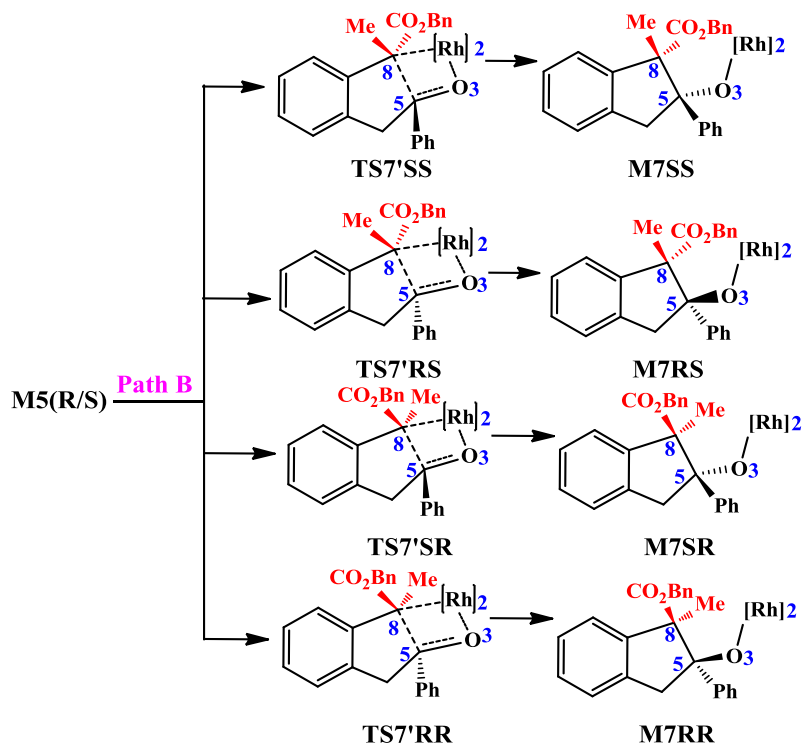


**Scheme S2** Different modes for the intramolecular aldol reaction transition states of Path A

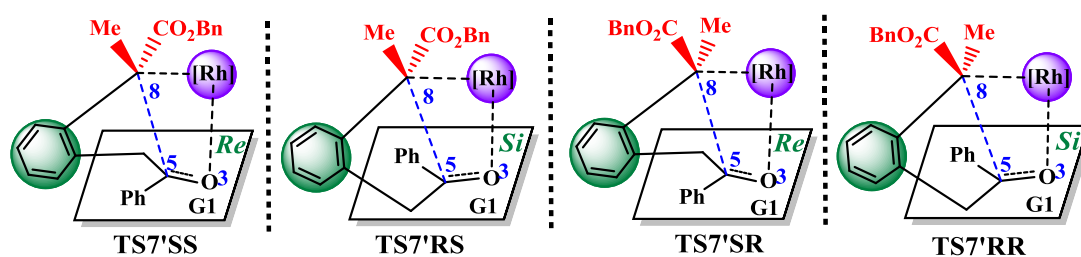
**Ketone-Type mechanism (Path B):** Scheme S3 depicts the detailed reaction process of the ketone-type aldol reaction pathway in the fourth stage, and the specific attack faces in **TS7'** are presented in Scheme S4. In this path, the *Re/Si*-face attack on C5 atom of carbonyl group by C8 atom in **M5(R/S)**, concerted with the breaking of C8–Rh2 bond leads to four diastereoisomers **M7(SR/RR/RS/SS)** via transition states **TS7'(SR/RR/RS/SS)**, respectively. In this stage, four possible reaction patterns should be involved: the C8 atom can attack either the *Re* or *Si* face of the carbonyl group to participate in the intramolecular aldol reaction. The attack on the *Re*- or *Si*-face of the carbonyl group (Scheme S4) by the *R*-configuration of the C8 atom can lead to the diastereoisomeric intermediates **M7SR** and **M7RR**, respectively. Whereas the attack on the *Re*- or *Si*-face of the carbonyl group (Scheme S4) by the *S*-configuration of the C8 atom can lead to the diastereoisomeric intermediates **M7RS** and **M7SS**, separately. The distance changes of C5–C8 and C8–Rh2 summarized in Table S3 (in the supporting information) and Fig.S4 reveal that the gradual accomplishment of this stage.

As shown in Fig.S1, the energy barriers of the tautomerism step are 9.6 (via **ESi-TS6**), 7.0 (via **ZRe-TS6**), 7.5 (via **ZSi-TS6**) and 9.5 (via **ERe-TS6**) kcal/mol, separately, and those of the following intramolecular aldol-type reaction processes via

**TS7RS**, **TS7SR**, **TS7RR**, **TS7SS** are 0.6, 0.6, 0.2, and 0.3 kcal/mol in Path A, separately, while those energy barriers via Path B are 21.8 (via **TS7'RS**), 17.3 (via **TS7'SS**), 17.2 (via **TS7'RR**), 16.8 (via **TS7'SR**) kcal/mol, respectively. Obviously, the enol-type mechanism (Path A) is more energy favorable than the ketone-type mechanism (Path B).

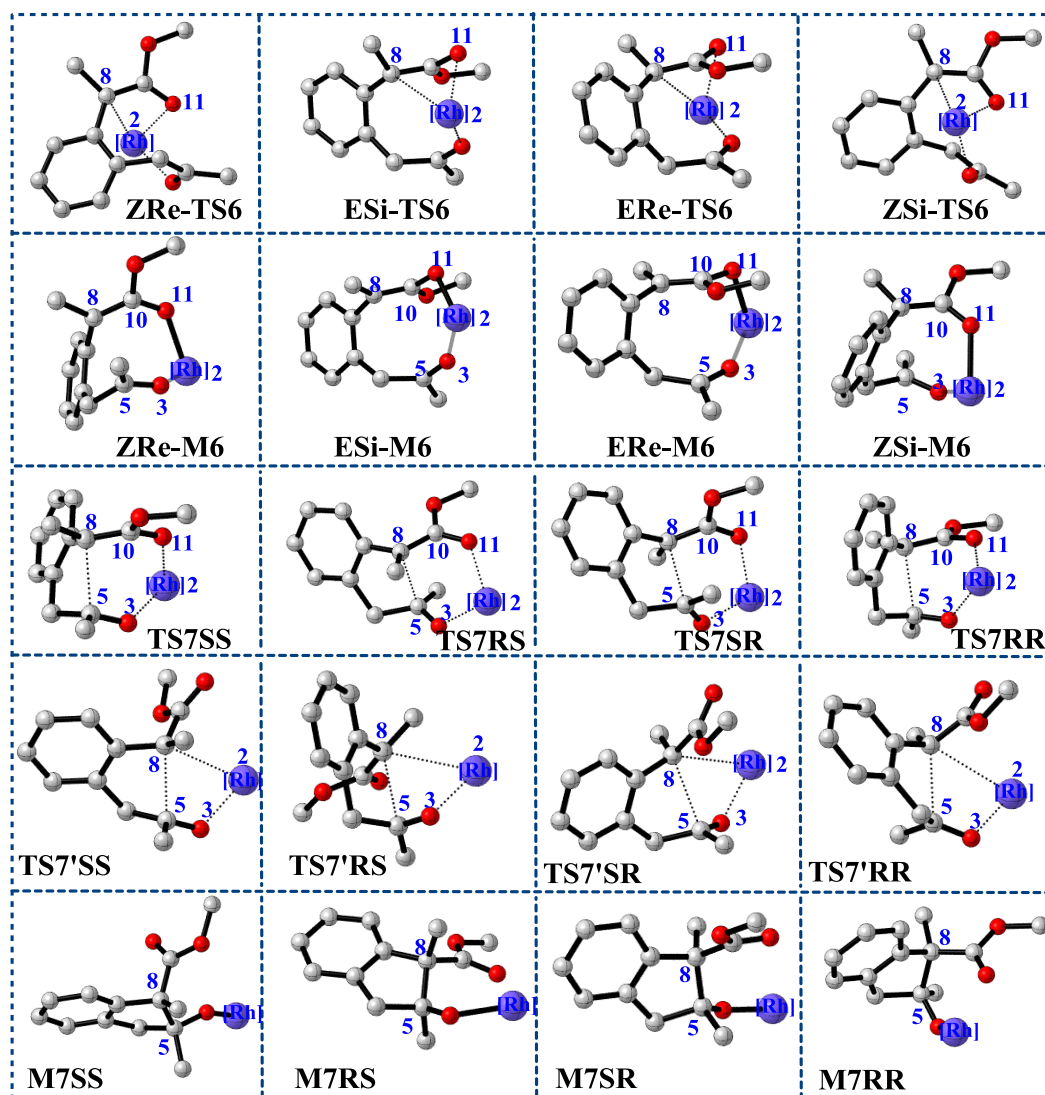


**Scheme S3** Possible reaction modes in Path B in the fourth stage



**Scheme S4** Different modes of Path B





**Fig.S4** Optimized geometries of all stationary points involved in the fourth stage (For parameters of bond lengths, please see **Tables S2** and **S3**, the hydrogen atoms and the ligand of Rh(I) which are not involved in the reaction are omitted; only the  $\alpha$ -carbon of phenyl and benzyl group are shown).

**Table S3** Some Geometrical Parameters of Several Stationary Points (SP) Along the Reaction Coordinate for the Path A in the Fourth Stage (distances in Å)

SP	Rh2–O11	Rh2–C8	C10–C8	C8–C5	C5–O3	O3–Rh2
<b>ERe-TS6</b>	2.44	2.84	--	--	--	2.31
<b>ESi-TS6</b>	2.40	2.91	--	--	--	2.16
<b>ZRe-TS6</b>	2.40	2.91	--	--	--	2.16
<b>ZSi-TS6</b>	2.43	2.84	--	--	--	2.31
<b>ERe-M6</b>	2.11	3.60	1.38	2.79	1.25	2.17
<b>ESi-M6</b>	2.15	3.55	1.39	2.59	1.27	2.21
<b>ZRe-M6</b>	2.15	3.55	1.39	2.58	1.27	2.20
<b>ZSi-M6</b>	2.14	3.60	1.39	2.72	1.25	2.16
<b>TS7SS</b>	2.15	--	1.42	2.32	1.28	2.12
<b>TS7RS</b>	2.17	--	1.41	2.37	1.28	2.18
<b>TS7SR</b>	2.17	--	1.41	2.37	1.28	2.18
<b>TS7RR</b>	2.16	--	1.42	2.32	1.29	2.12

**Table S4** Some geometrical parameters of several stationary points (SP) along the reaction coordinate for the Path B in the fourth stage (distances in Å)

SP	Rh2–C8	C8–C5	C5–O3	O3–Rh2
<b>TS7'SS</b>	3.05	2.45	1.29	2.05
<b>TS7'RS</b>	3.25	2.66	1.28	2.06
<b>TS7'SR</b>	3.01	2.61	1.28	2.09
<b>TS7'RR</b>	3.06	2.46	1.29	2.06
<b>M7RS</b>	--	1.63	1.39	1.98
<b>M7RR</b>	--	1.63	1.39	2.02
<b>M7SS</b>	--	1.64	1.38	1.99
<b>M7SR</b>	--	1.65	1.38	2.05

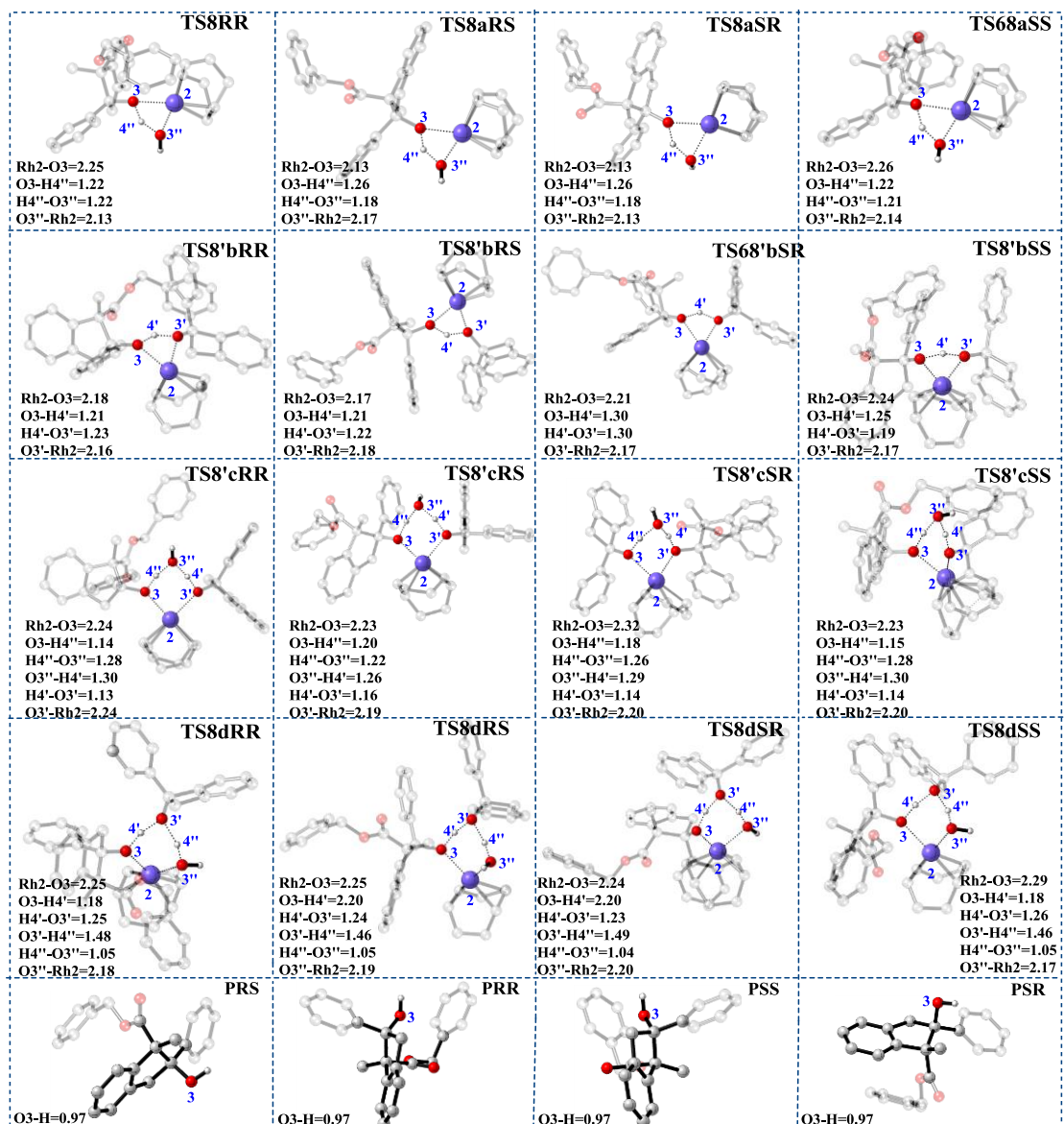
## 6. Additional Description for the Fifth Stage

The **R1**-assisted protonation process (Channel B, **Scheme 9** in the main text) is also taken into consideration due to the existence of free hydroxyl group in the reactant. Similar with the H<sub>2</sub>O-assisted the protonation channel, the **R1**-assisted protonation process for the formation of **M2** and product **PRR** via the transition state **TS8'bRR** is also a concerted process on the basis of distance change analyses (**Fig.S5**).

Additionally, we have also investigated the possible trimolecular protonation mechanism (**Scheme 9** in the main text), namely, two molecules (**R1** and H<sub>2</sub>O) react with **M7RR** to accomplish the catalytic cycle via the transition state **TS8'cRR** and **TS8dRR**. The trimolecular protonation process for the formation of final products associated with Channels C and D is proceeded via the transition states **TS8'cRR** (Channel C) and **TS8dRR** (Channel D), respectively.

The free energy barriers of the four RR-configurational channels (Channels A, B, C, and D) are 6.3 kcal/mol (**TS8aRR**), 20.9 kcal/mol (**TS8'bRR**), 23.8 kcal/mol (**TS8'cRR**), and 21.5 kcal/mol (**TS8dRR**), respectively. Obviously, the Channel A is the most energy favorable channel.

The free energy barriers of the four RR-configurational channels (Channels A, B, C, and D) are 6.3 kcal/mol (**TS8aRR**), 20.9 kcal/mol (**TS8'bRR**), 23.8 kcal/mol (**TS8'cRR**), and 21.5 kcal/mol (**TS8dRR**), respectively. Obviously, the Channel A is the most energy favorable channel. For the RR-configurational isomer pathway, the energy barrier of this stage (6.3 kcal/mol) is lower than that of the fourth stage in Path A (7.6 kcal/mol). The optimized structures of the transition states involved in this stage (**Fig.S5**) show that the less steric-hinder in **TS8a** leads to the lowest free energy barrier. Besides, the stronger acidity of H<sub>2</sub>O than the alcohol **R1** is also the controlling factor.



**Fig.S5** Optimized geometries of all stationary points involved in the fifth stage (the hydrogen atoms which are not involved in the reaction are omitted; the ligand of **Cat** and some atoms which are not involved in the reaction are shown in transparent; distances in Å)

## 7. Solvent Effect Analysis

**Table S4** Solvent Effect Analysis (Unit: kcal/mol)

Solvent	Re_TS4	Si_TS4	$\Delta\Delta G^\ddagger$
toluene	24.7	20.8	3.9
DMSO	32.2	28.9	3.3

## 8. Cartesian Coordinates of All the Optimized Structures Obtained at the B3LYP/6-31G(d)//LanL2DZ Level in the Solvent Toluene Using CPCM Model

### Cat

C	1.04127300	0.13823600	-1.41113200
C	0.94919800	-1.18400800	-0.95209300
C	-0.03228600	1.24243700	0.95145100
C	1.62281400	-1.74001800	0.29369500
C	0.11204200	-0.07005100	1.50444100
C	1.43083300	-0.84309000	1.54027200
H	0.78064600	0.32079600	-2.45411600
H	0.64205700	-1.93915400	-1.67912500
H	1.17980900	-2.72239000	0.49409200
H	-0.60388300	-0.34474400	2.27964600
H	-0.84118000	1.85066700	1.35912200
H	2.69467400	-1.91885700	0.11464100
H	1.45599600	-1.46733000	2.44009500
H	2.26363900	-0.13735800	1.63857100
C	1.88417600	1.21737900	-0.73707800
H	2.29572500	1.88724900	-1.50044900
H	2.74775100	0.75785800	-0.24383700
C	1.06479000	2.04721700	0.27923200
H	1.72701800	2.49964400	1.03496900
H	0.58320400	2.88291300	-0.24197400
Rh	-0.86571500	-0.16114600	-0.34803400
O	-2.70206000	0.04903400	0.29836900
H	-2.78882200	0.34140000	1.22022500

**H2O**

O	0.00000000	0.00000000	0.12025100
H	0.00000000	0.76009800	-0.48100500
H	0.00000000	-0.76009800	-0.48100500

**N<sub>2</sub>**

N	0.00000000	0.00000000	0.55268300
N	0.00000000	0.00000000	-0.55268300

**R1**

C	-3.08353100	-0.25315700	1.12878100
C	-1.84377500	0.31173200	0.85602600
C	-1.25052800	0.21517600	-0.40107600
C	-1.85509000	-0.43435200	-1.47037400
C	-3.11378900	-0.99762400	-1.21024100
C	-3.71006700	-0.91108700	0.05827100
H	-3.56127000	-0.19555500	2.10339100
H	-1.39639100	-0.51282600	-2.45238700
H	-3.64193400	-1.51753000	-2.00540500
H	-4.68545100	-1.36621000	0.21114600
C	0.00477100	0.99520100	0.02000600
C	-0.69826600	1.11110800	1.45806200
H	-0.92670300	2.14815600	1.73051000
H	-0.15303600	0.64073300	2.28324000
O	0.20091000	2.23359000	-0.64493700
H	-0.66546900	2.66606500	-0.70942600
C	1.32425700	0.24215900	0.00921100
C	2.51279000	0.87609500	-0.37301600
C	1.37814700	-1.10017500	0.41375300
C	3.72627600	0.18395200	-0.34981300
H	2.48357900	1.91187900	-0.69021900
C	2.58959900	-1.79001800	0.43912900
H	0.46478200	-1.61236100	0.70462100
C	3.77116400	-1.14997300	0.05623800
H	4.63831100	0.69250200	-0.65200900
H	2.60907600	-2.83019800	0.75388300
H	4.71548000	-1.68758300	0.07241000

**R2**

C	-2.92701500	0.30266100	0.00001200
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N	-2.49307000	1.53719200	-0.00087100
N	-2.13949500	2.62097900	-0.00189600
C	-4.41132600	0.03681600	0.00018400
H	-4.90566500	0.44626300	-0.88803000
H	-4.53836500	-1.04774800	-0.00081700
H	-4.90519800	0.44450900	0.88948100
C	-1.93682400	-0.77197400	0.00033300
O	-2.22863400	-1.95711200	0.00097900
O	-0.66582400	-0.30254600	-0.00009200
C	0.37655100	-1.31735800	0.00023500
H	0.24817200	-1.94628800	-0.88513900
H	0.24799200	-1.94584600	0.88589700
C	1.70634200	-0.61414200	0.00018100
C	2.33151400	-0.27639000	-1.20674900
C	2.33002900	-0.27352500	1.20709200
C	3.55779300	0.38968000	-1.20872900
H	1.85540300	-0.53928300	-2.14845500
C	3.55627800	0.39256800	1.20901300
H	1.85275300	-0.53420100	2.14882500
C	4.17219900	0.72505300	0.00012000
H	4.03455900	0.64336600	-2.15159800
H	4.03187400	0.64850800	2.15186300
H	5.12884900	1.24045400	0.00010200

## M1

C	1.45463600	0.33460200	1.37751400
C	1.79977700	1.29997200	0.40899200
C	3.05379000	-1.67326600	0.21726400
C	3.20428400	1.78294900	0.09693800
C	3.58869500	-0.63944900	-0.57286300
C	4.22753300	0.63028100	-0.01825500
H	0.42532100	0.35153700	1.72869000
H	1.00952800	1.97990400	0.09534500
H	3.16130400	2.31992900	-0.85794900
H	3.87575500	-0.89892600	-1.59207900
H	2.98061200	-2.65860000	-0.24449400
H	3.53140700	2.52028200	0.84717100
H	5.04727900	0.93896200	-0.67663100
H	4.68581100	0.42338800	0.95464900
C	2.44968800	-0.34863300	2.31386700
H	1.95985200	-0.54259100	3.27460600
H	3.27974700	0.33193800	2.53131000
C	2.97478800	-1.68159200	1.73351300

H	3.95203700	-1.93549300	2.17351400
H	2.29182500	-2.48936600	2.02121200
Rh	1.41454500	-0.54579000	-0.58225100
O	0.96257300	-1.97021000	-2.26318100
H	1.36546100	-1.64009200	-3.08389700
C	-4.46992000	-2.04041200	-0.28234400
C	-3.45370800	-1.14878200	-0.60157000
C	-2.37616200	-0.91364300	0.25036600
C	-2.23048000	-1.58492700	1.45963900
C	-3.24651300	-2.49678900	1.79179300
C	-4.34302100	-2.71412500	0.94391700
H	-5.31911100	-2.22934800	-0.93469800
H	-1.38632000	-1.43064100	2.12739500
H	-3.18662100	-3.04713400	2.72764800
H	-5.10662700	-3.42819400	1.24271300
C	-1.73150000	0.12572900	-0.69525500
C	-2.96125800	-0.19944500	-1.67784200
H	-2.62302600	-0.68088400	-2.60161600
H	-3.61268500	0.64611100	-1.92811500
O	-0.50884200	-0.21407400	-1.26454700
H	0.06393700	-1.52697900	-2.20200400
C	-1.75057500	1.57540800	-0.21175800
C	-1.85971300	1.92575700	1.13909100
C	-1.63362000	2.60427300	-1.16059300
C	-1.84599000	3.26756600	1.53678800
H	-1.96840800	1.14740600	1.88808300
C	-1.62160500	3.94281500	-0.76995900
H	-1.54551400	2.34691800	-2.21283800
C	-1.72609400	4.28041900	0.58468600
H	-1.93220300	3.51756200	2.59071400
H	-1.53385700	4.72428300	-1.51991200
H	-1.71806600	5.32260000	0.89075900

## M2

C	-2.88264100	0.79900700	0.10401400
C	-2.60421200	0.30212400	1.38644700
C	-2.12011400	-1.59086500	-1.20382800
C	-3.21906700	-0.93658500	2.01720300
C	-2.07149200	-2.16122500	0.09067600
C	-3.24416000	-2.15868000	1.06841100
H	-2.61813400	1.83889800	-0.08763000
H	-2.17816500	1.00342200	2.10340700
H	-2.61590000	-1.18728500	2.89798000



H	-1.31957700	-2.93191200	0.25277800
H	-1.40404400	-1.97342800	-1.92962100
H	-4.23252900	-0.72337900	2.39226400
H	-3.21382900	-3.07724400	1.66485600
H	-4.18726800	-2.19111200	0.51176500
C	-3.91823700	0.19271400	-0.84007500
H	-4.38560100	0.99271800	-1.42531000
H	-4.72572800	-0.26453700	-0.25832400
C	-3.29751700	-0.84460100	-1.80599900
H	-4.06490100	-1.55335200	-2.15587600
H	-2.93089200	-0.32692700	-2.70002000
Rh	-1.00379800	-0.30585600	0.05954100
C	0.43045600	3.21760700	-1.18033700
C	0.89622800	1.91341500	-1.12057400
C	0.94095900	1.19718600	0.08755500
C	0.50975300	1.75244600	1.29779600
C	0.01136100	3.06867500	1.23596900
C	-0.02496300	3.77778700	0.02933500
H	0.41872800	3.79974500	-2.09805500
H	0.58175500	1.22938000	2.24749400
H	-0.33792800	3.55077400	2.14507400
H	-0.40512300	4.79622100	0.03154000
C	1.60457600	-0.05224600	-0.57969900
C	1.57609700	0.82464700	-1.93009100
H	0.98194100	0.36078400	-2.72351000
H	2.56000300	1.10200300	-2.32536200
O	0.73091000	-1.12915900	-0.58241600
C	2.99460000	-0.46520200	-0.12550900
C	3.70177800	-1.40340200	-0.89525700
C	3.59313300	0.03507000	1.03859000
C	4.97454000	-1.82799900	-0.51212100
H	3.24785600	-1.80311100	-1.79549700
C	4.86949500	-0.38865400	1.42479700
H	3.06681300	0.76122500	1.64548700
C	5.56388100	-1.32030000	0.65076600
H	5.50684700	-2.55233500	-1.11865000
H	5.31926600	0.00918700	2.32789800
H	6.55331200	-1.64845500	0.94886900

### M3

C	-3.14805000	-1.77174200	-0.98012000
C	-3.93791900	-0.64777800	-1.12447200
C	-3.14433300	-2.67165500	0.24534000

C	-4.89253300	-0.07854700	-0.08971500
C	-1.81015500	-0.78806800	1.39487000
C	-2.80974200	0.23916300	1.39150600
C	-2.06300000	-2.28074200	1.28592600
C	-4.31654400	-0.02319500	1.34773400
H	-4.13431300	-2.66209600	0.70836700
H	-2.96776300	-3.70610700	-0.07462300
H	-5.84023400	-0.64235600	-0.09064400
H	-5.14979300	0.93982800	-0.40603400
H	-1.11550500	-2.75425000	1.01252500
H	-2.33553800	-2.69210200	2.27415900
H	-4.83081900	0.77028900	1.89613300
H	-4.54342800	-0.95424600	1.88386300
H	-2.52627200	1.17355800	1.87514700
H	-4.04844900	-0.24337400	-2.13238500
H	-0.87262800	-0.53907700	1.89089100
H	-2.66184900	-2.16333000	-1.87321300
Rh	-1.89080700	0.12652800	-0.49165800
C	0.95588200	1.15701100	-0.25930000
C	-0.41841900	1.45184700	-0.04038600
C	-0.75308700	2.76502300	0.33709800
C	0.21476200	3.77303300	0.45306100
C	1.55163600	3.47055400	0.21771800
C	1.91657900	2.16486500	-0.13355600
C	1.34565000	-0.27840100	-0.63122200
C	2.74067100	-0.46467200	-1.22247000
H	-1.79410300	3.01868300	0.53046300
H	-0.08183900	4.78302000	0.73205600
H	2.31829200	4.23892000	0.30520000
H	2.96654000	1.94499800	-0.31124100
H	1.22219700	-0.93183000	0.24511000
H	0.65294900	-0.65125000	-1.39715500
O	2.89174800	-0.45818900	-2.44029500
C	3.91755900	-0.68132400	-0.31709000
C	5.16226500	-0.97463400	-0.90018800
C	3.82196700	-0.60080700	1.08202000
C	6.28260100	-1.19154400	-0.10625200
H	5.22190600	-1.03020200	-1.98513600
C	4.94747800	-0.81154800	1.87992300
H	2.87329100	-0.35506900	1.55588900
C	6.17669100	-1.11088300	1.28665300
H	7.23939900	-1.42223700	-0.56540900
H	4.86739000	-0.74414900	2.96104800
H	7.05315300	-1.28162100	1.90949600

## Re\_M4

C	2.80135400	-2.05144800	-1.68930200
C	3.23660300	-2.72515400	-0.55635000
C	3.59652300	-1.00474600	-2.45431000
C	4.53553400	-2.51378600	0.19346700
C	3.18887000	0.60852000	-0.49085900
C	3.87644100	-0.05048900	0.49441500
C	3.33974600	0.44712000	-1.98683400
C	5.00571400	-1.04324500	0.28153800
H	4.66455700	-1.23657900	-2.39823400
H	3.33019100	-1.07544800	-3.51498200
H	5.33085100	-3.12865500	-0.25737000
H	4.39673700	-2.90343200	1.20904700
H	2.41733100	0.81104200	-2.45390800
H	4.14404400	1.10225500	-2.35709100
H	5.70823600	-0.95518400	1.11821200
H	5.57234200	-0.77305300	-0.61427500
H	3.73029300	0.29717400	1.51385400
H	2.74172800	-3.66656700	-0.32256800
H	2.58320900	1.45591900	-0.18018000
H	1.94725700	-2.47380000	-2.21172300
Rh	1.73806600	-1.16894500	0.17790500
C	-0.09524600	1.13037700	1.29389600
C	0.87809600	0.14358000	1.57750900
C	1.30777500	0.01690200	2.90978500
C	0.81021000	0.83058000	3.93504000
C	-0.15231700	1.79447600	3.64180300
C	-0.60125600	1.93452700	2.32699300
C	-0.64111700	1.26441900	-0.12669300
C	-1.46976500	2.50628700	-0.43389900
H	2.04986800	-0.73791100	3.16446000
H	1.17037800	0.70381400	4.95378000
H	-0.55674500	2.43102700	4.42467000
H	-1.36423500	2.67844200	2.10918300
H	0.19129800	1.20223200	-0.83864900
H	-1.29196800	0.40958200	-0.33309200
O	-2.68531800	2.41237700	-0.58135100
C	-0.79988800	3.83633200	-0.60278500
C	-1.57971100	4.92577200	-1.02660000
C	0.56942400	4.03107800	-0.36308600
C	-1.00270300	6.17840100	-1.21501700
H	-2.63730200	4.76370900	-1.20669300

C	1.14719000	5.28736500	-0.54724300
H	1.18146500	3.20868100	-0.00934600
C	0.36365300	6.36146500	-0.97613000
H	-1.61384900	7.01309900	-1.54710800
H	2.20701000	5.42786700	-0.35428600
H	0.81511300	7.33912900	-1.12194500
C	0.29038700	-2.36691200	0.23872200
C	0.08334500	-3.43782300	1.26909100
H	0.85936500	-3.45086900	2.03567800
H	-0.88865000	-3.25955600	1.75466300
H	0.01168800	-4.43123400	0.79933300
C	-0.70495800	-2.40175200	-0.87060000
O	-0.44834300	-2.75094600	-2.01222700
O	-1.93042500	-2.03018900	-0.44918400
C	-2.98438900	-1.99106400	-1.46412700
H	-2.95920800	-2.92935100	-2.02249000
H	-2.75179000	-1.17186000	-2.15099000
C	-4.29911400	-1.78587400	-0.76422000
C	-5.15095400	-2.87338400	-0.53280000
C	-4.68277800	-0.50926000	-0.32754700
C	-6.37009200	-2.69370400	0.12376900
H	-4.85934600	-3.86483800	-0.87195800
C	-5.89959700	-0.33089500	0.33246200
H	-4.03056500	0.34466400	-0.49847600
C	-6.74553700	-1.42060200	0.55823300
H	-7.02453700	-3.54445000	0.29342400
H	-6.18926300	0.66153800	0.66715700
H	-7.69442100	-1.27717100	1.06832300

### Si\_M4

C	-3.83952600	-1.04282300	-1.41925700
C	-4.14532500	0.11263900	-0.71440100
C	-4.30432500	-2.45008700	-1.07497000
C	-4.94729400	0.21762400	0.56595200
C	-2.70269100	-2.39117300	0.94470700
C	-3.28911700	-1.39112400	1.67656000
C	-3.33390000	-3.22317300	-0.15090300
C	-4.73327900	-0.93614900	1.57326400
H	-5.30288200	-2.41211100	-0.62891300
H	-4.41625600	-3.01802200	-2.00572500
H	-6.01932300	0.30317200	0.32588600
H	-4.67200100	1.16401300	1.04603200
H	-2.52094500	-3.63451700	-0.76059400

H	-3.85231700	-4.09113400	0.28659900
H	-5.06299600	-0.59606000	2.56173500
H	-5.37468200	-1.78509200	1.31968600
H	-2.72470000	-1.00146200	2.51993800
H	-4.00798300	1.06089900	-1.22970700
H	-1.73608100	-2.75065700	1.29055800
H	-3.46749000	-0.91194500	-2.43313300
Rh	-2.00201800	-0.39821600	-0.13858100
C	0.79980700	-1.17301700	1.06887200
C	-0.33502100	-0.33561500	1.13832000
C	-0.39907500	0.57878800	2.20860100
C	0.60331900	0.66680800	3.17966500
C	1.71366600	-0.17601400	3.10244300
C	1.80260100	-1.08753300	2.05188400
C	0.96062000	-2.19442100	-0.05713600
C	2.24904900	-1.98751600	-0.85542300
H	-1.25783700	1.24247000	2.29127800
H	0.51290500	1.38484200	3.99222600
H	2.50141200	-0.12644000	3.84998500
H	2.66930700	-1.74263600	1.99267100
H	0.89887200	-3.21440900	0.33690300
H	0.12904200	-2.06662500	-0.75719200
O	2.31603400	-1.07850800	-1.67761100
C	3.43955700	-2.87623900	-0.64216700
C	4.58965100	-2.62347900	-1.41226900
C	3.46197000	-3.93789000	0.27766900
C	5.72844500	-3.40897800	-1.26847200
H	4.56390500	-1.80079100	-2.11874500
C	4.60594100	-4.72460600	0.42379700
H	2.59432400	-4.15686000	0.89037200
C	5.73924400	-4.46334100	-0.34829300
H	6.60932500	-3.20221200	-1.86991200
H	4.60994600	-5.54124900	1.14010800
H	6.62832900	-5.07759800	-0.23440900
C	-1.18196300	0.70856400	-1.42210900
C	-0.51714500	0.26518800	-2.68621000
H	-0.88489600	-0.70823500	-3.02299400
H	-0.59278100	0.99832800	-3.50056300
H	0.55120400	0.12298500	-2.44903400
C	-1.26494600	2.18307500	-1.23997300
O	-2.28139900	2.82989600	-1.44350400
O	-0.09383200	2.71402400	-0.84967700
C	-0.09841900	4.14557200	-0.58051200
H	-0.83525000	4.33312400	0.20778000

H	-0.42377100	4.67526000	-1.47956600
C	1.28877500	4.55508200	-0.16449000
C	1.90168800	3.96714400	0.95199000
C	1.97435000	5.54691000	-0.87444900
C	3.17847200	4.36593100	1.34562800
H	1.38144900	3.18890900	1.50457900
C	3.24954100	5.95503300	-0.47418200
H	1.50855100	6.00347500	-1.74462400
C	3.85439000	5.36370700	0.63576400
H	3.64619500	3.89969400	2.20857800
H	3.76954700	6.72829600	-1.03318300
H	4.84790100	5.67569700	0.94647800

## M5R

C	-3.25265000	-1.86152400	-0.83472700
C	-3.59453300	-1.77856100	0.53070400
C	-4.18506200	-1.46778400	-1.97782100
C	-4.88617000	-1.22758000	1.10315400
C	-3.66574300	0.95488100	-1.29392000
C	-4.23310000	0.97856400	-0.02653600
C	-4.01667500	0.00510500	-2.42421200
C	-5.37307100	0.07817800	0.42713900
H	-5.22414400	-1.65901000	-1.68768300
H	-3.98885200	-2.11867300	-2.83731300
H	-5.68186500	-1.98890800	1.06047600
H	-4.71151000	-1.03193500	2.16817300
H	-3.20621000	0.06046900	-3.16053000
H	-4.92456200	0.34547800	-2.94716300
H	-6.00071400	0.62928300	1.13673500
H	-6.01807600	-0.15553700	-0.42628100
H	-4.04700500	1.85948800	0.58588800
H	-3.06535300	-2.44335900	1.20925900
H	-3.10104200	1.83610600	-1.59827600
H	-2.45017900	-2.55076000	-1.09270800
Rh	-2.26675300	-0.15179100	0.05826400
C	-0.44814400	1.50570500	0.31864700
C	-0.36931400	0.44705200	1.30525200
C	-0.48968000	0.83562200	2.67469800
C	-0.67790600	2.14681700	3.06803000
C	-0.80410300	3.16158100	2.10340000
C	-0.68595800	2.83305400	0.76709900
C	-0.09232400	1.37243900	-1.15586000
C	1.33299900	1.67802400	-1.66990800

H	-0.40691100	0.06926600	3.43654200
H	-0.73782200	2.38728700	4.12619800
H	-0.97493200	4.19151700	2.40288600
H	-0.74124000	3.61951400	0.01794600
H	-0.70698200	2.09380200	-1.71118600
H	-0.34309900	0.39683700	-1.58046200
O	1.55994600	1.39227000	-2.83888900
C	2.37500300	2.41454800	-0.88122000
C	3.20118000	3.29623200	-1.60227500
C	2.60397600	2.23840600	0.49309700
C	4.20916900	4.01088000	-0.96079800
H	3.03386700	3.41268300	-2.66809900
C	3.63238300	2.93756500	1.12799800
H	2.01062400	1.53436200	1.06100300
C	4.42765900	3.83188500	0.40878400
H	4.82822800	4.70121900	-1.52710800
H	3.81015700	2.78146600	2.18836800
H	5.21809400	4.38318400	0.91103400
C	-0.46204400	-0.98017900	0.93658800
C	-0.65987500	-1.99260600	2.07176300
H	-1.48739600	-1.71972500	2.73131400
H	0.24595800	-2.09356000	2.68909600
H	-0.87146400	-2.97592900	1.64620100
C	0.42558600	-1.60863900	-0.09057100
O	0.22391100	-2.71156200	-0.57882300
O	1.54340700	-0.88555700	-0.37671500
C	2.49915700	-1.48779600	-1.30321600
H	1.95176000	-2.13234800	-1.99157500
H	2.91801400	-0.64161300	-1.84859800
C	3.56997600	-2.24891200	-0.56197700
C	3.42080800	-3.61646100	-0.29016800
C	4.73035500	-1.59278600	-0.12897200
C	4.41432200	-4.31326500	0.39981300
H	2.51948400	-4.12589800	-0.61775700
C	5.72431200	-2.28766000	0.56244700
H	4.85459900	-0.53253900	-0.33708200
C	5.56799000	-3.65060200	0.82727900
H	4.28954500	-5.37398600	0.60102400
H	6.62085500	-1.76766900	0.88949000
H	6.34279300	-4.19421400	1.36148100

## M5S

C	3.25244900	-1.86139800	-0.83499000
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C	3.59443800	-1.77862800	0.53042400
C	4.18480900	-1.46763400	-1.97811000
C	4.88622800	-1.22791500	1.10282400
C	3.66579900	0.95497000	-1.29385500
C	4.23327900	0.97847300	-0.02651200
C	4.01658700	0.00532400	-2.42430100
C	5.37318600	0.07790400	0.42698800
H	5.22388800	-1.65905300	-1.68813200
H	3.98838300	-2.11836500	-2.83767200
H	5.68180700	-1.98935700	1.05996800
H	4.71171000	-1.03237600	2.16788500
H	3.20612000	0.06086400	-3.16059900
H	4.92450100	0.34565400	-2.94723700
H	6.00090500	0.62885500	1.13664200
H	6.01811900	-0.15573500	-0.42649600
H	4.04732000	1.85937500	0.58598500
H	3.06529400	-2.44349300	1.20893100
H	3.10114900	1.83627900	-1.59806800
H	2.44988800	-2.55053100	-1.09298200
Rh	2.26679800	-0.15170100	0.05832100
C	0.44820900	1.50583400	0.31886500
C	0.36938900	0.44704900	1.30534900
C	0.48975700	0.83550900	2.67482800
C	0.67806700	2.14666800	3.06828400
C	0.80425700	3.16151600	2.10377000
C	0.68605500	2.83312300	0.76742600
C	0.09242500	1.37268900	-1.15567700
C	-1.33290400	1.67809700	-1.66982800
H	0.40699200	0.06909400	3.43662000
H	0.73795700	2.38705400	4.12647400
H	0.97516700	4.19140900	2.40336200
H	0.74131100	3.61965700	0.01835300
H	0.70698900	2.09417600	-1.71092200
H	0.34334300	0.39715700	-1.58035400
O	-1.55973300	1.39226700	-2.83881800
C	-2.37506300	2.41452300	-0.88124100
C	-3.20162700	3.29571000	-1.60248600
C	-2.60387000	2.23867700	0.49314400
C	-4.20979800	4.01019600	-0.96111600
H	-3.03445000	3.41188900	-2.66836000
C	-3.63246800	2.93765400	1.12793700
H	-2.01030600	1.53492500	1.06118000
C	-4.42810800	3.83150500	0.40853300
H	-4.82917000	4.70013000	-1.52757600



H	-3.81011900	2.78176600	2.18835900
H	-5.21867400	4.38269100	0.91069900
C	0.46215800	-0.98015400	0.93653600
C	0.65999300	-1.99267700	2.07161500
H	1.48743700	-1.71979100	2.73125900
H	-0.24587500	-2.09376600	2.68887100
H	0.87172100	-2.97594900	1.64599500
C	-0.42557200	-1.60846600	-0.09062700
O	-0.22393700	-2.71133800	-0.57900500
O	-1.54340900	-0.88535400	-0.37657100
C	-2.49925100	-1.48749300	-1.30305400
H	-1.95190800	-2.13188200	-1.99161500
H	-2.91825500	-0.64124000	-1.84821200
C	-3.56994200	-2.24879800	-0.56183700
C	-3.42067600	-3.61635700	-0.29013900
C	-4.73042200	-1.59282500	-0.12885300
C	-4.41413300	-4.31328600	0.39979800
H	-2.51930600	-4.12569500	-0.61776000
C	-5.72432300	-2.28782500	0.56252000
H	-4.85481600	-0.53259500	-0.33696400
C	-5.56786400	-3.65076200	0.82730400
H	-4.28926000	-5.37400700	0.60094600
H	-6.62092900	-1.76793800	0.88955200
H	-6.34261300	-4.19447600	1.36147900

### **ERe-M6**

C	3.56354200	-1.71049800	0.11632000
C	3.38028100	-1.30305300	-1.21596000
C	4.76938700	-1.33486300	0.97352500
C	4.29946200	-0.39051900	-2.00935900
C	3.59899300	0.93309800	1.11535400
C	3.67365800	1.33178100	-0.23777800
C	4.51111600	-0.06134700	1.81054600
C	4.74612100	0.85939800	-1.21639200
H	5.65095000	-1.20419900	0.33685700
H	5.00561400	-2.16628300	1.64714800
H	5.17556700	-0.94637000	-2.37900300
H	3.74653700	-0.06661800	-2.89892000
H	4.02250100	-0.34558800	2.74982200
H	5.46257500	0.41685300	2.09261600
H	4.97266200	1.66875500	-1.91922500
H	5.67723000	0.65942200	-0.67546000
H	3.17430200	2.26485500	-0.49419500

H	2.70699100	-1.90594900	-1.82520200
H	3.06009100	1.60136600	1.78490400
H	3.01102000	-2.59170200	0.44097300
Rh	2.10049500	-0.09455600	0.02398200
C	-2.07084300	-1.68642900	1.86169600
C	-2.00749000	-0.32586000	2.25021800
C	-3.12763200	0.24244000	2.87634200
C	-4.29077800	-0.49296400	3.10617300
C	-4.34426500	-1.83459200	2.72601000
C	-3.23666400	-2.42202200	2.11306400
C	-0.84722000	-2.36630900	1.24254900
C	-0.58034000	-2.06465900	-0.23071700
H	-3.07616600	1.28561900	3.17786500
H	-5.14692500	-0.02384600	3.58442000
H	-5.23710600	-2.42560200	2.91241500
H	-3.27919400	-3.47524400	1.84680100
H	-0.95681800	-3.45308000	1.34506500
H	0.05789100	-2.07553200	1.78153300
O	0.41571500	-1.42242500	-0.58805000
C	-1.49538200	-2.57053500	-1.29089700
C	-1.42872400	-1.98125300	-2.56739900
C	-2.39407600	-3.62853800	-1.07703100
C	-2.25220700	-2.42692300	-3.59623200
H	-0.72957500	-1.16886300	-2.73063400
C	-3.20873400	-4.08353800	-2.11330300
H	-2.44867200	-4.11699100	-0.11201300
C	-3.14454500	-3.48064800	-3.37125300
H	-2.19991200	-1.95631000	-4.57379700
H	-3.89252800	-4.90876500	-1.93744600
H	-3.78550700	-3.83169200	-4.17520000
C	-0.74315400	0.43947000	2.07333900
C	0.19982100	0.48415900	3.25174100
H	0.61671900	-0.50444900	3.51072800
H	-0.31656200	0.84192500	4.15438200
H	1.03918000	1.15553600	3.05272300
C	-0.40026600	0.96192200	0.86394300
O	0.77266400	1.45058200	0.53887700
O	-1.38109500	0.92669600	-0.12521000
C	-1.16979800	1.69783900	-1.31576000
H	-0.10748400	1.69163800	-1.57294800
H	-1.72767800	1.17017900	-2.09503600
C	-1.68103800	3.11852700	-1.18808900
C	-0.94758100	4.08267100	-0.47959400
C	-2.89790600	3.49202700	-1.77173300

C	-1.42464000	5.38846500	-0.35884400
H	-0.00514900	3.79379500	-0.02268700
C	-3.37614600	4.79978700	-1.65638200
H	-3.47503500	2.75261400	-2.32315100
C	-2.63965700	5.75144700	-0.94815900
H	-0.84618800	6.12608100	0.19183100
H	-4.32128100	5.07387600	-2.11823000
H	-3.00836600	6.76986800	-0.85667900

## ESi-M6

C	-3.55990900	-1.71387800	0.11610700
C	-3.37788400	-1.30668000	-1.21638200
C	-4.76600900	-1.33947300	0.97349500
C	-4.29870400	-0.39543000	-2.00934500
C	-3.59856900	0.92993300	1.11460000
C	-3.67432800	1.32838200	-0.23844000
C	-4.50926400	-0.06547500	1.81021300
C	-4.74635700	0.85431900	-1.21665500
H	-5.64777600	-1.20994700	0.33683600
H	-5.00119900	-2.17105700	1.64727800
H	-5.17447700	-0.95237500	-2.37814000
H	-3.74679800	-0.07128600	-2.89943800
H	-4.02030800	-0.34878000	2.74958800
H	-5.46134700	0.41155800	2.09214300
H	-4.97393000	1.66313500	-1.91978800
H	-5.67717000	0.65362300	-0.67542300
H	-3.17611600	2.26198800	-0.49515600
H	-2.70435000	-1.90887600	-1.82602600
H	-3.05999200	1.59882200	1.78375100
H	-3.00603700	-2.59419200	0.44089300
Rh	-2.09889600	-0.09604500	0.02264600
C	2.07032400	-1.68519800	1.86132000
C	2.00621500	-0.32500100	2.25106500
C	3.12574700	0.24308500	2.87842200
C	4.28910800	-0.49209100	3.10805100
C	4.34340500	-1.83325100	2.72642700
C	3.23633000	-2.42054600	2.11238000
C	0.84707600	-2.36491600	1.24122700
C	0.58212200	-2.06360500	-0.23233800
H	3.07379400	1.28592400	3.18099200
H	5.14479400	-0.02310300	3.58724800
H	5.23643300	-2.42403700	2.91253700
H	3.27948600	-3.47340900	1.84485100

H	0.95625500	-3.45167900	1.34415200
H	-0.05844100	-2.07371100	1.77925300
O	-0.41285400	-1.42065300	-0.59155900
C	1.49823500	-2.57046900	-1.29117300
C	1.43538900	-1.97969800	-2.56718300
C	2.39412200	-3.63073900	-1.07669600
C	2.25994400	-2.42607600	-3.59488200
H	0.73835000	-1.16559300	-2.73091700
C	3.20974300	-4.08648200	-2.11188400
H	2.44568600	-4.12051400	-0.11216400
C	3.14943100	-3.48205200	-3.36929500
H	2.21067800	-1.95424700	-4.57200100
H	3.89126600	-4.91347900	-1.93560700
H	3.79119900	-3.83366300	-4.17234100
C	0.74159500	0.43980100	2.07392900
C	-0.20208100	0.48306700	3.25175900
H	-0.61548500	-0.50660300	3.51207800
H	0.31252100	0.84405000	4.15412100
H	-1.04367900	1.15116800	3.05131900
C	0.39950100	0.96322200	0.86471400
O	-0.77354300	1.45100200	0.53891200
O	1.38154200	0.93038400	-0.12329400
C	1.16975000	1.70060700	-1.31431500
H	0.10770800	1.69208300	-1.57252100
H	1.72946400	1.17387000	-2.09290600
C	1.67781700	3.12248500	-1.18686800
C	0.94395300	4.08415000	-0.47535400
C	2.89179700	3.49972400	-1.77405400
C	1.41792500	5.39109300	-0.35503500
H	0.00356300	3.79248800	-0.01603800
C	3.36686100	4.80872600	-1.65922300
H	3.46925300	2.76231100	-2.32780700
C	2.63011500	5.75782300	-0.94789200
H	0.83924100	6.12671700	0.19805900
H	4.30978800	5.08568600	-2.12384500
H	2.99638000	6.77715300	-0.85671300

### ZSi-M6

C	-3.01729100	-2.02621300	0.61814700
C	-2.19854100	-2.79149600	-0.23993300
C	-4.50134500	-1.75983900	0.37570500
C	-2.62209300	-3.40684600	-1.56155000
C	-3.60077300	-0.09392700	-1.33296400

C	-2.99263000	-0.97868800	-2.24562600
C	-4.73507800	-0.43254500	-0.38069200
C	-3.42565500	-2.42802600	-2.45052900
H	-4.94082300	-2.60018500	-0.17388900
H	-5.02213400	-1.72357900	1.33940800
H	-3.19263800	-4.33388100	-1.39463400
H	-1.70886600	-3.70162800	-2.09079200
H	-4.80147900	0.38287200	0.34663500
H	-5.69817600	-0.45350400	-0.91393600
H	-3.28640900	-2.70052600	-3.50277600
H	-4.49922700	-2.52401700	-2.25373600
H	-2.43837400	-0.52940600	-3.06933200
H	-1.30112700	-3.22347000	0.20053300
H	-3.48374200	0.97109000	-1.53214500
H	-2.68160100	-1.92239400	1.64925600
Rh	-1.73499400	-0.73817200	-0.51555900
C	-1.64478400	2.31226400	1.08440900
C	-0.90866800	1.45423900	1.92575600
C	-1.53037500	0.97688900	3.09387200
C	-2.83685400	1.34039000	3.42524000
C	-3.55202100	2.19754500	2.58504600
C	-2.95514000	2.67827100	1.41797000
C	-0.96188800	2.89169900	-0.13546200
C	-0.08498000	1.91887400	-0.92009700
H	-0.96788600	0.31579000	3.74912900
H	-3.29275200	0.96041400	4.33607700
H	-4.56824200	2.49262800	2.83639100
H	-3.51123600	3.34423900	0.76091700
H	-1.72182500	3.25724900	-0.84441500
H	-0.38037900	3.76812600	0.16274400
O	-0.58082000	0.86368300	-1.38291100
C	1.27085300	2.30924000	-1.38988000
C	1.86784000	3.55361700	-1.11148200
C	1.97726300	1.39378300	-2.19670000
C	3.12507600	3.87128900	-1.62742500
H	1.36073800	4.28927100	-0.49824000
C	3.22925700	1.71390600	-2.71138900
H	1.52038300	0.43494400	-2.41225400
C	3.80894700	2.95689000	-2.43104500
H	3.56614100	4.83808500	-1.40388700
H	3.75561700	0.99661100	-3.33656100
H	4.78477900	3.20924700	-2.83638800
C	0.50856200	1.11273500	1.61360400
C	1.58532000	2.04027700	2.12902400

H	1.29199200	3.09216800	2.00617200
H	1.79031700	1.89965500	3.20488600
H	2.52875600	1.89346800	1.59540000
C	0.80160800	-0.15109900	1.12814500
O	-0.02133200	-1.05049200	0.70530200
O	2.13843700	-0.48156700	1.10801600
C	2.49796200	-1.74580000	0.53230800
H	2.15329100	-1.78705500	-0.50860400
H	2.00330500	-2.55995700	1.07304700
C	3.99911700	-1.88506600	0.61457000
C	4.58113800	-2.93359700	1.33477900
C	4.83561000	-0.96602500	-0.03654000
C	5.97062400	-3.07312500	1.39905000
H	3.94171700	-3.64713900	1.84958900
C	6.22224300	-1.09706400	0.03170900
H	4.39440800	-0.14171300	-0.59021300
C	6.79487200	-2.15323100	0.74927000
H	6.40577200	-3.89342500	1.96273500
H	6.85950900	-0.37803200	-0.47676500
H	7.87559800	-2.25712600	0.79882400

### ZRe-M6

C	2.31510900	-2.74783300	-0.41565200
C	2.87777000	-2.01992600	0.65687400
C	3.09976900	-3.21917700	-1.63752200
C	4.31559800	-1.54707600	0.75686800
C	2.92319700	-0.76414100	-2.31494900
C	3.69414900	-0.17386600	-1.29371000
C	3.02922500	-2.20026100	-2.79816300
C	4.81999400	-0.88343400	-0.54516900
H	4.14127500	-3.40971100	-1.35710300
H	2.69692900	-4.18075100	-1.97487600
H	4.97683900	-2.37756500	1.05225300
H	4.36135500	-0.81619400	1.57140900
H	2.13763600	-2.40921000	-3.40080800
H	3.89093200	-2.32278500	-3.47341700
H	5.60131800	-0.15551300	-0.29835900
H	5.29356700	-1.62381000	-1.19825000
H	3.73194800	0.91410200	-1.27406100
H	2.34536100	-2.06861600	1.60584200
H	2.43705300	-0.08534100	-3.01639700
H	1.39110200	-3.28334700	-0.20337800
Rh	1.73677400	-0.69348600	-0.54381400

C	1.62514900	2.28132900	1.16951900
C	0.92503700	1.35489900	1.96920200
C	1.58936600	0.81256900	3.08494900
C	2.89942600	1.17200500	3.40526300
C	3.57834900	2.09396400	2.60441300
C	2.94080400	2.63811700	1.48909500
C	0.91602900	2.93557500	0.00499400
C	0.07425500	1.99567600	-0.85444000
H	1.05402600	0.10116400	3.70857300
H	3.38569400	0.74035400	4.27647200
H	4.59731800	2.38576700	2.84538600
H	3.46805900	3.35280400	0.86077400
H	0.30644000	3.76872700	0.36404400
H	1.66365300	3.37820500	-0.67080000
O	0.60407000	0.97525900	-1.34739000
C	-1.28402600	2.37489800	-1.32408500
C	-1.95708600	1.48072800	-2.18299000
C	-1.91290700	3.59164400	-1.00066300
C	-3.20893300	1.79338600	-2.70022200
H	-1.47672800	0.54088300	-2.43007000
C	-3.17066100	3.90194200	-1.51852700
H	-1.43191900	4.31054600	-0.34794500
C	-3.82086700	3.00926500	-2.37231700
H	-3.71119700	1.09328200	-3.36226600
H	-3.63952500	4.84624000	-1.25744900
H	-4.79624400	3.25775700	-2.78104400
C	-0.49952700	1.01139900	1.69110500
C	-1.56509100	1.92141500	2.25469900
H	-1.26081500	2.97451700	2.18344400
H	-2.51156300	1.81034300	1.71780900
H	-1.76907500	1.73162900	3.32152700
C	-0.80402500	-0.20477800	1.11382800
O	0.00241400	-1.07762000	0.60387800
O	-2.14406100	-0.53623100	1.09001600
C	-2.50651200	-1.75456800	0.43053100
H	-1.98773900	-2.60288200	0.89019100
H	-2.19676200	-1.71241100	-0.62117400
C	-4.00349900	-1.91893400	0.54603800
C	-4.86726600	-1.00502900	-0.07629700
C	-4.55477400	-2.97664200	1.27645000
C	-6.24982200	-1.15039400	0.02932000
H	-4.44989100	-0.17313500	-0.63789500
C	-5.94035700	-3.13010300	1.37932900
H	-3.89380600	-3.68686900	1.76833800

C	-6.79121500	-2.21548600	0.75737400
H	-6.90873100	-0.43645400	-0.45828200
H	-6.35168000	-3.95786600	1.95089200
H	-7.86897300	-2.33120100	0.83534000

## M7RR

C	-1.99299200	-2.78311200	0.44097200
C	-3.00196700	-1.86514300	0.77688100
C	-2.02525300	-3.75198200	-0.73018400
C	-4.33736900	-1.74772500	0.04694800
C	-2.10837500	-1.62253600	-2.13801800
C	-2.93078000	-0.55406300	-1.71920100
C	-2.49986300	-3.09631500	-2.04931500
C	-4.29456800	-0.67351400	-1.06414100
H	-1.00479700	-4.12845600	-0.86961000
H	-2.64579900	-4.63161400	-0.49552200
H	-5.12200200	-1.48961100	0.76747300
H	-4.62096100	-2.72038800	-0.36976200
H	-3.58511600	-3.19756900	-2.15822300
H	-2.06055600	-3.63565200	-2.89615500
H	-5.07453000	-0.86523900	-1.81876200
H	-4.52661900	0.30283400	-0.62328500
H	-2.72781800	0.41621000	-2.16962600
H	-2.98250400	-1.46127800	1.78867100
H	-1.33254300	-1.37882600	-2.86261200
H	-1.28008500	-3.04178100	1.22459600
Rh	-1.39076400	-0.84698100	-0.28356800
C	-1.74896300	2.67013300	0.08518200
C	-1.15487900	2.04957600	1.19274100
C	-1.86189200	1.89271300	2.38532900
C	-3.18461500	2.34328500	2.45669600
C	-3.78293600	2.95443400	1.34982700
C	-3.06539400	3.12422000	0.15985800
C	-0.76958400	2.77340200	-1.05348600
C	0.29854100	1.66889700	-0.74347300
H	-1.40166200	1.42021700	3.25011300
H	-3.74791100	2.21941200	3.37779600
H	-4.81021900	3.30348500	1.41529000
H	-3.53163400	3.60634800	-0.69612700
H	-1.20621700	2.57695100	-2.03741100
H	-0.34746700	3.78548300	-1.07854000
O	-0.14276400	0.46126200	-1.24261100
C	1.70314700	1.93540900	-1.31656800



C	2.17560700	3.20050100	-1.69555100
C	2.57134300	0.84121800	-1.46843900
C	3.46788100	3.36811600	-2.20374500
H	1.54198300	4.07668100	-1.60473400
C	3.86459100	1.00523200	-1.96335300
H	2.21176400	-0.14816200	-1.20970800
C	4.32064000	2.27260200	-2.33648300
H	3.80303600	4.36018800	-2.49628600
H	4.51483900	0.13945100	-2.06052100
H	5.32562100	2.40275800	-2.72969500
C	0.30972600	1.72978300	0.90750900
C	1.18927900	2.87382700	1.45614700
H	0.87388000	3.82727100	1.02322900
H	1.07977900	2.94953300	2.54324200
H	2.24519000	2.72446700	1.22405500
C	0.71567300	0.39020400	1.47823000
O	0.04116200	-0.64269400	1.37799000
O	1.87766400	0.39200900	2.12279600
C	2.37480300	-0.87079400	2.68060000
H	1.51909100	-1.47318200	2.98631100
H	2.93542100	-0.55024500	3.55997200
C	3.25686400	-1.59591800	1.69800300
C	2.73351600	-2.59455400	0.86474700
C	4.61567000	-1.26740200	1.59932700
C	3.55563600	-3.25079600	-0.05322100
H	1.68088500	-2.85230500	0.93548600
C	5.43828400	-1.92153000	0.68136600
H	5.02998200	-0.49667500	2.24492000
C	4.90861900	-2.91441700	-0.14742600
H	3.14066400	-4.02545200	-0.69213900
H	6.49093300	-1.66048800	0.61606300
H	5.54891300	-3.42735200	-0.85989100

## M7SR

C	-3.07105300	-1.68884500	-0.01660200
C	-2.89526500	-1.22998900	-1.35384900
C	-4.31895700	-2.41068500	0.48985400
C	-3.91864400	-1.33541800	-2.46760900
C	-5.29751000	-0.05727900	0.43185600
C	-5.26201400	0.18916000	-0.95298600
C	-5.35255300	-1.42806800	1.08557500
C	-5.33025200	-0.89791500	-2.02049100
H	-4.76391200	-2.99131200	-0.32589600

H	-4.02745300	-3.13807000	1.25523400
H	-3.93440400	-2.35887800	-2.87520200
H	-3.58224400	-0.68803000	-3.28593100
H	-5.14108100	-1.29190600	2.15245700
H	-6.36812700	-1.84962300	1.02589700
H	-5.88840300	-0.52181200	-2.88511800
H	-5.89894100	-1.75509000	-1.64422100
H	-5.54739200	1.18942100	-1.28143100
H	-1.86165700	-1.13856200	-1.67980800
H	-5.63122000	0.76395600	1.07053100
H	-2.15587300	-1.89457300	0.53584900
Rh	-3.27306000	0.42259200	-0.09493400
C	1.56267400	3.06768800	0.34315000
C	1.87782900	2.10087500	-0.62020900
C	3.07414800	2.19251300	-1.33639700
C	3.95925700	3.23939100	-1.06281800
C	3.65009600	4.19389100	-0.08789800
C	2.44653700	4.11219200	0.61791900
C	0.20427600	2.81909600	0.93802100
C	-0.18392300	1.34644300	0.53467300
H	3.33017900	1.44825000	-2.08365500
H	4.89669700	3.30709900	-1.60872800
H	4.34769700	5.00068800	0.12178200
H	2.20188400	4.85502400	1.37362600
H	0.16602100	2.95996300	2.02342800
H	-0.54541400	3.48781600	0.49576000
O	-1.53996200	1.32789200	0.28422600
C	0.22363500	0.40212400	1.69554600
C	-0.76052100	-0.25222900	2.44806400
C	1.56304400	0.24023900	2.09643700
C	-0.42777900	-1.05992300	3.53943300
H	-1.80104200	-0.12054100	2.17534900
C	1.89824700	-0.56295100	3.18868500
H	2.35911300	0.74102600	1.55851600
C	0.90524700	-1.22382300	3.91531200
H	-1.21739600	-1.55647000	4.09866900
H	2.94240900	-0.66263000	3.47597300
H	1.16744300	-1.84917100	4.76476300
C	0.72963300	1.11438000	-0.80233800
C	-0.06870600	1.51838900	-2.06489600
H	0.57383900	1.44539800	-2.95022600
H	-0.93761700	0.87466600	-2.20191600
H	-0.41231000	2.55272200	-1.97873800
C	1.11090400	-0.35567400	-0.95879400

O	0.31067000	-1.23554100	-1.22738500
O	2.42108700	-0.61181000	-0.78536200
C	2.80845900	-2.01207500	-0.87789900
H	2.49034400	-2.39723600	-1.85016600
H	2.27144000	-2.56250100	-0.10038700
C	4.29971200	-2.09629400	-0.70006400
C	5.14877400	-2.14172200	-1.81290800
C	4.86052300	-2.11988300	0.58423200
C	6.53370700	-2.20855800	-1.64781500
H	4.72230500	-2.12817400	-2.81326200
C	6.24404300	-2.18500500	0.75280800
H	4.20673300	-2.08644400	1.45249300
C	7.08345800	-2.22996700	-0.36397000
H	7.18149800	-2.24682400	-2.51941900
H	6.66714500	-2.20476300	1.75347800
H	8.16090400	-2.28487000	-0.23363500

## M7SS

C	-1.99299200	-2.78311200	-0.44097200
C	-3.00196700	-1.86514300	-0.77688100
C	-2.02525300	-3.75198200	0.73018400
C	-4.33736900	-1.74772500	-0.04694800
C	-2.10837500	-1.62253600	2.13801800
C	-2.93078000	-0.55406300	1.71920100
C	-2.49986300	-3.09631500	2.04931500
C	-4.29456800	-0.67351400	1.06414100
H	-1.00479700	-4.12845600	0.86961000
H	-2.64579900	-4.63161400	0.49552200
H	-5.12200200	-1.48961100	-0.76747300
H	-4.62096100	-2.72038800	0.36976200
H	-3.58511600	-3.19756900	2.15822300
H	-2.06055600	-3.63565200	2.89615500
H	-5.07453000	-0.86523900	1.81876200
H	-4.52661900	0.30283400	0.62328500
H	-2.72781800	0.41621000	2.16962600
H	-2.98250400	-1.46127800	-1.78867100
H	-1.33254300	-1.37882600	2.86261200
H	-1.28008500	-3.04178100	-1.22459600
Rh	-1.39076400	-0.84698100	0.28356800
C	-1.74896300	2.67013300	-0.08518200
C	-1.15487900	2.04957600	-1.19274100
C	-1.86189200	1.89271300	-2.38532900
C	-3.18461500	2.34328500	-2.45669600

C	-3.78293600	2.95443400	-1.34982700
C	-3.06539400	3.12422000	-0.15985800
C	-0.76958400	2.77340200	1.05348600
C	0.29854100	1.66889700	0.74347300
H	-1.40166200	1.42021700	-3.25011300
H	-3.74791100	2.21941200	-3.37779600
H	-4.81021900	3.30348500	-1.41529000
H	-3.53163400	3.60634800	0.69612700
H	-1.20621700	2.57695100	2.03741100
H	-0.34746700	3.78548300	1.07854000
O	-0.14276400	0.46126200	1.24261100
C	1.70314700	1.93540900	1.31656800
C	2.17560700	3.20050100	1.69555100
C	2.57134300	0.84121800	1.46843900
C	3.46788100	3.36811600	2.20374500
H	1.54198300	4.07668100	1.60473400
C	3.86459100	1.00523200	1.96335300
H	2.21176400	-0.14816200	1.20970800
C	4.32064000	2.27260200	2.33648300
H	3.80303600	4.36018800	2.49628600
H	4.51483900	0.13945100	2.06052100
H	5.32562100	2.40275800	2.72969500
C	0.30972600	1.72978300	-0.90750900
C	1.18927900	2.87382700	-1.45614700
H	0.87388000	3.82727100	-1.02322900
H	1.07977900	2.94953300	-2.54324200
H	2.24519000	2.72446700	-1.22405500
C	0.71567300	0.39020400	-1.47823000
O	0.04116200	-0.64269400	-1.37799000
O	1.87766400	0.39200900	-2.12279600
C	2.37480300	-0.87079400	-2.68060000
H	1.51909100	-1.47318200	-2.98631100
H	2.93542100	-0.55024500	-3.55997200
C	3.25686400	-1.59591800	-1.69800300
C	2.73351600	-2.59455400	-0.86474700
C	4.61567000	-1.26740200	-1.59932700
C	3.55563600	-3.25079600	0.05322100
H	1.68088500	-2.85230500	-0.93548600
C	5.43828400	-1.92153000	-0.68136600
H	5.02998200	-0.49667500	-2.24492000
C	4.90861900	-2.91441700	0.14742600
H	3.14066400	-4.02545200	0.69213900
H	6.49093300	-1.66048800	-0.61606300
H	5.54891300	-3.42735200	0.85989100

## M7RS

C	-3.07105300	-1.68884500	0.01660200
C	-2.89526500	-1.22998900	1.35384900
C	-4.31895700	-2.41068500	-0.48985400
C	-3.91864400	-1.33541800	2.46760900
C	-5.29751000	-0.05727900	-0.43185600
C	-5.26201400	0.18916000	0.95298600
C	-5.35255300	-1.42806800	-1.08557500
C	-5.33025200	-0.89791500	2.02049100
H	-4.76391200	-2.99131200	0.32589600
H	-4.02745300	-3.13807000	-1.25523400
H	-3.93440400	-2.35887800	2.87520200
H	-3.58224400	-0.68803000	3.28593100
H	-5.14108100	-1.29190600	-2.15245700
H	-6.36812700	-1.84962300	-1.02589700
H	-5.88840300	-0.52181200	2.88511800
H	-5.89894100	-1.75509000	1.64422100
H	-5.54739200	1.18942100	1.28143100
H	-1.86165700	-1.13856200	1.67980800
H	-5.63122000	0.76395600	-1.07053100
H	-2.15587300	-1.89457300	-0.53584900
Rh	-3.27306000	0.42259200	0.09493400
C	1.56267400	3.06768800	-0.34315000
C	1.87782900	2.10087500	0.62020900
C	3.07414800	2.19251300	1.33639700
C	3.95925700	3.23939100	1.06281800
C	3.65009600	4.19389100	0.08789800
C	2.44653700	4.11219200	-0.61791900
C	0.20427600	2.81909600	-0.93802100
C	-0.18392300	1.34644300	-0.53467300
H	3.33017900	1.44825000	2.08365500
H	4.89669700	3.30709900	1.60872800
H	4.34769700	5.00068800	-0.12178200
H	2.20188400	4.85502400	-1.37362600
H	0.16602100	2.95996300	-2.02342800
H	-0.54541400	3.48781600	-0.49576000
O	-1.53996200	1.32789200	-0.28422600
C	0.22363500	0.40212400	-1.69554600
C	-0.76052100	-0.25222900	-2.44806400
C	1.56304400	0.24023900	-2.09643700
C	-0.42777900	-1.05992300	-3.53943300
H	-1.80104200	-0.12054100	-2.17534900

C	1.89824700	-0.56295100	-3.18868500
H	2.35911300	0.74102600	-1.55851600
C	0.90524700	-1.22382300	-3.91531200
H	-1.21739600	-1.55647000	-4.09866900
H	2.94240900	-0.66263000	-3.47597300
H	1.16744300	-1.84917100	-4.76476300
C	0.72963300	1.11438000	0.80233800
C	-0.06870600	1.51838900	2.06489600
H	0.57383900	1.44539800	2.95022600
H	-0.93761700	0.87466600	2.20191600
H	-0.41231000	2.55272200	1.97873800
C	1.11090400	-0.35567400	0.95879400
O	0.31067000	-1.23554100	1.22738500
O	2.42108700	-0.61181000	0.78536200
C	2.80845900	-2.01207500	0.87789900
H	2.49034400	-2.39723600	1.85016600
H	2.27144000	-2.56250100	0.10038700
C	4.29971200	-2.09629400	0.70006400
C	5.14877400	-2.14172200	1.81290800
C	4.86052300	-2.11988300	-0.58423200
C	6.53370700	-2.20855800	1.64781500
H	4.72230500	-2.12817400	2.81326200
C	6.24404300	-2.18500500	-0.75280800
H	4.20673300	-2.08644400	-1.45249300
C	7.08345800	-2.22996700	0.36397000
H	7.18149800	-2.24682400	2.51941900
H	6.66714500	-2.20476300	-1.75347800
H	8.16090400	-2.28487000	0.23363500

**PRR**

C	2.18762300	-1.41895900	-1.00064600
C	1.79683600	-1.48039200	0.34230300
C	2.38638700	-2.39582000	1.21088100
C	3.37878100	-3.25347800	0.72335300
C	3.77133600	-3.19139800	-0.61681300
C	3.17723700	-2.27098600	-1.48741600
C	1.40414500	-0.35546900	-1.72893700
C	0.82831500	0.53933300	-0.58955300
H	2.08749300	-2.44781000	2.25455800
H	3.84951600	-3.96860900	1.39258600
H	4.54660000	-3.85847100	-0.98440700
H	3.48846800	-2.22081200	-2.52810000
H	1.99925800	0.21697000	-2.44865700

H	0.56029800	-0.80210500	-2.26722100
O	-0.49231300	0.99637700	-0.88248700
C	1.73607900	1.73620100	-0.27497900
C	1.16464200	2.94927000	0.13855900
C	3.13413600	1.66708500	-0.38657400
C	1.96095000	4.05925800	0.42563700
H	0.08613900	3.01934900	0.23111700
C	3.93139200	2.77519100	-0.09509500
H	3.61183700	0.74454400	-0.69921100
C	3.34915600	3.97747300	0.31069300
H	1.49258300	4.98853900	0.73954900
H	5.01117400	2.69695800	-0.19115900
H	3.97084400	4.84061500	0.53284200
C	0.69600600	-0.47061800	0.64681300
C	0.82914600	0.18850000	2.02652600
H	1.83446300	0.59687900	2.15519800
H	0.10495500	0.99649700	2.15208000
H	0.65074400	-0.54327600	2.82055600
C	-0.66734200	-1.18758500	0.48297400
O	-0.88338700	-2.05386500	-0.34175200
O	-1.58115200	-0.75360500	1.37014200
C	-2.90558700	-1.36203500	1.31555000
H	-3.23093800	-1.37997600	2.35767200
H	-2.79861600	-2.38265500	0.94507000
C	-3.85743700	-0.55871200	0.46511300
C	-4.65871800	0.43193000	1.04638500
C	-3.95255700	-0.78762300	-0.91487700
C	-5.54038300	1.18251000	0.26675300
H	-4.59384600	0.61349500	2.11684700
C	-4.83345000	-0.03879000	-1.69578200
H	-3.32672600	-1.54951800	-1.36982600
C	-5.62908800	0.94759300	-1.10696400
H	-6.15893800	1.94576300	0.73129700
H	-4.90166100	-0.22724300	-2.76395400
H	-6.31746800	1.52788800	-1.71567800
H	-0.43698800	1.58685600	-1.65179700

**PRS**

C	1.10065700	-1.82269900	1.14685900
C	1.56157800	-1.85817400	-0.17309400
C	1.76314400	-3.07217100	-0.82688000
C	1.50430700	-4.26276400	-0.13871000
C	1.04729700	-4.23034600	1.18187700

C	0.84271400	-3.00805700	1.83191400
C	0.94548400	-0.40059000	1.62032300
C	1.78993500	0.42239700	0.60834600
H	2.11759900	-3.10246100	-1.85382300
H	1.66243500	-5.21687700	-0.63420700
H	0.85372700	-5.16055100	1.70958900
H	0.49297600	-2.98709500	2.86128600
H	1.32102600	-0.24375500	2.63604100
H	-0.10307400	-0.08849200	1.59058200
O	3.12336400	0.35542400	1.15073700
C	1.39516100	1.89779100	0.51542700
C	1.20019300	2.60261100	1.71624800
C	1.30838100	2.61400700	-0.68625300
C	0.90548900	3.96413100	1.71596100
H	1.28685900	2.07864900	2.66314000
C	1.01488500	3.98156300	-0.68977100
H	1.46075100	2.12054700	-1.63931900
C	0.80964300	4.66187700	0.50880000
H	0.75276700	4.48152500	2.65944600
H	0.94968400	4.51003700	-1.63711000
H	0.58050700	5.72403900	0.50551500
C	1.75744600	-0.44608800	-0.73413000
C	3.03796200	-0.31995800	-1.57348300
H	3.89447600	-0.67632000	-0.99796100
H	3.22406300	0.71409800	-1.88189600
H	2.95522800	-0.91618400	-2.48486500
C	0.53848300	-0.15602400	-1.62871900
O	0.58246200	-0.02662900	-2.83681900
O	-0.60907900	-0.10632500	-0.92565200
C	-1.82606100	0.09575900	-1.69292100
H	-1.79398700	1.08888100	-2.14997100
H	-1.84404300	-0.64511100	-2.49830300
C	-2.99990400	-0.05107200	-0.76175800
C	-3.91621900	0.99372400	-0.60337900
C	-3.20239500	-1.24732800	-0.05806800
C	-5.02262900	0.84768000	0.23732700
H	-3.76420700	1.92708700	-1.14022700
C	-4.30027300	-1.39141300	0.78862900
H	-2.49088800	-2.06147700	-0.16921700
C	-5.21573800	-0.34455000	0.93579000
H	-5.72756000	1.66699200	0.34927300
H	-4.44533500	-2.32170700	1.33122300
H	-6.07361700	-0.45938000	1.59281600
H	3.67940200	0.96595100	0.63984800



## PSR

C	1.10065700	-1.82269900	-1.14685900
C	1.56157800	-1.85817400	0.17309400
C	1.76314400	-3.07217100	0.82688000
C	1.50430700	-4.26276400	0.13871000
C	1.04729700	-4.23034600	-1.18187700
C	0.84271400	-3.00805700	-1.83191400
C	0.94548400	-0.40059000	-1.62032300
C	1.78993500	0.42239700	-0.60834600
H	2.11759900	-3.10246100	1.85382300
H	1.66243500	-5.21687700	0.63420700
H	0.85372700	-5.16055100	-1.70958900
H	0.49297600	-2.98709500	-2.86128600
H	1.32102600	-0.24375500	-2.63604100
H	-0.10307400	-0.08849200	-1.59058200
O	3.12336400	0.35542400	-1.15073700
C	1.39516100	1.89779100	-0.51542700
C	1.20019300	2.60261100	-1.71624800
C	1.30838100	2.61400700	0.68625300
C	0.90548900	3.96413100	-1.71596100
H	1.28685900	2.07864900	-2.66314000
C	1.01488500	3.98156300	0.68977100
H	1.46075100	2.12054700	1.63931900
C	0.80964300	4.66187700	-0.50880000
H	0.75276700	4.48152500	-2.65944600
H	0.94968400	4.51003700	1.63711000
H	0.58050700	5.72403900	-0.50551500
C	1.75744600	-0.44608800	0.73413000
C	3.03796200	-0.31995800	1.57348300
H	3.89447600	-0.67632000	0.99796100
H	3.22406300	0.71409800	1.88189600
H	2.95522800	-0.91618400	2.48486500
C	0.53848300	-0.15602400	1.62871900
O	0.58246200	-0.02662900	2.83681900
O	-0.60907900	-0.10632500	0.92565200
C	-1.82606100	0.09575900	1.69292100
H	-1.79398700	1.08888100	2.14997100
H	-1.84404300	-0.64511100	2.49830300
C	-2.99990400	-0.05107200	0.76175800
C	-3.91621900	0.99372400	0.60337900
C	-3.20239500	-1.24732800	0.05806800
C	-5.02262900	0.84768000	-0.23732700

H	-3.76420700	1.92708700	1.14022700
C	-4.30027300	-1.39141300	-0.78862900
H	-2.49088800	-2.06147700	0.16921700
C	-5.21573800	-0.34455000	-0.93579000
H	-5.72756000	1.66699200	-0.34927300
H	-4.44533500	-2.32170700	-1.33122300
H	-6.07361700	-0.45938000	-1.59281600
H	3.67940200	0.96595100	-0.63984800

## PSS

C	2.18762300	-1.41895900	1.00064600
C	1.79683600	-1.48039200	-0.34230300
C	2.38638700	-2.39582000	-1.21088100
C	3.37878100	-3.25347800	-0.72335300
C	3.77133600	-3.19139800	0.61681300
C	3.17723700	-2.27098600	1.48741600
C	1.40414500	-0.35546900	1.72893700
C	0.82831500	0.53933300	0.58955300
H	2.08749300	-2.44781000	-2.25455800
H	3.84951600	-3.96860900	-1.39258600
H	4.54660000	-3.85847100	0.98440700
H	3.48846800	-2.22081200	2.52810000
H	1.99925800	0.21697000	2.44865700
H	0.56029800	-0.80210500	2.26722100
O	-0.49231300	0.99637700	0.88248700
C	1.73607900	1.73620100	0.27497900
C	1.16464200	2.94927000	-0.13855900
C	3.13413600	1.66708500	0.38657400
C	1.96095000	4.05925800	-0.42563700
H	0.08613900	3.01934900	-0.23111700
C	3.93139200	2.77519100	0.09509500
H	3.61183700	0.74454400	0.69921100
C	3.34915600	3.97747300	-0.31069300
H	1.49258300	4.98853900	-0.73954900
H	5.01117400	2.69695800	0.19115900
H	3.97084400	4.84061500	-0.53284200
C	0.69600600	-0.47061800	-0.64681300
C	0.82914600	0.18850000	-2.02652600
H	1.83446300	0.59687900	-2.15519800
H	0.10495500	0.99649700	-2.15208000
H	0.65074400	-0.54327600	-2.82055600
C	-0.66734200	-1.18758500	-0.48297400
O	-0.88338700	-2.05386500	0.34175200

O	-1.58115200	-0.75360500	-1.37014200
C	-2.90558700	-1.36203500	-1.31555000
H	-3.23093800	-1.37997600	-2.35767200
H	-2.79861600	-2.38265500	-0.94507000
C	-3.85743700	-0.55871200	-0.46511300
C	-4.65871800	0.43193000	-1.04638500
C	-3.95255700	-0.78762300	0.91487700
C	-5.54038300	1.18251000	-0.26675300
H	-4.59384600	0.61349500	-2.11684700
C	-4.83345000	-0.03879000	1.69578200
H	-3.32672600	-1.54951800	1.36982600
C	-5.62908800	0.94759300	1.10696400
H	-6.15893800	1.94576300	-0.73129700
H	-4.90166100	-0.22724300	2.76395400
H	-6.31746800	1.52788800	1.71567800
H	-0.43698800	1.58685600	1.65179700

## TS1

C	1.72461800	0.89998500	1.08903400
C	2.19690300	1.38892200	-0.13940900
C	2.71857100	-1.70881400	0.66026200
C	3.64033700	1.38292800	-0.61001400
C	3.41311500	-1.14790400	-0.43044900
C	4.36239300	0.04346400	-0.33609400
H	0.73917500	1.24075900	1.40341400
H	1.54807000	2.08748300	-0.66711300
H	3.63166900	1.56778000	-1.69062500
H	3.55668400	-1.78977900	-1.29926800
H	2.38714300	-2.74155800	0.55125000
H	4.19803800	2.21993800	-0.16108100
H	5.17105200	-0.08418100	-1.06429300
H	4.84308700	0.05888900	0.64765300
C	2.60970500	0.33111000	2.19377000
H	2.17688300	0.58858000	3.16692600
H	3.59407000	0.81022300	2.16654000
C	2.75015800	-1.20504200	2.09158800
H	3.66569700	-1.54425900	2.60147100
H	1.91474800	-1.67674800	2.62209200
Rh	1.34212200	-0.55373100	-0.49129100
O	0.45039500	-2.13920700	-1.59935800
H	0.93625000	-2.27098000	-2.42986000
C	-4.31418000	-2.18204600	-0.29514200
C	-3.40119000	-1.18941000	-0.62909800

C	-2.28596600	-0.91450200	0.15894200
C	-1.99835000	-1.62329900	1.31943700
C	-2.90823000	-2.63603000	1.66356700
C	-4.03954000	-2.90542100	0.87697400
H	-5.19069500	-2.40856500	-0.89686300
H	-1.12398200	-1.42445900	1.93378400
H	-2.73699000	-3.22733100	2.55956900
H	-4.71559100	-3.69970400	1.18378800
C	-1.78716500	0.20988500	-0.76384300
C	-3.06840200	-0.13373300	-1.66916600
H	-2.78858400	-0.51122800	-2.65869300
H	-3.78881000	0.68356200	-1.78590100
O	-0.56677600	-0.03432400	-1.43651500
H	-0.34084200	-1.16757900	-1.71231900
C	-1.79452500	1.62885400	-0.21428500
C	-1.29665500	2.67380500	-1.01016800
C	-2.32292400	1.94099900	1.04453400
C	-1.32470600	3.99255200	-0.55689200
H	-0.88426400	2.44178200	-1.98725500
C	-2.35047500	3.26293100	1.50095100
H	-2.71542500	1.14807900	1.67413400
C	-1.85201700	4.29313600	0.70310800
H	-0.93604000	4.78775400	-1.18813200
H	-2.76140800	3.48310000	2.48295700
H	-1.87323500	5.32035300	1.05726500

## TS2

C	-2.29274300	-1.67864300	-1.04540700
C	-2.32667000	-0.39363400	-1.66546100
C	-2.59069100	-0.59732600	1.55636300
C	-3.45983000	0.61232200	-1.56774300
C	-2.86588800	0.61555700	0.91074000
C	-3.97310800	0.80364800	-0.12260700
H	-1.62436700	-2.41046400	-1.49953400
H	-1.68112000	-0.26466200	-2.53304900
H	-3.07810800	1.57034100	-1.94222400
H	-2.49673200	1.52379500	1.38408500
H	-2.05179000	-0.54960500	2.50276300
H	-4.28756000	0.33076700	-2.23866400
H	-4.39599400	1.80890500	-0.01876600
H	-4.79447000	0.10989400	0.08737700
C	-3.43808600	-2.25287800	-0.21029800
H	-3.46085800	-3.34180900	-0.33346900

H	-4.39577500	-1.88747300	-0.59806400
C	-3.29942200	-1.91869600	1.29493200
H	-4.28592900	-1.93476500	1.78339400
H	-2.71038100	-2.70718000	1.77999000
Rh	-1.07838500	-0.31448600	0.01790300
C	0.94868100	3.67151300	-0.60533200
C	1.22207600	2.33417000	-0.85466900
C	1.08064500	1.35666700	0.13609400
C	0.67172100	1.65846100	1.43532100
C	0.36655200	3.00977500	1.68513600
C	0.50105600	3.98767300	0.69039500
H	1.07407500	4.45110300	-1.35365800
H	0.61110400	0.90881000	2.21910000
H	0.03621200	3.30685500	2.67733900
H	0.26661800	5.02161300	0.93471300
C	1.54006700	0.20313500	-0.81300600
C	1.74485000	1.36887400	-1.90457700
H	1.11578300	1.21783400	-2.78638100
H	2.78096800	1.53671300	-2.21844000
O	0.53614300	-0.69113700	-1.14181500
C	2.83367500	-0.50930900	-0.40806300
C	3.91142900	0.18581800	0.16602900
C	2.96877300	-1.88904200	-0.62578300
C	5.08940100	-0.47772600	0.50641200
H	3.82452300	1.25359800	0.35023300
C	4.15025500	-2.55566200	-0.28278400
H	2.13797300	-2.42448000	-1.07449300
C	5.21395100	-1.85290200	0.28353700
H	5.90957000	0.07928800	0.95291200
H	4.23580100	-3.62454000	-0.46254100
H	6.13166800	-2.36966900	0.55439100
O	0.72457200	-1.53927800	1.98360000
H	0.13333200	-2.20487000	1.59047100
H	1.46687100	-1.49559700	1.34722900

### TS3

C	-2.63426200	1.12205500	0.34778900
C	-2.29310900	0.41925800	1.51518800
C	-2.59607000	-1.21264000	-1.27969800
C	-3.05856300	-0.74509100	2.11965800
C	-2.50508000	-1.92610700	-0.07290200
C	-3.49868900	-1.79744600	1.07517700
H	-2.19399700	2.11073000	0.22654200

H	-1.63953700	0.93318000	2.21785100
H	-2.39817500	-1.22685100	2.85091900
H	-1.90617100	-2.83583100	-0.08491100
H	-2.07155100	-1.63078200	-2.13816900
H	-3.93078200	-0.38522600	2.68864700
H	-3.60525700	-2.77005700	1.56875100
H	-4.48954300	-1.55026000	0.67920200
C	-3.88624200	0.85317900	-0.48447800
H	-4.23496800	1.79558900	-0.92173800
H	-4.69565300	0.50854200	0.16831900
C	-3.64125900	-0.16720500	-1.62223800
H	-4.58887800	-0.64787700	-1.91316600
H	-3.28737100	0.36789400	-2.51121000
Rh	-1.04502300	-0.30115600	-0.09902200
C	1.45371000	3.22072600	-0.85102200
C	1.16474300	1.86094500	-0.94614100
C	0.78393900	1.09443500	0.17304300
C	0.81477100	1.68286700	1.44881600
C	1.07105200	3.05450800	1.55142100
C	1.36239600	3.81935400	0.41159000
H	1.77640300	3.79787400	-1.71438400
H	0.62753900	1.10185400	2.34802400
H	1.05427600	3.53492900	2.52682700
H	1.56693200	4.88151800	0.52020200
C	1.38869900	-0.36561500	-0.93505600
C	1.45183400	0.80080400	-1.97485300
H	0.68457800	0.66220700	-2.74371000
H	2.42688300	0.89634400	-2.46614600
O	0.45871600	-1.27690100	-1.10340600
C	2.69442600	-0.84844500	-0.33836500
C	3.81977000	-0.01817700	-0.21528200
C	2.78954500	-2.18078900	0.08562500
C	5.01117600	-0.51229400	0.31401200
H	3.76419500	1.02437100	-0.51608300
C	3.98221700	-2.67487900	0.61657100
H	1.92082600	-2.82220900	-0.01810400
C	5.09777600	-1.84341600	0.73275900
H	5.87293500	0.14456600	0.40311400
H	4.03976400	-3.71247400	0.93664500
H	6.02717300	-2.22696500	1.14614600

**Re\_TS4**

C	1.91706100	0.98562100	-1.60892000
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C	2.46196600	1.69878100	-0.55929000
C	1.37529700	1.58416100	-2.89654700
C	2.55205800	3.20545900	-0.43432300
C	-0.64494400	2.36256400	-1.52094900
C	-0.00822500	3.25107500	-0.66169200
C	-0.14352600	1.86045300	-2.85643700
C	1.30730400	3.96680000	-0.94545700
H	1.92033200	2.50331900	-3.13332100
H	1.58358100	0.89148900	-3.72044100
H	3.45311100	3.57653600	-0.94925500
H	2.69764300	3.43736000	0.62765200
H	-0.68025400	0.93120300	-3.08254300
H	-0.41424000	2.56858600	-3.65658300
H	1.28033300	4.95100400	-0.46372800
H	1.39792300	4.16387100	-2.01876500
H	-0.62284300	3.69771100	0.11610300
H	3.10873100	1.14911700	0.11937200
H	-1.70871600	2.20898100	-1.35752600
H	2.12729900	-0.07952500	-1.64527400
Rh	0.31883200	1.15420200	0.12160200
C	-2.67422700	0.67363100	0.80318100
C	-1.45548500	1.30398800	1.16331600
C	-1.48012700	2.14777000	2.29379400
C	-2.63576800	2.35565300	3.05247900
C	-3.82621500	1.72912100	2.68059500
C	-3.83788600	0.89960800	1.55997000
C	-2.74678700	-0.22321200	-0.43454600
C	-3.53371000	-1.51692400	-0.22682900
H	-0.56677700	2.66018300	2.59368100
H	-2.60602000	3.00638300	3.92417800
H	-4.73680600	1.88311300	3.25412900
H	-4.77016600	0.41897000	1.27110100
H	-3.14467300	0.33796100	-1.28806700
H	-1.72703700	-0.51897500	-0.70363200
O	-3.00755700	-2.45907000	0.35498800
C	-4.93765600	-1.65005700	-0.74210500
C	-5.56938000	-2.89965700	-0.60937900
C	-5.64522400	-0.59307900	-1.33820000
C	-6.86940700	-3.09029300	-1.06621700
H	-5.01513000	-3.70760100	-0.14353800
C	-6.95221800	-0.78259100	-1.79074200
H	-5.18962000	0.38598300	-1.44206200
C	-7.56474700	-2.03026900	-1.65917000
H	-7.34473900	-4.06164400	-0.96087600

H	-7.49012500	0.04409400	-2.24615000
H	-8.58073100	-2.17745000	-2.01553500
C	1.05016700	-0.37488400	1.31941100
C	1.80757200	0.06387500	2.56924200
H	1.20320400	0.75242000	3.16492300
H	2.14470700	-0.76802500	3.19916400
H	2.69735700	0.60467900	2.23475200
C	1.64479900	-1.54649300	0.57794900
O	1.03728200	-2.49707500	0.12447500
O	2.97766500	-1.37100800	0.43491300
C	3.66871200	-2.39012700	-0.35100100
H	3.25357500	-2.38285400	-1.36274200
H	3.45794900	-3.36397100	0.09750400
C	5.13712900	-2.06853300	-0.33992900
C	5.69216100	-1.23461900	-1.31982900
C	5.96886700	-2.59010900	0.65975700
C	7.05318400	-0.92570000	-1.30022500
H	5.05538200	-0.82795000	-2.10185000
C	7.33022700	-2.28314500	0.68196400
H	5.54724900	-3.24186900	1.42129800
C	7.87447100	-1.44982300	-0.29865500
H	7.47268000	-0.28102500	-2.06767400
H	7.96559900	-2.69678300	1.46025700
H	8.93493000	-1.21332500	-0.28492400
N	-0.27357000	-1.26501400	2.08311000
N	-1.29827500	-1.42186100	2.48345400

#### Si\_TS4

C	-0.53289600	3.08699600	-1.17668600
C	0.83661800	3.00354900	-1.03917200
C	-1.43984500	4.02956200	-0.40133300
C	1.69889800	3.74925300	-0.04322900
C	-1.08120400	2.48135900	1.61848400
C	0.28649100	2.66311400	1.80459800
C	-2.02745700	3.40992200	0.88643700
C	1.08109100	3.88590600	1.36578600
H	-0.89251600	4.94672200	-0.16153400
H	-2.26674300	4.33669400	-1.05246600
H	1.95534200	4.74625000	-0.43677500
H	2.64808000	3.20579700	0.03669300
H	-2.92461000	2.83399800	0.62713700
H	-2.37095500	4.21130700	1.56077700
H	1.88991400	4.05486300	2.08611300



H	0.44689900	4.77714800	1.41700800
H	0.75555300	2.05501000	2.57397800
H	1.38554900	2.55093800	-1.85837200
H	-1.57449900	1.78195300	2.28947500
H	-0.96725400	2.65360300	-2.07443100
Rh	-0.03038600	1.16950700	0.13641900
C	-1.35043600	-0.99450100	1.89835300
C	-0.15311000	-0.32553800	1.54446800
C	1.01695500	-0.68509300	2.24846200
C	1.01592700	-1.65843500	3.25187200
C	-0.17487700	-2.30512100	3.58916900
C	-1.34475000	-1.96884400	2.91045700
C	-2.67040500	-0.66561300	1.23112800
C	-3.22543800	-1.74273700	0.29875300
H	1.95627600	-0.18965700	2.00900400
H	1.93990500	-1.90387600	3.77168100
H	-0.19312500	-3.06032000	4.37100100
H	-2.27675100	-2.46853200	3.17115000
H	-3.43942700	-0.44431300	1.98441600
H	-2.55712600	0.24922400	0.63077600
O	-2.57000400	-2.72739500	-0.01709100
C	-4.61008000	-1.55593500	-0.25766800
C	-5.13544500	-2.57300700	-1.07264100
C	-5.39018500	-0.41535600	-0.00651100
C	-6.41003200	-2.45690300	-1.61992700
H	-4.52277900	-3.44840600	-1.26122600
C	-6.66630700	-0.29679600	-0.55911600
H	-5.00845700	0.38668500	0.61658500
C	-7.17892600	-1.31665500	-1.36409500
H	-6.80637400	-3.25208500	-2.24534000
H	-7.26018000	0.59077600	-0.35963200
H	-8.17403700	-1.22405000	-1.79072400
C	0.29339700	-0.12633600	-1.46939800
C	-0.80607700	-0.28609400	-2.51198500
H	-1.76398200	-0.53109900	-2.05025900
H	-0.90287800	0.68029400	-3.01439900
H	-0.57240600	-1.02886000	-3.28362300
C	1.65110100	0.05164100	-2.10236400
O	1.80984300	0.71579400	-3.11408900
O	2.66030900	-0.51208600	-1.41458100
C	3.99543400	-0.30294100	-1.96364700
H	4.17771100	0.77322700	-2.02088300
H	4.01330000	-0.70807800	-2.97941900
C	4.98193600	-0.99201000	-1.06248200

C	5.64705400	-0.27687000	-0.05842700
C	5.24067400	-2.36164500	-1.20809900
C	6.55422300	-0.91805000	0.78735900
H	5.45613500	0.78748000	0.05763800
C	6.14485500	-3.00571800	-0.36300500
H	4.73209200	-2.92341700	-1.98803500
C	6.80372100	-2.28401400	0.63627700
H	7.06666400	-0.35183400	1.56022000
H	6.33883400	-4.06762500	-0.48632900
H	7.51130800	-2.78402000	1.29201200
N	0.41346300	-2.60687800	-0.16150900
N	0.45243300	-1.78693000	-0.91218900

### Re\_TS5

C	-3.17010700	-0.90736400	-1.95544200
C	-3.51857500	-1.89825800	-1.02757100
C	-4.10149400	0.19801600	-2.44241200
C	-4.83657200	-2.02324600	-0.29097200
C	-3.78477000	1.28632700	-0.12768800
C	-4.35307200	0.31091700	0.66088000
C	-4.01694600	1.50249500	-1.60936200
C	-5.41506000	-0.67649000	0.20334800
H	-5.13310600	-0.16946800	-2.46440200
H	-3.84828400	0.43740900	-3.48140400
H	-5.58143200	-2.53797700	-0.91957300
H	-4.66940200	-2.67768800	0.57341500
H	-3.18394400	2.10558500	-1.98905700
H	-4.92519700	2.10446100	-1.77273700
H	-6.09680400	-0.87266900	1.03929400
H	-6.02589600	-0.21811900	-0.58040800
H	-4.21685300	0.40123300	1.73680100
H	-2.93779200	-2.81984800	-1.05112600
H	-3.28275300	2.10279900	0.38737600
H	-2.32148400	-1.12028800	-2.60226900
Rh	-2.23502300	-0.44153600	-0.00825400
C	-0.36169200	1.67209800	1.47665300
C	-0.89703600	0.35769200	1.58725400
C	-0.96726500	-0.21348100	2.86967700
C	-0.55783900	0.46274900	4.02217200
C	-0.05421100	1.75513000	3.90817000
C	0.02449000	2.34651000	2.64567300
C	-0.35029100	2.47556400	0.17392600
C	0.68764000	2.17829500	-0.91971900

H	-1.36925000	-1.21478200	2.98546100
H	-0.64254500	-0.01575700	4.99473000
H	0.26158800	2.30971500	4.78786700
H	0.36640600	3.37709900	2.57378700
H	-0.26169300	3.53839900	0.42961700
H	-1.30785800	2.33403500	-0.32964100
O	0.34613200	1.56113000	-1.92147000
C	2.07368100	2.74624200	-0.83680000
C	2.83754100	2.78388600	-2.01677400
C	2.63349200	3.23908200	0.35150200
C	4.12683200	3.30846800	-2.01016500
H	2.39578900	2.39934800	-2.93009600
C	3.93207700	3.75109600	0.36110000
H	2.07011600	3.20089500	1.27555100
C	4.67853000	3.79194200	-0.81876000
H	4.70371500	3.34095000	-2.93027300
H	4.35914900	4.11974900	1.28954400
H	5.68613300	4.19871600	-0.81106600
C	-0.55659300	-1.33622500	0.22144500
C	-0.43380600	-2.61788800	1.02203900
H	-1.32018900	-2.83988100	1.61773000
H	0.45776700	-2.63328200	1.66253700
H	-0.31216800	-3.42488600	0.28442300
C	0.69832200	-1.16225300	-0.57439800
O	0.78290800	-1.65341300	-1.68668300
O	1.71111200	-0.56732700	0.08009400
C	3.01431800	-0.58417100	-0.58718100
H	2.85636600	-0.44822200	-1.65743100
H	3.52248600	0.28916200	-0.17832600
C	3.76900900	-1.85407400	-0.28469100
C	3.76722600	-2.92547600	-1.18846100
C	4.48133200	-1.97911000	0.91660700
C	4.46744500	-4.09795400	-0.89730700
H	3.20864400	-2.83720100	-2.11536400
C	5.17776500	-3.15186100	1.21149800
H	4.49233000	-1.15053600	1.62111200
C	5.17262900	-4.21392900	0.30309600
H	4.46227300	-4.92024600	-1.60777700
H	5.72827200	-3.23490400	2.14478100
H	5.71846200	-5.12617500	0.52879800

### Si\_TS5

C	3.00252600	-1.96656200	-1.66285800
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C	2.15642800	-3.06320400	-1.45990700
C	4.40224300	-1.81274700	-1.07806200
C	2.42936400	-4.26125400	-0.57352700
C	3.25061500	-1.38479500	1.18392300
C	2.66533400	-2.61451800	1.37940200
C	4.42835300	-1.07386500	0.28296000
C	3.12984400	-3.92483800	0.76594800
H	4.87645600	-2.79516100	-0.98405700
H	5.02104300	-1.25148000	-1.78787100
H	3.02086900	-5.01367600	-1.12011800
H	1.46315000	-4.73373000	-0.36086500
H	4.42515400	0.00707200	0.09701600
H	5.37615300	-1.28650400	0.80317100
H	2.92994300	-4.73583700	1.47587700
H	4.21574200	-3.90586600	0.63112500
H	1.94159500	-2.69581400	2.18754900
H	1.36503600	-3.22544800	-2.18920500
H	2.97988600	-0.59258600	1.88001400
H	2.79416000	-1.34538400	-2.53208700
Rh	1.39530100	-1.42967200	-0.21367100
C	0.13425500	0.74571500	1.74844400
C	-0.06037900	-0.53135100	1.17580100
C	-0.96805200	-1.41225100	1.79613400
C	-1.63939800	-1.06739400	2.97029000
C	-1.43498200	0.19493400	3.53377000
C	-0.55503500	1.08690600	2.92228900
C	1.12242000	1.73995400	1.17760100
C	0.50470400	3.02638900	0.62085600
H	-1.14720700	-2.39134700	1.35834900
H	-2.31720000	-1.77653800	3.43958700
H	-1.95759200	0.48375300	4.44192900
H	-0.39329500	2.06694600	3.36539200
H	1.84406600	2.03855000	1.95264900
H	1.72050900	1.25982800	0.39250700
O	-0.69925900	3.23602800	0.67448000
C	1.42368500	4.03914500	0.00133500
C	0.85540900	5.21603100	-0.51512900
C	2.81434000	3.86054800	-0.08295900
C	1.65627600	6.19093200	-1.10279300
H	-0.21982200	5.34260100	-0.44392000
C	3.61705700	4.83840400	-0.67199700
H	3.27930800	2.96244600	0.31042700
C	3.04036500	6.00359800	-1.18260200
H	1.20560300	7.09659500	-1.49913700

H	4.69160700	4.69037300	-0.73168900
H	3.66680000	6.76380700	-1.64133900
C	-0.18293000	-0.71044500	-1.02558800
C	-0.31952500	0.62975900	-1.69987200
H	0.59700100	1.21895900	-1.65471000
H	-0.54908200	0.44382500	-2.76099900
H	-1.15422200	1.21555100	-1.29791100
C	-1.43473400	-1.55483900	-1.17017800
O	-1.42738800	-2.73928600	-1.45588200
O	-2.56948500	-0.85036800	-0.98899900
C	-3.80899300	-1.60634300	-1.05391200
H	-3.72865800	-2.44226700	-0.35099600
H	-3.91656600	-2.02304000	-2.05928100
C	-4.94620200	-0.68322700	-0.70708300
C	-5.00626100	-0.07391200	0.55507000
C	-5.96625600	-0.43518700	-1.63194800
C	-6.06727500	0.76993400	0.88090800
H	-4.21441800	-0.25674800	1.27716900
C	-7.03532600	0.40278200	-1.30350300
H	-5.92510500	-0.90035700	-2.61403500
C	-7.08648100	1.00792700	-0.04701400
H	-6.10174700	1.24041700	1.85980200
H	-7.82217300	0.58516000	-2.03042300
H	-7.91480600	1.66280700	0.20968900

## ESi-TS6

C	3.49722000	-0.93760800	-1.06164300
C	3.12470200	0.08575900	-1.99184000
C	4.82282800	-0.94179400	-0.29948100
C	3.93513200	1.32502700	-2.32323000
C	3.62948400	0.83620500	1.08365100
C	3.48932300	1.85151000	0.12104200
C	4.68465200	-0.25668400	1.07542800
C	4.44109600	2.04650800	-1.05618500
H	5.59921000	-0.45470100	-0.90073700
H	5.15802300	-1.97521600	-0.15783200
H	4.77342900	1.07943900	-2.99509500
H	3.28187000	2.00302100	-2.88465200
H	4.38321900	-1.00441200	1.81781400
H	5.65201000	0.14330400	1.41886100
H	4.54428700	3.11801500	-1.25966700
H	5.44076100	1.69157300	-0.78265900
H	2.88976100	2.71529500	0.40027600

H	2.42492300	-0.20977300	-2.77488900
H	3.17281100	1.01182100	2.05310600
H	3.06633700	-1.92292700	-1.23866700
Rh	2.00557800	0.31232200	-0.23335200
C	-0.70345100	-2.04388500	1.90899400
C	-0.68316900	-0.75614000	2.51028000
C	-1.39792400	-0.60540300	3.71875900
C	-2.11594300	-1.64411700	4.30468700
C	-2.12716100	-2.90301000	3.70290100
C	-1.41539800	-3.08797400	2.51957100
C	0.16424600	-2.38275700	0.70165000
C	-0.20288400	-1.81788100	-0.66266200
H	-1.40279200	0.36707400	4.20139800
H	-2.66352200	-1.47029800	5.22780500
H	-2.66445600	-3.73297400	4.15357500
H	-1.38103400	-4.08139600	2.07645400
H	0.20047700	-3.47380100	0.59781000
H	1.18297100	-2.02148700	0.89415000
O	0.47260700	-0.89935800	-1.16330900
C	-1.29015900	-2.40221800	-1.48643400
C	-1.40026300	-2.01459100	-2.83649900
C	-2.20652600	-3.33246600	-0.96708300
C	-2.39695800	-2.54988900	-3.64541200
H	-0.69177700	-1.29681200	-3.23472600
C	-3.21054200	-3.85941200	-1.77805700
H	-2.15523900	-3.62626800	0.07338000
C	-3.30562800	-3.47358500	-3.11699000
H	-2.46836000	-2.24927000	-4.68664500
H	-3.91882900	-4.57062200	-1.36349100
H	-4.08580400	-3.88999900	-3.74813300
C	0.09802900	0.39019900	1.97135900
C	0.86199800	1.23080000	2.98297100
H	1.61721400	0.65266700	3.53194600
H	0.19872600	1.67208000	3.74444900
H	1.35828800	2.06799400	2.48718400
C	-0.32135700	1.04902100	0.79685300
O	0.32163900	1.96582000	0.18867600
O	-1.53203100	0.63058200	0.28607500
C	-1.98306500	1.22387900	-0.95003500
H	-1.11678100	1.59636300	-1.49914300
H	-2.44900600	0.40979700	-1.51107900
C	-2.98352900	2.33097900	-0.70213000
C	-2.55965500	3.58640500	-0.24005900
C	-4.34865900	2.12081900	-0.93058500

C	-3.48449300	4.60545800	-0.01127100
H	-1.50078100	3.74930100	-0.05962600
C	-5.27684900	3.14102900	-0.70586000
H	-4.68759000	1.15089700	-1.28831300
C	-4.84597500	4.38617200	-0.24451800
H	-3.14350800	5.57406300	0.34551800
H	-6.33318600	2.96231800	-0.88964500
H	-5.56511000	5.18195400	-0.06844200

### **ERe-TS6**

C	-3.49768800	-0.93849100	-1.05894500
C	-3.12476500	0.08271400	-1.99131800
C	-4.82308000	-0.94078900	-0.29638500
C	-3.93346600	1.32244800	-2.32502100
C	-3.62890300	0.83992400	1.08294000
C	-3.48832400	1.85302600	0.11816700
C	-4.68472000	-0.25238900	1.07692700
C	-4.44018700	2.04564000	-1.05936800
H	-5.59966300	-0.45528800	-0.89866400
H	-5.15809700	-1.97389900	-0.15210600
H	-4.77104400	1.07736500	-2.99797800
H	-3.27847900	1.99919100	-2.88597500
H	-4.38389300	-0.99852700	1.82114000
H	-5.65193500	0.14893800	1.41917800
H	-4.54409900	3.11675800	-1.26458900
H	-5.43961300	1.69042800	-0.78543500
H	-2.88778500	2.71687300	0.39504400
H	-2.42552500	-0.21519200	-2.77394700
H	-3.17213400	1.01724800	2.05201000
H	-3.06760600	-1.92444200	-1.23449600
Rh	-2.00529800	0.31203200	-0.23328700
C	0.70287100	-2.04476300	1.90804800
C	0.68275100	-0.75716800	2.50966000
C	1.39761500	-0.60696600	3.71819700
C	2.11555900	-1.64592400	4.30375300
C	2.12665100	-2.90462600	3.70155300
C	1.41477700	-3.08910900	2.51822900
C	-0.16505400	-2.38316700	0.70076100
C	0.20257100	-1.81790400	-0.66319300
H	1.40262200	0.36534900	4.20114700
H	2.66320500	-1.47244700	5.22689800
H	2.66390500	-3.73479200	4.15190500
H	1.38017200	-4.08241500	2.07487100

H	-0.20199900	-3.47415600	0.59673100
H	-1.18351600	-2.02123400	0.89342500
O	-0.47202000	-0.89837400	-1.16325800
C	1.28992600	-2.40208600	-1.48694800
C	1.40207500	-2.01192200	-2.83612600
C	2.20439800	-3.33470100	-0.96849900
C	2.39891300	-2.54699300	-3.64500900
H	0.69506600	-1.29233800	-3.23371100
C	3.20852300	-3.86149300	-1.77943300
H	2.15154500	-3.63058200	0.07129000
C	3.30566300	-3.47307600	-3.11746700
H	2.47190100	-2.24435900	-4.68554700
H	3.91529400	-4.57459700	-1.36553700
H	4.08594100	-3.88933000	-3.74858900
C	-0.09842900	0.38959200	1.97142500
C	-0.86185000	1.22985200	2.98376400
H	-1.61663700	0.65142800	3.53300600
H	-0.19830100	1.67131800	3.74491600
H	-1.35861500	2.06699400	2.48839100
C	0.32119200	1.04942300	0.79736800
O	-0.32126200	1.96723600	0.19039400
O	1.53163300	0.63104700	0.28613100
C	1.98222300	1.22506200	-0.94985500
H	1.11574500	1.59813000	-1.49824900
H	2.44764700	0.41120100	-1.51163100
C	2.98308900	2.33171700	-0.70161800
C	2.55928200	3.58805900	-0.24196900
C	4.34851300	2.12019000	-0.92704400
C	3.48445800	4.60667800	-0.01260000
H	1.50019300	3.75193400	-0.06368500
C	5.27704900	3.13995600	-0.70174900
H	4.68737000	1.14957600	-1.28296200
C	4.84622500	4.38602900	-0.24287300
H	3.14353500	5.57600300	0.34228500
H	6.33361200	2.96020500	-0.88320500
H	5.56563100	5.18147800	-0.06639200

### ZSi-TS6

C	-2.33878200	-1.87397700	-1.90367200
C	-1.55536100	-0.94075100	-2.64287200
C	-2.22032300	-3.38995100	-2.05307300
C	-0.43379000	-1.29832900	-3.60244500
C	-0.17173800	-2.99938800	-0.60184200



C	0.62911700	-2.24064900	-1.48863600
C	-1.26890700	-3.97393400	-0.99092100
H	-1.87931300	-3.63992300	-3.06373900
H	-3.21161700	-3.84428100	-1.94729500
H	-0.84061300	-1.64792700	-4.56443700
H	0.11563600	-0.37531500	-3.82071300
H	-1.84049900	-4.19434700	-0.08227600
H	-0.83648800	-4.93082700	-1.32383500
H	1.57715600	-1.87585400	-1.09335600
H	-1.99092600	0.04455900	-2.80231200
H	0.23098900	-3.15656100	0.39618800
H	-3.30142300	-1.51362900	-1.54166100
Rh	-0.87840700	-0.98595700	-0.65099200
C	-1.97541200	0.11589700	2.26764300
C	-0.99405700	-0.91852000	2.22922700
C	-1.42315500	-2.19261700	2.70532200
C	-2.71490000	-2.44414000	3.14744900
C	-3.66900100	-1.42339500	3.14669600
C	-3.27769300	-0.16277000	2.70593900
C	-1.69486000	1.53348800	1.84843400
C	-1.96598000	1.78072800	0.36768800
H	-0.71533100	-3.01355400	2.71097100
H	-2.97523900	-3.44164500	3.49390300
H	-4.68209300	-1.59885100	3.49702100
H	-3.99773300	0.65358700	2.72227700
H	-0.67188800	1.83995800	2.08639700
H	-2.35619500	2.20669900	2.40959300
O	-2.25403700	0.85174200	-0.40567800
C	-1.99769700	3.17984400	-0.13815200
C	-2.35120900	3.41052500	-1.47986700
C	-1.67442000	4.27811600	0.67826400
C	-2.38213700	4.70404100	-1.99183600
H	-2.60277300	2.56088500	-2.10502900
C	-1.70107600	5.57310500	0.16258000
H	-1.39256500	4.12752400	1.71477900
C	-2.05642000	5.78907800	-1.17128500
H	-2.65920700	4.86958200	-3.02916300
H	-1.44514700	6.41328800	0.80165300
H	-2.07945900	6.79933500	-1.57063600
C	0.43604800	-0.78447600	1.86316700
C	1.38804200	-1.72305600	2.59210900
H	1.06365100	-1.88508500	3.62734800
H	2.39830900	-1.31536000	2.61391000
H	1.46001600	-2.72168900	2.12897500

C	1.01750900	0.18227500	0.99808000
O	0.44828800	0.90707700	0.12892400
O	2.39234000	0.26856200	1.09430600
C	3.05162000	1.12509700	0.15247000
H	2.62864400	0.95753700	-0.84438400
H	2.86520200	2.17490400	0.40716500
C	4.53241600	0.82610600	0.17615400
C	5.00323400	-0.49454000	0.18009000
C	5.46118600	1.87274500	0.14446100
C	6.37249200	-0.76010900	0.15171800
H	4.29108800	-1.31378200	0.21819000
C	6.83313000	1.60965400	0.10731600
H	5.10902400	2.90190600	0.15080700
C	7.29281100	0.29168100	0.11202300
H	6.72242700	-1.78918900	0.16004900
H	7.54038700	2.43457200	0.08387000
H	8.35930600	0.08417000	0.08935700
C	0.54345600	-2.33892000	-3.01148000
H	1.54067000	-2.18449700	-3.43746100
H	0.24674200	-3.35429700	-3.29644100

### ZRe-TS6

C	2.86800100	-1.48949800	-1.68527700
C	1.99006100	-0.74356200	-2.52448300
C	3.06800600	-3.00024800	-1.79385300
C	1.05792900	-1.33023800	-3.56954700
C	0.85173000	-3.00722100	-0.55203500
C	0.00442700	-2.43985400	-1.53305000
C	2.15265600	-3.74749500	-0.80499000
H	2.88335700	-3.32845300	-2.82284500
H	4.11469200	-3.24478800	-1.58188600
H	1.61392600	-1.60243000	-4.48058700
H	0.35907500	-0.53840500	-3.86289600
H	2.66566500	-3.83641600	0.15938800
H	1.95230900	-4.77614000	-1.14445200
H	-1.03065700	-2.26889500	-1.23739800
H	2.23804000	0.30579300	-2.67780400
H	0.39392700	-3.22626800	0.40976700
H	3.70081700	-0.93735700	-1.25040100
Rh	1.14612900	-0.89254100	-0.60495000
C	1.69304500	0.45114300	2.35535500
C	0.94403900	-0.75988900	2.26247400
C	1.56528200	-1.91255100	2.82851600

C	2.82941500	-1.89177100	3.40178000
C	3.55903200	-0.70113100	3.45197200
C	2.97343200	0.44697100	2.92694800
C	1.18150600	1.77756800	1.86144100
C	1.54739600	2.05589700	0.40675400
H	1.03629000	-2.85815800	2.79998600
H	3.24445800	-2.81004400	3.81092500
H	4.54588700	-0.66357200	3.90428600
H	3.51273100	1.39113500	2.98028900
H	0.09911400	1.87491500	1.98780600
H	1.63433100	2.57725200	2.46216600
O	2.08347700	1.19248400	-0.30798900
C	1.36168700	3.42909700	-0.13595000
C	1.79621200	3.70828600	-1.44427900
C	0.75648000	4.45422700	0.61230300
C	1.63238000	4.97794600	-1.98958900
H	2.26507900	2.91570400	-2.01701600
C	0.58814500	5.72440400	0.06271900
H	0.40756400	4.26476300	1.62167400
C	1.02693800	5.98972900	-1.23691300
H	1.97490200	5.18164700	-3.00023400
H	0.11547700	6.50704700	0.64913000
H	0.89769600	6.98117900	-1.66227200
C	-0.43998100	-0.92181300	1.75876200
C	-1.25405800	-2.02379000	2.42305300
H	-1.02549900	-2.09126300	3.49402900
H	-2.32264600	-1.84101200	2.31440600
H	-1.06211200	-3.02467500	2.00109200
C	-1.10998300	-0.10492000	0.80748300
O	-0.60782500	0.70269600	-0.02920300
O	-2.47660400	-0.29442600	0.76377300
C	-3.18798900	0.43418300	-0.24867200
H	-2.83060000	0.14485900	-1.24269500
H	-2.98436100	1.50488500	-0.13135400
C	-4.66155400	0.14181900	-0.09731600
C	-5.29532200	0.27764300	1.14659400
C	-5.42709000	-0.23156500	-1.20741800
C	-6.66413800	0.04321400	1.27455600
H	-4.70776300	0.55981600	2.01581000
C	-6.80076700	-0.45879200	-1.08417100
H	-4.94586000	-0.34615900	-2.17608400
C	-7.42238900	-0.32328300	0.15792400
H	-7.14140500	0.14862800	2.24537800
H	-7.38077600	-0.74803300	-1.95660400

H	-8.48937500	-0.50372900	0.25796300
C	0.25430800	-2.53844100	-3.03766900
H	-0.70800000	-2.59263900	-3.55808200
H	0.77252200	-3.47727900	-3.26190500

## TS7'RR

C	2.56589000	-2.41271200	-1.55881500
C	3.49793200	-1.51977800	-0.96819000
C	2.44472500	-3.88653200	-1.18307200
C	4.46475200	-1.85288800	0.15262500
C	1.26408200	-2.94671900	0.88025400
C	2.32720500	-2.25574200	1.48389600
C	1.38805400	-4.11738700	-0.07953000
C	3.79801700	-2.62504100	1.31439600
H	3.42230300	-4.26575000	-0.86558300
H	2.17040700	-4.46271400	-2.07345300
H	5.32946600	-2.41108300	-0.23928700
H	4.86166800	-0.90474100	0.53344100
H	0.40845900	-4.26190800	-0.55017800
H	1.60297800	-5.04700100	0.47013700
H	4.33348400	-2.40793400	2.24513600
H	2.07426500	-1.66513500	2.36318800
H	3.77393400	-0.65011300	-1.56346500
H	0.29595100	-2.84188100	1.36472000
H	2.19982300	-2.14462600	-2.54901600
Rh	1.57092200	-1.10044300	-0.19972500
C	-1.59652000	2.28000200	-0.58338100
C	-1.29239700	2.00052500	0.75780000
C	-2.05369400	2.62261400	1.76046300
C	-3.09836100	3.49171500	1.43614300
C	-3.40131200	3.75012100	0.09748100
C	-2.64599600	3.14434100	-0.90897900
C	-0.72957900	1.61025900	-1.61440500
C	0.70440600	1.41713100	-1.13962800
H	-1.83462700	2.42023500	2.80567300
H	-3.67416400	3.96332000	2.22843400
H	-4.21263900	4.42506200	-0.16187800
H	-2.86651900	3.35288700	-1.95361000
H	-0.71130900	2.19052500	-2.54888500
H	-1.11294100	0.61517300	-1.86416700
O	1.32911100	0.38396500	-1.60036600
C	1.54466400	2.60875700	-0.79784700
C	2.89875800	2.41907100	-0.46265200

C	1.05659700	3.92590300	-0.86736200
C	3.73052300	3.50176100	-0.19302500
H	3.28827600	1.40869300	-0.40810500
C	1.89361600	5.01200300	-0.60432400
H	0.02327200	4.11335400	-1.13255200
C	3.23096200	4.80652800	-0.26289000
H	4.77103300	3.33011800	0.06974500
H	1.49611300	6.02115400	-0.67023900
H	3.87960000	5.65313300	-0.05494700
C	-0.20160400	1.01459600	1.11092500
C	0.78703200	1.50403800	2.15847800
H	1.22506900	2.46018800	1.86153500
H	1.60140200	0.78966800	2.31011800
H	0.30567800	1.64550900	3.13793400
C	-0.79014900	-0.29458800	1.46022100
O	-0.53750400	-0.95537900	2.46705700
O	-1.73941200	-0.70587600	0.55610000
C	-2.55821200	-1.82745900	0.93799400
H	-2.01955700	-2.76063700	0.73879100
H	-2.73565200	-1.77615500	2.01753200
C	-3.84893800	-1.77729600	0.15770000
C	-4.34423800	-2.92934300	-0.46320000
C	-4.59205900	-0.59017400	0.08038100
C	-5.56534900	-2.90423200	-1.14253800
H	-3.77202900	-3.85317700	-0.41519800
C	-5.80649200	-0.56151000	-0.60486100
H	-4.20959100	0.31165100	0.54992400
C	-6.29891700	-1.71917600	-1.21584500
H	-5.93692400	-3.80750800	-1.61911500
H	-6.37116100	0.36545100	-0.66109500
H	-7.24639000	-1.69498800	-1.74755700
H	3.89084800	-3.70524900	1.15802900

## TS7'RS

C	4.06557400	-0.74928400	1.35152000
C	3.91440900	0.64139100	1.48748200
C	5.21761800	-1.43003900	0.61690200
C	4.82208200	1.70754000	0.89768900
C	3.95251800	-0.68314700	-1.46767400
C	4.08309000	0.72466500	-1.32641700
C	4.85892900	-1.73305400	-0.85464300
C	5.21268600	1.41833000	-0.56914900
H	6.11705400	-0.80824800	0.67424500

H	5.46592600	-2.36627300	1.12688000
H	5.71917300	1.84281100	1.52062400
H	4.27679600	2.65857800	0.93769000
H	4.32381800	-2.68916700	-0.90301600
H	5.76827300	-1.86075300	-1.46295800
H	5.45590600	2.36138100	-1.07154600
H	6.12083500	0.80866000	-0.61548000
H	3.57365400	1.33166100	-2.07218200
H	3.28670700	0.98421000	2.31274700
H	3.36145700	-1.03069000	-2.31532500
H	3.54483200	-1.37116200	2.07489700
Rh	2.54492300	-0.00502800	-0.03947000
C	-0.96854200	-1.89518200	-0.98402600
C	-0.61096400	-1.97031500	0.38380900
C	-0.41785400	-3.25644400	0.93143900
C	-0.59406600	-4.41483900	0.17312400
C	-0.96417300	-4.32045300	-1.16909600
C	-1.14844200	-3.05554200	-1.73655300
C	-1.16598600	-0.53091000	-1.60809800
C	-0.10541400	0.46542200	-1.16766100
H	-0.14565200	-3.35091100	1.97886500
H	-0.44400600	-5.38788000	0.63367900
H	-1.09109400	-5.21496100	-1.77228600
H	-1.41718600	-2.97110500	-2.78656900
H	-1.09792800	-0.61082300	-2.70213500
H	-2.16226400	-0.16697300	-1.35940900
O	1.09820500	0.17983700	-1.50083400
C	-0.45822600	1.87832900	-0.85914800
C	0.48777100	2.73753700	-0.26453600
C	-1.70773800	2.41846200	-1.22072300
C	0.19410800	4.07491500	-0.02660000
H	1.46059700	2.34294400	0.02362300
C	-1.99845600	3.76542200	-0.99085500
H	-2.45491700	1.80006500	-1.70593200
C	-1.05277200	4.59793600	-0.38949100
H	0.93691000	4.71316000	0.44772000
H	-2.96629400	4.16137400	-1.28854900
H	-1.28236100	5.64318300	-0.20429500
C	-0.37516100	-0.74934000	1.18836500
C	0.58950000	-0.89090600	2.36628300
H	1.46742900	-1.48633700	2.10165400
H	0.90962900	0.08559900	2.73750600
H	0.11097700	-1.39808500	3.22139500
C	-1.45234300	0.16787900	1.52960800

O	-1.37103300	1.07752200	2.35431400
O	-2.64258800	-0.06752500	0.87345400
C	-3.74226700	0.76249400	1.27701600
H	-3.54003300	1.80651700	1.01550300
H	-3.83514300	0.71778900	2.36893400
C	-4.99962300	0.26958100	0.59988400
C	-5.97276400	1.18750900	0.18642800
C	-5.24255200	-1.09956800	0.42110300
C	-7.17027300	0.75009200	-0.38637500
H	-5.79178200	2.25318900	0.31210600
C	-6.43452600	-1.53794000	-0.15916300
H	-4.48764600	-1.81753400	0.72582200
C	-7.40419300	-0.61534300	-0.56116600
H	-7.91396000	1.47693200	-0.70321400
H	-6.60761400	-2.60271100	-0.29467700
H	-8.33201800	-0.95804800	-1.01128300

### TS7'SR

C	-3.21539800	-0.84529100	-1.76058500
C	-2.54370200	-1.83276100	-1.02415000
C	-4.73029700	-0.67305600	-1.79026700
C	-3.19070600	-2.86342100	-0.11589200
C	-4.36763300	0.33374900	0.52867200
C	-3.90430900	-0.81564600	1.22218500
C	-5.22076500	0.33514400	-0.72544400
C	-4.24582100	-2.25270800	0.83615200
H	-5.21782100	-1.64394300	-1.65139000
H	-5.03252700	-0.32207900	-2.78303300
H	-3.63537400	-3.67568500	-0.71152000
H	-2.39557800	-3.32391700	0.48136100
H	-5.18151100	1.34686300	-1.14507800
H	-6.27645100	0.14938200	-0.47174000
H	-4.30796700	-2.86239200	1.74417300
H	-3.62182900	-0.66359500	2.26302700
H	-1.53210400	-2.06450600	-1.35679900
H	-4.40242800	1.26158900	1.10058900
H	-2.65526600	-0.41005200	-2.58404900
Rh	-2.33358600	0.02401300	0.04815200
C	1.20790200	3.12977400	0.48282500
C	1.23221800	2.35063500	-0.68714500
C	2.29804400	2.54790300	-1.58478800
C	3.30559400	3.47867800	-1.32868400
C	3.26267400	4.25016100	-0.16519300

C	2.21201900	4.07170100	0.73536700
C	0.06957400	2.91130600	1.45159900
C	-0.43208800	1.47727300	1.52232000
H	2.33271700	1.96664700	-2.50244400
H	4.11758900	3.60560000	-2.04021300
H	4.04238700	4.97776900	0.04327500
H	2.17757700	4.65746000	1.65144800
H	-0.79936000	3.52541700	1.18726500
H	0.37258000	3.21668400	2.46349700
O	-1.70103900	1.32275600	1.56365100
C	0.46144700	0.40267000	2.05176600
C	-0.09401100	-0.83115800	2.44462600
C	1.83759200	0.60670900	2.26562100
C	0.69760300	-1.83063200	3.00205600
H	-1.15744700	-0.99757900	2.31213400
C	2.62983300	-0.39632900	2.82394700
H	2.29950200	1.54669100	1.99183400
C	2.06734000	-1.61990400	3.19025500
H	0.24516000	-2.77336900	3.29819500
H	3.69132300	-0.21845200	2.97109900
H	2.68718300	-2.39980600	3.62384100
C	0.08411400	1.44701800	-1.03822600
C	-1.03516000	2.22847900	-1.72047900
H	-1.47655100	2.96720500	-1.04098900
H	-1.83911100	1.58085100	-2.07904200
H	-0.65518700	2.78710600	-2.59220500
C	0.43361400	0.17715800	-1.66517800
O	-0.18473000	-0.40316500	-2.56340500
O	1.57802000	-0.37334100	-1.14190200
C	2.00734800	-1.60860400	-1.73210200
H	1.27627100	-2.39719300	-1.52094500
H	2.04097200	-1.48863600	-2.82198300
C	3.36462700	-1.97424800	-1.18031800
C	3.66675400	-3.31283000	-0.90298800
C	4.35593100	-1.00213900	-0.98553900
C	4.93661500	-3.67949900	-0.45032400
H	2.90278600	-4.07485500	-1.04091700
C	5.62213200	-1.36557600	-0.52497900
H	4.12654500	0.04047500	-1.18374600
C	5.91845200	-2.70567500	-0.25911200
H	5.15419500	-4.72343600	-0.24006500
H	6.38006800	-0.60100300	-0.37462600
H	6.90571300	-2.98702200	0.09768300
H	-5.24193000	-2.28610200	0.38178400



## TS7'SS

C	-2.32026900	-2.26310800	1.48373400
C	-1.25321200	-2.94848700	0.88062300
C	-3.78950100	-2.63795700	1.31305900
C	-1.36979000	-4.11858300	-0.08060300
C	-3.49253600	-1.53093800	-0.96910500
C	-2.55620100	-2.41950600	-1.55904700
C	-4.45865500	-1.86851100	0.15087400
C	-2.42806900	-3.89276500	-1.18341900
H	-3.87860300	-3.71852200	1.15708000
H	-4.32625200	-2.42235100	2.24341800
H	-1.57814200	-5.05056200	0.46763900
H	-0.38939700	-4.25579300	-0.55187300
H	-4.86006000	-0.92219800	0.53154700
H	-5.32065200	-2.43039300	-0.24179000
H	-2.15125700	-4.46750800	-2.07398300
H	-3.40348700	-4.27711700	-0.86554800
H	-2.19034400	-2.14928300	-2.54873800
H	-0.28643000	-2.83974000	1.36683300
H	-3.77154200	-0.66208900	-1.56416500
H	-2.07040600	-1.67234400	2.36380900
Rh	-1.56792500	-1.10279500	-0.19900600
C	1.58898300	2.28394800	-0.58418100
C	1.28562100	2.00285300	0.75673900
C	2.04754600	2.62327800	1.75989300
C	3.09198900	3.49281900	1.43612500
C	3.39412300	3.75310700	0.09761000
C	2.63826100	3.14875900	-0.90926700
C	0.72134200	1.61529500	-1.61529700
C	-0.71051800	1.41649700	-1.13618100
H	1.82947100	2.41921600	2.80497800
H	3.66829200	3.96329700	2.22872300
H	4.20532300	4.42840000	-0.16124700
H	2.85823100	3.35865800	-1.95374100
H	0.69779500	2.19958500	-2.54715000
H	1.10725000	0.62264000	-1.87085000
O	-1.33478700	0.38306100	-1.59825400
C	-1.55376100	2.60650000	-0.79482000
C	-2.90830700	2.41348100	-0.46346600
C	-1.06861400	3.92486000	-0.86160300
C	-3.74332600	3.49395200	-0.19485000
H	-3.29571400	1.40214900	-0.41159400

C	-1.90882300	5.00875500	-0.59958300
H	-0.03502800	4.11515300	-1.12370300
C	-3.24660100	4.79991600	-0.26190900
H	-4.78417600	3.31958000	0.06478300
H	-1.51342100	6.01887700	-0.66336600
H	-3.89775300	5.64482500	-0.05489300
C	0.19637300	1.01428300	1.10812200
C	-0.79349800	1.49977200	2.15626100
H	-1.24744900	2.44641200	1.85300400
H	-1.59574300	0.77441500	2.31961000
H	-0.30864700	1.65825800	3.13137800
C	0.78987700	-0.29309100	1.45833700
O	0.53959600	-0.95417800	2.46544300
O	1.74105000	-0.70058600	0.55502000
C	2.56220200	-1.82080800	0.93605900
H	2.02556800	-2.75476900	0.73521400
H	2.73881100	-1.77059500	2.01581800
C	3.85337300	-1.76696600	0.15672100
C	4.35293500	-2.91800900	-0.46264500
C	4.59278300	-0.57756600	0.07902000
C	5.57450400	-2.88957700	-1.14101000
H	3.78361300	-3.84362200	-0.41436500
C	5.80770200	-0.54564400	-0.60522700
H	4.20721800	0.32343300	0.54757500
C	6.30435200	-1.70224800	-1.21477200
H	5.94937200	-3.79209600	-1.61644800
H	6.36941000	0.38310100	-0.66180100
H	7.25218800	-1.67549900	-1.74572100

## TS7RR

C	-3.09520300	-1.99531800	0.62639800
C	-2.29474100	-2.78059900	-0.22602900
C	-4.56828200	-1.68207600	0.37433800
C	-2.72329600	-3.37681300	-1.55576800
C	-3.60554300	-0.03641200	-1.32158100
C	-3.01470500	-0.93698200	-2.23268600
C	-4.75430600	-0.34507500	-0.37804500
C	-3.49017500	-2.37245100	-2.44660900
H	-5.03208600	-2.50524600	-0.17998100
H	-5.09346300	-1.63199500	1.33468600
H	-3.32040100	-4.28925800	-1.40028900
H	-1.81316500	-3.69295200	-2.07879300
H	-4.80100700	0.46999400	0.35248200

H	-5.71517000	-0.33342800	-0.91684200
H	-3.35126200	-2.64471400	-3.49882600
H	-4.56722900	-2.43588900	-2.25742000
H	-2.44311000	-0.49970500	-3.05056300
H	-1.41329300	-3.24236500	0.21818800
H	-3.45893800	1.02443900	-1.52226200
H	-2.76366900	-1.90022600	1.65955900
Rh	-1.76552500	-0.73194600	-0.50554000
C	-1.65293100	2.32609000	1.11653700
C	-0.87652400	1.42482800	1.86606600
C	-1.40165000	0.90419200	3.05822800
C	-2.67675300	1.27225000	3.49436800
C	-3.43970200	2.17108500	2.74297900
C	-2.92759100	2.69669500	1.55359400
C	-0.99206100	2.86829800	-0.12606300
C	-0.05579700	1.83390000	-0.76214200
H	-0.80562500	0.21032800	3.64628600
H	-3.07242500	0.86310400	4.42049300
H	-4.43070000	2.46194300	3.08183900
H	-3.52148000	3.39400900	0.96692100
H	-1.73591400	3.14780500	-0.88413000
H	-0.44685800	3.78337700	0.12564800
O	-0.60310500	0.82670300	-1.34431900
C	1.27048200	2.25594100	-1.32162300
C	1.87514300	3.49771900	-1.05802100
C	1.94254400	1.36137000	-2.17672600
C	3.10486100	3.83175300	-1.62879200
H	1.39433100	4.22050500	-0.40826100
C	3.16919400	1.69467300	-2.74603700
H	1.47606400	0.40655600	-2.39088700
C	3.75799600	2.93435700	-2.47489700
H	3.54940500	4.79939400	-1.41196700
H	3.66447900	0.98971200	-3.40893700
H	4.71284300	3.19800800	-2.92152000
C	0.50721600	1.14276700	1.37575500
C	1.59851200	2.02855900	1.94848000
H	1.27136500	3.07407100	1.97573600
H	1.85363000	1.74731300	2.98173800
H	2.51593500	1.97581900	1.35659300
C	0.82670200	-0.19650000	1.03166300
O	0.01619800	-1.09452200	0.65706100
O	2.14834900	-0.50019400	1.06424800
C	2.54264700	-1.79361600	0.55283300
H	2.17663800	-1.89123700	-0.47469000

H	2.07170800	-2.57996500	1.15016100
C	4.04600800	-1.88506800	0.62025100
C	4.66311800	-2.87916400	1.38722200
C	4.84707100	-0.98499600	-0.09792600
C	6.05633700	-2.98087200	1.43466500
H	4.05046700	-3.57858800	1.95136500
C	6.23725100	-1.07945700	-0.04585900
H	4.37610700	-0.20649700	-0.69255300
C	6.84606100	-2.07985100	0.71929200
H	6.52119400	-3.75913200	2.03398000
H	6.84780700	-0.37478700	-0.60431000
H	7.92962700	-2.15407500	0.75674600

### TS7RS

C	4.35891700	0.64828300	0.08656000
C	4.01214000	-0.15273200	1.19393500
C	5.31661800	0.22000700	-1.02231900
C	4.47332400	-1.57857900	1.44280500
C	3.31744000	-1.17075400	-1.79865800
C	3.20465000	-2.06281700	-0.71315100
C	4.57394600	-0.42639200	-2.21516300
C	4.36856100	-2.47258500	0.18598900
H	6.06728100	-0.46743100	-0.61775400
H	5.87032900	1.09675000	-1.37577800
H	5.49971900	-1.59080400	1.84192400
H	3.83588300	-1.99574500	2.23112900
H	4.26934600	0.36125100	-2.91388400
H	5.24996600	-1.08933500	-2.77767900
H	4.23443800	-3.51525400	0.49476500
H	5.30349000	-2.44468000	-0.38384100
H	2.35195000	-2.73998700	-0.72642700
H	3.65579000	0.37342200	2.07947200
H	2.55045200	-1.24188900	-2.56920800
H	4.21490800	1.72155300	0.20064200
Rh	2.38252100	-0.14773100	-0.18190900
C	-1.56425400	3.25725300	0.11286900
C	-1.71920300	2.32201100	-0.93388300
C	-2.89969200	2.33312900	-1.68621600
C	-3.90706800	3.26384400	-1.41594500
C	-3.73908200	4.19936600	-0.39282400
C	-2.56905400	4.19250500	0.37313900
C	-0.28077500	3.17091900	0.92206400
C	0.27588900	1.74273000	1.02923400

H	-3.02936900	1.60610000	-2.48296200
H	-4.82087000	3.25864800	-2.00469100
H	-4.51994600	4.92542900	-0.18200700
H	-2.44872800	4.90591600	1.18563500
H	-0.44103900	3.57547800	1.93121300
H	0.51189900	3.77308900	0.46216400
O	1.53067300	1.57203200	0.84212500
C	-0.46790600	0.76767700	1.89973500
C	0.22936300	-0.31968400	2.45815300
C	-1.81796500	0.93875200	2.26137100
C	-0.39827300	-1.21538200	3.32224100
H	1.27972200	-0.44824100	2.22214400
C	-2.44650000	0.04311600	3.12644000
H	-2.38785400	1.76932600	1.86455300
C	-1.74312100	-1.04044900	3.65915000
H	0.16694400	-2.04289300	3.74328700
H	-3.48982400	0.19743200	3.38815200
H	-2.23327500	-1.73180400	4.33957200
C	-0.54486600	1.44356600	-1.16973500
C	0.59163200	2.06575900	-1.95461700
H	0.49414200	1.85468700	-3.03034000
H	1.57466400	1.69480800	-1.63864900
H	0.59543300	3.15450800	-1.83900000
C	-0.56449400	0.04563000	-1.01852500
O	0.46429400	-0.71112200	-1.03819400
O	-1.77992500	-0.51511300	-0.79301200
C	-1.82415400	-1.91661400	-0.43307700
H	-1.14716200	-2.46962300	-1.08916800
H	-1.47664600	-2.03184200	0.59765700
C	-3.24827800	-2.38579400	-0.58870000
C	-3.79763700	-2.55973500	-1.86717300
C	-4.04443000	-2.64933300	0.53140000
C	-5.11601400	-2.98716300	-2.02208000
H	-3.18643500	-2.35594800	-2.74331900
C	-5.36413600	-3.08376300	0.38029300
H	-3.62818000	-2.50906700	1.52580000
C	-5.90259600	-3.25230200	-0.89650200
H	-5.52943200	-3.11823800	-3.01860600
H	-5.97046800	-3.28743700	1.25897000
H	-6.92880500	-3.58947400	-1.01605100

## TS7SR

C	-4.35891700	0.64828300	0.08656000
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C	-4.01214000	-0.15273200	1.19393500
C	-5.31661800	0.22000700	-1.02231900
C	-4.47332400	-1.57857900	1.44280500
C	-3.31744000	-1.17075400	-1.79865800
C	-3.20465000	-2.06281700	-0.71315100
C	-4.57394600	-0.42639200	-2.21516300
C	-4.36856100	-2.47258500	0.18598900
H	-6.06728100	-0.46743100	-0.61775400
H	-5.87032900	1.09675000	-1.37577800
H	-5.49971900	-1.59080400	1.84192400
H	-3.83588300	-1.99574500	2.23112900
H	-4.26934600	0.36125100	-2.91388400
H	-5.24996600	-1.08933500	-2.77767900
H	-4.23443800	-3.51525400	0.49476500
H	-5.30349000	-2.44468000	-0.38384100
H	-2.35195000	-2.73998700	-0.72642700
H	-3.65579000	0.37342200	2.07947200
H	-2.55045200	-1.24188900	-2.56920800
H	-4.21490800	1.72155300	0.20064200
Rh	-2.38252100	-0.14773100	-0.18190900
C	1.56425400	3.25725300	0.11286900
C	1.71920300	2.32201100	-0.93388300
C	2.89969200	2.33312900	-1.68621600
C	3.90706800	3.26384400	-1.41594500
C	3.73908200	4.19936600	-0.39282400
C	2.56905400	4.19250500	0.37313900
C	0.28077500	3.17091900	0.92206400
C	-0.27588900	1.74273000	1.02923400
H	3.02936900	1.60610000	-2.48296200
H	4.82087000	3.25864800	-2.00469100
H	4.51994600	4.92542900	-0.18200700
H	2.44872800	4.90591600	1.18563500
H	0.44103900	3.57547800	1.93121300
H	-0.51189900	3.77308900	0.46216400
O	-1.53067300	1.57203200	0.84212500
C	0.46790600	0.76767700	1.89973500
C	-0.22936300	-0.31968400	2.45815300
C	1.81796500	0.93875200	2.26137100
C	0.39827300	-1.21538200	3.32224100
H	-1.27972200	-0.44824100	2.22214400
C	2.44650000	0.04311600	3.12644000
H	2.38785400	1.76932600	1.86455300
C	1.74312100	-1.04044900	3.65915000
H	-0.16694400	-2.04289300	3.74328700

H	3.48982400	0.19743200	3.38815200
H	2.23327500	-1.73180400	4.33957200
C	0.54486600	1.44356600	-1.16973500
C	-0.59163200	2.06575900	-1.95461700
H	-0.49414200	1.85468700	-3.03034000
H	-1.57466400	1.69480800	-1.63864900
H	-0.59543300	3.15450800	-1.83900000
C	0.56449400	0.04563000	-1.01852500
O	-0.46429400	-0.71112200	-1.03819400
O	1.77992500	-0.51511300	-0.79301200
C	1.82415400	-1.91661400	-0.43307700
H	1.14716200	-2.46962300	-1.08916800
H	1.47664600	-2.03184200	0.59765700
C	3.24827800	-2.38579400	-0.58870000
C	3.79763700	-2.55973500	-1.86717300
C	4.04443000	-2.64933300	0.53140000
C	5.11601400	-2.98716300	-2.02208000
H	3.18643500	-2.35594800	-2.74331900
C	5.36413600	-3.08376300	0.38029300
H	3.62818000	-2.50906700	1.52580000
C	5.90259600	-3.25230200	-0.89650200
H	5.52943200	-3.11823800	-3.01860600
H	5.97046800	-3.28743700	1.25897000
H	6.92880500	-3.58947400	-1.01605100

## TS7SS

C	2.42606000	-2.74812700	-0.32047700
C	2.96765300	-1.96274800	0.71658500
C	3.21731900	-3.22871800	-1.53437500
C	4.38884400	-1.43314900	0.78657100
C	2.93744500	-0.80723600	-2.29646500
C	3.69808100	-0.15330900	-1.30444600
C	3.09243200	-2.25496500	-2.72912000
C	4.85563200	-0.79402800	-0.54140700
H	4.26872600	-3.36644000	-1.25985500
H	2.85146700	-4.21697400	-1.83466100
H	5.08519100	-2.22661700	1.10121000
H	4.41251500	-0.67302300	1.57500900
H	2.20223000	-2.51853900	-3.31215300
H	3.94990100	-2.36741900	-3.41134100
H	5.61100100	-0.02961900	-0.32750500
H	5.35111900	-1.53741900	-1.17529500
H	3.70056200	0.93518200	-1.33040500

H	2.44775600	-1.99263600	1.67404500
H	2.42282200	-0.17020100	-3.01617700
H	1.52282200	-3.31055100	-0.08815200
Rh	1.77182100	-0.70780900	-0.52429400
C	1.63736300	2.33369600	1.14802700
C	0.87422100	1.40027300	1.87268100
C	1.40933800	0.85318400	3.04788700
C	2.68119200	1.22534800	3.49127600
C	3.43084400	2.15457300	2.76374500
C	2.90851200	2.70726700	1.59121800
C	0.96460600	2.90240500	-0.07581500
C	0.05318500	1.86510200	-0.74212200
H	0.82399600	0.13602200	3.61829700
H	3.08392200	0.79615200	4.40521600
H	4.41917600	2.44808800	3.10806200
H	3.49184700	3.42813300	1.02271200
H	0.39739000	3.79487100	0.20707500
H	1.70153700	3.22274000	-0.82433400
O	0.62575000	0.88144400	-1.33752300
C	-1.27742900	2.27114500	-1.30255600
C	-1.93484400	1.37053000	-2.16271500
C	-1.89997900	3.50319100	-1.03517900
C	-3.16564100	1.68789700	-2.73200000
H	-1.45418800	0.42351900	-2.38056300
C	-3.13374700	3.82151400	-1.60642800
H	-1.42912500	4.23117500	-0.38402900
C	-3.77288200	2.91778600	-2.45639100
H	-3.64993600	0.97834200	-3.39808000
H	-3.59235600	4.78205700	-1.38733400
H	-4.73109500	3.16913200	-2.90292400
C	-0.50864100	1.11952200	1.37849800
C	-1.60206400	1.99178400	1.96792100
H	-1.27616700	3.03702200	2.01552700
H	-2.51943800	1.94987400	1.37489200
H	-1.85729000	1.69043000	2.99543100
C	-0.82633600	-0.21302200	1.00858200
O	-0.01634300	-1.10276800	0.61078800
O	-2.14704200	-0.52024600	1.04128600
C	-2.54106200	-1.80740800	0.51406900
H	-2.05647200	-2.60077200	1.09053300
H	-2.19091400	-1.88455000	-0.52076700
C	-4.04262200	-1.90854400	0.60297500
C	-4.85915000	-1.00268300	-0.09003300
C	-4.64275600	-2.91559100	1.36656000



C	-6.24795400	-1.10435000	-0.01681700
H	-4.40147500	-0.21398800	-0.68177600
C	-6.03449800	-3.02447800	1.43504300
H	-4.01775400	-3.61919200	1.91160200
C	-6.83971700	-2.11768800	0.74455900
H	-6.87055200	-0.39526600	-0.55605200
H	-6.48631700	-3.81286000	2.03110400
H	-7.92217400	-2.19773300	0.79839300

## TS8aRR

C	2.37342800	0.97618000	0.98342400
C	2.96460900	-0.22721000	0.57649100
C	3.01804900	2.34948700	0.94800300
C	4.40015400	-0.36537600	0.07650700
C	3.09448000	1.94733300	-1.56119900
C	3.44647600	0.66892800	-2.05437300
C	3.76831500	2.63017300	-0.37391200
C	4.49748500	-0.25259700	-1.46247400
H	2.21741700	3.08870800	1.06635800
H	3.68988800	2.48333600	1.81051700
H	4.79123300	-1.33963800	0.39063000
H	5.03578100	0.38518400	0.55822200
H	4.81280200	2.30761400	-0.30187400
H	3.79724200	3.71119400	-0.55100800
H	5.50696000	0.06847800	-1.76439100
H	4.34952000	-1.24559900	-1.90390000
H	3.21411700	0.46866200	-3.10190300
H	2.49931800	-1.14345300	0.92971800
H	2.58646700	2.61437400	-2.25713500
H	1.49813300	0.89318100	1.62613900
Rh	1.62391600	0.50303900	-0.98980000
C	0.56647300	-3.04599400	0.19439700
C	0.05670200	-2.49379700	1.37477100
C	0.68377800	-2.74264500	2.59713400
C	1.83297100	-3.53990800	2.62384500
C	2.34407100	-4.08951600	1.44261900
C	1.71019400	-3.84494700	0.22030100
C	-0.29707700	-2.68038800	-0.98517200
C	-1.17072300	-1.49114400	-0.47457500
H	0.29790600	-2.30938400	3.51412100
H	2.33276700	-3.73097100	3.56996400
H	3.23725300	-4.70797700	1.47521800
H	2.10538200	-4.27308700	-0.69828900

H	0.27258500	-2.36203100	-1.86527700
H	-0.89982000	-3.54145700	-1.29437800
O	-0.47181400	-0.27420300	-0.66590200
C	-2.53722200	-1.39139700	-1.17482200
C	-3.28257500	-2.52074900	-1.55178000
C	-3.07949800	-0.12823300	-1.46267200
C	-4.51703800	-2.39473900	-2.19372400
H	-2.91087900	-3.52002600	-1.34857200
C	-4.31071600	0.00123400	-2.10717100
H	-2.52508800	0.75622100	-1.17671900
C	-5.03731200	-1.13185000	-2.47760400
H	-5.06637800	-3.28938400	-2.47561700
H	-4.70007500	0.99324000	-2.32220300
H	-5.99440300	-1.03223700	-2.98327700
C	-1.24522500	-1.74916600	1.10826100
C	-2.42784700	-2.65222100	1.54304300
H	-2.37032500	-3.62477700	1.04519500
H	-2.37699200	-2.83347800	2.62261900
H	-3.39068000	-2.19471600	1.31013700
C	-1.34270800	-0.41904300	1.86266200
O	-0.48179300	0.05168200	2.58262200
O	-2.55227400	0.14971400	1.69335700
C	-2.82026400	1.37706700	2.42876700
H	-2.34272800	1.30632000	3.40760900
H	-3.90560200	1.36775700	2.54980600
C	-2.36945800	2.61295300	1.68858100
C	-1.17996300	3.26432600	2.03871200
C	-3.14764000	3.13296800	0.64485600
C	-0.77587100	4.41517000	1.35837800
H	-0.57195200	2.86313300	2.84409200
C	-2.74109200	4.27710200	-0.04310200
H	-4.07695100	2.63787500	0.37202800
C	-1.55327600	4.92157000	0.31360200
H	0.14338400	4.91871700	1.64652600
H	-3.35323900	4.67016500	-0.85025600
H	-1.23939800	5.81755300	-0.21552700
O	0.31779200	0.64696000	-2.67452400
H	-0.34414700	0.08367600	-1.83034600
H	0.57890700	0.00142300	-3.35228700

**TS8aRS**

C	3.21895800	-0.97941600	-1.55967200
C	3.32727000	-1.55137900	-0.28417300

C	4.40523700	-0.73063800	-2.49051200
C	4.61113500	-1.97403100	0.40856000
C	4.86544500	1.22278100	-0.90795800
C	5.16700400	0.50664000	0.27396500
C	4.98841400	0.69097200	-2.32551700
C	5.73126600	-0.91106700	0.30093300
H	5.17847800	-1.48507300	-2.31818400
H	4.07770600	-0.86653300	-3.52876100
H	4.95743800	-2.94301700	0.01793700
H	4.37211600	-2.13714200	1.46383100
H	4.44313600	1.37952300	-2.97943700
H	6.03835500	0.72047500	-2.65667400
H	6.40533300	-1.01579800	1.16058900
H	6.34487100	-1.08572700	-0.58886600
H	5.35295300	1.09982300	1.16978200
H	2.41969900	-1.99750400	0.12942400
H	4.86760600	2.31118800	-0.83894500
H	2.24285100	-1.02385900	-2.04129600
Rh	3.04724000	0.56994800	-0.03312100
C	-0.49209600	-1.78405000	-0.37291200
C	-0.58526600	-1.79011500	1.02462800
C	-0.45980600	-2.98296900	1.73564700
C	-0.23259000	-4.17539400	1.03554400
C	-0.13865400	-4.16649600	-0.36150200
C	-0.26962000	-2.96823800	-1.07147700
C	-0.69619100	-0.39307300	-0.91088000
C	-0.45847700	0.53710600	0.31717700
H	-0.53358100	-2.99826500	2.82210900
H	-0.12962400	-5.11005000	1.57891700
H	0.04083800	-5.09720100	-0.89679900
H	-0.19372800	-2.96604000	-2.15846800
H	-0.00583500	-0.13080100	-1.71841000
H	-1.71609400	-0.28141100	-1.29017200
O	0.92727900	0.83303600	0.37257900
C	-1.19712200	1.88191600	0.20880800
C	-1.37280200	2.47151500	-1.05411600
C	-1.61709100	2.60552000	1.33090300
C	-1.96750700	3.72718500	-1.19341100
H	-1.04214600	1.94843100	-1.94527300
C	-2.21571100	3.86208000	1.19902100
H	-1.49898200	2.19953300	2.32910900
C	-2.39751300	4.43097100	-0.06314200
H	-2.09317200	4.15513300	-2.18360700
H	-2.54071900	4.39845100	2.08794100

H	-2.86187500	5.40691000	-0.16707700
C	-0.83421400	-0.38823900	1.58211300
C	0.02195200	-0.11421300	2.82794700
H	1.07657500	-0.27496300	2.59580100
H	-0.09612700	0.90894000	3.19450700
H	-0.27103000	-0.78794400	3.63880700
C	-2.32084700	-0.28427800	1.95683000
O	-2.74540800	-0.08805400	3.08014000
O	-3.12603700	-0.46497200	0.88908800
C	-4.55296200	-0.33648100	1.13558000
H	-4.72962100	0.63219100	1.61093200
H	-4.86101500	-1.11910000	1.83752000
C	-5.26647800	-0.45788100	-0.18203300
C	-5.15572200	0.55493600	-1.14525700
C	-6.05005500	-1.58155300	-0.46741500
C	-5.81520000	0.44478700	-2.37067500
H	-4.54721700	1.43078600	-0.93357300
C	-6.71714600	-1.69430300	-1.69174400
H	-6.14084400	-2.37634500	0.27222600
C	-6.59956700	-0.67991100	-2.64583500
H	-5.72133100	1.23611200	-3.10884400
H	-7.32502200	-2.57083500	-1.89893300
H	-7.11592200	-0.76464700	-3.59816700
O	2.54719900	2.30479900	1.09988600
H	1.42207100	1.78897000	0.85116100
H	2.68954500	3.13356300	0.61125900

## TS8aSR

C	-3.14662500	0.86092900	1.66776600
C	-3.41985000	1.54381600	0.47085500
C	-4.20777400	0.41968100	2.67431600
C	-4.79400800	1.91556700	-0.05495100
C	-4.67347000	-1.40042200	0.94668500
C	-5.14793900	-0.60115600	-0.12007800
C	-4.69567300	-1.02266500	2.41662800
C	-5.81537600	0.76177600	0.05279000
H	-5.05006300	1.11982000	2.65794700
H	-3.78425500	0.48046800	3.68377800
H	-5.17056000	2.81682800	0.45329800
H	-4.67754200	2.19072200	-1.11153600
H	-4.03630400	-1.72308800	2.94642600
H	-5.70175300	-1.17111800	2.84007300
H	-6.58360000	0.88498800	-0.71628700

H	-6.34097200	0.79848300	1.01470700
H	-5.37158500	-1.11674200	-1.05202400
H	-2.59461400	2.10570100	0.02972500
H	-4.60549900	-2.47479500	0.76261000
H	-2.13810400	0.94987200	2.06052300
Rh	-3.01092200	-0.51513900	-0.02578400
C	0.54782100	1.92084500	0.30774100
C	0.79245300	2.03908500	-1.06641500
C	0.82743700	3.29505300	-1.67486500
C	0.60463500	4.43673300	-0.89428300
C	0.35607900	4.31616000	0.47818300
C	0.32574200	3.05536800	1.08614700
C	0.59809200	0.47829200	0.73103500
C	0.41206700	-0.32014100	-0.59159400
H	1.01653100	3.39287700	-2.73890100
H	0.62743100	5.41589900	-1.35648700
H	0.17948300	5.20877600	1.07494400
H	0.13306100	2.96729700	2.15062700
H	-0.17832400	0.20220200	1.45083800
H	1.57265100	0.25332600	1.17975100
O	-0.97718600	-0.46368200	-0.84755900
C	1.02024800	-1.73045200	-0.53396500
C	1.00690300	-2.43813800	0.68122400
C	1.50106100	-2.39576700	-1.67127800
C	1.47313500	-3.75138600	0.75958000
H	0.63253200	-1.95726700	1.57807000
C	1.97212900	-3.71235500	-1.59573700
H	1.52593900	-1.89625700	-2.63279200
C	1.96274700	-4.39430400	-0.37889400
H	1.45637300	-4.26802400	1.71719800
H	2.34605500	-4.19778300	-2.49084800
H	2.32748900	-5.41600000	-0.31926200
C	0.99757100	0.67100900	-1.72090200
C	0.26770700	0.57957900	-3.06987500
H	-0.79217400	0.80082200	-2.92867100
H	0.34869400	-0.41448100	-3.51684300
H	0.69500900	1.29166400	-3.78114700
C	2.50576400	0.47153700	-1.94985100
O	3.03180600	0.33052200	-3.03854100
O	3.20368200	0.49184100	-0.79652800
C	4.63225500	0.25535000	-0.91245500
H	4.77725900	-0.67374600	-1.46978600
H	5.07671800	1.07380900	-1.48701300
C	5.20725700	0.17430500	0.47757800

C	4.93759700	-0.93950200	1.28917500
C	6.01706800	1.19985000	0.97750500
C	5.46396100	-1.01670800	2.57847300
H	4.30594300	-1.74053000	0.90912000
C	6.55065500	1.11753300	2.26593200
H	6.22924700	2.06710000	0.35560600
C	6.27555000	0.01100000	3.06849000
H	5.24773000	-1.88360300	3.19849600
H	7.18106500	1.92006800	2.64149300
H	6.69257600	-0.05479200	4.06998100
O	-2.52100900	-2.12768700	-1.33158300
H	-1.45140500	-1.46859400	-1.24528300
H	-2.43322400	-2.95342800	-0.82415000

### TS8aSS

C	-2.43798600	0.75587500	1.01935600
C	-2.99795400	-0.39040000	0.43257700
C	-3.10200100	2.11742500	1.14278300
C	-4.41335300	-0.47037900	-0.13241900
C	-3.08416100	2.05953300	-1.40317300
C	-3.40109100	0.85309400	-2.07507000
C	-3.80705300	2.56850700	-0.15855700
C	-4.46159800	-0.14832600	-1.64626800
H	-2.31575900	2.83946400	1.38919300
H	-3.80561400	2.12623500	1.98832000
H	-4.80229200	-1.48464700	0.02879700
H	-5.07687400	0.19896100	0.42263500
H	-4.84875600	2.23234300	-0.17151000
H	-3.83995000	3.66520900	-0.18795600
H	-5.46419300	0.20757300	-1.93849600
H	-4.29114000	-1.07086200	-2.21546100
H	-3.12619800	0.79442400	-3.13010300
H	-2.53424500	-1.34284400	0.67599200
H	-2.56194600	2.81792100	-1.98645400
H	-1.57984300	0.59776500	1.67260400
Rh	-1.61389100	0.56443500	-0.97113000
C	-0.52263500	-3.08836900	0.12907000
C	-0.00481700	-2.57272100	1.31990700
C	-0.59401800	-2.89719000	2.54522900
C	-1.71016700	-3.73705600	2.56232900
C	-2.22946200	-4.25508500	1.37060000
C	-1.63543400	-3.93274900	0.14479900
C	0.28566800	-2.63240800	-1.05650900

C	1.16223000	-1.46145700	-0.50947400
H	-0.20049600	-2.49252900	3.47036800
H	-2.17965600	-3.98750200	3.50842400
H	-3.09788000	-4.91037500	1.39607100
H	-2.03878300	-4.33547200	-0.78115200
H	-0.32773000	-2.26482600	-1.88464400
H	0.88342500	-3.45881400	-1.44928600
O	0.45893200	-0.23552800	-0.63429700
C	2.52105300	-1.32722100	-1.22370900
C	3.25028300	-2.43459300	-1.68367900
C	3.07416400	-0.05147500	-1.43095700
C	4.48064900	-2.28058000	-2.32679800
H	2.87389500	-3.44095000	-1.54071600
C	4.30137900	0.10608400	-2.07987400
H	2.53519700	0.81702200	-1.08266300
C	5.01092400	-1.00469900	-2.53500600
H	5.01693800	-3.15770100	-2.67495000
H	4.69741100	1.10889900	-2.23129400
H	5.96510300	-0.88316500	-3.04090400
C	1.27095300	-1.77858100	1.06175000
C	2.48713300	-2.66175200	1.44208400
H	2.45169600	-3.61120300	0.89924900
H	2.45483600	-2.89103000	2.51261500
H	3.43045900	-2.16303400	1.21745300
C	1.33605900	-0.47667700	1.86461100
O	0.46184800	-0.05000000	2.59572800
O	2.53099000	0.12524600	1.71949700
C	2.76863300	1.34130200	2.48607900
H	2.27181300	1.24271000	3.45113500
H	3.85156800	1.34893100	2.62572000
C	2.31144300	2.58258700	1.75544200
C	1.07085400	3.16758100	2.04465400
C	3.13201100	3.17293900	0.78604100
C	0.66139400	4.32085100	1.37258200
H	0.43263400	2.71410800	2.79366500
C	2.72082600	4.31734000	0.10335500
H	4.10187300	2.72882700	0.56167400
C	1.48191800	4.89724200	0.39810700
H	-0.29968200	4.77369000	1.61001600
H	3.36503700	4.76630700	-0.64626400
H	1.16105200	5.79426900	-0.12561900
O	-0.20384600	0.98343500	-2.51523800
H	0.40629500	0.26638500	-1.74007800
H	-0.42156400	0.51725000	-3.34022500

## TS8'bRR

C	-2.82473200	0.24093800	-1.84409900
C	-3.14907800	1.27111500	-0.94421500
C	-2.84997600	0.33796700	-3.35816400
C	-3.64085400	2.65488400	-1.35513400
C	-1.04600800	2.08414600	-2.98549200
C	-1.18267700	3.01015500	-1.92780900
C	-2.19059400	1.63072400	-3.88738400
C	-2.47817800	3.66303500	-1.48308600
H	-2.30444300	-0.52767500	-3.75108700
H	-3.88196000	0.24589600	-3.73182600
H	-4.35086900	3.01646500	-0.60319600
H	-4.20143400	2.58975300	-2.29386500
H	-2.93101400	2.43185700	-3.98299400
H	-1.80398600	1.45406900	-4.89728000
H	-2.74692000	4.48630200	-2.16373900
H	-2.29377100	4.12374300	-0.50568100
H	-0.28857400	3.54971500	-1.61872400
H	-3.39610000	0.97170100	0.06941900
H	-0.04862700	1.95813900	-3.40519300
H	-2.84388400	-0.77350100	-1.44839700
Rh	-0.98835700	1.05922900	-1.09989900
C	-2.53585700	0.44384000	2.48905900
C	-2.92077000	-0.85065700	2.12756300
C	-4.27397600	-1.18936200	2.05645200
C	-5.23664400	-0.21757400	2.34541500
C	-4.85044900	1.07694300	2.71300800
C	-3.49555300	1.41297600	2.78775700
C	-1.03655700	0.57453500	2.52620100
C	-0.49825900	-0.70382300	1.80575000
H	-4.57841600	-2.18974300	1.76589300
H	-6.29195100	-0.47024200	2.28456500
H	-5.60693600	1.82381400	2.93985200
H	-3.19411300	2.41876400	3.07151400
H	-0.66587900	1.46276600	2.00424100
H	-0.69187800	0.65210000	3.56275100
O	-0.34111600	-0.44848900	0.41901700
C	0.83795200	-1.21654100	2.37372400
C	1.18348800	-1.09692900	3.73103700
C	1.75562200	-1.85737300	1.52586300
C	2.39612200	-1.59006300	4.21896600
H	0.50625000	-0.62403900	4.43435600



C	2.96907300	-2.34885000	2.00940300
H	1.51577300	-1.96740700	0.47632400
C	3.29795000	-2.21803700	3.35939400
H	2.63250900	-1.47746900	5.27401200
H	3.66307400	-2.82347200	1.32113100
H	4.24467600	-2.59638400	3.73582300
C	-1.70819200	-1.75659700	1.96924400
C	-1.59686600	-2.64803500	3.23299000
H	-1.55670600	-2.02947900	4.13455700
H	-2.48260500	-3.28860600	3.31345100
H	-0.70937500	-3.28191100	3.20291300
C	-1.80172000	-2.66411600	0.73806800
O	-2.69744600	-2.64478500	-0.08588900
O	-0.79693300	-3.56139000	0.70918500
C	-0.82049000	-4.55782900	-0.35216000
H	-1.86093600	-4.80704400	-0.56756500
H	-0.32219100	-5.42047600	0.09512200
C	-0.09787400	-4.10449800	-1.59710700
C	-0.80217600	-3.53617300	-2.66750600
C	1.29051000	-4.26248600	-1.70529500
C	-0.13069800	-3.13381500	-3.82366700
H	-1.87760000	-3.41083000	-2.58664500
C	1.96479800	-3.85707000	-2.85875900
H	1.84441900	-4.71087500	-0.88376500
C	1.25466200	-3.29125200	-3.92102900
H	-0.68920600	-2.70477700	-4.65145000
H	3.04024100	-3.99394200	-2.93300400
H	1.77665400	-2.98301500	-4.82291800
C	2.23899700	5.06747100	0.19108700
C	2.28992500	3.75437200	-0.26128600
C	2.17133300	2.66802300	0.60321700
C	2.00352400	2.81925800	1.97481300
C	1.93907300	4.14204900	2.44379300
C	2.05224500	5.23771500	1.57320400
H	2.33634300	5.92689800	-0.46754300
H	1.93109700	1.97768400	2.65860600
H	1.80513100	4.32622100	3.50681600
H	1.99922800	6.24292700	1.98400000
C	2.30529200	1.63004200	-0.52564800
C	2.46482800	2.89061800	-1.49928800
H	1.68210100	2.95281000	-2.25993900
H	3.44168300	2.95797900	-1.99038900
O	1.15264600	0.86383800	-0.79511800
C	3.54243900	0.73611900	-0.51187500

C	3.59887300	-0.38327000	-1.35559600
C	4.66421000	1.04285700	0.27003600
C	4.74874300	-1.17162600	-1.41702700
H	2.73111300	-0.63748400	-1.95494900
C	5.81479100	0.25244300	0.21100300
H	4.63869200	1.90102100	0.93518900
C	5.86328400	-0.85747400	-0.63440200
H	4.77324600	-2.03409100	-2.07858200
H	6.67187100	0.50472200	0.83030600
H	6.75827700	-1.47239800	-0.68176000
H	0.68850400	0.13819700	0.03143600

### TS8'bRS

C	1.32706000	3.37154600	1.15083800
C	1.27354900	3.62992500	-0.23192800
C	2.40612500	3.91197000	2.08413800
C	2.28940000	4.42588200	-1.03087700
C	3.81500100	2.08106300	1.00185800
C	3.87345000	2.57110500	-0.32070400
C	3.57240000	2.91431100	2.24793400
C	3.74956600	4.04545800	-0.69719400
H	2.77090000	4.87500600	1.71172100
H	1.96361900	4.11631400	3.06540500
H	2.12722300	5.50655600	-0.89446800
H	2.10224000	4.21777400	-2.09015900
H	3.33620600	2.21945200	3.06202100
H	4.49376900	3.43729400	2.54893300
H	4.38253600	4.24776900	-1.56822000
H	4.13878200	4.67304500	0.11163100
H	4.37176600	1.94515100	-1.05930600
H	0.30144900	3.52245700	-0.71198100
H	4.26553600	1.11212400	1.21087100
H	0.39213600	3.09074400	1.63120800
Rh	1.97554400	1.62807700	0.03122000
C	-2.22471400	2.28990200	-0.05326600
C	-2.30355200	1.90639600	-1.39606400
C	-2.71669600	2.81517000	-2.37044900
C	-3.04383100	4.12104300	-1.98813500
C	-2.95726200	4.50809700	-0.64700900
C	-2.54806500	3.59171600	0.32826100
C	-1.79802500	1.13042800	0.80529300
C	-1.16364200	0.11528800	-0.19168300
H	-2.78475000	2.52182100	-3.41470300

H	-3.36433200	4.83800100	-2.73932400
H	-3.20791500	5.52609600	-0.36045800
H	-2.47255300	3.89770900	1.36896600
H	-1.07415900	1.39824500	1.58046000
H	-2.67160800	0.69039300	1.29801000
O	0.20986800	0.42877400	-0.33836500
C	-1.25606800	-1.33729300	0.29902600
C	-1.21377300	-1.60750300	1.67743600
C	-1.29736300	-2.43145000	-0.57819400
C	-1.23711700	-2.91701800	2.16190200
H	-1.16609600	-0.78787400	2.38732500
C	-1.32145500	-3.74381800	-0.09791500
H	-1.32046300	-2.27668100	-1.64990000
C	-1.29390900	-3.99440400	1.27378000
H	-1.21359100	-3.09311600	3.23441500
H	-1.35528000	-4.56857000	-0.80434300
H	-1.31360800	-5.01453500	1.64748100
C	-1.90344300	0.44224700	-1.58994400
C	-1.00520800	0.26055800	-2.82220900
H	-0.11838000	0.88759000	-2.72212300
H	-0.67985000	-0.77490000	-2.94872800
H	-1.54644500	0.54469100	-3.72877900
C	-3.19027400	-0.37675500	-1.77771600
O	-3.47539900	-1.00673500	-2.77767900
O	-4.00074700	-0.30361600	-0.70203200
C	-5.22015300	-1.09113700	-0.76892700
H	-4.94189800	-2.12593200	-0.99100400
H	-5.83362700	-0.72082000	-1.59480900
C	-5.92959600	-0.96840800	0.55293500
C	-5.40380600	-1.58291600	1.69921900
C	-7.12146100	-0.24240000	0.65728900
C	-6.05791800	-1.46784200	2.92573700
H	-4.47768500	-2.14805800	1.62862700
C	-7.78198900	-0.13151000	1.88350200
H	-7.53509100	0.23811000	-0.22616100
C	-7.25010200	-0.74301300	3.02009300
H	-5.64152200	-1.94793600	3.80728100
H	-8.70829800	0.43270900	1.94972100
H	-7.76183800	-0.65805800	3.97501200
C	5.65077500	-1.86817100	1.85303600
C	4.75694800	-1.67002700	0.80729500
C	3.38112800	-1.82956100	0.96548800
C	2.80535800	-2.17851700	2.18149700
C	3.69671700	-2.36672400	3.25122100

C	5.08396600	-2.21859200	3.09006500
H	6.72664700	-1.75620800	1.74429300
H	1.73473300	-2.31109600	2.31242100
H	3.30752800	-2.63972000	4.22905800
H	5.73282600	-2.37951300	3.94754800
C	3.07736400	-1.51158600	-0.51116900
C	4.65673700	-1.28328200	-0.65756200
H	4.90796600	-0.24331800	-0.88824800
H	5.15689500	-1.93997700	-1.37762500
O	2.31559300	-0.36170700	-0.78110100
C	2.57481300	-2.67585800	-1.36557900
C	2.02715400	-2.41594700	-2.63121400
C	2.69695900	-4.00919400	-0.95161500
C	1.60901000	-3.45998300	-3.45783300
H	1.92740500	-1.38675000	-2.95894100
C	2.27890900	-5.05538800	-1.77839900
H	3.11091100	-4.23450400	0.02663800
C	1.73238600	-4.78604400	-3.03454600
H	1.18667300	-3.23671600	-4.43446100
H	2.37745200	-6.08222200	-1.43520400
H	1.40531100	-5.59967000	-3.67661700
H	1.10234400	-0.33665900	-0.62122300

### TS8'bSR

C	1.25395400	3.22995100	-0.29209400
C	1.53695400	2.67929400	-1.55413400
C	2.12938900	4.25582900	0.42044300
C	2.76748400	2.96018700	-2.39605000
C	3.60932000	2.22994300	0.88161800
C	4.00784800	1.92178700	-0.43328600
C	3.14108900	3.58543900	1.37689000
C	4.07860300	2.92673700	-1.57918700
H	2.64926300	4.87680400	-0.31658500
H	1.48910900	4.93730600	0.99161000
H	2.66279900	3.92175800	-2.92287900
H	2.81337600	2.19027200	-3.17504200
H	2.66525200	3.43399800	2.35293400
H	4.00273400	4.24757700	1.55631200
H	4.90861400	2.65563300	-2.24105600
H	4.31745800	3.92209700	-1.18997000
H	4.61807700	1.02895400	-0.55516600
H	0.69208800	2.27306600	-2.10787600
H	3.95740800	1.55529000	1.66296900

H	0.21649100	3.18875900	0.03442300
Rh	1.99938500	1.19798000	-0.07258500
C	-1.92005500	-0.18141200	2.75454700
C	-2.59179700	-1.09917900	1.93609500
C	-3.69948400	-1.79410600	2.42397600
C	-4.13836200	-1.55088200	3.72896500
C	-3.47253800	-0.62711700	4.54170000
C	-2.35683400	0.06222000	4.05705300
C	-0.73719200	0.40703300	2.03158500
C	-0.99653800	0.10869400	0.52402500
H	-4.23038300	-2.50254400	1.79526100
H	-5.00658300	-2.08080700	4.11165600
H	-3.82480400	-0.44319800	5.55331600
H	-1.83736200	0.77927100	4.68854900
H	-0.58372300	1.47552400	2.21670100
H	0.19091100	-0.09970000	2.32692900
O	0.19619800	-0.07452400	-0.20656500
C	-1.81060000	1.21772300	-0.16438700
C	-1.77040500	1.32213800	-1.56544300
C	-2.61651100	2.12313100	0.54106200
C	-2.50334500	2.30225700	-2.23651700
H	-1.15911200	0.62347300	-2.12481400
C	-3.34717800	3.10957000	-0.12886200
H	-2.69164000	2.06427400	1.62133600
C	-3.29362600	3.20568300	-1.52035400
H	-2.45204200	2.36266000	-3.32071800
H	-3.95722900	3.80349500	0.44373500
H	-3.85884900	3.97445600	-2.04051800
C	-1.87390100	-1.26259400	0.60306000
C	-0.95523800	-2.50180500	0.66725100
H	-1.55901200	-3.40359100	0.81719100
H	-0.39050800	-2.61569200	-0.25955200
H	-0.26285600	-2.42343300	1.51060100
C	-2.76529500	-1.42454500	-0.62914700
O	-2.38109300	-1.89986300	-1.68147300
O	-4.02307300	-0.98195600	-0.44116000
C	-4.89238900	-1.03764900	-1.60587500
H	-4.85001000	-2.04378600	-2.02991600
H	-4.49550000	-0.33744900	-2.34778300
C	-6.28558900	-0.67120800	-1.17031600
C	-7.28504900	-1.64796800	-1.09040900
C	-6.60045100	0.65385800	-0.83603200
C	-8.57911600	-1.31073400	-0.68594900
H	-7.04937800	-2.67775700	-1.34867500

C	-7.89004700	0.99203900	-0.42634600
H	-5.82888700	1.41760500	-0.89366200
C	-8.88305200	0.01018500	-0.35192900
H	-9.34638400	-2.07834200	-0.63168400
H	-8.12304400	2.02180700	-0.16873900
H	-9.88880000	0.27532000	-0.03696500
C	2.40511400	-4.27420900	-2.03707600
C	2.70318300	-3.38943400	-1.00779700
C	3.08843900	-2.07306700	-1.25138400
C	3.18532500	-1.54940200	-2.53550800
C	2.87715300	-2.43038400	-3.58477200
C	2.49950500	-3.76031900	-3.34064700
H	2.10520100	-5.30471500	-1.86524700
H	3.47709100	-0.52188000	-2.73572900
H	2.93230200	-2.07870100	-4.61192200
H	2.26942900	-4.40450300	-4.18557800
C	3.24203600	-1.73674900	0.24097600
C	2.78468300	-3.25408900	0.50252300
H	3.53069100	-3.87808400	1.00701700
H	1.83575300	-3.32505800	1.04193500
O	2.33700400	-0.78045500	0.76300600
H	1.10963600	-0.82436600	0.33849200
C	4.64540700	-1.45255400	0.76034300
C	4.81550200	-1.07796500	2.10339200
C	5.78487000	-1.61210600	-0.03853200
C	6.08969400	-0.86465100	2.62943400
H	3.93831400	-0.95315400	2.73077100
C	7.06282900	-1.39627100	0.48709300
H	5.67523900	-1.90561900	-1.07831400
C	7.22059800	-1.02159300	1.82184200
H	6.20082400	-0.57661200	3.67181300
H	7.93375500	-1.52117900	-0.15125300
H	8.21338400	-0.85416800	2.23089800

**TS8'bSS**

C	-2.60532000	-2.69713000	-0.63796500
C	-2.54636100	-2.45485800	0.74847000
C	-2.36370200	-4.05863700	-1.28312800
C	-2.18613900	-3.46851600	1.81822700
C	0.08069700	-3.51280300	-0.79886600
C	0.05047300	-3.52333800	0.60906800
C	-0.89105000	-4.23557000	-1.71458700
C	-0.94673700	-4.31493800	1.45052600

H	-2.66096000	-4.85510100	-0.59292800
H	-3.01264300	-4.16122800	-2.15995700
H	-3.04713500	-4.11827600	2.04111800
H	-1.97647200	-2.90937300	2.73675300
H	-0.76121400	-3.82154400	-2.72141600
H	-0.63223100	-5.30370300	-1.78728100
H	-0.45256200	-4.64815200	2.36985600
H	-1.24235600	-5.22615100	0.91975200
H	0.96995100	-3.24408100	1.12034600
H	-3.08471500	-1.58069200	1.11333900
H	1.02673200	-3.25086400	-1.27180900
H	-3.18352700	-1.99277000	-1.23111300
Rh	-0.76868600	-1.66780800	-0.13256400
C	4.46680800	-0.91699600	-0.01871000
C	4.45040000	0.46067700	0.23096900
C	5.63806500	1.15734800	0.44115600
C	6.85150400	0.45970200	0.40084200
C	6.86861600	-0.91628500	0.15549400
C	5.67315700	-1.61330200	-0.05811300
C	3.06296000	-1.42670800	-0.22371600
C	2.23473900	-0.15479600	-0.57303800
H	5.63315800	2.22730600	0.63216000
H	7.78523900	0.99304100	0.55810600
H	7.81609600	-1.44786700	0.12371600
H	5.69024700	-2.68231900	-0.25719200
H	2.98364300	-2.20045800	-0.99342800
H	2.66946900	-1.83538300	0.71203600
O	0.91417900	-0.28723800	-0.09143800
C	2.25943300	0.13915500	-2.08632000
C	1.25329200	0.92685200	-2.66820500
C	3.27308500	-0.34249000	-2.93130600
C	1.25206100	1.21773100	-4.03299300
H	0.45742500	1.32830700	-2.05364200
C	3.27436100	-0.05621800	-4.29903400
H	4.08068400	-0.94518300	-2.53163300
C	2.26354400	0.72479900	-4.85917600
H	0.45727400	1.83227100	-4.44779900
H	4.07162800	-0.44924000	-4.92466800
H	2.26431700	0.94763900	-5.92275500
C	3.02112200	0.99374300	0.25354400
C	2.89498100	2.41570000	-0.30685700
H	3.35718300	2.47314000	-1.29525200
H	1.85311400	2.73161700	-0.39162200
H	3.40077000	3.13168600	0.34909600

C	2.52935900	0.90539500	1.71932700
O	2.84921700	0.02245500	2.49150200
O	1.74168300	1.94235900	2.07416200
C	1.36603900	2.03920200	3.48238800
H	1.24359300	3.11318400	3.63620900
H	2.20437500	1.67735500	4.08030100
C	0.09277000	1.30516500	3.82811400
C	-1.14183000	1.96492800	3.75634300
C	0.12690200	-0.02670000	4.26650300
C	-2.32265200	1.30787500	4.10817900
H	-1.17798800	3.00026200	3.42625000
C	-1.05165000	-0.68293600	4.62570500
H	1.08111200	-0.54060100	4.31891300
C	-2.27905700	-0.01792100	4.54628200
H	-3.27180500	1.83432600	4.05351900
H	-1.01095000	-1.71015900	4.97851300
H	-3.19499600	-0.52762100	4.83345400
H	-0.03767800	0.44479700	-0.25398600
C	-5.08340800	0.09303000	-2.53594700
C	-3.83782300	0.48234700	-2.05591400
C	-3.64234700	0.84450300	-0.72508900
C	-4.66320700	0.83050500	0.21653100
C	-5.92242100	0.42198000	-0.25257200
C	-6.12728000	0.06641000	-1.59577100
H	-5.26114000	-0.18252800	-3.57245400
H	-4.51561200	1.11854200	1.25412200
H	-6.76373700	0.38613600	0.43499900
H	-7.12218800	-0.23596100	-1.91302100
C	-2.15967700	1.20094700	-0.93161800
C	-2.38660700	0.71166600	-2.44500900
H	-1.81438300	-0.19765000	-2.65747300
H	-2.19084100	1.44965800	-3.23013700
O	-1.26621700	0.43481800	-0.16721300
C	-1.87721400	2.69962800	-0.78608000
C	-0.96397400	3.17070500	0.16438500
C	-2.56136600	3.63979500	-1.57498000
C	-0.72372500	4.54147700	0.30916600
H	-0.43856800	2.46537800	0.79571000
C	-2.32406600	5.00606500	-1.43017200
H	-3.29602700	3.30512300	-2.30216400
C	-1.39954100	5.46529100	-0.48709800
H	-0.00253000	4.88096600	1.04846300
H	-2.86387800	5.71349800	-2.05447000
H	-1.21316300	6.53002900	-0.37499000



## TS8'cRR

C	1.90950700	-0.60754600	2.80348400
C	1.88828900	0.77726000	2.56102200
C	1.26639100	-1.32009500	3.97743800
C	1.24737400	1.81585000	3.47650300
C	-0.88783100	-0.40954100	2.99272800
C	-0.91402800	0.90269600	2.47941200
C	-0.16491600	-0.82317200	4.27068000
C	-0.21442000	2.11037700	3.07303800
H	1.23018200	-2.38835100	3.73343300
H	1.90421000	-1.23222600	4.87118600
H	1.82913600	2.74319500	3.42895800
H	1.30131300	1.47841500	4.51683100
H	-0.14818400	0.01079900	4.98044400
H	-0.73067300	-1.62333500	4.76098500
H	-0.78457000	2.49647000	3.93272000
H	-0.22771200	2.90407800	2.31778600
H	-1.73311300	1.13962200	1.80083000
H	2.65764700	1.15324500	1.89230200
H	-1.70763900	-1.05266100	2.68919000
H	2.69031400	-1.17660400	2.30278200
Rh	0.44288000	-0.21725900	1.28626400
C	-3.55270500	-2.03369300	0.93059300
C	-4.09673600	-1.29285800	-0.12326200
C	-5.34231700	-0.68124000	0.01216000
C	-6.03403700	-0.80579400	1.22229400
C	-5.48974300	-1.54548500	2.27700700
C	-4.24518400	-2.16926700	2.13325500
C	-2.23722400	-2.63775100	0.51532100
C	-1.78184800	-1.77915600	-0.69616300
H	-5.77388600	-0.10699700	-0.80364600
H	-7.00142100	-0.32500000	1.34119900
H	-6.03588400	-1.63781900	3.21205200
H	-3.82763700	-2.75288200	2.95067000
H	-1.47162000	-2.63489300	1.29618600
H	-2.38749800	-3.68144700	0.21261000
O	-1.18742200	-0.58308100	-0.18498800
C	-0.80366600	-2.51330700	-1.62689200
C	-0.10932800	-3.65231500	-1.18984500
C	-0.52671400	-2.03740500	-2.91997700
C	0.81877800	-4.29925100	-2.01116600
H	-0.28156500	-4.05070200	-0.19566600

C	0.39552600	-2.68374700	-3.74440600
H	-1.03080900	-1.15530800	-3.29394000
C	1.07386800	-3.81928500	-3.29585700
H	1.33526100	-5.18251300	-1.64391300
H	0.57989600	-2.29726600	-4.74347900
H	1.78940200	-4.32357800	-3.93987300
C	-3.20801700	-1.38805000	-1.36058000
C	-3.74216800	-2.52226700	-2.26625600
H	-3.74655200	-3.47457500	-1.72768200
H	-4.77100100	-2.30203600	-2.56865100
H	-3.13801500	-2.63129500	-3.16762900
C	-3.18099500	-0.09633900	-2.18711200
O	-3.18387100	-0.06182800	-3.40428200
O	-3.17173100	1.01467800	-1.42931000
C	-3.03887200	2.26806900	-2.14461200
H	-3.99956200	2.48871800	-2.62440600
H	-2.28717500	2.14859500	-2.92687500
C	-2.64582800	3.33442100	-1.15488900
C	-3.39019800	3.54065300	0.01615600
C	-1.53380600	4.14779900	-1.40439100
C	-3.02477200	4.53885900	0.91934900
H	-4.25050200	2.90926700	0.22100600
C	-1.17003300	5.15355200	-0.50344400
H	-0.95217900	3.99909900	-2.31133700
C	-1.91387300	5.34962800	0.66108300
H	-3.60870400	4.68833800	1.82358300
H	-0.30595400	5.77826000	-0.71259000
H	-1.63366800	6.13007800	1.36333900
C	4.11588300	2.44159100	-3.15092400
C	3.69653100	1.37495400	-2.36643700
C	3.42977800	1.50992000	-1.00443800
C	3.54063000	2.73334600	-0.35034500
C	3.95314100	3.82343000	-1.13417100
C	4.23858200	3.67981900	-2.50032100
H	4.33147400	2.34594500	-4.21200200
H	3.32691100	2.86954800	0.70621200
H	4.05753200	4.80244000	-0.67322000
H	4.55666300	4.55185200	-3.06634900
C	3.07220100	0.01683600	-0.83353500
C	3.34457100	-0.09875600	-2.41214100
H	2.43900600	-0.34936900	-2.97293000
H	4.14782300	-0.78816100	-2.69413700
O	1.72747100	-0.27869000	-0.50048800
C	4.01589600	-0.84638800	-0.01287900

C	3.77314900	-2.22891500	0.05742500
C	5.14012000	-0.32796600	0.63923900
C	4.63065100	-3.06635400	0.76975500
H	2.90335600	-2.63905100	-0.44739200
C	5.99920300	-1.16700900	1.35719500
H	5.34834500	0.73655800	0.58816000
C	5.74756100	-2.53732600	1.42624800
H	4.42956800	-4.13391500	0.81198200
H	6.86455200	-0.74500100	1.86178900
H	6.41527500	-3.18977400	1.98263700
O	-0.02074900	0.83183100	-1.75944400
H	1.00882900	0.28242700	-1.17967500
H	-0.75909300	0.10259900	-1.00317400
H	-0.08153200	1.73589500	-1.40816900

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C	0.75212700	-2.99017400	-1.39035400
C	0.72993600	-3.38561500	-0.04263700
C	1.69933800	-3.55574800	-2.44449200
C	1.66644600	-4.38188000	0.61375100
C	3.39958500	-2.05667200	-1.28253300
C	3.44443900	-2.68631800	-0.02094000
C	2.98112400	-2.70697000	-2.58702600
C	3.14289400	-4.16125500	0.22296300
H	1.94875300	-4.59339800	-2.19863300
H	1.17940700	-3.59095000	-3.40832000
H	1.35110000	-5.41207600	0.38510300
H	1.56194400	-4.26494200	1.69859600
H	2.79969300	-1.90423600	-3.31153300
H	3.80413400	-3.31115100	-3.00013700
H	3.79020000	-4.53121200	1.02569600
H	3.39994700	-4.74541700	-0.66698100
H	4.05662600	-2.20090300	0.73594800
H	-0.19825200	-3.21500000	0.49777400
H	4.01941200	-1.16963200	-1.40099500
H	-0.15791400	-2.54307400	-1.77718600
Rh	1.68364700	-1.46179900	-0.15786200
C	-2.54972000	-2.05618400	-0.51168800
C	-2.69515800	-2.17235600	0.87393400
C	-3.17935500	-3.35128000	1.44244600
C	-3.51552200	-4.42111000	0.60579500
C	-3.37777700	-4.30398600	-0.78136900
C	-2.89641400	-3.11837500	-1.34673800

C	-2.03690200	-0.69040300	-0.88178000
C	-1.49598000	-0.07977600	0.44630900
H	-3.29844600	-3.44319300	2.51877500
H	-3.89007800	-5.34570500	1.03682500
H	-3.64606200	-5.13847200	-1.42391100
H	-2.79222700	-3.03064400	-2.42581100
H	-1.24935800	-0.70449100	-1.64201100
H	-2.85995300	-0.08129200	-1.26989100
O	-0.10443300	-0.35626900	0.58601600
C	-1.64654800	1.45502600	0.47708700
C	-1.51687300	2.18794200	-0.71405300
C	-1.81655200	2.17828800	1.66900000
C	-1.58283400	3.58232500	-0.72160500
H	-1.36290700	1.66770500	-1.65405100
C	-1.88549600	3.57475800	1.66616100
H	-1.90945800	1.66173900	2.61691000
C	-1.77186900	4.28475600	0.47059400
H	-1.48117000	4.11877500	-1.66120000
H	-2.02812600	4.10320900	2.60508800
H	-1.82582200	5.36993000	0.46746000
C	-2.30939600	-0.87964900	1.59226200
C	-1.48904600	-1.14697600	2.86323500
H	-0.63270700	-1.77946400	2.62514500
H	-1.10911200	-0.22572000	3.31074000
H	-2.10788200	-1.64960900	3.61117600
C	-3.62289500	-0.17717700	1.97928700
O	-3.97916600	0.05784200	3.11774000
O	-4.37153400	0.12924400	0.90024100
C	-5.61036800	0.84022400	1.16678200
H	-5.36813300	1.73235200	1.75239900
H	-6.25870500	0.20232800	1.77378400
C	-6.24505200	1.18830000	-0.15293900
C	-5.67057700	2.16601300	-0.97889500
C	-7.41544900	0.54625500	-0.57262500
C	-6.25665200	2.49033600	-2.20224600
H	-4.76035200	2.66899100	-0.66196100
C	-8.00808100	0.87452700	-1.79464600
H	-7.86610400	-0.21392200	0.06098600
C	-7.42864800	1.84649600	-2.61194400
H	-5.80323000	3.24924800	-2.83427300
H	-8.91870800	0.37041700	-2.10671000
H	-7.88755000	2.10373800	-3.56281800
C	2.30516000	4.06827400	-1.83446000
C	2.74636600	2.85563600	-1.31944900

C	3.06625900	2.69865300	0.02631800
C	2.95541300	3.73022100	0.95081100
C	2.49177300	4.95608900	0.44574200
C	2.18008900	5.12138900	-0.91314900
H	2.06417100	4.21509700	-2.88427000
H	3.21410600	3.61808000	2.00046100
H	2.37950300	5.80245700	1.11850800
H	1.83432900	6.09265800	-1.25801400
C	3.53621300	1.23818100	-0.15349500
C	3.08944200	1.41977100	-1.67802100
H	2.22914400	0.78494000	-1.91678400
H	3.86786600	1.26424700	-2.43253100
O	2.80078500	0.27696500	0.57448000
C	5.03977700	1.06217600	0.07846800
C	5.98698400	1.70633800	-0.73410900
C	5.50185900	0.29686800	1.15726200
C	7.35342300	1.56689100	-0.49063300
H	5.65978600	2.33356200	-1.55866600
C	6.87053600	0.15865600	1.40484200
H	4.77719400	-0.18724800	1.80220300
C	7.80292500	0.78821200	0.57943200
H	8.06789200	2.07023800	-1.13699900
H	7.20530500	-0.44185500	2.24703500
H	8.86742500	0.67961100	0.76921700
O	1.13616400	1.01656800	2.13061000
H	0.40305400	0.35562100	1.41048300
H	0.89962800	1.94317600	1.95826500
H	2.09932200	0.73748100	1.37229200

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C	-1.38729700	-3.21117400	0.36256100
C	-1.58952600	-2.78034300	-0.95763700
C	-2.26352800	-4.22340400	1.09394100
C	-2.72103700	-3.19980600	-1.87609400
C	-3.87286200	-2.25417200	1.23971100
C	-4.16980600	-2.07807000	-0.13029500
C	-3.39611300	-3.53794600	1.89065200
C	-4.09514900	-3.18416900	-1.17636200
H	-2.67643100	-4.94230800	0.37833400
H	-1.63940400	-4.80479300	1.78155400
H	-2.51022700	-4.19066000	-2.30885100
H	-2.74164900	-2.49712300	-2.71702200
H	-3.02951300	-3.28525500	2.89216600

H	-4.24066700	-4.22930300	2.03825200
H	-4.87979700	-3.02385900	-1.92395800
H	-4.30700600	-4.15513000	-0.71584300
H	-4.80893900	-1.23799600	-0.38433800
H	-0.72400300	-2.36848600	-1.47027000
H	-4.30988100	-1.52919200	1.92612300
H	-0.38186300	-3.09388200	0.75377700
Rh	-2.25907500	-1.20852400	0.35754800
C	2.57736600	-1.03047500	2.75203900
C	3.10113500	0.12032800	2.15022200
C	4.39067100	0.55108500	2.46668900
C	5.15575200	-0.18952500	3.37276700
C	4.63485400	-1.34512900	3.96457500
C	3.33911300	-1.77045700	3.65686900
C	1.16595500	-1.27599500	2.29051800
C	1.00647400	-0.42928800	0.99038400
H	4.80862100	1.43871400	2.00199700
H	6.16490300	0.13382600	3.61406300
H	5.23990200	-1.91512600	4.66482200
H	2.93151200	-2.66735000	4.11763700
H	0.93797100	-2.33454000	2.13299300
H	0.44072400	-0.90409000	3.02529700
O	-0.32678200	-0.00661000	0.79155100
C	1.48661900	-1.16665700	-0.27167600
C	1.09177800	-0.68940800	-1.53403500
C	2.34045500	-2.27788500	-0.22895100
C	1.53370500	-1.30034200	-2.70877300
H	0.42650500	0.16397900	-1.58862700
C	2.77478100	-2.90011800	-1.40365300
H	2.68463100	-2.66816700	0.72221100
C	2.37505500	-2.41510100	-2.64979700
H	1.21059200	-0.91073700	-3.67090900
H	3.42757200	-3.76676300	-1.33860000
H	2.71217000	-2.89897600	-3.56261000
C	2.04637500	0.80668000	1.29173700
C	1.39709700	1.93141200	2.12907900
H	2.15943000	2.67361000	2.39147400
H	0.61017000	2.43456100	1.56724100
H	0.98454600	1.53281500	3.05876000
C	2.54460100	1.44954800	-0.00324600
O	1.91610900	2.28506600	-0.62995800
O	3.75478500	1.01018700	-0.39294200
C	4.25189900	1.55032600	-1.64862200
H	4.21971200	2.64165700	-1.60073300

H	3.57212600	1.22447300	-2.44215100
C	5.65253400	1.04071000	-1.85906500
C	6.74468900	1.91299600	-1.78677200
C	5.88126600	-0.31538800	-2.13452700
C	8.04517100	1.44358400	-1.98929600
H	6.57638600	2.96599700	-1.57321100
C	7.17886400	-0.78732700	-2.33030300
H	5.03860100	-0.99988700	-2.18950000
C	8.26417800	0.09192300	-2.26016200
H	8.88369500	2.13248900	-1.93366100
H	7.34482900	-1.84030500	-2.54194400
H	9.27450400	-0.27610200	-2.41761600
C	-3.16693100	5.13489700	1.18069800
C	-3.48986200	3.81120700	0.90911800
C	-2.60167900	2.94190800	0.27799600
C	-1.31822400	3.33126000	-0.09249000
C	-0.97654200	4.66493900	0.18662700
C	-1.87927300	5.54674500	0.80101500
H	-3.85352400	5.82471800	1.66492600
H	-0.59032900	2.66354700	-0.54168200
H	0.01612500	5.02047700	-0.07707400
H	-1.56762600	6.57044400	0.99365200
C	-3.61979100	1.78138600	0.25460300
C	-4.59129300	2.77707000	1.04279200
H	-5.54270900	3.01311800	0.55511700
H	-4.78840400	2.43409700	2.06398000
O	-3.29353100	0.61965200	1.01464000
C	-4.11192200	1.37827100	-1.12830800
C	-5.45984400	1.05997200	-1.34802900
C	-3.21980600	1.27611900	-2.20463900
C	-5.90411200	0.64495400	-2.60587100
H	-6.17106500	1.13216100	-0.52974700
C	-3.65880700	0.85986800	-3.46363800
H	-2.17587300	1.53832900	-2.06358400
C	-5.00371900	0.54217500	-3.66884400
H	-6.95426500	0.40778700	-2.75512200
H	-2.95151300	0.79554800	-4.28645000
H	-5.34857800	0.22682600	-4.64993300
O	-1.54922500	0.95869500	2.64663200
H	-1.35308400	1.90253100	2.75422300
H	-0.79719000	0.51580200	1.73550800
H	-2.57376200	0.87709000	1.85921100

C	3.34720800	-2.16403200	-0.91055200
C	3.00268800	-1.56609300	-2.13832300
C	3.45002400	-3.66780600	-0.67897000
C	2.62820300	-2.29674000	-3.41362700
C	0.90903800	-3.52064200	-0.66822300
C	0.68986400	-3.14134600	-2.00738300
C	2.12854300	-4.24987000	-0.13749000
C	1.63505400	-3.45234500	-3.16443300
H	3.74528400	-4.16984700	-1.60606900
H	4.25358900	-3.86291500	0.03969200
H	3.53044400	-2.66180700	-3.92887900
H	2.16528500	-1.56629700	-4.08718300
H	2.11590800	-4.15539900	0.95435400
H	2.05612600	-5.32741300	-0.35326800
H	1.04443500	-3.62450800	-4.07088100
H	2.16929500	-4.38770900	-2.96821000
H	-0.33429100	-2.92316100	-2.29624500
H	3.32299800	-0.53547100	-2.28373000
H	0.03832800	-3.59450300	-0.02097300
H	3.90391500	-1.55068200	-0.20958100
Rh	1.30940900	-1.42766900	-0.84826600
C	-3.97774700	-2.58062300	-0.42012100
C	-4.35734400	-1.40640400	0.23912800
C	-5.68614800	-1.19001100	0.59908000
C	-6.63893800	-2.17054600	0.29825100
C	-6.26108900	-3.34615800	-0.35708400
C	-4.92546800	-3.55805300	-0.71910200
C	-2.49738300	-2.57501800	-0.70071600
C	-1.91505100	-1.49576300	0.26482600
H	-5.98622000	-0.27849700	1.10889300
H	-7.67734800	-2.01679500	0.57919200
H	-7.00771600	-4.10291900	-0.58303500
H	-4.63358300	-4.47656700	-1.22280700
H	-2.03358600	-3.55733400	-0.57057200
H	-2.31126400	-2.23764200	-1.72405000
O	-0.78028100	-0.85040600	-0.29428300
C	-1.53848000	-2.09397600	1.63621200
C	-0.53526700	-1.47645000	2.40076500
C	-2.16121200	-3.23247300	2.17125600
C	-0.16456900	-1.97500800	3.64989800
H	-0.04068500	-0.59585100	2.00691300
C	-1.78918300	-3.73717300	3.42097500
H	-2.94653300	-3.73701700	1.61923500
C	-0.78913000	-3.11253900	4.16682700



H	0.61468300	-1.47365500	4.21854000
H	-2.28518600	-4.62380600	3.80743600
H	-0.49996800	-3.50606900	5.13760900
C	-3.16322500	-0.47114900	0.43262400
C	-3.21498000	0.28255400	1.76928900
H	-3.29959000	-0.42126400	2.59994000
H	-2.32177500	0.89332400	1.92256500
H	-4.07515700	0.95532700	1.79589800
C	-3.19937800	0.48947500	-0.78220800
O	-3.08134500	0.13603600	-1.93911600
O	-3.45385600	1.76052400	-0.42435700
C	-3.48345400	2.73291900	-1.50501000
H	-4.43394100	2.62771400	-2.03735800
H	-2.67455900	2.49019100	-2.19760600
C	-3.32265700	4.10701700	-0.91222200
C	-4.38938000	5.01197300	-0.89146400
C	-2.08308000	4.49655900	-0.38259500
C	-4.22430000	6.29130700	-0.35323300
H	-5.35285300	4.71634200	-1.30058100
C	-1.91836300	5.77158400	0.15775400
H	-1.25846900	3.78795000	-0.39434400
C	-2.98846700	6.67265900	0.17232900
H	-5.05938200	6.98680800	-0.34515700
H	-0.95214400	6.06383200	0.56085100
H	-2.85788500	7.66767700	0.58980700
H	-0.71401600	0.26792700	-0.08437400
C	5.64108000	-0.10014400	2.04030300
C	4.43224800	0.38107100	1.55254400
C	4.30380200	0.87475300	0.25554100
C	5.36706700	0.92802600	-0.63657900
C	6.59010300	0.42817800	-0.16107800
C	6.72324200	-0.07211100	1.14439300
H	5.76443900	-0.48155200	3.05071400
H	5.27994100	1.33150600	-1.64189100
H	7.45992800	0.43536700	-0.81294900
H	7.69280100	-0.44167600	1.46865200
C	2.83762500	1.29360600	0.45749800
C	2.97572800	0.63439100	1.90706000
H	2.36413600	-0.27149300	1.97945300
H	2.76595500	1.27410000	2.77020200
O	1.87283300	0.68870000	-0.38522400
C	2.69210900	2.82116000	0.41969200
C	2.13565300	3.44435400	-0.70686500
C	3.18506300	3.63438700	1.45189400

C	2.04982900	4.83618600	-0.78748700
H	1.75602300	2.83272500	-1.51699200
C	3.09858100	5.02513400	1.37370600
H	3.65512900	3.18807000	2.32283900
C	2.52677100	5.63412000	0.25421400
H	1.60867200	5.29489600	-1.66853900
H	3.48203900	5.63233100	2.18961900
H	2.46078800	6.71706000	0.19199900
O	-0.37663200	1.49568800	-0.00078200
H	-0.48338300	1.82280600	0.90567400
H	0.86882700	1.16299900	-0.18051200

### TS8dRR

C	1.17976000	3.45517000	-1.82716200
C	-0.16693800	3.49799900	-2.26473000
C	1.81870900	4.37712500	-0.80478400
C	-1.18283100	4.53309100	-1.79001400
C	0.13092400	3.29847700	0.76313300
C	-1.18498200	3.10006500	0.32281100
C	0.95534900	4.54689300	0.46331100
C	-1.98482700	4.02649400	-0.57205000
H	2.78259700	3.93665700	-0.52631300
H	2.04619000	5.35499300	-1.25738000
H	-1.87239500	4.76287900	-2.60958300
H	-0.66847700	5.47101200	-1.55380000
H	0.28960400	5.41091200	0.36308800
H	1.60533000	4.76287000	1.31838300
H	-2.38323800	4.87197800	0.01024000
H	-2.85129600	3.45668800	-0.92339000
H	-1.78613400	2.37942500	0.86552200
H	-0.38405800	3.04394400	-3.23194400
H	0.44802000	2.71446200	1.62414000
H	1.90123400	2.99368700	-2.50420000
Rh	0.11215400	1.88317400	-0.89402800
C	-0.94032500	0.66515800	3.12339400
C	-2.15020100	0.46431500	2.45135300
C	-3.28100300	1.21043300	2.79255500
C	-3.18119200	2.17948200	3.79482200
C	-1.96632300	2.39138300	4.45735800
C	-0.84092100	1.63075500	4.12736400
C	0.11063100	-0.30523800	2.65000400
C	-0.45370300	-0.89869200	1.32053900
H	-4.22211600	1.05625800	2.27356900

H	-4.05274200	2.77208700	4.06023900
H	-1.89902500	3.14745300	5.23535900
H	0.09933500	1.78713000	4.65123200
H	1.08403600	0.15480100	2.45304900
H	0.27819300	-1.06782100	3.41729900
O	0.02614300	-0.10995600	0.23069600
C	-0.08328800	-2.37450000	1.07135300
C	0.15822400	-3.28428700	2.11249000
C	-0.02493400	-2.86440300	-0.24396000
C	0.45056600	-4.62637700	1.85409400
H	0.11920800	-2.96407700	3.14788000
C	0.26526800	-4.20273100	-0.50669400
H	-0.19887500	-2.18389100	-1.06594900
C	0.50686300	-5.09390300	0.54141800
H	0.63489300	-5.30228400	2.68529300
H	0.30749300	-4.54799100	-1.53669400
H	0.73588000	-6.13662500	0.33717200
C	-2.04878100	-0.69550900	1.47226900
C	-2.76495400	-1.91994000	2.10073500
H	-2.32816000	-2.15800900	3.07501200
H	-3.82253100	-1.68195900	2.26131300
H	-2.69859600	-2.80095000	1.46146500
C	-2.69849000	-0.39583800	0.11735200
O	-3.15051200	0.68193800	-0.22417400
O	-2.74960200	-1.49471300	-0.65668100
C	-3.33941400	-1.35901700	-1.98212400
H	-2.79305100	-2.08631900	-2.58563100
H	-3.13945600	-0.35181800	-2.35038300
C	-4.81693300	-1.66451100	-1.96463200
C	-5.26476900	-2.98534000	-2.10211700
C	-5.76002600	-0.64026800	-1.80013600
C	-6.62879800	-3.28021200	-2.07488500
H	-4.53988300	-3.78541000	-2.23358400
C	-7.12479300	-0.93280600	-1.77510500
H	-5.41631200	0.38327600	-1.68409600
C	-7.56176500	-2.25296300	-1.91194000
H	-6.96292500	-4.30835900	-2.18513200
H	-7.84704900	-0.13033100	-1.65075500
H	-8.62440500	-2.47996700	-1.89455200
C	4.50691100	0.16708300	2.86077400
C	4.06666600	0.05717400	1.54714100
C	3.74406100	-1.17120700	0.97250800
C	3.79934800	-2.36215600	1.68782900
C	4.23879700	-2.26478300	3.01843500

C	4.59098000	-1.03165400	3.58875500
H	4.76805100	1.11698400	3.32132600
H	3.51081600	-3.32109200	1.26636000
H	4.30686000	-3.16418600	3.62566200
H	4.92664200	-1.00622600	4.62274200
C	3.39262200	-0.55249700	-0.39455800
C	3.71627300	0.86050900	0.30900100
H	2.82379800	1.48927000	0.40410500
H	4.52492500	1.44911500	-0.14030100
O	2.08515700	-0.76711100	-0.83667700
C	4.35013700	-0.87912700	-1.53951800
C	4.47286300	0.01850900	-2.61189300
C	5.07215300	-2.07647600	-1.59315600
C	5.28864300	-0.27120400	-3.70561900
H	3.92686700	0.95932900	-2.58544300
C	5.89150700	-2.37273500	-2.68660300
H	5.00212500	-2.78179300	-0.77063200
C	6.00292400	-1.47229100	-3.74694200
H	5.37273500	0.44150300	-4.52242000
H	6.44464800	-3.30840600	-2.70621100
H	6.64233700	-1.70023800	-4.59565100
O	0.73516100	0.52526700	-2.46404800
H	1.20420800	0.95117300	-3.19922600
H	1.08706200	-0.47116200	-0.12617400
H	1.43998600	-0.05189000	-1.93576300

## TS8dRS

C	-1.79885900	-2.64720700	1.78192700
C	-1.04850800	-3.48752500	0.94457500
C	-3.14685700	-3.03056500	2.38510100
C	-1.45777700	-4.86365000	0.45226900
C	-3.98639500	-2.56125600	0.02108100
C	-3.32760700	-3.58153200	-0.69873600
C	-4.33115000	-2.58536400	1.49809500
C	-2.90418500	-4.91292500	-0.08660400
H	-3.17593800	-4.11259100	2.55398600
H	-3.24212500	-2.56601800	3.37246400
H	-1.31361600	-5.61169100	1.24761700
H	-0.76507500	-5.13676200	-0.35177700
H	-4.62821700	-1.57018400	1.78079200
H	-5.20936500	-3.22559100	1.67643400
H	-2.98018300	-5.69982900	-0.84492600
H	-3.60350500	-5.19217300	0.70924300

H	-3.45754100	-3.57777900	-1.78043500
H	0.01757400	-3.30321400	0.87829700
H	-4.56252800	-1.84722100	-0.56610800
H	-1.26449800	-1.84521000	2.28800000
Rh	-1.96839700	-1.97204100	-0.27515700
C	2.08311500	-2.33289200	-0.27309800
C	2.07923700	-1.81851400	-1.57235200
C	2.43434700	-2.62207200	-2.65628300
C	2.79460800	-3.95469900	-2.42677800
C	2.80848900	-4.46879500	-1.12611900
C	2.45575300	-3.65750100	-0.04162800
C	1.69338400	-1.26871800	0.71702100
C	1.01872300	-0.14544200	-0.12919400
H	2.43751800	-2.22518100	-3.66803700
H	3.07036900	-4.59055500	-3.26380000
H	3.09680800	-5.50269400	-0.95550500
H	2.47342300	-4.05916800	0.96905300
H	1.02089000	-1.61667600	1.50583200
H	2.59273400	-0.87915100	1.20435000
O	-0.38750900	-0.37693500	-0.21112700
C	1.22163700	1.24118100	0.50987500
C	1.30564500	1.35695900	1.90855000
C	1.26063500	2.42375000	-0.24244200
C	1.45577500	2.59898200	2.52831000
H	1.25789100	0.46811800	2.52950600
C	1.41400500	3.66950200	0.37273300
H	1.17610800	2.39121600	-1.32087800
C	1.51717000	3.76448400	1.75992500
H	1.52554000	2.65350300	3.61186100
H	1.43629600	4.56534200	-0.24108600
H	1.63632600	4.73290800	2.23820300
C	1.69236900	-0.34013800	-1.59009500
C	0.76948100	-0.00982800	-2.77055400
H	-0.07060400	-0.70475800	-2.78295800
H	0.36641200	1.00206400	-2.71395800
H	1.31701100	-0.10451600	-3.71183100
C	2.99025100	0.47626600	-1.73897900
O	3.23530200	1.23100200	-2.66002100
O	3.85881500	0.24215400	-0.73474300
C	5.08483700	1.02192400	-0.75990800
H	4.80948000	2.08004100	-0.80449100
H	5.63970700	0.77670400	-1.66956500
C	5.87271400	0.69618500	0.48058600
C	5.43483600	1.14437300	1.73574300

C	7.05120000	-0.05432500	0.40037500
C	6.16172300	0.84189700	2.88707100
H	4.52051900	1.72809700	1.80845200
C	7.78472900	-0.35253000	1.55163700
H	7.39720500	-0.40638400	-0.56855500
C	7.34013700	0.09420900	2.79716500
H	5.81329500	1.19435900	3.85422400
H	8.69966400	-0.93365600	1.47444300
H	7.90875500	-0.13632800	3.69409800
C	-5.32952300	1.46254700	1.46454600
C	-4.37672000	1.73792900	0.49055000
C	-3.02533900	1.88713200	0.79513500
C	-2.53719400	1.76633000	2.09166600
C	-3.48781300	1.47529200	3.08430100
C	-4.85075700	1.32878200	2.77897800
H	-6.38908800	1.35638500	1.24447500
H	-1.48748500	1.89164700	2.34093900
H	-3.16601400	1.37015700	4.11772700
H	-5.55048900	1.11331400	3.58302000
C	-2.62392700	2.18990100	-0.66417500
C	-4.18959000	1.99525600	-0.99308600
H	-4.38395400	1.14364600	-1.65347300
H	-4.69080200	2.88239200	-1.39569200
O	-1.79617200	1.25178000	-1.29757500
C	-2.15454100	3.61680700	-0.95238700
C	-1.47512500	3.89165900	-2.14773000
C	-2.43973400	4.68369400	-0.08895200
C	-1.08817700	5.19351200	-2.47015100
H	-1.24806800	3.07031500	-2.81871500
C	-2.05220100	5.98774700	-0.40791800
H	-2.96010900	4.49511000	0.84571200
C	-1.37394700	6.24945600	-1.60008000
H	-0.56134500	5.38341300	-3.40233600
H	-2.27750300	6.79873700	0.28041900
H	-1.07069100	7.26333500	-1.84836100
H	-1.01681500	0.54456100	-0.64697700
O	-2.69760400	-0.93996400	-2.06290600
H	-2.39790100	0.04734000	-1.85586300
H	-2.17807500	-1.22950300	-2.83061700

### TS8dSR

C	0.41830800	3.15374800	0.35784600
C	0.04516200	2.44574700	1.51010700

C	0.19180200	4.64812500	0.14773500
C	-0.68058100	3.01006800	2.71571800
C	-2.22557600	3.92876600	-0.24293100
C	-2.54108200	3.43775100	1.04250100
C	-1.14394500	4.94151600	-0.57182500
C	-1.87651700	3.90819700	2.33248800
H	0.23227600	5.16843700	1.11077500
H	1.01649300	5.05265400	-0.44933100
H	0.02327800	3.55605900	3.36370200
H	-1.04329200	2.16160900	3.30646400
H	-0.97830800	4.90197200	-1.65456000
H	-1.48907200	5.96363900	-0.34986400
H	-2.61489700	3.89618400	3.14198900
H	-1.55918400	4.95121700	2.22818500
H	-3.52161700	2.97784400	1.15773900
H	0.57405900	1.51152300	1.67876500
H	-3.00475700	3.84124500	-1.00145100
H	1.19116400	2.69628100	-0.25285000
Rh	-1.37373200	1.99317000	-0.04238900
C	1.34567400	-2.40016500	-2.63259200
C	2.31893900	-2.15276000	-1.65404100
C	3.49308600	-2.91198200	-1.63715300
C	3.69926300	-3.87933500	-2.62580000
C	2.74049300	-4.09867500	-3.61974200
C	1.55361800	-3.36130300	-3.62169800
C	0.12010200	-1.56426800	-2.39964900
C	0.60504600	-0.39579400	-1.46557400
H	4.24668200	-2.74845200	-0.87589300
H	4.61651500	-4.46258500	-2.62077300
H	2.91546400	-4.84766600	-4.38777000
H	0.79763800	-3.53824200	-4.38320000
H	-0.33311200	-1.17898400	-3.31854100
H	-0.65556300	-2.14495500	-1.88754100
O	-0.44003400	0.03625500	-0.61680100
C	1.05620600	0.74427400	-2.40281100
C	0.06542900	1.57766800	-2.95071100
C	2.37214700	0.92827400	-2.84981200
C	0.37721200	2.58284300	-3.86532700
H	-0.96822900	1.42302200	-2.66118100
C	2.69157000	1.93812900	-3.76498200
H	3.16974600	0.28147100	-2.50665600
C	1.70008400	2.77609400	-4.27214600
H	-0.41564200	3.20919400	-4.26698700
H	3.72393000	2.05907100	-4.08305800

H	1.94965400	3.55871100	-4.98355700
C	1.81276100	-1.10797800	-0.65924100
C	1.24475700	-1.84261900	0.58556500
H	2.05293300	-2.36396900	1.11079200
H	0.76814600	-1.13619500	1.26608200
H	0.50799800	-2.58982400	0.28186500
C	2.83134600	-0.12056100	-0.08537300
O	2.52786800	0.80138200	0.64772700
O	4.11241800	-0.40055100	-0.40585800
C	5.14722500	0.44933500	0.17583300
H	4.74932500	1.45980700	0.27634200
H	5.94195300	0.43759100	-0.57240700
C	5.63256500	-0.09476400	1.49623500
C	5.08308900	0.35577000	2.70473800
C	6.63813500	-1.07089400	1.52813000
C	5.53179500	-0.16118800	3.92143900
H	4.29851800	1.10611500	2.68443000
C	7.08573900	-1.59102400	2.74350200
H	7.07504600	-1.42069500	0.59546000
C	6.53272300	-1.13580200	3.94323500
H	5.10067100	0.19758800	4.85218900
H	7.86770900	-2.34547600	2.75470800
H	6.88251600	-1.53673600	4.89077300
C	-1.56540600	-3.02835400	3.32416600
C	-2.12448300	-2.74826100	2.08275800
C	-2.71819700	-1.52032200	1.79811900
C	-2.78610100	-0.49147800	2.73081300
C	-2.21433800	-0.75749500	3.98645400
C	-1.61987400	-1.99624800	4.27544600
H	-1.10379500	-3.98273600	3.56500900
H	-3.25146200	0.46788900	2.52020100
H	-2.23840100	0.00769300	4.75873600
H	-1.19333900	-2.15720900	5.26252500
C	-3.10200900	-1.92387100	0.35984500
C	-2.39576000	-3.32768200	0.70568300
H	-3.05371900	-4.20320600	0.66912400
H	-1.51566200	-3.51887100	0.08282700
O	-2.49936200	-1.20552400	-0.68245700
H	-1.38133800	-0.70463100	-0.55880900
C	-4.59704100	-2.07896900	0.08076700
C	-5.04702600	-2.15537200	-1.24621700
C	-5.53991400	-2.20020000	1.11117500
C	-6.39923000	-2.34635400	-1.53438200
H	-4.32450700	-2.05964300	-2.04988100



C	-6.89417900	-2.39054400	0.82465100
H	-5.21653800	-2.13820300	2.14612500
C	-7.33052400	-2.46466100	-0.49943300
H	-6.72608000	-2.40196900	-2.56999500
H	-7.60859000	-2.47527000	1.63979000
H	-8.38423500	-2.60997800	-0.72282900
O	-3.21979400	1.18978800	-0.92271400
H	-3.28268700	1.41124100	-1.86589900
H	-3.06346900	0.15966900	-0.87428900

## TS8dSS

C	1.04548000	3.96426400	-0.53270700
C	-0.33338500	3.86745800	-0.28337000
C	1.67084100	4.87042500	-1.58811900
C	-1.43023800	4.56639000	-1.06568100
C	0.87230600	3.04677400	-3.16225100
C	-0.52652800	3.18082200	-3.00799700
C	1.91551000	4.11763400	-2.90990800
C	-1.23227100	4.47111400	-2.59656100
H	1.02933700	5.74244000	-1.75207500
H	2.62168700	5.25947600	-1.20774800
H	-1.51771800	5.61833200	-0.75279000
H	-2.37933200	4.08766900	-0.80050000
H	2.89051700	3.61890100	-2.86362900
H	1.96638500	4.81807400	-3.75795700
H	-2.20962600	4.51319900	-3.08876200
H	-0.66849700	5.33401500	-2.96746100
H	-1.14827700	2.46300500	-3.54264200
H	-0.61630500	3.53911300	0.71402000
H	1.21591500	2.25892600	-3.83454500
H	1.70751200	3.67118500	0.27770100
Rh	0.27380600	2.10080600	-1.34640100
C	-1.19289600	-1.49525600	2.83796100
C	-2.29232800	-0.70039700	2.49106000
C	-3.55306300	-0.96511700	3.02548000
C	-3.70445500	-2.03450300	3.91663100
C	-2.60522200	-2.82408500	4.26728000
C	-1.34119400	-2.55618100	3.72899700
C	0.04295900	-1.03654700	2.11347000
C	-0.28601200	0.43035300	1.65546000
H	-4.41182300	-0.35292000	2.76319800
H	-4.68163600	-2.24638600	4.34243900
H	-2.73117100	-3.64685800	4.96615800

H	-0.48596800	-3.16729700	4.00722800
H	0.95582500	-1.08018400	2.71436400
H	0.20034000	-1.65561600	1.22492000
O	0.35281300	0.71722500	0.42552000
C	0.21567600	1.38276900	2.76561300
C	1.38492900	2.12415300	2.54868300
C	-0.36636400	1.45022100	4.04477500
C	1.93772000	2.92875200	3.54885400
H	1.87068900	2.05092100	1.58441100
C	0.18117500	2.25451200	5.04594900
H	-1.25159600	0.86873400	4.27513300
C	1.33430000	3.00416100	4.80382800
H	2.84527700	3.49119900	3.34340700
H	-0.29780100	2.28993200	6.02113100
H	1.75863800	3.62981500	5.58446900
C	-1.89801700	0.40233300	1.51092700
C	-2.62835700	1.72936400	1.77046200
H	-2.44042300	2.10032300	2.77799000
H	-2.32362500	2.48761700	1.04976200
H	-3.70774400	1.59322100	1.64998600
C	-2.25598600	-0.02349600	0.06917000
O	-2.74205900	0.71919300	-0.75999100
O	-2.00925400	-1.32796900	-0.17008400
C	-2.36424000	-1.81891000	-1.48746700
H	-1.79485400	-2.74915200	-1.56977300
H	-2.00226300	-1.11567500	-2.23871000
C	-3.84599500	-2.08024200	-1.63158200
C	-4.56291900	-2.72673800	-0.61520000
C	-4.51078600	-1.72180800	-2.80962400
C	-5.92047800	-3.00651600	-0.77661200
H	-4.05772500	-2.99810800	0.30758400
C	-5.86689900	-2.01136400	-2.97725500
H	-3.96504800	-1.20972600	-3.59862400
C	-6.57566200	-2.65347400	-1.95990600
H	-6.46683400	-3.50393900	0.02047700
H	-6.37019000	-1.72615400	-3.89728700
H	-7.63218900	-2.87450700	-2.08579300
H	1.16676300	-0.05240500	0.05415800
C	2.32876400	-4.44331500	-2.93968600
C	2.26393400	-3.49914600	-1.92145200
C	3.15667300	-2.43293000	-1.84652200
C	4.15908400	-2.22711400	-2.78601700
C	4.22834300	-3.16818000	-3.82638400
C	3.33738400	-4.25114600	-3.89853100

H	1.64595600	-5.28636300	-3.01243000
H	4.86115600	-1.39882800	-2.73231200
H	4.99190200	-3.06321800	-4.59337300
H	3.43308300	-4.95656500	-4.72041700
C	2.54198600	-1.86653200	-0.54948500
C	1.49892800	-3.08971000	-0.67429400
H	0.47971300	-2.73136600	-0.85085500
H	1.48659800	-3.80496600	0.15554000
O	1.99858200	-0.59346000	-0.71170300
C	3.47289800	-1.95034500	0.66260100
C	4.07354300	-3.16370600	1.03733000
C	3.76888700	-0.80595400	1.41159800
C	4.92982700	-3.23073600	2.13587100
H	3.87948700	-4.06418700	0.46024800
C	4.62502500	-0.87004500	2.51529000
H	3.31954500	0.13654000	1.12239200
C	5.20858900	-2.08234900	2.88367400
H	5.38170100	-4.18139400	2.40800500
H	4.83252400	0.03194100	3.08582700
H	5.87442500	-2.13461400	3.74110000
O	0.31322200	0.18167300	-2.37912100
H	1.05347600	-0.29671100	-1.81418800
H	0.65569400	0.24907000	-3.28481200