

## Supporting information

### DFT Study on Rh(II)/Guanidine-Catalyzed Asymmetric N-H bond Insertion of Benzophenone Imine

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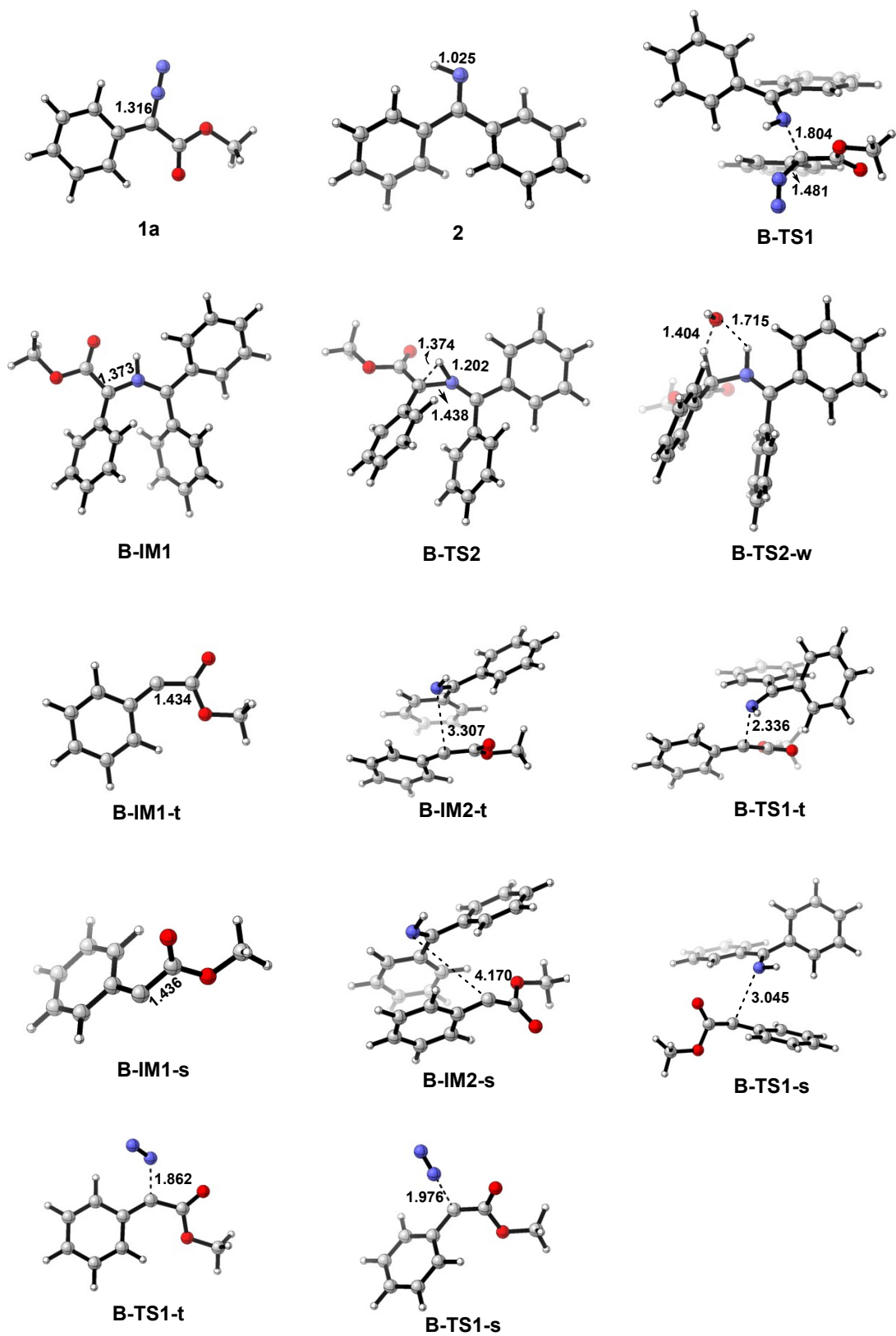
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National and Local Joint Engineering Laboratory of Energy Plant Biofuel Preparation and Utilization ; College of Chemistry, Sichuan University, Chengdu, Sichuan 610064, P. R. China.

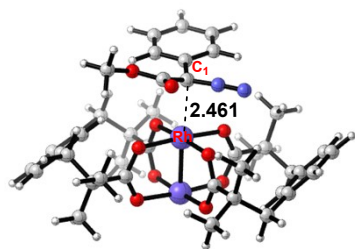
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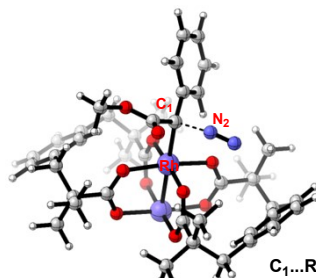
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**Figure S1** Optimized geometries of intermediates and transition states in the non-catalytic reaction.

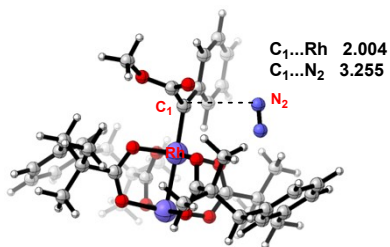


IM1



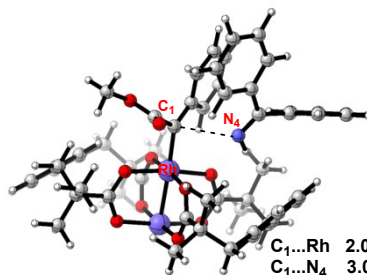
TS1

C<sub>1</sub>...Rh 2.146  
C<sub>1</sub>...N<sub>2</sub> 1.759



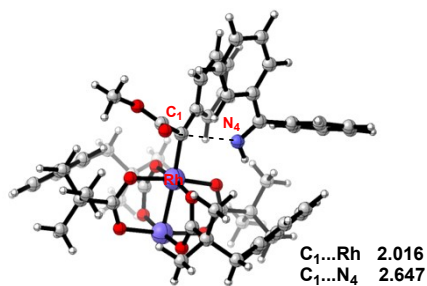
IM2

C<sub>1</sub>...Rh 2.004  
C<sub>1</sub>...N<sub>2</sub> 3.255



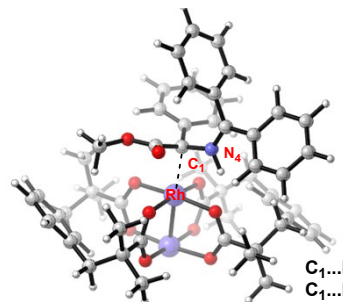
IM3

C<sub>1</sub>...Rh 2.000  
C<sub>1</sub>...N<sub>4</sub> 3.005



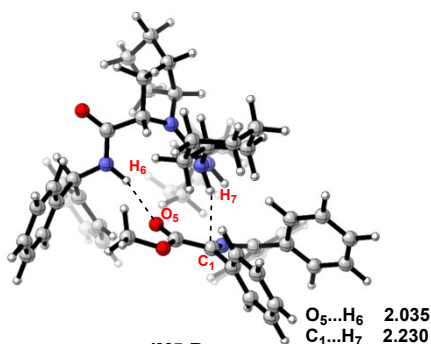
TS2

C<sub>1</sub>...Rh 2.016  
C<sub>1</sub>...N<sub>4</sub> 2.647



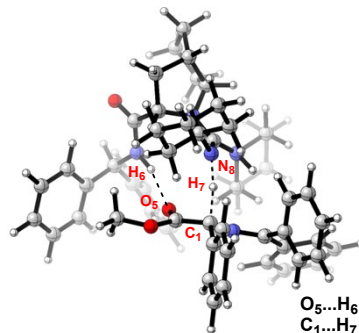
IM4

C<sub>1</sub>...Rh 2.280  
C<sub>1</sub>...N<sub>4</sub> 1.476



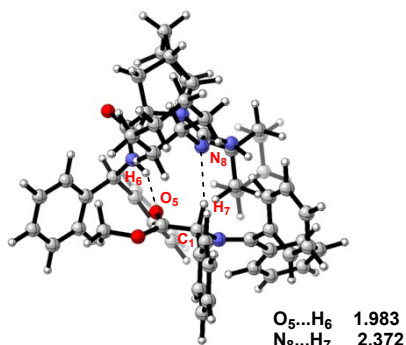
IM5-R

O<sub>5</sub>...H<sub>6</sub> 2.035  
C<sub>1</sub>...H<sub>7</sub> 2.230



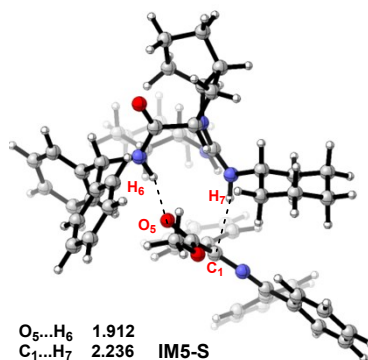
TS3-R

O<sub>5</sub>...H<sub>6</sub> 1.922  
C<sub>1</sub>...H<sub>7</sub> 1.433  
N<sub>8</sub>...H<sub>7</sub> 1.323



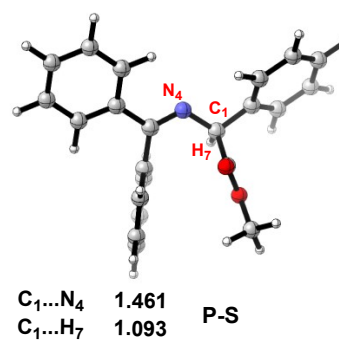
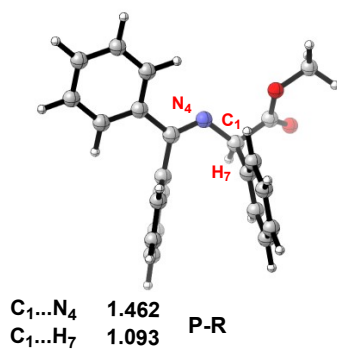
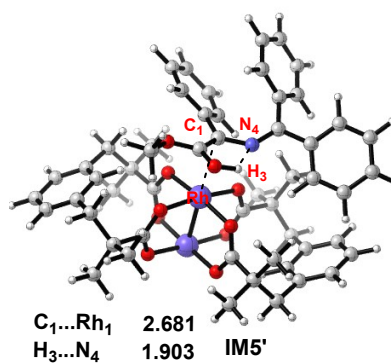
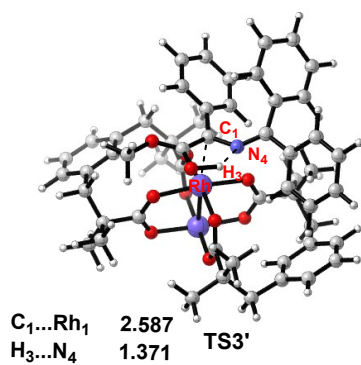
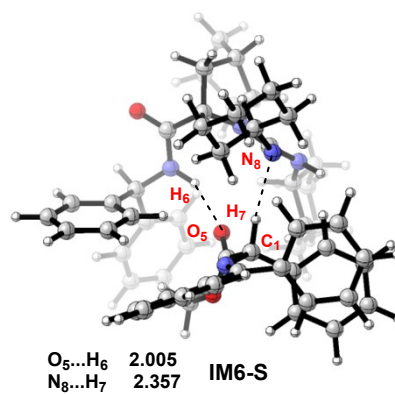
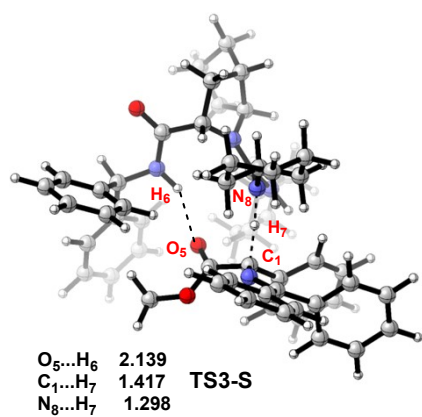
IM6-R

O<sub>5</sub>...H<sub>6</sub> 1.983  
N<sub>8</sub>...H<sub>7</sub> 2.372

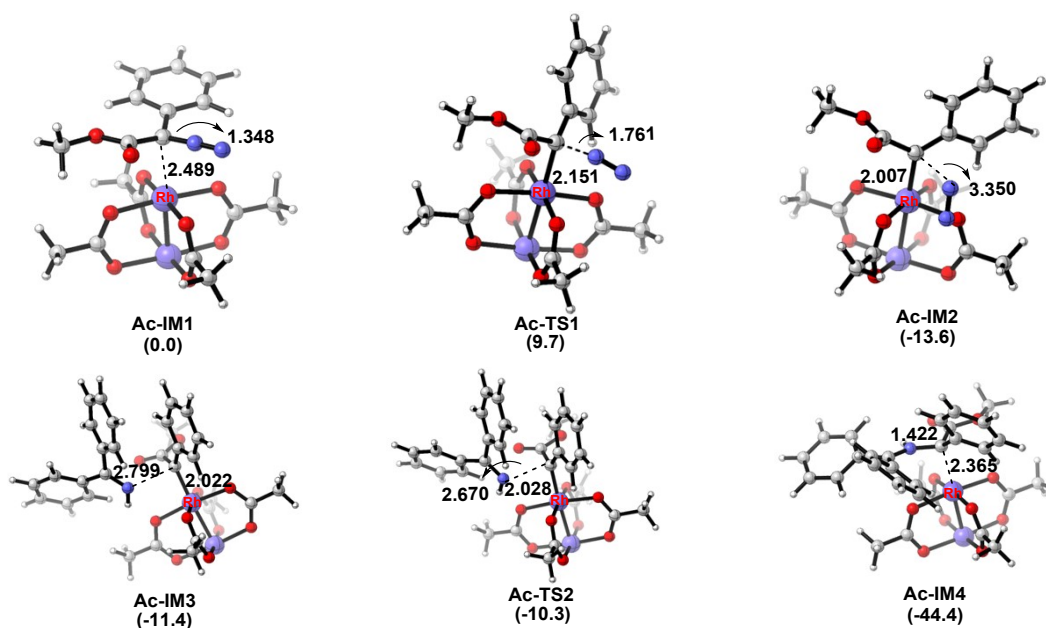


O<sub>5</sub>...H<sub>6</sub> 1.912  
C<sub>1</sub>...H<sub>7</sub> 2.236

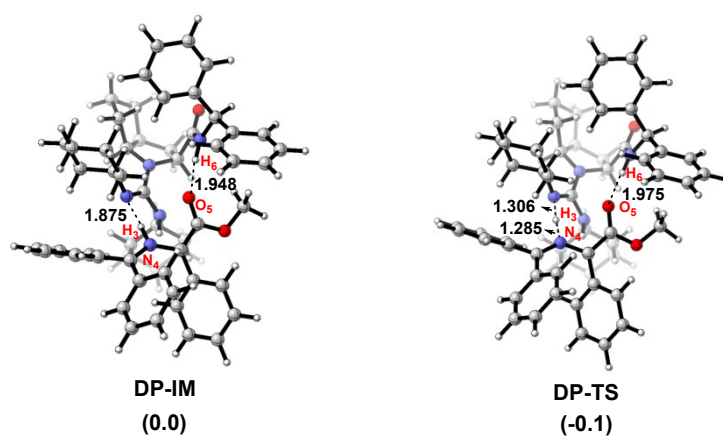
IM5-S



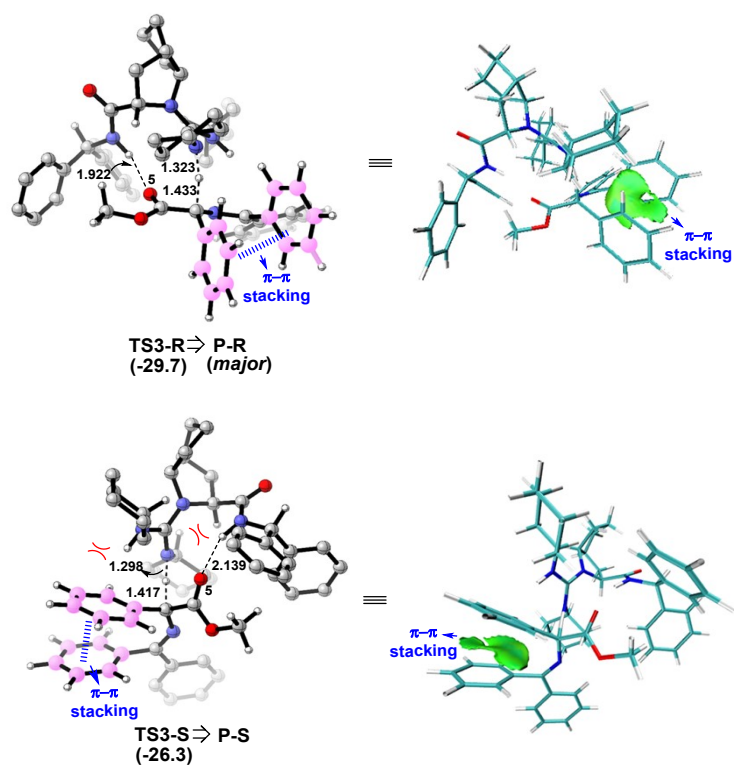
**Figure S2** Optimized geometries of intermediates and transition states in the catalytic reaction.



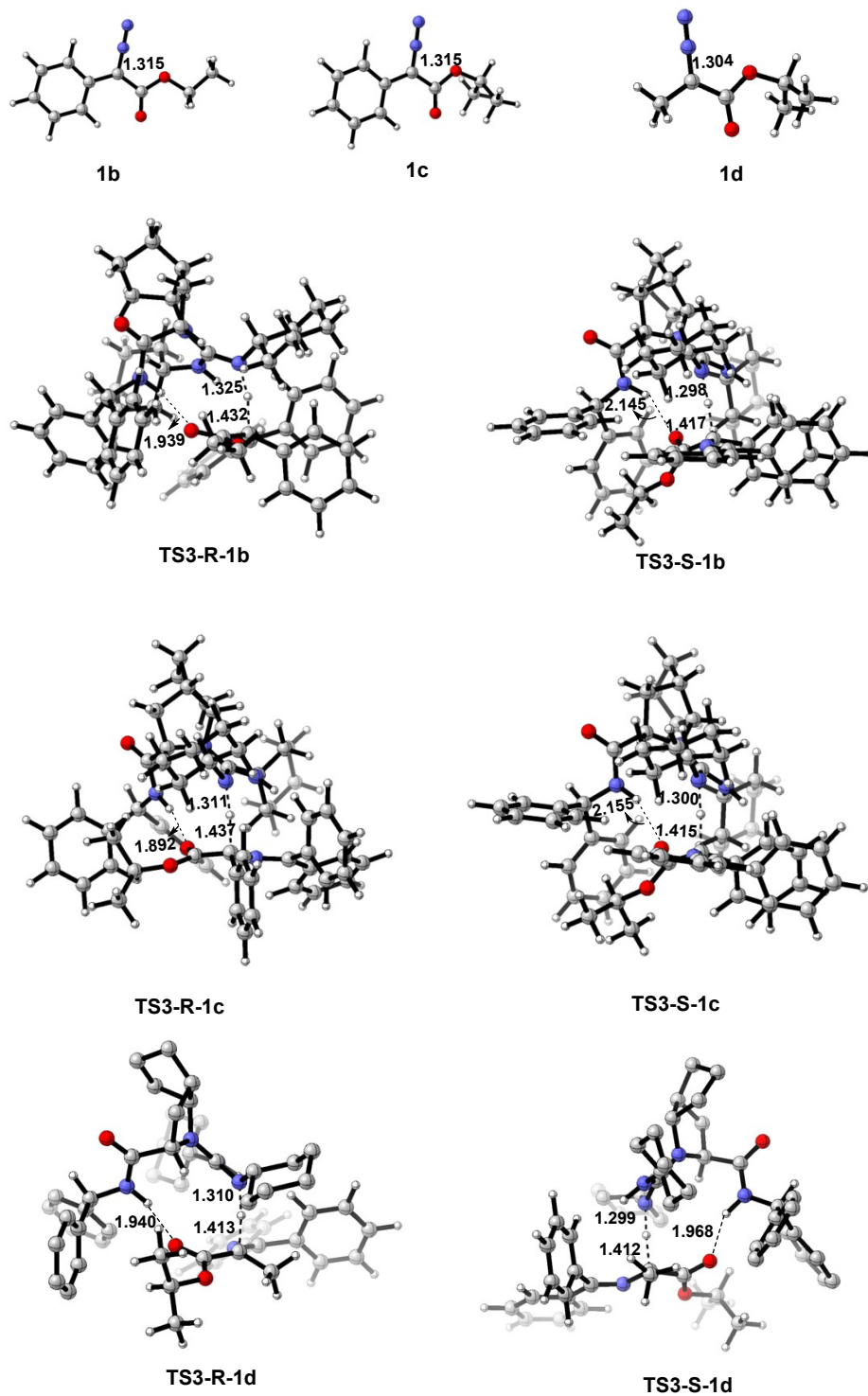
**Figure S3** Optimized geometries of transition states in the C-N bond formation step, catalyzed by  $\text{Rh}_2(\text{OAc})_4$ . Relative Gibbs energy was in  $\text{kcal mol}^{-1}$ .



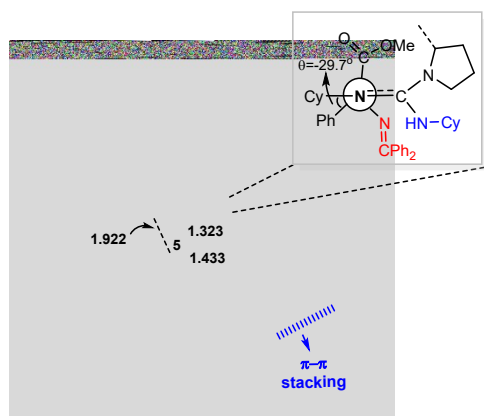
**Figure S4** Optimized geometries of intermediate DP-IM and transition state DP-TS in the proton transfer from ylide to the guanidine catalyst G1. The Gibbs free energy of DP-IM was set to zero.



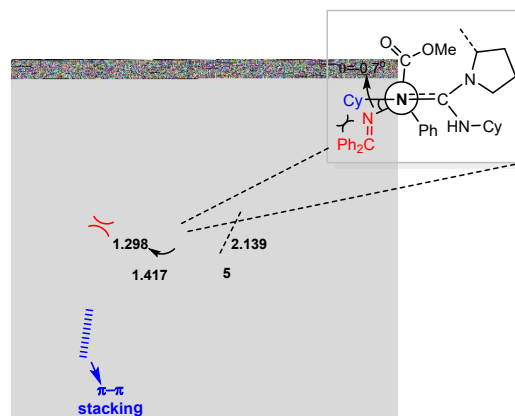
**Figure S5** Optimized geometries of transition states TS3-R and TS3-S. the noncovalent analysis was performed by Multiwfn 3.8 (dev).



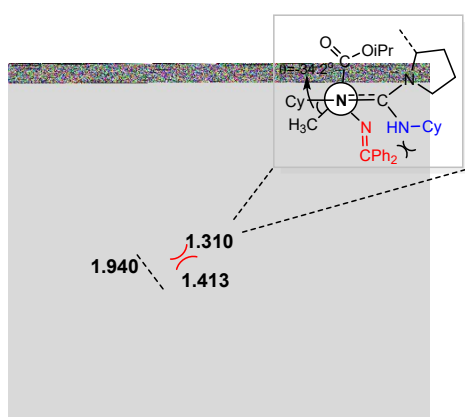
**Figure S6** Optimized geometries of transition states in the C-H formation step in the catalytic reactions using 1b~1d as substrates.



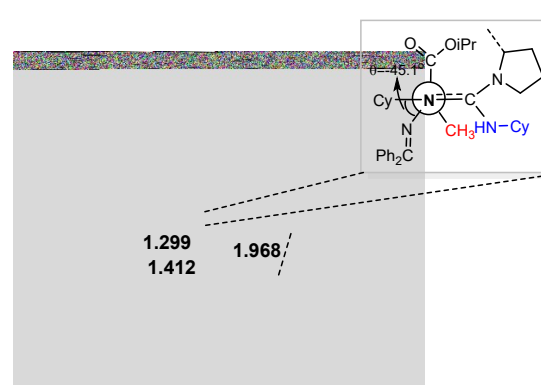
TS3-R  $\Rightarrow$  P-R  
(-29.7) (major)



TS3-S  $\Rightarrow$  P-S  
(-26.3)



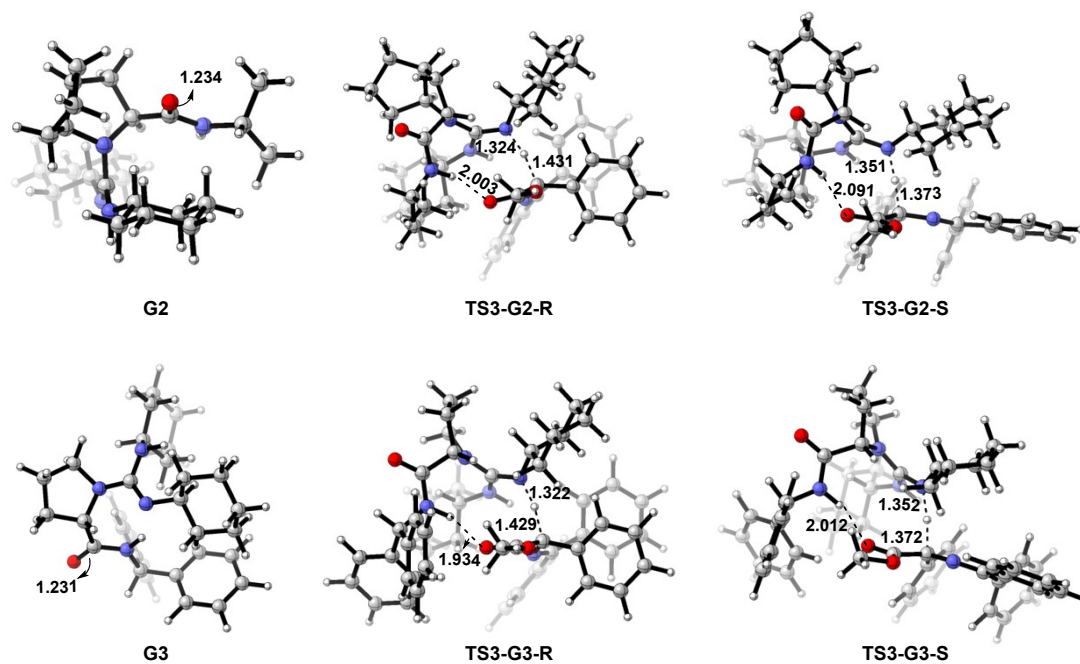
TS3-R-1d  $\Rightarrow$  P-R  
(-29.2)



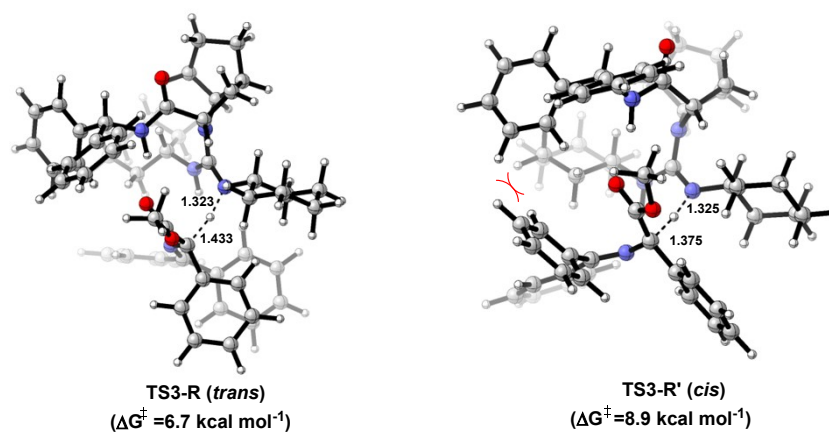
TS3-S-1d  $\Rightarrow$  P-S  
(-32.1) (major)

**Figure S7** Optimized geometries of transition states of TS3-R, TS3-S, TS3-R-1d and TS3-S-1d.



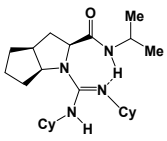
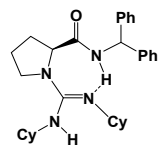


**Figure S8** Optimized geometries of transition states in the C-H formation step in the reaction catalyzed by G2 and G3, respectively.



**Figure S9** The optimized geometries of TS3-R and TS3-R', with the CPh<sub>2</sub> moiety of the enolate ion oriented either *trans* or *cis* to the COOMe group, respectively.

**Table S1** Relative Gibbs free energies of two competing transition states in the H-shift step ( $\Delta G$ ) and their energy difference ( $\Delta\Delta G$ , in kcal mol<sup>-1</sup>) catalyzed by G2 and G3 respectively.

Catalysts	TSs	$\Delta G$	$\Delta\Delta G$
	TS3-G2-R	-29.9	0.5
	TS3-G2-S	-29.4	
	TS3-G3-R	-22.0	0.9
	TS3-G3-S	-21.1	

**Table S2** Electronic energies ( $E_e$ ), enthalpies ( $H$ ) and Gibbs free energies ( $G$ ) for all stationary points (in Hartree), obtained at the B3LYP-D3(BJ)/6-31G(d)(SMD, CHCl<sub>3</sub>) theoretical level.

Structures	<sup>a</sup> ZPE	$E_e$	<sup>b</sup> H <sub>corr</sub>	$H$	<sup>c</sup> G <sub>corr</sub>	<sup>d</sup> G
<b>1a</b>	0.15871	-607.72983	0.16963	-607.71891	0.12401	-607.76453
<b>2</b>	0.20466	-556.75395	0.21467	-556.74394	0.17119	-556.78742
<b>B-TS1</b>	0.36200	-1164.41485	0.38273	-1164.39413	0.31533	-1164.46152
<b>N<sub>2</sub></b>	0.00561	-109.54574	0.00863	-109.54271	-0.01102	-109.56236
<b>B-IM1</b>	0.35729	-1055.00388	0.37629	-1054.98488	0.31131	-1055.04986
<b>B-TS2</b>	0.35098	-1054.92098	0.36982	-1054.90215	0.30567	-1054.96630
<b>P-R</b>	0.35671	-1055.01084	0.37588	-1054.99167	0.30901	-1055.05853
<b>H<sub>2</sub>O</b>	0.02104	-76.43346	0.02363	-76.43086	0.00516	-76.44934
<b>B-TS2-w</b>	0.37748	-1131.40303	0.39812	-1131.38238	0.33021	-1131.45030
<b>B-TS1-s</b>	0.15444	-607.67806	0.16605	-607.66644	0.11829	-607.71421
<b>B-TS1-t</b>	0.15365	-607.66725	0.16522	-607.65568	0.11667	-607.70423
<b>B-IM1-s</b>	0.14729	-498.14390	0.15683	-498.13435	0.11455	-498.17664
<b>B-IM1-t</b>	0.14678	-498.14086	0.15632	-498.13133	0.11206	-498.17558
<b>B-IM2-s</b>	0.35306	-1054.91270	0.37336	-1054.89240	0.30458	-1054.96117
<b>B-IM2-t</b>	0.35271	-1054.90926	0.37290	-1054.88906	0.30364	-1054.95833
<b>B-TS2-s</b>	0.35236	-1054.90343	0.37145	-1054.88434	0.30395	-1054.95185
<b>B-TS2-t</b>	0.35258	-1054.90613	0.37205	-1054.88665	0.30459	-1054.95412
<b>G1</b>	0.75569	-1617.47921	0.78665	-1617.44825	0.69161	-1617.54329
<b>Rh<sub>2</sub>(esp)<sub>2</sub></b>	0.67716	-2066.80557	0.71263	-2066.77009	0.61709	-2066.86564
<b>IM1</b>	0.83732	-2674.56330	0.88435	-2674.51627	0.76316	-2674.63746
<b>TS1</b>	0.83551	-2674.54780	0.88224	-2674.50108	0.76274	-2674.62057
<b>IM2</b>	0.83482	-2674.57956	0.88305	-2674.53134	0.75895	-2674.65544
<b>IM3</b>	1.03435	-3121.79760	1.08997	-3121.74198	0.94949	-3121.88246
<b>TS2</b>	1.03456	-3121.79696	1.08926	-3121.74226	0.95198	-3121.87953
<b>IM4</b>	1.03755	-3121.84003	1.09216	-3121.78542	0.95496	-3121.92262
<b>TS3'</b>	1.03300	-3121.82394	1.08702	-3121.76992	0.95289	-3121.90405

<b>IM5'</b>	1.03653	-3121.82727	1.09089	-3121.77291	0.95589	-3121.90791
<b>IM5-R</b>	1.11720	-2672.50967	1.16593	-2672.46095	1.03598	-2672.59090
<b>TS3-R</b>	1.11139	-2672.49767	1.16070	-2672.44836	1.02887	-2672.58019
<b>IM6-R</b>	1.11572	-2672.51524	1.16579	-2672.46517	1.03021	-2672.60076
<b>IM5-S</b>	1.11718	-2672.51274	1.16654	-2672.46338	1.03515	-2672.59477
<b>TS3-S</b>	1.11077	-2672.49067	1.16023	-2672.44121	1.02666	-2672.57478
<b>IM6-S</b>	1.11683	-2672.50913	1.16650	-2672.45946	1.03307	-2672.59289
<b>P-S</b>	0.35673	-1055.01108	0.37588	-1054.99193	0.30890	-1055.05891
<b>G3</b>	0.69231	-1500.77750	0.72070	-1500.74911	0.63390	-1500.83591
<b>TS3-G3-R</b>	1.04543	-2555.78101	1.09239	-2555.73404	0.96584	-2555.86059
<b>TS3-G3-S</b>	1.04647	-2555.77972	1.09380	-2555.73238	0.96701	-2555.85917
<b>G2</b>	0.65014	-1233.97380	0.67556	-1233.94838	0.59628	-1234.02766
<b>TS3-G2-R</b>	1.00495	-2288.99037	1.04902	-2288.94630	0.93045	-2289.06487
<b>TS3-G2-S</b>	1.00431	-2288.99078	1.04763	-2288.94746	0.93103	-2289.06407
<b>1b</b>	0.18720	-647.03722	0.19920	-647.02522	0.15095	-647.07346
<b>TS3-R-1b</b>	1.13937	-2711.80621	1.18996	-2711.75562	1.05572	-2711.88987
<b>TS3-S-1b</b>	1.13952	-2711.79956	1.18999	-2711.74909	1.05495	-2711.88412
<b>1c</b>	0.21532	-686.34140	0.22840	-686.32832	0.17782	-686.37890
<b>TS3-R-1c</b>	1.16848	-2751.11204	1.21970	-2751.06082	1.08559	-2751.19493
<b>TS3-S-1c</b>	1.16780	-2751.10830	1.21915	-2751.05695	1.08311	-2751.19299
<b>1d</b>	0.16162	-494.58704	0.17252	-494.57614	0.12762	-494.62104
<b>TS3-R-1d</b>	1.11588	-2559.35572	1.16440	-2559.30720	1.03572	-2559.43588
<b>TS3-S-1d</b>	1.11497	-2559.35647	1.16394	-2559.30750	1.03090	-2559.44054
<b>Rh-IM-R</b>	1.79717	-4739.35807	1.88167	-4739.27357	1.68171	-4739.47353
<b>Rh-TS-R</b>	1.79154	-4739.33456	1.87667	-4739.24943	1.67305	-4739.45305
<b>Rh<sub>2</sub>(OAc)<sub>4</sub></b>	0.21159	-1135.42184	0.23092	-1135.40252	0.16514	-1135.46830
<b>Ac-IM1</b>	0.37151	-1743.17248	0.40228	-1743.14170	0.31113	-1743.23285
<b>Ac-TS1</b>	0.36923	-1743.15789	0.39995	-1743.12717	0.30977	-1743.21735
<b>Ac-IM2</b>	0.36843	-1743.18990	0.40096	-1743.15737	0.30379	-1743.25453
<b>Ac-IM3</b>	0.56877	-2190.40588	0.60799	-2190.36667	0.49865	-2190.47601
<b>Ac-TS2</b>	0.56859	-2190.40600	0.60700	-2190.36760	0.50029	-2190.47431
<b>Ac-IM4</b>	0.57117	-2190.45939	0.60963	-2190.42092	0.50191	-2190.52865
<b>DP-TS</b>	1.11107	-2672.50901	1.15961	-2672.46047	1.02934	-2672.59074
<b>DP-IM</b>	1.11578	-2672.51041	1.16385	-2672.46234	1.03570	-2672.59049
<b>G-IM1</b>	1.59782	-4292.07983	1.67476	-4292.00288	1.49072	-4292.18692
<b>G-TS1</b>	1.59617	-4292.05663	1.67362	-4291.97918	1.48743	-4292.16537
<b>TS3-R'</b>	1.11176	-2672.49533	1.16108	-2672.44602	1.02880	-2672.57830

<sup>a</sup> Zero-point correction energy;

<sup>b</sup> Thermal correction to enthalpy;

<sup>c</sup> Thermal correction to Gibbs free energy.

<sup>d</sup> Gibbs free energy obtained at the B3LYP-D3(BJ)/6-311G(d,p)(SMD, CHCl<sub>3</sub>)/B3LYP-D3(BJ)/6-31G(d)(SMD, CHCl<sub>3</sub>) theoretical level.

**Cartesian coordinates of all structures.****1a**

C	-1.66033200	-1.27540800	-0.13752300
C	-1.30914600	0.08264900	-0.04200000
C	-2.32851800	1.02921800	0.17149400
C	-3.65694100	0.62936700	0.28353700
C	-3.99993900	-0.72086200	0.18941100
C	-2.99403200	-1.66428200	-0.02051800
H	-0.88873900	-2.01574200	-0.29803700
H	-2.08898400	2.08558200	0.25330300
H	-4.42570300	1.37929800	0.44793600
H	-5.03686000	-1.03165000	0.27809600
H	-3.24348300	-2.71916200	-0.09703700
C	0.09599600	0.51549600	-0.16845500
C	1.28594600	-0.34197900	-0.23227300
O	2.41470700	0.39455400	-0.33057000
O	1.27601600	-1.56017700	-0.20085200
C	3.64045700	-0.35571900	-0.40878800
H	4.42938200	0.39170600	-0.49596900
H	3.63658100	-1.00891100	-1.28512700
N	0.34172700	1.80705100	-0.21492600
N	0.53241700	2.92713400	-0.25449100
H	3.78295400	-0.95439200	0.49472200

**1b**

C	-1.39443300	-1.24879000	0.12403400
C	-0.94758900	0.07974500	0.01433200
C	-1.90374800	1.10428300	-0.11568200
C	-3.26364100	0.80830300	-0.13365600
C	-3.70184200	-0.51313700	-0.02606400
C	-2.75900000	-1.53336100	0.10153700
H	-0.67206800	-2.04751800	0.22119100
H	-1.58948500	2.14026100	-0.20596900
H	-3.98233500	1.61667800	-0.23564300
H	-4.76326500	-0.74290100	-0.04161300
H	-3.08283500	-2.56708400	0.18735300
C	0.49201200	0.40205300	0.04186100
C	1.61529300	-0.54396000	-0.01126700
O	2.79922900	0.10198600	0.01709000
O	1.50514500	-1.75652400	-0.07602600
C	3.98420200	-0.73199400	-0.04334200
H	3.94777400	-1.32385300	-0.96274700
H	3.97201600	-1.42044800	0.80694100

N	0.83932300	1.66940100	0.09658700
N	1.12115100	2.76991100	0.14495600
C	5.18290800	0.19084300	-0.01083300
H	6.10163100	-0.40336900	-0.06704400
H	5.16765300	0.88366200	-0.85879900
H	5.20583500	0.77368600	0.91598000

**1c**

C	-1.49768700	-1.27485200	0.09193600
C	-1.01080600	0.04127400	0.00209400
C	-1.93698400	1.09643800	-0.09864300
C	-3.30534200	0.84342700	-0.10591100
C	-3.78333800	-0.46556300	-0.01666200
C	-2.87084200	-1.51628900	0.08035200
H	-0.79924600	-2.09687500	0.16615000
H	-1.59160100	2.12331400	-0.17559100
H	-3.99899800	1.67597900	-0.18428900
H	-4.85149000	-0.66209500	-0.02348400
H	-3.22593900	-2.54092900	0.15004800
C	0.43715600	0.32471700	0.01911700
C	1.53937000	-0.65095800	-0.01462900
O	2.72897400	-0.02002100	0.00304200
O	1.38168200	-1.85976600	-0.05510200
C	3.97790200	-0.78828300	-0.04283100
N	0.81401200	1.58400700	0.05599900
N	1.11789000	2.67926700	0.08990400
H	4.71603200	0.01791700	-0.01668500
C	4.14510400	-1.65184200	1.20061700
H	3.45328900	-2.49668800	1.19927000
H	5.17008700	-2.03829100	1.23268500
H	3.97825700	-1.05697600	2.10504900
C	4.11543400	-1.54166000	-1.35922800
H	5.13560100	-1.93272600	-1.44357300
H	3.41485600	-2.37705700	-1.41841300
H	3.93923700	-0.86950000	-2.20586100

**1d**

C	-0.01336100	0.41794800	-0.02743000
C	-1.06245500	-0.59697800	0.02966400
O	-2.29492900	-0.05058400	0.00937500
O	-0.80332700	-1.78957800	0.08734800
C	-3.48283200	-0.90615600	0.05793400
N	-0.37269500	1.67048000	-0.08401100
N	-0.68591900	2.76656900	-0.13480400

H	-4.28117200	-0.15899200	0.02587900	O	1.36520500	3.12131800	1.60545000
C	1.44572100	0.05113600	-0.01335600	O	2.21568100	2.70598400	-0.44810400
H	1.70809900	-0.45697600	0.92146200	C	1.89725200	4.05872600	-0.83233700
H	1.67511500	-0.62814000	-0.84136200	H	2.12443700	4.11304400	-1.89700900
H	2.06999300	0.94323400	-0.11138900	H	2.51523000	4.76638800	-0.27372800
C	-3.58216700	-1.78860200	-1.17978000	C	3.03869100	-0.04815500	0.46679300
H	-2.81740500	-2.56794100	-1.17586600	C	3.65671000	0.21042700	-0.76663700
H	-4.56903500	-2.26456100	-1.20406100	C	3.32855100	-1.25597500	1.12585900
H	-3.47290200	-1.18781400	-2.08913800	C	4.54135500	-0.71652500	-1.31661100
C	-3.56802200	-1.66374900	1.37676600	H	3.43546400	1.12260200	-1.30073000
H	-3.44868800	-0.97734700	2.22200600	C	4.21070100	-2.17684900	0.56697300
H	-4.55448200	-2.13415900	1.45831100	H	2.85677200	-1.49383600	2.07291400
H	-2.80322400	-2.44045600	1.44025400	C	4.82351600	-1.91440000	-0.65967000
				H	5.00914600	-0.49515100	-2.27202300
<b>2</b>				H	4.41725300	-3.10239600	1.09696600
C	-1.37716800	-0.64521500	-0.61323100	H	5.51190200	-2.63279600	-1.09507200
C	-2.59633200	-1.31996100	-0.67818200	N	1.72412500	0.65536600	2.34323900
C	-3.74182800	-0.75294300	-0.11806200	N	1.40345300	0.42087500	3.39579300
C	-3.66530900	0.49815600	0.50138400	H	0.84075800	4.25939300	-0.65167800
C	-2.45159000	1.17726100	0.55712500	Rh	-2.22467900	-0.77056500	-0.64258600
C	-1.29134800	0.61203600	0.00400300	C	-0.75333200	-2.58673400	1.07852700
C	-0.01143100	1.37461900	0.04018800	C	-0.52802200	-3.84011100	1.88171900
C	1.27563300	0.61592900	0.02904200	O	-1.82259400	-2.50633000	0.39303100
C	2.35228300	1.07562100	-0.74438600	O	0.75260600	-0.65034600	-1.51183700
C	3.57477500	0.40658900	-0.72555900	C	0.75199200	-1.76751500	-3.60305100
C	3.74077100	-0.72535500	0.07561200	C	0.04705600	-1.27776500	-2.36552000
C	2.67617400	-1.18858600	0.85170500	O	-1.20439300	-1.49965000	-2.27495700
C	1.44799300	-0.52956200	0.82132100	O	0.13977500	-1.68011800	1.17045400
N	-0.06980300	2.65911500	0.08050800	O	-2.51255300	1.01603200	-1.62913700
H	-0.49280500	-1.08972500	-1.05738400	O	-1.15280100	0.80500000	1.82611000
H	-2.64991800	-2.28798000	-1.16837100	O	-3.12561700	0.00978800	1.04517500
H	-4.55332800	0.94260400	0.94228000	C	-3.10980900	1.21334500	3.10052000
H	-2.38264100	2.15000400	1.03238900	C	-2.41292900	0.62235700	1.90357400
H	2.22081900	1.94901200	-1.37721900	O	-0.55974800	1.84528800	-0.83191300
H	4.39572200	0.76541500	-1.33988900	C	-1.63675900	1.93190300	-1.50719600
H	2.80105300	-2.06592500	1.48007000	C	-1.89490700	3.24617300	-2.19638300
H	0.62257300	-0.89281400	1.42526500	Rh	-0.13505700	0.10351500	0.18478200
H	0.87607400	3.05087000	0.13835200	H	0.24420700	-2.64307800	-4.01375900
H	4.69414900	-1.24586200	0.09237500	H	0.73087900	-0.97054500	-4.35688200
H	-4.68972300	-1.28212700	-0.16240400	H	1.79545200	-1.99983500	-3.37859700
				H	-1.15763500	-4.65364500	1.51673700
				H	-0.78436600	-3.63576100	2.92844600
<b>Ac-IM1</b>				H	0.52590400	-4.12844400	1.84373500
C	2.05306400	0.90385600	1.05960400	H	-3.28127900	2.28065500	2.91443400
C	1.84748000	2.35886900	0.78685800				

H	-2.47836600	1.12453800	3.98829500	C	-2.41174800	3.35426900	-1.79596700
H	-4.07302200	0.72713900	3.26753700	Rh	-0.09426500	0.10603400	-0.14289000
H	-2.20024200	3.98472600	-1.44559100	H	-0.22674300	-2.81160900	-3.75358300
H	-2.68835000	3.14762800	-2.93955000	H	-1.95272400	-2.49089800	-4.09289500
H	-0.97720100	3.60744600	-2.66880700	H	-0.69669000	-1.29230700	-4.52276700

### Ac-IM2

C	1.83286000	0.65964900	-0.22829100
C	2.06418500	2.08637700	0.09642600
O	2.21755000	2.49180400	1.23516000
O	2.03521300	2.85770600	-0.99688100
C	2.07367800	4.28101700	-0.76310400
H	2.03492100	4.73703400	-1.75197100
H	2.99579300	4.56235100	-0.24841100
C	2.97452800	-0.16349900	-0.45495500
C	4.29101900	0.31853100	-0.20291300
C	2.81958100	-1.49587100	-0.92636500
C	5.39108200	-0.49989200	-0.39493500
H	4.42850900	1.32643200	0.17407100
C	3.93020500	-2.29928000	-1.13829700
H	1.82500300	-1.86032200	-1.13788200
C	5.21181100	-1.80805900	-0.86565500
H	6.38937200	-0.12966900	-0.18400400
H	3.80519600	-3.31150000	-1.51019100
H	6.07768700	-2.44499700	-1.02248600
N	2.47497500	-0.34172700	2.90312000
N	1.51212400	-0.62578000	3.36330200
H	1.20890300	4.58679700	-0.16892100
Rh	-2.45727400	-0.57483700	0.01942400
C	-0.56960600	-2.48464500	1.12527200
C	-0.13228600	-3.72420700	1.86231100
O	-1.81160800	-2.30641900	0.94353900
O	-0.07660000	-0.82001700	-1.98997900
C	-1.00607500	-2.04231800	-3.78724100
C	-1.13159700	-1.39516800	-2.43171000
O	-2.24676900	-1.46431100	-1.83426900
O	0.36411600	-1.69042100	0.76186900
O	-2.93734000	1.21364500	-0.89361800
O	-0.35186300	0.98048400	1.70188500
O	-2.52461600	0.34778900	1.85986200
C	-1.52834000	1.51051100	3.68324700
C	-1.47474100	0.90553400	2.30446400
O	-0.76076400	1.84728800	-1.02305400
C	-2.01423500	2.02892000	-1.19736400

H	-0.90918400	-4.49049700	1.82431000
H	0.05105900	-3.46080300	2.91123300
H	0.80244500	-4.10685500	1.44425100
H	-0.89446800	2.39901800	3.73596700
H	-1.14342200	0.77661300	4.40174100
H	-2.55707200	1.75750700	3.95417400
H	-2.37233700	4.12064700	-1.01221500
H	-3.42796000	3.30871600	-2.19235800
H	-1.70919200	3.64146000	-2.58271500

### Ac-IM3

H	-1.36275000	1.19736400	-1.18299400
C	-5.14053300	-0.34209400	0.39542300
C	-6.03161400	-1.40548600	0.54245500
C	-5.99511100	-2.47905200	-0.35019300
C	-5.05380200	-2.49169600	-1.38363100
C	-4.15273600	-1.43933800	-1.52094100
C	-4.19073100	-0.34935900	-0.63821100
C	-3.18515600	0.74233700	-0.77307700
C	-3.59815500	2.14896900	-0.50003400
C	-2.66856500	3.07127200	0.00938100
C	-3.03001000	4.40345900	0.19786600
C	-4.31941100	4.83710300	-0.12467600
C	-5.24930200	3.92770000	-0.63210200
C	-4.89357000	2.59101700	-0.81302800
N	-2.00121700	0.40031000	-1.13733500
H	-5.16981400	0.49027700	1.09141900
H	-6.75579800	-1.39341700	1.35237600
H	-5.01901900	-3.32577200	-2.07892900
H	-3.41009100	-1.44497400	-2.31123200
H	-1.67802700	2.72733200	0.28250700
H	-2.30672900	5.10492400	0.60459200
H	-6.25183600	4.25756800	-0.89010100
H	-5.61850400	1.89032200	-1.21426500
H	-4.59774800	5.87715000	0.02182000
H	-6.69726400	-3.30122600	-0.24174900
C	-0.90188100	-0.09878700	2.02226800
O	-0.49039000	-0.71774300	3.14427600
O	-1.47960000	0.97087000	2.00571900

C	-0.57780800	0.06083400	4.35333300	H	1.21535000	-2.04761900	-4.15276000
H	-0.04623100	1.00699500	4.23073200	H	0.57465800	-0.43652700	-4.49146900
H	-0.10418300	-0.54663400	5.12463700				
H	-1.62263700	0.25417600	4.61058900				
C	-0.70876000	-2.94554200	-0.49597000	H	1.46597900	-0.92985700	1.85446200
C	-1.15710800	-2.08762000	0.54195000	C	4.56457200	0.56714300	-0.85917200
C	-2.29419000	-2.47967800	1.30087500	C	5.07367000	1.44898500	-1.80927600
C	-2.93169600	-3.68414400	1.05112100	C	4.20408100	2.17357900	-2.62792900
C	-2.46059100	-4.52058900	0.03265700	C	2.82390300	2.01130000	-2.48829100
C	-1.35451600	-4.14811600	-0.74089300	C	2.30797400	1.14701000	-1.52652400
H	0.13728100	-2.63810700	-1.09410600	C	3.17486000	0.41626300	-0.69823200
H	-2.66974700	-1.82822900	2.08193300	C	2.69154500	-0.48081300	0.36394000
H	-3.80090900	-3.96965100	1.63395400	C	3.33874300	-1.79292900	0.56381600
H	-2.96348100	-5.46341100	-0.16383400	C	3.41914600	-2.38418700	1.83855000
H	-1.00317100	-4.80110200	-1.53411600	C	3.97791100	-3.65005500	1.99548100
C	-0.46641000	-0.87148800	0.82756400	C	4.47417000	-4.34254600	0.88824900
O	1.84467000	0.46979100	1.96872900	C	4.41419800	-3.75765500	-0.37895200
C	2.99233200	0.99927700	2.15193900	C	3.85513900	-2.49241500	-0.54192900
O	3.88781500	1.16345900	1.26931500	N	1.71876500	-0.18506100	1.19627100
C	3.27739800	1.48777900	3.55000000	H	5.24298100	0.01037000	-0.22092200
H	2.92355600	0.75886900	4.28430900	H	6.14833800	1.57024300	-1.90895200
H	4.34484600	1.67232400	3.68476100	H	2.14006300	2.57105500	-3.11971800
H	2.73180100	2.42451600	3.71603200	H	1.23847800	1.04171800	-1.42755000
Rh	3.49851600	0.59573900	-0.67932700	H	3.07532800	-1.84427700	2.71616100
Rh	1.28492100	-0.18238600	0.08715700	H	4.03837700	-4.08907700	2.98681300
C	3.41677700	-2.17755800	0.18515800	H	4.79857300	-4.28920000	-1.24451400
O	4.20971300	-1.30188800	-0.27432300	H	3.79806100	-2.04808700	-1.52865800
O	2.17158600	-2.01252200	0.42729600	H	4.91287900	-5.32807300	1.01380100
C	3.97077300	-3.54422200	0.49913900	H	4.60063000	2.86062200	-3.37008500
H	3.34351400	-4.31527900	0.04095900	C	0.21104500	0.69681700	2.73731600
H	4.99833500	-3.63719200	0.14317700	O	-0.50394900	1.75252300	3.14752700
H	3.94647800	-3.69963800	1.58382600	O	0.36192600	-0.31738000	3.41312500
O	2.64163100	2.44177400	-1.03462300	C	-1.27251500	1.55869700	4.34296900
O	0.60540400	1.72568700	-0.33607800	H	-1.97142100	0.72761000	4.21724000
C	1.40996500	2.61152600	-0.78879500	H	-1.81623000	2.49221200	4.49187700
C	0.82617800	3.98255300	-1.01899200	H	-0.62036400	1.36251300	5.19870500
H	0.69692900	4.47847600	-0.04956500	C	0.31888700	3.24700200	0.64950000
H	1.49312000	4.58532300	-1.63835100	C	1.24094100	2.27706300	1.06504200
H	-0.15805200	3.90456800	-1.48794800	C	2.57597300	2.66447600	1.26346400
O	0.93211900	-0.72536600	-1.87145300	C	2.98967400	3.96890300	0.99999300
O	2.97044600	-0.02091600	-2.57900300	C	2.06890300	4.91914800	0.55409200
C	1.82799500	-0.53963400	-2.76386600	C	0.73009100	4.55450300	0.39440800
C	1.46490800	-0.98119700	-4.15919300	H	-0.71758300	2.96570200	0.52216300
H	2.28883000	-0.79880800	-4.85121200	H	3.30037900	1.94076800	1.62261700

**Ac-IM4**

H	4.03121300	4.24174500	1.14717900	C	4.35939500	0.26677500	0.06188000
H	2.38920200	5.93592400	0.34336200	C	2.88927800	-1.66316800	-0.01822900
H	0.00058000	5.29026000	0.06565000	C	5.43175800	-0.53431500	-0.31520600
C	0.79689000	0.88152100	1.37891000	H	4.51994900	1.32378500	0.24516000
O	-1.19727800	-1.57905200	1.39607000	C	3.96810200	-2.46340100	-0.38293800
C	-2.09023800	-2.46257100	1.18250800	H	1.90437200	-2.09150300	0.10860000
O	-2.91647600	-2.47157800	0.21553700	C	5.23773700	-1.90111600	-0.53784700
C	-2.14357200	-3.61677900	2.15160500	H	6.41973000	-0.09755900	-0.42563300
H	-1.81251800	-3.30027700	3.14341600	H	3.81892700	-3.52608800	-0.55007300
H	-3.15335300	-4.03079000	2.19973600	H	6.07740400	-2.52693100	-0.82681600
H	-1.46532000	-4.40345900	1.79833000	N	1.84506800	0.33418300	2.34156300
Rh	-2.81469200	-0.97622200	-1.20246400	N	1.53056900	-0.19640700	3.26410300
Rh	-0.97933200	-0.00185100	0.09112800	H	1.27565500	4.17673400	-0.72683600
C	-3.63910100	0.94781300	0.80769200	Rh	-2.42889700	-0.51049100	-0.46386200
O	-4.11339100	0.16719100	-0.07757300	C	-1.07055100	-2.49257900	1.18153900
O	-2.40711900	1.09221000	1.09989800	C	-0.94941300	-3.75129800	2.00068000
C	-4.61547200	1.81452700	1.56287200	O	-2.17362100	-2.26472500	0.59987500
H	-4.74046300	2.75902100	1.01888400	O	0.43445400	-0.88755700	-1.63796900
H	-5.59044400	1.32649200	1.63128100	C	0.04582300	-2.10042400	-3.63171000
H	-4.23226500	2.04314300	2.56005200	C	-0.45530900	-1.41391300	-2.38648000
O	-1.40429900	-2.06477600	-2.25223000	O	-1.70647500	-1.42445500	-2.16524700
O	0.29135500	-1.18773100	-1.02890400	O	-0.04117100	-1.73304300	1.15458700
C	-0.17710700	-1.93674900	-1.94999400	O	-2.53241500	1.28503100	-1.47779300
C	0.83275400	-2.71763500	-2.75215800	O	-0.86316100	0.94420800	1.81811100
H	1.50622800	-3.25536100	-2.07852200	O	-3.00755700	0.45120600	1.26911400
H	0.33659900	-3.41933800	-3.42492400	C	-2.59420300	1.71054700	3.24437700
H	1.43833900	-2.01843800	-3.34040200	C	-2.12394400	0.96915600	2.01999800
O	-0.88943000	1.46096800	-1.37438800	O	-0.39686700	1.81013500	-0.92400900
O	-2.60763000	0.57064200	-2.55586200	C	-1.51711100	2.04762400	-1.48650400
C	-1.69111500	1.43016300	-2.36505400	C	-1.63565300	3.37009700	-2.20118200
C	-1.49725700	2.49374800	-3.41644100	Rh	-0.11813700	0.05120200	0.11940100
H	-2.43375700	2.69494000	-3.94170100	H	0.57385800	-3.01779900	-3.34609000
H	-1.10656100	3.40935300	-2.96602700	H	-0.78209100	-2.35489900	-4.29584500
H	-0.76407600	2.13117000	-4.14785600	H	0.76102300	-1.45510100	-4.15030500
				H	-1.76457500	-4.44035700	1.77251100
				H	-0.99257000	-3.48674300	3.06400700
<b>Ac-TS1</b>				H	0.01576800	-4.23213500	1.81676300
C	1.91819500	0.55299700	0.59603400	H	-1.84067900	1.66566700	4.03402300
C	2.05676300	2.04419900	0.54636600	H	-3.54426200	1.30369300	3.59787800
O	1.82823800	2.81818500	1.45632100	H	-2.74716600	2.76376000	2.97791600
O	2.38247300	2.40869600	-0.70181700	H	-1.78463300	4.16261500	-1.45788800
C	2.27195500	3.81604900	-0.98792400	H	-2.48565800	3.36495700	-2.88636000
H	2.44516100	3.90699700	-2.06007900	H	-0.71292400	3.58839500	-2.74571800
H	3.02860000	4.37635800	-0.43200000				
C	3.06884600	-0.28419100	0.20022700				



**Ac-TS2**

			C	-0.49848600	-0.86003200	0.78937600	
H	-1.32750700	1.23234700	-1.06977300	O	1.82601400	0.43992300	1.97274800
C	-5.13655300	-0.36252800	0.37977700	C	2.97541500	0.95932000	2.17232500
C	-6.01483600	-1.44037000	0.49374800	O	3.87597600	1.13793800	1.29742100
C	-5.93090400	-2.51053300	-0.40008800	C	3.25722300	1.41622300	3.58167500
C	-4.95466800	-2.50619300	-1.40038500	H	2.89025600	0.67690700	4.29904700
C	-4.06548800	-1.44017000	-1.50384700	H	4.32591800	1.58542300	3.72657400
C	-4.15156400	-0.35325400	-0.62045700	H	2.72214500	2.35614700	3.76326300
C	-3.16056900	0.75311500	-0.72291600	Rh	3.49452300	0.60684400	-0.66252400
C	-3.60097700	2.15495000	-0.47537900	Rh	1.27174900	-0.17296800	0.07614400
C	-2.69570900	3.09432200	0.04758300	C	3.38995900	-2.18134400	0.15397200
C	-3.07930500	4.42252400	0.21718500	O	4.19057500	-1.30246400	-0.28618900
C	-4.36734000	4.83518200	-0.13719800	O	2.14453700	-2.01375800	0.39178400
C	-5.27320000	3.90895300	-0.65772800	C	3.93537600	-3.55589700	0.44836500
C	-4.89518200	2.57616200	-0.82093100	H	3.30129800	-4.31674500	-0.01727600
N	-1.95709700	0.42813400	-1.03844200	H	4.96130000	-3.65138100	0.08828000
H	-5.20195500	0.46764500	1.07597800	H	3.91364500	-3.72475100	1.53114200
H	-6.76626900	-1.44258500	1.27852200	O	2.65009400	2.46559000	-0.98893900
H	-4.88253800	-3.33781500	-2.09558900	O	0.60768600	1.74860000	-0.31207400
H	-3.29590600	-1.43154900	-2.26785400	C	1.41916900	2.63882900	-0.74294400
H	-1.70737100	2.76615600	0.34668500	C	0.84395600	4.01837600	-0.94259400
H	-2.37458300	5.13682200	0.63396300	H	0.71633500	4.49261500	0.03796500
H	-6.27423800	4.22303300	-0.93994900	H	1.51453400	4.63154800	-1.54768900
H	-5.60099800	1.86261300	-1.23340300	H	-0.14058200	3.95677500	-1.41360600
H	-4.66323200	5.87229000	-0.00507500	O	0.92766100	-0.68119600	-1.89419700
H	-6.62342700	-3.34380000	-0.31773900	O	2.97401600	0.02659600	-2.57581100
C	-0.92400200	-0.10100200	1.99884600	C	1.83016500	-0.48295000	-2.77733300
O	-0.52130300	-0.75793900	3.10443000	C	1.47467500	-0.89729900	-4.18297200
O	-1.47384700	0.98280900	2.01659300	H	2.30102400	-0.69842100	-4.86753900
C	-0.58284900	-0.00674900	4.33169900	H	1.22946600	-1.96466200	-4.19882700
H	-0.04406300	0.93689700	4.22350700	H	0.58386300	-0.34955800	-4.50853800
H	-0.10497700	-0.63692600	5.08200900				
H	-1.62204300	0.19067800	4.60847500				
C	-0.71409700	-2.93945800	-0.53166300	<b>B-IM1</b>			
C	-1.16687100	-2.09423800	0.51346200	H	-0.44055300	-2.03405800	-0.26128100
C	-2.28293900	-2.51381500	1.28651400	C	1.23628200	-1.03405700	-0.06647600
C	-2.89175500	-3.73597600	1.04752200	C	1.77859900	-2.34040300	-0.35397400
C	-2.41533600	-4.56080200	0.02266300	O	1.08134700	-3.31430500	-0.66967900
C	-1.33263600	-4.15821700	-0.76857300	O	3.12372500	-2.42896000	-0.21559600
H	0.11396200	-2.60949300	-1.14321100	C	3.68370800	-3.72538300	-0.46208800
H	-2.66468000	-1.87223000	2.07246200	H	3.46720200	-4.05888400	-1.48120600
H	-3.74399400	-4.04344300	1.64438400	H	3.29284100	-4.46170300	0.24631700
H	-2.89609100	-5.51673000	-0.16580200	N	-0.13454300	-1.06160200	-0.14029500
H	-0.97712500	-4.80074500	-1.56855100	C	-1.11584300	-0.15480900	-0.14974500
				C	1.99674500	0.11988800	0.41462900

C	3.20326500	0.50618900	-0.19853000	C	-1.28159700	0.74451800	0.56743600
C	1.52984000	0.88932200	1.49823300	C	-3.55021700	-0.33604100	-0.69200400
C	3.90849500	1.62062900	0.24995500	H	-2.26126400	-1.97385800	-1.25917800
H	3.57802300	-0.06924700	-1.03763500	C	-2.48761600	1.42126600	0.62816300
C	2.23295500	2.00539700	1.94094800	H	-0.40037900	1.15009700	1.05546500
H	0.60780500	0.60686900	1.99569800	C	-3.61743600	0.88204600	-0.00549700
C	3.42473400	2.38148800	1.31656600	H	-4.43586600	-0.73686000	-1.17482300
H	4.83391300	1.90319500	-0.24520400	H	-2.56315700	2.36660100	1.15657400
H	1.84762800	2.58435100	2.77590100	H	-4.56070800	1.41933100	0.03954900
H	3.96975100	3.25722300	1.65780200	H	3.89326600	0.74724300	-0.67068800
C	-2.47823400	-0.67340000	0.00620100				
C	-2.72844300	-1.85866600	0.72928700				
C	-3.57272500	-0.01384600	-0.59025700				
C	-4.01828100	-2.37494800	0.82850600				
H	-1.91435800	-2.35870300	1.24687800				
C	-4.86021800	-0.52787500	-0.47670300				
H	-3.40221600	0.89363200	-1.15935500				
C	-5.09092400	-1.71336800	0.22790400				
H	-4.18699500	-3.28711100	1.39402000				
H	-5.68743500	-0.00718000	-0.95104300				
C	-0.85286900	1.27660400	-0.33530300				
C	-1.55030400	2.23242700	0.42529000				
C	0.09513600	1.72488900	-1.27321700				
C	-1.29351500	3.59185000	0.26600700				
H	-2.28221100	1.90184300	1.15525100				
C	0.34341200	3.08392800	-1.43613500				
H	0.63421700	1.00304300	-1.87634100				
C	-0.34325500	4.02287800	-0.66233800				
H	-1.83151400	4.31506500	0.87239600				
H	1.08011600	3.41063700	-2.16431600				
H	-0.13930700	5.08308800	-0.78279100				
H	4.75986500	-3.60749100	-0.32495500				
H	-6.09768000	-2.11181300	0.31406700				

**B-IM1-t**

C	-0.54001000	-0.99612900	0.05724800
C	-1.92439400	-0.62246200	0.05310700
O	-2.84578100	-1.43049800	0.05418600
O	-2.11372100	0.72342900	0.04994400
C	-3.48759100	1.15452600	0.04078400
H	-4.00392200	0.81254500	0.94203700
H	-4.00584300	0.77102900	-0.84225400
C	0.74507600	-0.43950900	0.03292700
C	1.88071200	-1.29736500	0.08576800
C	0.96448300	0.96857800	-0.04918100
C	3.16376700	-0.77347300	0.06018800
H	1.72223800	-2.36932800	0.14730200
C	2.25630000	1.47195700	-0.07439100
H	0.10877600	1.63157400	-0.09117300
C	3.36046100	0.61124600	-0.01999100
H	4.01866300	-1.44208800	0.10226300
H	2.41005500	2.54554500	-0.13707200
H	4.36735500	1.01731800	-0.04018600
H	-3.44896400	2.24427000	0.01578000

**B-IM2-s**

H	-0.05687900	-1.87963400	-2.98616900
N	-0.85548400	-1.72553300	-2.36214600
C	-0.44560500	-1.62532900	-1.14607300
C	0.99800200	-1.66657900	-0.77052400
C	1.93430900	-0.97838200	-1.55597100
C	1.44643200	-2.39420300	0.34230300
C	3.28856000	-1.00307800	-1.22761800
H	1.59268800	-0.38313800	-2.39573400
C	2.80310300	-2.43307200	0.65917800
H	0.73156100	-2.93643200	0.95309900
C	3.72681200	-1.73127700	-0.12085300

**B-IM1-s**

C	0.02562200	-1.23788400	-0.24716500
C	1.22550200	-0.76007600	0.37999600
O	1.49087600	-1.07711200	1.53918400
O	2.05955000	-0.07722500	-0.43237300
C	3.34370400	0.25292800	0.13118600
H	3.87169100	-0.64962100	0.45049000
H	3.23228200	0.92854000	0.98394300
C	-1.17866500	-0.50056400	-0.12040300
C	-2.34658600	-1.02378000	-0.74177300

H	3.99846200	-0.44404500	-1.83041400	C	-1.05255100	-1.06398400	-0.75836100
H	3.14018400	-3.00966400	1.51619300	C	2.44406000	-1.44388800	0.70222900
C	-1.46153800	-1.42983800	-0.07330600	C	2.97342500	-2.48413000	-0.11057700
C	-1.13082900	-0.83140700	1.15238600	C	3.06501100	-0.16237800	0.65336500
C	-2.79435300	-1.80475400	-0.30579400	C	4.07273800	-2.25351600	-0.92320500
C	-2.10736800	-0.63015300	2.12809500	H	2.49143700	-3.45596500	-0.09097800
H	-0.11713000	-0.49002900	1.32766100	C	4.16352200	0.04817500	-0.16594100
C	-3.76798200	-1.60215900	0.66818500	H	2.65884200	0.64121500	1.25509700
H	-3.04870800	-2.25841100	-1.25746900	C	4.67656300	-0.98990700	-0.95371100
C	-3.42637200	-1.01803200	1.89177000	H	4.46259200	-3.05721400	-1.54136500
H	-1.83655600	-0.15983600	3.06938200	H	4.62379600	1.03160100	-0.19941600
H	-4.79401900	-1.90427900	0.47675800	H	5.53749100	-0.81341500	-1.59194400
C	0.63795200	1.98200600	-1.17405400	C	-2.37526500	-0.53448300	-0.31092200
C	1.34552400	2.31706800	0.02993000	C	-2.93863100	-0.98825000	0.89243000
O	1.70886300	3.46921300	0.26154100	C	-3.09393000	0.38031100	-1.09607500
O	1.67700500	1.25188400	0.79643900	C	-4.19085000	-0.53287800	1.30243900
C	2.63463400	1.49738500	1.84052900	H	-2.37675200	-1.66873200	1.52416400
H	2.81111800	0.52597700	2.30283000	C	-4.35390000	0.82056200	-0.69265800
H	2.23878600	2.20135400	2.57784900	H	-2.66906600	0.73540400	-2.02961400
C	-0.77400400	1.91794500	-1.18598000	C	-4.90374600	0.36901900	0.50912700
C	-1.40940800	1.48922800	-2.38519400	H	-4.60652100	-0.87965200	2.24431600
C	-1.59436200	2.18910000	-0.05009200	H	-4.90592400	1.51790500	-1.31656300
C	-2.78199100	1.30479800	-2.43747000	C	-0.07349300	-0.12657200	-1.37340100
H	-0.78397200	1.28782200	-3.24786800	C	-0.05047100	1.23399900	-1.03281000
C	-2.96723300	2.03854000	-0.11670600	C	0.88758400	-0.61832200	-2.27034100
H	-1.12405000	2.52016000	0.87059100	C	0.90980100	2.08382500	-1.58085600
C	-3.55557700	1.57952200	-1.30478100	H	-0.77319400	1.62401700	-0.32490900
H	-3.25484400	0.94442800	-3.34516700	C	1.83745700	0.23245000	-2.82615700
H	-3.58648900	2.24132800	0.75081900	H	0.87438000	-1.67299000	-2.52122000
H	-4.63150200	1.43420700	-1.34417800	C	1.85172900	1.58727100	-2.48259300
H	3.56644400	1.89135000	1.42539900	H	0.92237300	3.13350000	-1.30080700
H	4.78231400	-1.75152900	0.13622100	H	2.57280900	-0.16104300	-3.52165400
H	-4.18633300	-0.86472000	2.65326700	H	-5.88099400	0.72105800	0.82755100
				H	2.59665700	2.25064600	-2.91357000
				H	-0.37316900	2.12265500	2.66182500

**B-IM2-t**

H	-1.47715100	-2.83429300	-0.20813600
C	1.34515000	-1.70513400	1.53037300
C	0.36691800	-1.02098300	2.31835800
O	-0.42576000	-1.58173500	3.06973800
O	0.38751800	0.32585500	2.13340000
C	-0.57724600	1.07619800	2.89189600
H	-0.45434900	0.89257900	3.96267900
H	-1.59388500	0.81282300	2.58993700
N	-0.71022300	-2.29804600	-0.62597100

**B-TS1**

H	0.38921600	-2.20749600	0.00381000
N	-0.02753200	-1.32627900	-0.30460900
C	0.83285000	-0.36845400	-0.61688000
C	0.23593900	0.89758400	-1.04811700
C	-1.01698600	0.87506500	-1.69107700
C	0.81378600	2.14053100	-0.72441800
C	-1.68640900	2.06186100	-1.97741500

H	-1.44040400	-0.08031800	-1.98050600	O	-1.68077700	-1.03743300	0.17480900
C	0.14057100	3.32124400	-1.01130700	C	-3.00357400	-1.48706700	-0.16922000
H	1.76049700	2.16983600	-0.19716100	H	-3.08776700	-2.48943200	0.25245500
C	-1.11484700	3.28640000	-1.63005100	H	-3.13051000	-1.52123000	-1.25478800
H	-2.65537000	2.02972400	-2.46704000	C	1.11404400	0.00854700	0.21727800
H	0.58190200	4.27319100	-0.73090700	C	2.21380300	0.37747900	1.02739900
C	2.28283300	-0.57653400	-0.53444900	C	1.30743000	-0.98249300	-0.77555700
C	2.83399500	-1.51113600	0.36679700	C	3.45827500	-0.21261400	0.84921600
C	3.15908400	0.13220800	-1.38104600	H	2.06076400	1.13458200	1.79046200
C	4.20829300	-1.70945500	0.43285800	C	2.54492500	-1.59367200	-0.93116200
H	2.18532500	-2.06705100	1.03818200	H	0.47231000	-1.27487900	-1.40367400
C	4.53372000	-0.07738900	-1.31712700	C	3.62115400	-1.20229500	-0.12659800
H	2.75431800	0.83458500	-2.10140300	H	4.29822100	0.08208500	1.47089500
C	5.06654700	-0.99505700	-0.40898800	H	2.68244500	-2.36241100	-1.68571500
H	4.61313400	-2.42201900	1.14579600	H	4.59141300	-1.67282500	-0.25949100
H	5.19085500	0.47497800	-1.98283100	N	0.00589900	2.45537200	-0.28208800
C	-1.33550500	-0.98838300	0.89105300	N	0.13039500	3.53820000	-0.06628000
C	-2.60040000	-1.18660400	0.15048300	H	-3.76273000	-0.82944700	0.26332700
O	-3.62648500	-0.53996100	0.30646000				
O	-2.53147900	-2.29072700	-0.62299500				
C	-3.76126900	-2.67002300	-1.26434100	<b>B-TS1-t</b>			
H	-4.10430400	-1.88152200	-1.93955500	C	0.08954900	0.76290000	0.03014500
H	-4.53563500	-2.87321800	-0.51977800	C	1.48314800	0.42894800	0.24514900
C	-1.01518600	0.25157900	1.62071900	O	2.34544600	1.24605200	0.53317800
C	0.22982400	0.33504200	2.27239100	O	1.73715200	-0.89115500	0.07136000
C	-1.86666500	1.37155700	1.64689500	C	3.10397500	-1.28758300	0.29376300
C	0.60982700	1.49864400	2.93826500	H	3.12166200	-2.36563600	0.13159400
H	0.90634100	-0.51209200	2.24920600	H	3.41246200	-1.05063600	1.31554600
C	-1.47235300	2.53228000	2.30318900	C	-1.11981000	0.03717400	-0.00387000
H	-2.82172300	1.32568200	1.14394300	C	-2.31424700	0.61874800	-0.51513200
C	-0.23505700	2.60747500	2.95131100	C	-1.18762600	-1.29651000	0.49909500
H	1.57699400	1.53912800	3.43181600	C	-3.50171200	-0.09654300	-0.52494300
H	-2.13806900	3.39103300	2.30146000	H	-2.29116400	1.62382600	-0.91799500
H	0.06555600	3.52175700	3.45513000	C	-2.38556000	-1.99349700	0.48575500
N	-0.97155700	-2.15712400	1.72445000	H	-0.29089400	-1.75665500	0.89376100
N	-1.43817400	-2.91686200	2.47862500	C	-3.54852800	-1.40280200	-0.02370500
H	-3.52806000	-3.57429300	-1.82742200	H	-4.39927100	0.36349300	-0.92757900
H	6.13937900	-1.15671500	-0.35980800	H	-2.41763400	-3.00627600	0.87710100
H	-1.64128200	4.21256700	-1.84258800	H	-4.48280700	-1.95608300	-0.03108000
				N	-0.79270100	3.22493400	0.32871200
				N	0.04907400	2.61732800	-0.13344900
				H	3.76884400	-0.78462800	-0.41331000
<b>B-TS1-s</b>							
C	-0.15927800	0.63501000	0.46977000				
C	-1.38286700	0.23665400	-0.21175300	<b>B-TS2</b>			
O	-2.13063100	0.92126900	-0.89429600	H	0.20578000	-1.75669300	0.83651500

C	1.17405200	-1.18027600	0.05051100	<b>B-TS2-s</b>			
C	1.78508900	-2.44018900	-0.41572400	H	-0.52605600	-1.10966900	-1.50242800
O	1.19981400	-3.36789900	-0.95401200	C	2.25735200	0.04109600	0.52145800
O	3.10998200	-2.48318400	-0.11949600	C	3.23282700	0.57527200	-0.39200900
C	3.78150000	-3.69042500	-0.50542000	O	2.96987300	1.17176300	-1.43234400
H	3.70643000	-3.85243100	-1.58463700	O	4.49182300	0.47447400	0.11478600
H	3.35887200	-4.55399500	0.01630000	C	5.50154600	1.22032300	-0.58857900
N	-0.25348500	-1.19695800	-0.12344300	H	5.25038300	2.28456800	-0.61657500
C	-1.14702800	-0.23063000	-0.11071500	H	5.62132400	0.85017300	-1.61052200
C	1.97525200	0.02897400	0.34043500	N	-0.28033100	-0.18012000	-1.14742700
C	3.04488500	0.41612200	-0.48338200	C	-1.30039400	0.38230700	-0.60403200
C	1.64226900	0.84640500	1.43252700	C	1.95424500	-1.34590600	0.54684700
C	3.74547100	1.59418300	-0.23247000	C	1.01352400	-1.79955400	1.50989800
H	3.31788300	-0.20412100	-1.33022200	C	2.53325000	-2.30218400	-0.33288100
C	2.33692800	2.02657900	1.67925200	C	0.67055400	-3.14151200	1.59520400
H	0.82485800	0.55665300	2.08560500	H	0.56857600	-1.06107400	2.16867700
C	3.38898300	2.40878600	0.84393900	C	2.18372200	-3.64106200	-0.25186400
H	4.56470400	1.88206200	-0.88580000	H	3.24802500	-1.96622500	-1.07793000
H	2.05475400	2.64967000	2.52308900	C	1.25426100	-4.05800700	0.71149900
H	3.92857700	3.33242100	1.03378600	H	-0.04659100	-3.48157700	2.33591100
C	-2.55400100	-0.64034600	0.07451200	H	2.62443400	-4.36668900	-0.92869100
C	-2.87283100	-1.90437400	0.60927300	H	0.98328600	-5.10853500	0.77251900
C	-3.61472700	0.20808600	-0.29703200	C	-2.62810200	-0.29703500	-0.50655500
C	-4.19670700	-2.29829300	0.77240100	C	-2.68923300	-1.64464700	-0.11992300
H	-2.07146600	-2.57774300	0.89312500	C	-3.81563100	0.36574300	-0.85186900
C	-4.94002600	-0.18870600	-0.12948300	C	-3.91098600	-2.31413600	-0.07614700
H	-3.39989100	1.17652700	-0.73427700	H	-1.77538500	-2.15989600	0.16299600
C	-5.23959500	-1.44143600	0.40793900	C	-5.03525300	-0.30930600	-0.82112800
H	-4.41700300	-3.27701400	1.18995200	H	-3.77899000	1.40588100	-1.16001800
H	-5.74053500	0.48239600	-0.42859100	C	-5.08715200	-1.64868000	-0.42899000
C	-0.81505700	1.19983800	-0.30774200	H	-3.94554400	-3.35401300	0.23686700
C	-1.31596900	2.17838500	0.56668800	H	-5.94577100	0.21207600	-1.10293100
C	0.03385100	1.59755100	-1.35203500	C	-1.13049500	1.75092400	-0.04255000
C	-0.95098500	3.51483200	0.41943000	C	-2.01737500	2.27532200	0.90990800
H	-1.97224200	1.88237300	1.37926200	C	-0.01912200	2.51893900	-0.43216400
C	0.39303700	2.93439300	-1.50265700	C	-1.80653200	3.54330000	1.45278500
H	0.41436100	0.85222400	-2.04258100	H	-2.86577800	1.68732800	1.24257600
C	-0.09093400	3.89574500	-0.61270000	C	0.18544400	3.78475100	0.10781000
H	-1.33184200	4.25755400	1.11493300	H	0.68448900	2.10198900	-1.14404900
H	1.05838000	3.22472900	-2.31050100	C	-0.70840400	4.30355400	1.04994400
H	-6.27303800	-1.74924100	0.53996700	H	-2.49927900	3.93276400	2.19370500
H	0.19787600	4.93690700	-0.72569000	H	1.04808500	4.36764500	-0.20326400
H	4.82404100	-3.54970200	-0.21639000	H	-0.54617100	5.29248000	1.47026600
				H	-6.03941300	-2.17067400	-0.39760100

H	6.42226400	1.06689900	-0.02381800	H	-1.91714600	-2.60866800	2.31916600
				H	-1.22177400	-4.18410600	-1.46912400
				H	6.37789900	1.12634300	0.44642000
<b>B-TS2-t</b>							
H	0.91391400	2.46150400	-0.57654900				
C	-1.34199100	1.39669000	0.72217000	<b>B-TS2-w</b>			
C	-0.86711200	0.38101800	1.61477600	H	0.60414700	-2.19338100	-0.27998700
O	0.19633400	0.43844400	2.22747100	C	-1.17608200	-1.25084600	-0.39844400
O	-1.68543900	-0.70766100	1.67158400	C	-2.07550100	-1.58455300	0.72481100
C	-1.20055300	-1.79968500	2.46796600	O	-1.71807300	-1.90672500	1.84943800
H	-1.15735500	-1.52101500	3.52538500	O	-3.37142800	-1.59875900	0.33633700
H	-0.20723700	-2.10861300	2.13437000	C	-4.31405600	-2.00822900	1.33932400
N	0.40167800	1.60933900	-0.81819600	H	-5.29574300	-1.90954400	0.87408500
C	1.17580600	0.57275000	-0.78323900	H	-4.24670400	-1.36741400	2.22276000
C	-2.58889600	1.79140100	0.20509700	N	0.23634600	-1.25283900	0.03179200
C	-2.65885600	2.65173000	-0.92524800	C	1.02370300	-0.26209600	0.32453100
C	-3.81297800	1.37766300	0.80718700	C	-1.49941600	-0.13440100	-1.34744800
C	-3.88452700	3.06534400	-1.42688400	C	-2.44983000	0.86186000	-1.08899700
H	-1.73139300	2.96019800	-1.39371300	C	-0.76846700	-0.06384400	-2.54480700
C	-5.03004300	1.80123000	0.29294100	C	-2.65495500	1.90232200	-1.99511600
H	-3.77878200	0.71918000	1.66768100	H	-3.02434300	0.83136700	-0.17090400
C	-5.07698800	2.64536100	-0.82389800	C	-0.96370100	0.98080400	-3.44542400
H	-3.91732600	3.71665000	-2.29612400	H	-0.03643700	-0.83756500	-2.76083700
H	-5.95320800	1.47211400	0.76246700	C	-1.90986000	1.97194700	-3.17328500
H	-6.03399900	2.97143000	-1.22090900	H	-3.39105700	2.66933300	-1.76935000
C	2.61527100	0.67684400	-0.42683200	H	-0.38317800	1.01699400	-4.36359100
C	2.99807800	1.44019500	0.68728900	H	-2.06533500	2.78866900	-3.87281000
C	3.60336000	0.06652100	-1.21443300	C	2.47781000	-0.47303000	0.28743100
C	4.34668600	1.59522800	1.00159100	C	3.03360000	-1.52728600	-0.46471000
H	2.22823400	1.86692300	1.32249300	C	3.32884200	0.38196600	1.00981400
C	4.95205500	0.23682600	-0.90531000	C	4.41039600	-1.71585000	-0.48552400
H	3.31232400	-0.52778800	-2.07531600	H	2.39471300	-2.18809200	-1.04404500
C	5.32666200	1.00132200	0.20228400	C	4.70627400	0.18221200	0.98801900
H	4.63298200	2.17407200	1.87523400	H	2.90704400	1.18899000	1.59780400
H	5.71069700	-0.22749900	-1.52918400	C	5.24911500	-0.86439900	0.24049600
C	0.56926900	-0.75316900	-1.04509000	H	4.83217600	-2.52486000	-1.07398300
C	1.15639800	-1.92960100	-0.55205800	H	5.35500800	0.84207000	1.55588800
C	-0.67260500	-0.83541100	-1.69833100	C	0.46023000	1.06081100	0.65676100
C	0.51399000	-3.15795500	-0.70516100	C	0.87417100	2.19528900	-0.05598200
H	2.10266200	-1.87843900	-0.02485800	C	-0.50961100	1.17708600	1.66294000
C	-1.31007900	-2.06177900	-1.85195100	C	0.29373600	3.43210500	0.21398500
H	-1.12840900	0.07347600	-2.07381800	H	1.61901200	2.09672800	-0.83890200
C	-0.72073600	-3.22711400	-1.35249400	C	-1.06047300	2.42356200	1.94923600
H	0.97472500	-4.05884000	-0.30984400	H	-0.81789000	0.29430800	2.21210900
H	-2.26988000	-2.11025800	-2.35845600	C	-0.66921800	3.54822200	1.21889800

H	0.59487200	4.30477200	-0.35758200	N	-1.33025400	-0.85680900	0.38725600
H	-1.80240800	2.51526100	2.73701100	H	-1.06574900	-1.68449700	-0.13047000
O	-0.05658200	-3.36460300	-1.34485000	C	3.09897900	0.36686200	1.65955800
H	-0.97747100	-2.35361400	-1.02805100	H	4.02935500	-0.06471400	1.26404600
H	0.13856100	-3.17956700	-2.27819500	C	1.51932000	-1.43016400	2.16070800
H	-4.13874100	-3.04683600	1.63382500	H	2.02671900	-2.35968900	1.88326500
H	6.32428900	-1.01708500	0.22087200	H	0.68407000	-1.69515000	2.81592300
H	-1.11347000	4.51584000	1.43404400	H	2.42840600	2.26410000	-1.92633000
				C	1.06106300	2.81336700	-0.43186000
<b>G1</b>				C	1.43132300	4.29527600	-0.31797700
C	-2.75277100	-0.54664600	0.50560800	C	-0.21257300	2.63024600	-1.27044400
C	-3.52016600	-1.83190300	0.79115700	H	0.86573200	2.41755000	0.56512900
C	-4.00040900	-2.64413100	-0.24196100	C	0.26437100	5.11170900	0.25597000
C	-3.70060800	-2.24144500	2.11782900	H	1.69491900	4.68077700	-1.31499400
C	-4.64743400	-3.84697200	0.04666300	H	2.32356800	4.40352400	0.31058300
H	-3.88045300	-2.32923800	-1.27441500	C	-1.38142100	3.43536300	-0.69177900
C	-4.35267300	-3.43955100	2.40860200	H	-0.01275000	2.95039200	-2.30496700
H	-3.32769100	-1.61414300	2.92376900	H	-0.47317200	1.56863500	-1.31066600
C	-4.82664700	-4.24720800	1.37198200	C	-1.01983700	4.92051500	-0.56283500
H	-5.01729100	-4.46768900	-0.76494400	H	0.53583600	6.17409800	0.29991800
H	-4.49319800	-3.74104800	3.44304800	H	0.08052100	4.78985500	1.29104000
H	-5.33759200	-5.17949700	1.59618600	H	-2.27251100	3.30628000	-1.31680100
C	-3.29610700	0.22266500	-0.69057000	H	-1.62713900	3.02858600	0.29801400
C	-4.45019900	0.99762500	-0.52531200	H	-1.84690900	5.47619400	-0.10248800
C	-2.69750200	0.16128400	-1.95160600	H	-0.87439000	5.34603600	-1.56713400
C	-4.99410100	1.70163200	-1.59814200	C	3.28697200	-1.41298100	-1.32271300
H	-4.92073300	1.04990500	0.45354800	C	2.48858000	-2.42181000	-2.16594400
C	-3.23985600	0.86536300	-3.02958100	C	4.78893400	-1.55173600	-1.62699100
H	-1.79436800	-0.42449800	-2.09259000	H	3.14981300	-1.67279100	-0.26222300
C	-4.38852400	1.63804500	-2.85630400	C	2.96575200	-3.85995300	-1.92960800
H	-5.88588500	2.30488500	-1.45154600	H	2.60793900	-2.15617900	-3.22546300
H	-2.75861700	0.81297500	-4.00235700	H	1.41829200	-2.32710900	-1.93953100
H	-4.80811000	2.18949100	-3.69309900	C	5.28157500	-2.98564400	-1.39227600
H	-2.82847000	0.10269100	1.38116700	H	4.96111100	-1.26039500	-2.67245800
C	2.51417100	-0.46572400	2.82541500	H	5.35130500	-0.84445300	-1.00445800
H	3.31048800	-1.03616100	3.31204700	C	4.46838400	-4.00002500	-2.20725800
N	2.18869400	2.04236400	-0.96375000	H	2.39530100	-4.55566600	-2.55801300
N	2.84995900	-0.06067300	-1.62314700	H	2.76277900	-4.14171000	-0.88544800
N	2.03558200	0.32397900	0.63513000	H	6.34716500	-3.06310500	-1.64229300
C	2.36574400	0.69594800	-0.70054100	H	5.19284900	-3.22791600	-0.32273900
C	1.04943000	-0.72252000	0.86577200	H	4.80272600	-5.02177900	-1.98678600
H	1.02416100	-1.43977200	0.03800200	H	4.65214300	-3.83091100	-3.27823500
O	-0.61823500	0.84962300	1.71067600	C	1.92229000	0.56878700	3.82817900
C	-0.36665700	-0.14464700	1.02907800	H	0.86234400	0.38203500	4.02195200

H	2.44927800	0.48796600	4.78593000	H	5.71362000	-0.67879600	-1.66126600
C	3.32324200	1.76828700	2.23919400	H	4.67994500	-0.90018100	-3.07278500
H	3.39186800	2.53218900	1.45932700	C	-2.93396700	-0.06782000	-0.89892100
H	4.27357800	1.76804000	2.79076400	C	-3.32742200	1.38089300	-1.23395600
C	2.14337400	1.96316000	3.20257600	C	-4.06014700	-1.02742200	-1.32313200
H	2.33482300	2.73828900	3.95253900	H	-2.83336300	-0.15230600	0.19365000
H	1.24985600	2.24615700	2.64289200	C	-4.66387000	1.77387100	-0.59252300
<b>G2</b>				H	-3.39548800	1.47249700	-2.32680200
C	2.09870200	3.23739900	0.49866700	H	-2.52904700	2.06330200	-0.91321300
H	2.93134700	2.53939700	0.37047200	C	-5.40012900	-0.64685500	-0.68047300
C	-0.86522200	-1.35292400	2.71531500	H	-4.14727400	-0.99805900	-2.41821400
H	-1.70430400	-1.76582100	3.28253500	H	-3.78148700	-2.05437500	-1.05487600
N	0.38774400	-1.35283300	-1.66153600	C	-5.78172300	0.80440300	-0.99858900
N	-1.71008500	-0.41793200	-1.59858900	H	-4.92932000	2.80129000	-0.87272200
N	-0.44746300	-0.75011900	0.45293400	H	-4.55825900	1.76444500	0.50269300
C	-0.65921000	-0.78877400	-0.95378700	H	-6.18778500	-1.33153400	-1.01953300
C	-0.53463800	0.52893300	1.15549500	H	-5.32655900	-0.76952600	0.41035500
H	-1.24279400	1.20730200	0.66712800	H	-6.71913400	1.07151800	-0.49437600
O	1.82949900	0.70326300	1.72052700	H	-5.96507900	0.89946100	-2.07863300
C	0.84155100	1.21356200	1.18461300	C	0.47656200	-1.84480900	3.33412700
N	0.88710200	2.41622100	0.56302700	H	1.06571900	-1.01506400	3.73300400
H	0.03557100	2.79213100	0.16519000	H	0.26383100	-2.52831000	4.16455400
C	-0.88672600	-1.90127600	1.26793800	C	0.11819800	-3.05955800	1.26278400
H	-1.88932700	-2.22837000	0.95778200	H	0.46314600	-3.30581000	0.25479900
C	-1.04040300	0.16829300	2.56998100	H	-0.37647900	-3.95065500	1.67332100
H	-2.10113400	0.43092100	2.63769400	C	1.22934900	-2.58336200	2.20869900
H	-0.51242600	0.72478300	3.34899300	H	1.85141100	-3.40509900	2.57976400
H	0.19367900	-1.36619300	-2.65905100	H	1.87903800	-1.87328600	1.69238100
C	1.79501900	-1.12889700	-1.32431000	C	2.01751600	4.15724700	-0.71684400
C	2.64275800	-2.33374200	-1.74736200	H	1.89409700	3.58233200	-1.64126900
C	2.34457400	0.16767100	-1.94183700	H	1.17366300	4.85425700	-0.62917000
H	1.83608100	-1.03064400	-0.23867500	H	2.93248200	4.75217200	-0.80367800
C	4.11961300	-2.12835100	-1.38355200	C	2.30712800	4.00758300	1.80565900
H	2.54737100	-2.47662000	-2.83460000	H	3.24092200	4.58060700	1.76991200
H	2.25111300	-3.24100600	-1.27243100	H	1.48076400	4.70657800	1.98343300
C	3.81545300	0.37701600	-1.55896700	H	2.36342700	3.31273300	2.64908700
H	2.24940000	0.11227400	-3.03701500	<b>G3</b>			
H	1.73695800	1.01554900	-1.60811400	O	2.17767200	0.32932200	3.17610100
C	4.67247700	-0.82515400	-1.97529300	H	-0.19750600	0.70382200	1.13205100
H	4.71318900	-2.98554300	-1.72515200	N	0.72757500	0.89542600	1.51629500
H	4.21522100	-2.09450300	-0.28884400	N	-0.03576200	-1.88972900	1.65079300
H	4.19915100	1.29919300	-2.01388600	N	-1.23289600	-2.44685200	-0.28061500
H	3.87838400	0.50793300	-0.46989500	H	-2.05250800	-2.20514800	-0.82737600



N	-1.81765100	-0.53813600	1.05964900	H	0.32553700	-2.51649400	-4.52916600
C	0.77034500	-2.01779800	3.90319500	C	0.72805000	-4.10205700	-3.11555500
H	0.44016700	-1.75731400	4.91205300	H	0.44069400	-4.89246800	-3.81964400
H	1.86250100	-1.95782000	3.88657800	H	1.58831400	-4.48499600	-2.54771200
C	0.19271000	-1.05395200	2.85600700	C	-0.42893200	-3.82491700	-2.14564100
H	-0.77143800	-0.64117100	3.17219200	H	-0.68450600	-4.72658400	-1.57639600
C	1.13766000	0.12296100	2.55008700	H	-1.32597400	-3.54290900	-2.71773000
C	2.76364900	1.59729900	0.25365900	C	4.79606100	2.26627200	-0.89705600
C	3.64501800	2.59467500	-0.18388500	H	5.46742300	3.05309300	-1.23053100
H	3.42047700	3.63662400	0.03119600	C	1.50440000	2.02036800	1.00980100
C	5.08589200	0.92882900	-1.18215700	H	1.82726100	2.61774200	1.87070000
H	5.98300600	0.67002600	-1.73784300	C	0.36648700	-3.28456400	1.91938900
C	4.21671200	-0.06948500	-0.74381600	H	1.39338700	-3.45679900	1.57096200
H	4.43586400	-1.11317600	-0.95255100	H	-0.29498500	-3.97334400	1.39226700
C	3.06219600	0.26325400	-0.02948800	C	0.28996400	-3.39813100	3.44302800
H	2.39277200	-0.51899600	0.30906900	H	0.90061500	-4.21737200	3.83465800
C	-1.08932700	-1.58003200	0.80579000	H	-0.74971100	-3.56723200	3.74755900
C	-2.82434400	-0.08341800	0.11047300	C	0.57935200	2.87178800	0.15055800
H	-2.49078600	-0.23798500	-0.93277000	C	-0.09887100	3.95673500	0.71439600
C	-3.03405600	1.42513200	0.30338800	C	0.33675600	2.53828700	-1.18779400
H	-2.08591500	1.94665300	0.14505400	C	-1.00389600	4.70039800	-0.04514500
H	-3.32035200	1.59712600	1.35057200	H	0.08053400	4.21500300	1.75504200
C	-4.11274700	1.98210800	-0.63098400	C	-0.57157500	3.27587300	-1.94715200
H	-4.24963200	3.05451800	-0.44530200	H	0.86897800	1.70536700	-1.63671300
H	-3.77282200	1.88809100	-1.67299900	C	-1.24345100	4.36030500	-1.37786800
C	-5.44046600	1.23267400	-0.46112500	H	-1.52124500	5.54337300	0.40453500
H	-6.18766400	1.60947500	-1.17130800	H	-0.75261800	3.00566400	-2.98393000
H	-5.83608200	1.42544400	0.54660600	H	-1.94883200	4.93683300	-1.96967200
C	-5.24911300	-0.27847000	-0.64362200				
H	-4.96359200	-0.48156300	-1.68664600				
H	-6.19488400	-0.80753500	-0.47029400	<b>H<sub>2</sub>O</b>			
C	-4.16295500	-0.82568000	0.29210500	O	0.00000000	0.00000000	0.12063000
H	-4.47479700	-0.70772700	1.33916700	H	0.00000000	0.76066100	-0.48251800
H	-4.02751400	-1.90267500	0.12740300	H	0.00000000	-0.76066100	-0.48251800
C	-0.08405800	-2.68933000	-1.17820800				
H	0.75964500	-3.01100800	-0.56126600	<b>IMI</b>			
C	0.32934400	-1.42188900	-1.94189900	C	-1.75991500	1.40477600	-1.36371500
H	-0.53980100	-1.05612200	-2.50842700	C	-2.82229900	2.46116900	-1.67864100
H	0.60038600	-0.63725400	-1.22802200	C	-2.19000000	3.84313000	-1.41457500
C	1.49138000	-1.69852700	-2.90277700	H	-1.85969400	3.93563600	-0.37679900
H	1.75076800	-0.78555600	-3.45240500	H	-2.92146500	4.63299400	-1.62149400
H	2.38186200	-1.97328200	-2.32051800	H	-1.32486700	4.00440100	-2.06884800
C	1.14903500	-2.83592700	-3.87368600	C	-3.27422600	2.36539300	-3.13996900
H	2.00540300	-3.05253800	-4.52421100	H	-2.43700000	2.54981300	-3.81994300
				H	-4.04470900	3.12028800	-3.33498300

H	-3.68725900	1.38117500	-3.37388100	H	1.77756900	3.04716300	2.53051100
O	-1.34211500	0.66615900	-2.31127300	H	-2.35071100	1.82172800	2.64451300
O	-1.32350400	-1.46382800	0.75647700	H	-3.04304600	4.17377500	2.49685500
C	-5.69295700	-1.71606100	-0.89316700	H	-1.33858800	5.98521900	2.34084400
H	-6.10188900	-2.72152200	-0.95034500	H	1.08249200	5.38251800	2.35281100
C	-4.63355900	-1.44882400	-0.01627100	C	0.19493100	0.82316500	2.71166400
C	-4.00178100	-2.54402700	0.81242400	Rh	0.11258700	-0.72966700	-1.90236000
H	-4.74012800	-3.32383000	1.03300700	Rh	0.09050000	-0.00638600	0.39691000
H	-3.66590300	-2.13157300	1.76745500	O	1.54661300	-2.11763600	-1.35870800
C	-2.78463500	-3.24920300	0.13683900	C	4.26924500	-2.96240800	-0.67317500
C	-3.22158100	-4.01916200	-1.11440600	H	4.00555500	-3.15938800	-1.71709600
H	-3.66085200	-3.35751600	-1.86495100	H	5.01662300	-3.70776600	-0.37745400
H	-3.96852200	-4.77183400	-0.83655700	C	4.84202600	-1.56899600	-0.55154800
H	-2.37268800	-4.53425600	-1.57421400	C	5.80879900	-1.25240500	0.41173000
C	-2.14851400	-4.22003200	1.15251500	H	6.19374800	-2.03231800	1.06333500
H	-1.29081500	-4.74017300	0.71008300	C	6.28547700	0.05408900	0.53041300
H	-2.88259600	-4.97501000	1.45620800	H	7.04454100	0.28727400	1.27260700
H	-1.80155100	-3.68974300	2.04394200	C	4.37851900	-0.54939900	-1.39190300
C	-1.73388000	-2.18967800	-0.20802000	H	3.64083600	-0.78795300	-2.15058000
O	-1.33386900	-2.10667200	-1.41150200	O	1.52207000	1.37867600	-0.07343600
O	-1.35658100	1.35239100	-0.15686900	O	1.54426200	0.73709900	-2.23993300
C	-4.02480600	2.26480800	-0.70330000	C	5.79861800	1.06108600	-0.30479500
H	-3.67313500	2.47720100	0.31034900	H	6.17807200	2.07522900	-0.21017000
H	-4.77210000	3.02516200	-0.95885000	C	4.83122400	0.77044800	-1.27574600
C	-4.64652500	0.88739600	-0.75012400	C	4.25075700	1.84568200	-2.16526600
C	-5.70669300	0.59371300	-1.61794000	H	4.99359900	2.63148200	-2.34559300
H	-6.12659500	1.38121900	-2.23835300	H	3.98912300	1.41449000	-3.13665100
C	-6.22991300	-0.69859400	-1.68331000	C	2.98006300	2.54333000	-1.58713100
H	-7.05971000	-0.91350800	-2.35159300	C	3.32241300	3.35334400	-0.33067200
C	-4.13770600	-0.14064200	0.05429300	H	3.72221100	2.71791300	0.46336500
H	-3.32602700	0.07801900	0.73906400	H	4.07386700	4.11164200	-0.57937900
C	-0.47885500	-0.29863600	3.43488500	H	2.43604300	3.86300800	0.05723700
O	-1.79849100	-0.11633600	3.53767800	C	2.39126700	3.47719800	-2.66282200
O	0.11976000	-1.26547500	3.87029400	H	1.48472800	3.97193500	-2.29459200
C	-2.51630700	-1.15438000	4.23465500	H	3.12063000	4.25377000	-2.91943600
H	-3.56331200	-0.85577400	4.18932900	H	2.13641300	2.92432100	-3.57148700
H	-2.18093900	-1.21163600	5.27331000	C	1.93539600	1.46808800	-1.27437800
H	-2.36742700	-2.11750000	3.74416000	O	1.54637100	-1.39529300	0.78194100
C	0.71778100	3.27674800	2.52960200	C	1.95090900	-2.15907000	-0.15161400
C	-0.23723100	2.25091400	2.62722400	C	3.00206500	-3.21442500	0.20268300
C	-1.59845600	2.59482500	2.60186500	C	2.42011200	-4.59771100	-0.14885700
C	-1.98413500	3.93094800	2.50883000	H	2.16092400	-4.66019200	-1.20960500
C	-1.03103800	4.94642000	2.41724300	H	3.15446500	-5.37910600	0.07749000
C	0.32316200	4.60881300	2.42320400	H	1.51757100	-4.80077200	0.43965000

C	3.34607600	-3.15938500	1.69607600	C	-6.45425200	-0.32281000	-1.37381900
H	2.45978800	-3.34870700	2.30898300	H	-7.31721800	-0.53769600	-1.99869600
H	4.09460000	-3.92615400	1.92733000	C	-4.27745000	0.23898300	0.25439500
H	3.74815100	-2.18520900	1.98360900	H	-3.43521700	0.46169500	0.90050900
N	1.53243000	0.63852200	2.78021300	C	-0.15251000	-0.16129900	3.30994300
N	2.64356500	0.46992000	2.78205300	O	-1.43281500	-0.25932100	3.69430100

## IM2

C	-1.88396000	1.52551700	-1.40110700	H	-2.80694900	-1.32777100	4.73390200
C	-2.88549800	2.64205400	-1.71441800	H	-1.27422700	-1.05643000	5.62010400
C	-2.15893000	3.99101600	-1.53822800	H	-1.33479900	-2.25877500	4.30148800
H	-1.78628100	4.10964200	-0.51664800	C	0.35380800	3.23583500	1.67991100
H	-2.84870700	4.81521400	-1.75277700	C	0.24733800	2.19747800	2.64548200
H	-1.31156200	4.07278100	-2.22933100	C	0.36658100	2.54057900	4.02274700
C	-3.40690700	2.51656500	-3.15010100	C	0.58987700	3.85139700	4.40922500
H	-2.58817200	2.59385300	-3.87207900	C	0.68623200	4.85688500	3.43738100
H	-4.11915000	3.32484600	-3.35226300	C	0.56247000	4.54812800	2.07800400
H	-3.91084500	1.56143800	-3.31572600	H	0.26009200	2.98539900	0.63452500
O	-1.59437200	0.68967200	-2.30554000	H	0.30297100	1.76300400	4.77699800
O	-1.51243600	-1.23166300	0.90020400	H	0.68909000	4.09976400	5.46121900
C	-5.95387700	-1.30617000	-0.51905800	H	0.85726500	5.88511200	3.74336300
H	-6.42553200	-2.28468800	-0.48331400	H	0.63458700	5.33500400	1.33340700
C	-4.85109100	-1.03781900	0.30245200	C	0.03786300	0.84601800	2.23933700
C	-4.25143800	-2.10117900	1.19389300	Rh	-0.21512400	-0.79844800	-1.90187600
H	-5.02710800	-2.80270300	1.52263600	Rh	-0.03196500	0.10759100	0.37733900
H	-3.82927100	-1.63192300	2.08781100	O	1.13678300	-2.25053500	-1.33683500
C	-3.12668200	-2.94551800	0.51627200	C	3.79594900	-3.30939700	-0.79044300
C	-3.68547700	-3.78572900	-0.63768200	H	3.41828800	-3.56066700	-1.78653700
H	-4.12052800	-3.16107100	-1.42134000	H	4.48980200	-4.10424300	-0.49307400
H	-4.46350500	-4.45803600	-0.25771200	C	4.51799300	-1.98204100	-0.84755900
H	-2.89955800	-4.39667600	-1.09221300	C	5.63051900	-1.71163800	-0.04046100
C	-2.49231300	-3.86992100	1.57379100	H	6.01317500	-2.48284000	0.62316300
H	-1.67768200	-4.45990800	1.13713200	C	6.25337000	-0.46355100	-0.09181900
H	-3.24504400	-4.56574400	1.96179100	H	7.12319100	-0.26698300	0.52971100
H	-2.08783700	-3.29260000	2.40904300	C	4.05854300	-0.97726500	-1.70763000
C	-2.03744800	-1.99088100	0.01563500	H	3.21178800	-1.18379600	-2.35265700
O	-1.72873500	-2.01695400	-1.21151300	O	1.47188400	1.32120700	-0.34185900
O	-1.39753500	1.53710500	-0.21762600	O	1.30858500	0.49590200	-2.44108800
C	-4.05410400	2.56982700	-0.68167900	C	5.76628400	0.53335900	-0.93877300
H	-3.65025400	2.81998600	0.30426700	H	6.25601100	1.50319200	-0.97390900
H	-4.76907000	3.35544100	-0.95272200	C	4.65541200	0.28822600	-1.75632600
C	-4.75146000	1.23056000	-0.61375900	C	4.08266600	1.35540700	-2.66154500
C	-5.85385300	0.93608500	-1.42679900	H	4.87018000	2.05543400	-2.96416300
H	-6.24816600	1.69757100	-2.09466900	H	3.69134700	0.88976400	-3.57145600

C	2.93924200	2.20511500	-2.02395800	C	-5.31531600	0.78852100	2.89854000
C	3.47093400	3.04325500	-0.85538500	H	-5.87659900	0.22178800	2.15156800
H	3.89176600	2.41760800	-0.06590900	H	-6.00009400	1.49245800	3.38577300
H	4.25546300	3.71757700	-1.21795800	H	-4.95565000	0.08387700	3.65429800
H	2.67750000	3.65187400	-0.41138200	C	-3.36875500	2.31390000	3.36421900
C	2.34980800	3.13442500	-3.10352000	H	-2.98836500	1.61785200	4.12102500
H	1.53637000	3.74326000	-2.69092800	H	-4.02706300	3.03348200	3.86424900
H	3.12568100	3.81386500	-3.47417300	H	-2.51657700	2.85330500	2.94183100
H	1.95622000	2.56153000	-3.94802100	C	-3.17207500	0.60271200	1.57918900
C	1.82032100	1.26033600	-1.56727600	O	-3.37832600	-0.64310400	1.66691100
O	1.33325700	-1.38475500	0.74443600	O	-1.87070300	-0.06667700	-1.72336000
C	1.61248700	-2.23843200	-0.15846800	C	-4.17845700	0.54274400	-3.35783400
C	2.59611300	-3.35629800	0.20690500	H	-3.35514600	1.25587400	-3.46544000
C	1.85734900	-4.69861700	0.03030500	H	-4.73640000	0.54031100	-4.30146800
H	1.49800300	-4.82140300	-0.99543000	C	-5.07729200	0.97735800	-2.22300800
H	2.53342800	-5.52884200	0.26481800	C	-6.45655000	0.73241600	-2.24504200
H	0.99651700	-4.76192100	0.70686900	H	-6.90421000	0.25576300	-3.11327000
C	3.08131700	-3.22034300	1.65451300	C	-7.25757900	1.10740500	-1.16516700
H	2.24306900	-3.25836800	2.35591200	H	-8.32842600	0.92389800	-1.19627100
H	3.76391300	-4.04630400	1.88693300	C	-4.52916700	1.61404100	-1.10252000
H	3.60938800	-2.27934900	1.81925300	H	-3.46588700	1.82513900	-1.08363200
N	3.27000400	0.92050400	2.61926000	H	2.80756500	-0.31280000	0.07758400
N	3.53242900	0.39661100	1.68272700	C	3.59526300	3.24231000	1.25170700

### IM3

C	-2.79965200	-0.93518900	-1.86174700	C	3.82031500	4.59267500	1.50327800
C	-3.56410900	-0.88250300	-3.18914600	C	4.83592500	5.27620000	0.82521700
C	-2.54945600	-1.11712400	-4.32615600	C	5.62495900	4.59831900	-0.10580100
H	-1.76986800	-0.34980200	-4.32340400	C	5.40325200	3.24339800	-0.35737700
H	-3.06229400	-1.08811800	-5.29419700	C	4.38431200	2.55283800	0.31605400
H	-2.07063700	-2.09868100	-4.22666200	C	4.07233300	1.13182700	0.00291000
C	-4.65334400	-1.95971400	-3.23321000	C	5.09494300	0.31861700	-0.72108100
H	-4.21889700	-2.96064600	-3.14956500	C	4.76095000	-0.29333300	-1.93501300
H	-5.18923900	-1.89870500	-4.18753300	C	5.68223100	-1.11110000	-2.59044000
H	-5.37558700	-1.83785700	-2.42240400	C	6.94447200	-1.32929400	-2.03365500
O	-3.11574800	-1.81406800	-1.00867800	C	7.28877900	-0.71015200	-0.82834500
O	-2.19783500	1.15484500	0.96294600	C	6.37376700	0.12026300	-0.18094600
C	-6.68999200	1.71919800	-0.04641900	N	2.92329900	0.66950600	0.33737100
H	-7.31881300	2.00833000	0.79162200	H	2.79338400	2.71018000	1.74833500
C	-5.31328500	1.97467100	0.00047700	H	3.20109200	5.11468500	2.22778700
C	-4.66496100	2.59273700	1.21801300	H	6.41241100	5.12334700	-0.63948800
H	-5.37614200	3.24864900	1.73382500	H	6.01143000	2.72684100	-1.09232700
H	-3.81728700	3.20850200	0.90458100	H	3.78169800	-0.11352200	-2.36504300
C	-4.15002000	1.56030400	2.26896800	H	5.41286800	-1.57818200	-3.53366800
				H	8.27060300	-0.87352000	-0.39287400
				H	6.64065100	0.60433800	0.75403500

H	7.65991400	-1.97220300	-2.53869800	H	2.89097600	-2.11094300	-1.74060900
H	5.01047100	6.33038800	1.02280400	H	2.93739200	-3.44259600	-2.90684100
C	-0.03139200	2.82150100	0.32278800	H	1.78723700	-2.10881600	-3.12082200
O	-0.89906800	3.65243400	-0.28996300	C	0.41935200	-4.43060700	-2.49726100
O	0.41920200	3.00670000	1.43486000	H	-0.09077400	-3.83274500	-3.26236500
C	-1.33286800	4.78695100	0.48614400	H	1.07783400	-5.14172500	-3.00910500
H	-2.06574300	5.30014400	-0.13630500	H	-0.33597100	-4.99294600	-1.94191900
H	-0.48603000	5.44547500	0.69828100	C	0.29572500	-2.59248900	-0.81457300
H	-1.78715000	4.46001400	1.42342200	O	0.21119800	-0.13181600	1.81255700
C	0.99728100	0.90057700	-2.77832500	C	-0.06832700	-1.03855200	2.65797400
C	1.00151300	1.85579400	-1.72942600	C	0.73280000	-1.02210400	3.96496100
C	1.80408000	3.01964300	-1.87444600	C	-0.26077400	-0.97119400	5.14079900
C	2.58863000	3.20086300	-3.00232600	H	-0.95701200	-1.81425600	5.11162900
C	2.55850900	2.25134000	-4.03182500	H	0.28590900	-1.00248800	6.09047600
C	1.75435100	1.11074200	-3.92313500	H	-0.84321600	-0.04258200	5.11643700
H	0.38417600	0.01803700	-2.67508100	C	1.66142100	0.19809600	4.01761300
H	1.83559600	3.75218600	-1.07578600	H	1.08589700	1.12691600	3.96041400
H	3.22258800	4.07778600	-3.08613700	H	2.21606600	0.19237400	4.96362800
H	3.16395500	2.40247500	-4.92105400	H	2.37441400	0.20393800	3.19095900
H	1.73196800	0.38328000	-4.72901900				
C	0.22144400	1.64138600	-0.55043100	<b>IM4</b>			
Rh	-2.06661800	-1.95616200	0.76720400	C	0.96157800	2.06988700	-1.74759400
Rh	-0.76767000	0.00017700	0.02265000	C	2.11150700	2.50722100	-2.66254200
O	-0.94141700	-1.95131200	2.50786300	C	2.01257900	1.67459600	-3.95716300
C	1.55046200	-2.34878500	4.05417000	H	2.05545800	0.60400100	-3.74748400
H	0.84577100	-3.17294700	4.20485100	H	2.83754100	1.93213700	-4.63121300
H	2.17171100	-2.28097100	4.95486800	H	1.07080200	1.88087300	-4.47893600
C	2.40836200	-2.64320200	2.84512400	C	1.99124600	3.99637500	-3.01012900
C	3.71855100	-2.15979100	2.72836500	H	1.05734600	4.19834800	-3.54219300
H	4.15442700	-1.58299300	3.53959000	H	2.82483500	4.28852800	-3.65952300
C	4.46920100	-2.42521400	1.58243400	H	2.01358900	4.62564000	-2.11738700
H	5.48494300	-2.05110600	1.50120400	O	0.02386000	2.88812600	-1.53715300
C	1.88170800	-3.39906000	1.79138700	O	0.49178500	1.13414500	1.63258800
H	0.87052200	-3.78421300	1.87549400	C	3.86125300	4.36926500	1.76383200
O	0.55275900	-1.34176400	-0.84085300	H	3.94172200	4.92342900	2.69561800
O	-0.68003400	-3.13313700	-0.21279500	C	3.19241400	3.13849800	1.74795200
C	3.92152800	-3.16725500	0.53422800	C	2.53551900	2.58545300	2.99232100
H	4.51511000	-3.36551200	-0.35377600	H	3.03291800	2.98642800	3.88336300
C	2.61390100	-3.66226800	0.62715500	H	2.64534700	1.49919500	3.01749100
C	1.96394900	-4.42970100	-0.50115100	C	1.01770200	2.91243000	3.13179700
H	2.70854500	-5.03051100	-1.03649300	C	0.79117800	4.42174700	3.27446800
H	1.22200800	-5.11996100	-0.08781400	H	1.14103800	4.96938600	2.39528100
C	1.25008200	-3.53255800	-1.56189500	H	1.33516900	4.79299900	4.15116900
C	2.27728700	-2.74554100	-2.37774900	H	-0.27043200	4.64691000	3.41180600

C	0.47305300	2.18136100	4.37655200	O	-0.07167100	-3.05503400	-1.46385300
H	-0.59855600	2.37661300	4.50316100	C	-2.42070900	-3.62661400	-0.28843900
H	0.99014500	2.53920900	5.27477800	H	-3.04024900	-4.09697300	0.47609600
H	0.62077000	1.10112800	4.29633400	H	-2.06522800	-4.37311400	-1.00166200
C	0.26408100	2.35413400	1.91812900	H	-2.98914600	-2.85048600	-0.80258100
O	-0.54055900	3.11943200	1.30332300	C	2.10754300	-1.15933800	2.35105200
O	1.02074000	0.88026500	-1.26764600	C	0.95305600	-1.79745500	1.85532300
C	3.46992200	2.20953100	-1.95792400	C	0.11794400	-2.43133200	2.79359100
H	3.54743000	1.13013000	-1.79655900	C	0.44459500	-2.45065700	4.15010800
H	4.26518500	2.48550400	-2.66012600	C	1.60808700	-1.83983700	4.61901500
C	3.65766300	2.94714900	-0.65019400	C	2.43581000	-1.18686700	3.70296200
C	4.32353300	4.17928300	-0.60471700	H	2.75888500	-0.62503200	1.66855000
H	4.75850700	4.58816700	-1.51310300	H	-0.78923100	-2.91125800	2.45960000
C	4.42883900	4.88199600	0.59631400	H	-0.21993200	-2.96056800	4.84337100
H	4.95304200	5.83377200	0.62213400	H	1.86202100	-1.86538100	5.67506800
C	3.11788300	2.43646800	0.53717600	H	3.34137000	-0.68971600	4.04144000
H	2.60430100	1.48317800	0.51845800	C	0.65667800	-1.73283800	0.39379000
H	1.91591300	-0.77272300	-1.01443300	Rh	-1.57473400	2.37877900	-0.31983000
C	2.10352700	-4.83080200	-0.06695000	Rh	-0.45899300	0.22347500	0.03898500
C	2.13246400	-5.96925800	0.73905700	O	-3.06058700	1.70988100	0.95788200
C	2.91574600	-5.99648300	1.89387800	C	-5.44243200	0.15494000	1.62395800
C	3.68287800	-4.88289400	2.24175000	H	-5.65548000	1.20330500	1.39282900
C	3.66280700	-3.74172900	1.44240200	H	-6.22452700	-0.19407100	2.30858000
C	2.85990300	-3.70975200	0.29448000	C	-5.47257300	-0.65411700	0.34671500
C	2.83056000	-2.48899200	-0.55578800	C	-5.90705500	-1.98647200	0.32508500
C	3.87606800	-2.26357300	-1.56183100	H	-6.25966500	-2.45187100	1.24193500
C	3.56825500	-1.57328000	-2.74948900	C	-5.90594900	-2.71143300	-0.86808000
C	4.55928800	-1.32984400	-3.69410400	H	-6.25579100	-3.74058500	-0.87546000
C	5.86601400	-1.76912200	-3.46420800	C	-5.04828900	-0.07376100	-0.85456700
C	6.17322400	-2.47774400	-2.29965700	H	-4.72384200	0.96104200	-0.85333600
C	5.18251100	-2.74107900	-1.35807700	O	-1.51438600	-0.47748600	-1.59886700
N	1.87740100	-1.61434900	-0.42767600	O	-2.50415100	1.52615700	-1.95820500
H	1.48615700	-4.79890100	-0.95627200	C	-5.46048700	-2.12078500	-2.05240400
H	1.53736000	-6.83426000	0.46165400	H	-5.46308500	-2.68908700	-2.97889200
H	4.29239700	-4.89574500	3.14014300	C	-5.02171300	-0.79025400	-2.05764000
H	4.24483500	-2.87142800	1.72212000	C	-4.50172600	-0.12756200	-3.31277800
H	2.54526100	-1.27823000	-2.95325400	H	-4.97237400	-0.57188000	-4.19773200
H	4.31010400	-0.80708200	-4.61208000	H	-4.76879700	0.93387700	-3.29847700
H	7.18487400	-2.83186600	-2.12800700	C	-2.95743000	-0.23409700	-3.51029400
H	5.42097100	-3.30148600	-0.46167500	C	-2.54243700	-1.68173200	-3.79438500
H	6.64019100	-1.57555100	-4.20069200	H	-2.80597000	-2.35290900	-2.97594600
H	2.92933600	-6.88284700	2.52137700	H	-3.04401300	-2.03139900	-4.70474000
C	-0.24754300	-2.67237700	-0.31103000	H	-1.46210700	-1.75774700	-3.94613400
O	-1.32652600	-3.02186000	0.41447500	C	-2.54794300	0.65950200	-4.69765800

H	-1.46507400	0.61073500	-4.86536900	C	2.93539200	-1.65986400	-1.00109400
H	-3.04651300	0.31784900	-5.61222400	O	2.91324500	-2.22630800	0.13595300
H	-2.82096800	1.70335200	-4.52042800	O	1.71444300	1.13935500	0.75235700
C	-2.26827000	0.31054400	-2.25152600	C	4.08076600	2.63742500	1.24347100
O	-2.01012800	-0.27078300	1.28381600	H	3.34844700	3.09480900	0.57198200
C	-2.96229800	0.54836900	1.47174400	H	4.64382400	3.44891600	1.71941800
C	-4.09319200	0.09753000	2.40570500	C	5.02072100	1.74875700	0.46074900
C	-4.16045200	1.09080300	3.58196400	C	6.36179000	1.60071400	0.84035200
H	-4.33273800	2.11163500	3.22849000	H	6.74948300	2.17809500	1.67582700
H	-4.97684900	0.81387700	4.25907000	C	7.19990100	0.72188100	0.15326900
H	-3.22528100	1.07850800	4.15412600	H	8.24056300	0.62181300	0.45070500
C	-3.83167900	-1.31730200	2.93675600	C	4.55105500	1.01100700	-0.63358200
H	-2.89279900	-1.35864900	3.49604700	H	3.52254300	1.13696400	-0.95184100
H	-4.64681300	-1.61243300	3.60845600	H	-1.27225100	0.07352700	-2.97041000
H	-3.76885400	-2.04644200	2.12601000	C	-2.71953400	4.30846800	-1.64040500

**IMS'**

C	2.42688500	0.80588500	1.75312000	C	-4.13977800	4.83998000	0.70210000
C	3.30471000	1.89773000	2.37552600	C	-3.98318900	3.52585800	0.26432100
C	2.36249800	2.90231000	3.06845900	C	-3.24267400	3.24399400	-0.89317000
H	1.67364700	3.35596200	2.35322400	C	-3.04186800	1.83256100	-1.33045400
H	2.95066600	3.69860700	3.53945800	C	-4.26144100	1.00395000	-1.51160100
H	1.77470400	2.40748100	3.85109800	C	-4.17516700	-0.39795900	-1.46360200
C	4.26556800	1.29972300	3.41043300	C	-5.29862900	-1.18203800	-1.71185100
H	3.71289500	0.83687400	4.23310400	C	-6.53094300	-0.58428300	-1.99191800
H	4.89478500	2.09502700	3.82661200	C	-6.63171900	0.80789500	-2.02163000
H	4.91664100	0.54020900	2.97109200	C	-5.50716500	1.59661500	-1.78203900
O	2.44720200	-0.34964600	2.28473600	N	-1.91694000	1.26941000	-1.63793900
O	2.07542000	-0.81668800	-1.41885200	H	-2.17094200	4.10262200	-2.55315200
C	6.70542900	-0.03248100	-0.91183400	H	-2.46104000	6.43674500	-1.78998200
H	7.35894900	-0.72408100	-1.43768200	H	-4.69645200	5.04249100	1.61296600
C	5.37057300	0.10103000	-1.31509300	H	-4.41894200	2.70902100	0.82946900
C	4.80190900	-0.74388100	-2.43192500	H	-3.22087200	-0.85367500	-1.22374100
H	5.60437700	-1.05972700	-3.10858300	H	-5.21596000	-2.26217700	-1.66949500
H	4.09740200	-0.15173500	-3.01832900	H	-7.58433600	1.28296900	-2.23965100
C	4.07349900	-2.03766700	-1.95710000	H	-5.58987600	2.67702100	-1.82622800
C	5.06210900	-2.99390600	-1.27829500	H	-7.40628900	-1.19989300	-2.18058700
H	5.50848200	-2.54918000	-0.38554800	H	-3.70014600	6.91621700	0.31204200
H	5.86720900	-3.24114000	-1.98003800	C	0.15124700	1.17161200	-2.60245500
H	4.56908000	-3.92447100	-0.98220600	O	1.36582400	1.58417200	-2.91781300
C	3.44106400	-2.73611800	-3.17801100	O	-0.37869600	0.23295600	-3.38192700
H	2.91558500	-3.64909500	-2.87456600	C	1.97630600	1.05135900	-4.10903000
H	4.22360400	-3.01683800	-3.89224100	H	2.96632900	1.50417400	-4.14174200
H	2.72466500	-2.08486700	-3.68627600	H	1.39997500	1.34721800	-4.99045300

H	2.04977700	-0.03316500	-4.05051300	O	-0.62786000	-1.77439400	-1.01133800
C	-0.63030200	3.17693300	0.47901700	C	-0.49022100	-2.95423300	-0.55468300
C	-0.16824100	2.97217700	-0.83124400	C	-1.25479900	-4.09990500	-1.22711000
C	0.62465700	3.96965400	-1.41930400	C	-0.20301300	-5.03457900	-1.86070400
C	0.92398700	5.14465300	-0.72707200	H	0.48296900	-5.42964900	-1.10566900
C	0.42374200	5.35296300	0.55826700	H	-0.70250900	-5.87703500	-2.35267200
C	-0.35419600	4.35843700	1.15835200	H	0.38576400	-4.50169500	-2.61688200
H	-1.21345900	2.39939700	0.95359800	C	-2.20061000	-3.58103000	-2.31383300
H	0.99017600	3.84140100	-2.43083000	H	-1.65278000	-3.02974800	-3.08398200
H	1.53233400	5.90709000	-1.20659600	H	-2.70682400	-4.42679400	-2.79339300
H	0.63986700	6.27569200	1.08973000	H	-2.96198800	-2.91810900	-1.90129400
H	-0.74518800	4.50236400	2.16191400				
C	-0.60613400	1.76195300	-1.57656400				
Rh	1.35727800	-1.85217900	1.41239900				
Rh	0.50094700	-0.24404800	-0.18385500				
O	0.26006300	-3.28393700	0.42067500				
C	-2.03920000	-4.89469300	-0.13690300				
H	-1.30918300	-5.34870500	0.54017600				
H	-2.56162100	-5.71076700	-0.64932700				
C	-3.02652100	-4.06960900	0.65873000				
C	-4.38354500	-4.02191800	0.31630700				
H	-4.74894800	-4.62040900	-0.51462500				
C	-5.26668300	-3.21605300	1.03733500				
H	-6.31831700	-3.18836300	0.76551700				
C	-2.58870900	-3.30945900	1.75135500				
H	-1.54857600	-3.36512800	2.04732700				
O	-1.03941300	0.10828800	1.13745500				
O	-0.23990900	-1.38773800	2.63031900				
C	-4.80434400	-2.43626900	2.09767400				
H	-5.49578600	-1.80231800	2.64690200				
C	-3.45368400	-2.47354600	2.46844200				
C	-2.92365900	-1.62160300	3.60058100				
H	-3.73705900	-1.38013800	4.29463600				
H	-2.17083900	-2.18223600	4.16322100				
C	-2.28974100	-0.26792900	3.15833600				
C	-3.32926800	0.62397300	2.47137100				
H	-3.70685800	0.17325900	1.55064600				
H	-4.17504600	0.78908000	3.14916000				
H	-2.90164300	1.59755400	2.22114300				
C	-1.73026800	0.45084600	4.40387500				
H	-1.24979900	1.39581700	4.12380400				
H	-2.54478500	0.67865400	5.10096100				
H	-0.99251700	-0.16989400	4.92132200				
C	-1.10223400	-0.54056000	2.22936400				
				<b>IM5-R</b>			
				C	4.07869500	-0.19174300	1.29846700
				C	4.09595400	-1.28261700	2.37358200
				C	4.06709800	-1.00204200	3.74271500
				C	4.17838000	-2.62324100	1.96743400
				C	4.08677200	-2.03618700	4.68342700
				H	4.02170100	0.02544000	4.08423100
				C	4.19756700	-3.65546600	2.90266100
				H	4.23085700	-2.85937400	0.90898200
				C	4.14312200	-3.36551200	4.26909100
				H	4.05228500	-1.79527400	5.74252000
				H	4.25648600	-4.68707000	2.56572700
				H	4.15111600	-4.16854000	5.00093200
				C	3.85645600	1.21870200	1.81156600
				C	4.84984000	2.18339300	1.61336400
				C	2.68558300	1.57909700	2.49347300
				C	4.68653600	3.48571100	2.09104600
				H	5.75958500	1.91080200	1.08390900
				C	2.52353000	2.87811000	2.97418900
				H	1.89412400	0.84924000	2.62783400
				C	3.52345100	3.83427400	2.77858500
				H	5.46818400	4.22303600	1.92914200
				H	1.60803700	3.14394600	3.49547100
				H	3.39271400	4.84573600	3.15358500
				H	5.05049600	-0.21362200	0.79905400
				C	2.61287100	-0.75179100	-4.31916700
				H	1.85869000	-1.12016000	-5.02038400
				N	-0.23391400	0.98922300	-1.50328700
				N	-0.35892800	-1.30160200	-1.24599100
				N	1.53867600	-0.34741400	-2.23849300
				C	0.31542400	-0.21578000	-1.67143500
				C	2.45560100	-1.45680900	-1.94576600



H	1.92120500	-2.26055000	-1.45037100	H	-0.53243000	5.41953500	-0.76136200
O	4.75635100	-1.18298000	-1.21597500	C	3.80436400	-0.10193700	-5.03294900
C	3.56189100	-1.02575500	-0.94897700	H	4.50914500	-0.84017800	-5.43007500
N	3.12199000	-0.53431500	0.23302300	H	3.44480600	0.50018900	-5.87743000
H	2.12889200	-0.53239200	0.47968800	C	3.20690400	1.37382100	-3.19069200
C	2.02716000	0.37736200	-3.42574700	H	2.92401200	2.35562400	-3.58407500
H	1.17617100	0.87730000	-3.88859500	H	3.42097100	1.50199500	-2.12619400
C	3.00168200	-1.87768200	-3.32117900	C	4.42092100	0.80619500	-3.95665600
H	2.55821000	-2.83000700	-3.62234400	H	5.05173300	1.59457700	-4.37878900
H	4.08202000	-2.01429700	-3.25693300	H	5.04057900	0.21352100	-3.27750100
H	-1.16898500	0.99262200	-1.10151700	H	-1.06297800	-1.12839300	-0.52274500
C	-0.45662800	-2.59531500	-1.94217200	C	-5.70987500	1.12038000	0.31331200
C	-0.07518600	-3.76585700	-1.02212900	C	-6.81702100	0.50211700	-0.26667900
C	-1.87971300	-2.78237100	-2.49339300	C	-6.64413600	-0.55636000	-1.16108900
H	0.23240400	-2.55982500	-2.79137600	C	-5.35174400	-0.98455600	-1.47603000
C	-0.22944700	-5.11250500	-1.74016700	C	-4.25063200	-0.36723500	-0.89034100
H	-0.71608800	-3.73812400	-0.13432900	C	-4.40617100	0.68707300	0.02213900
H	0.95032400	-3.65173100	-0.65486400	C	-3.21055500	1.34000200	0.62480800
C	-2.02855200	-4.12741100	-3.21540200	C	-3.18721800	2.82240800	0.63649200
H	-2.58865700	-2.74122000	-1.65664400	C	-2.50885100	3.50852700	1.66325100
H	-2.12201300	-1.95030100	-3.16515900	C	-2.44160100	4.89936100	1.67857300
C	-1.64475900	-5.29582400	-2.30006800	C	-3.05880700	5.64733600	0.67141600
H	0.01906100	-5.92653900	-1.04928900	C	-3.74589900	4.98326300	-0.34902500
H	0.49691600	-5.16696700	-2.56444700	C	-3.81443300	3.59078000	-0.36375300
H	-3.05953900	-4.23990900	-3.57137000	N	-2.15687200	0.73511500	1.12476800
H	-1.38405300	-4.13566700	-4.10633000	H	-5.85316400	1.93890500	1.01247000
H	-1.71678100	-6.24490000	-2.84499800	H	-7.81774200	0.84330000	-0.01425100
H	-2.35966800	-5.35310800	-1.46689300	H	-5.20275500	-1.80154000	-2.17763300
C	0.46347400	2.28451700	-1.45774000	H	-3.25037200	-0.70427400	-1.13519700
C	-0.14603200	3.24076900	-2.49036300	H	-2.02755700	2.92363800	2.44005600
C	0.41746000	2.87566400	-0.04869500	H	-1.91197300	5.40301600	2.48331600
H	1.50265500	2.09689100	-1.71207300	H	-4.22744700	5.55229100	-1.14034700
C	0.54780400	4.60842300	-2.44558300	H	-4.34737900	3.08871800	-1.16535900
H	-1.21510700	3.36302500	-2.26742600	H	-3.01204200	6.73279300	0.68564900
H	-0.07374200	2.80117400	-3.49297400	H	-7.50669500	-1.04089700	-1.61037000
C	1.11126400	4.24146100	-0.00750600	C	-0.65481600	-0.98670600	1.72416700
H	-0.62582600	2.98940700	0.25086800	O	-0.55186900	-2.25374800	2.24741700
H	0.87134100	2.17485800	0.65417400	O	0.37898900	-0.32605400	1.49815300
C	0.50993800	5.20791100	-1.03493400	C	0.77740600	-2.72648500	2.46184500
H	0.07435000	5.28634200	-3.16622900	H	1.36393800	-2.69730100	1.54141500
H	1.59469400	4.49169700	-2.76270900	H	0.67185100	-3.75955800	2.80022900
H	1.02715900	4.65874400	1.00202300	H	1.29321100	-2.13905200	3.22612700
H	2.18580700	4.11596500	-0.20325400	C	-3.23192200	-2.82462300	1.30835100
H	1.04599300	6.16540000	-1.01797500	C	-3.15022500	-1.49304000	1.75013400

C	-4.22153800	-1.00925400	2.52448300	O	-4.30888300	-2.37236300	0.85150600
C	-5.32318900	-1.80635100	2.82413800	C	-3.21891900	-1.82004600	0.67392400
C	-5.38834500	-3.12442900	2.36512000	N	-2.88094300	-1.20032600	-0.47995400
C	-4.32924000	-3.62994300	1.60950000	H	-1.91892000	-0.89110900	-0.65628100
H	-2.42537900	-3.23368300	0.71353000	C	-2.67613700	-0.17953900	3.43601700
H	-4.18718000	0.01328800	2.88791000	H	-2.14819000	0.55446000	4.04534100
H	-6.13434100	-1.39671400	3.42110800	C	-2.54409600	-2.61030500	3.03470900
H	-6.25028500	-3.74560500	2.59361000	H	-1.74771000	-3.29720200	3.33145200
H	-4.35946300	-4.65360500	1.24297800	H	-3.43762900	-3.19762200	2.81930600
C	-2.00670200	-0.59640400	1.42637200	H	0.19124700	1.97065400	1.71859900

### IM5-S

C	-3.81426800	-1.18926200	-1.62068100	C	1.01430500	-1.54959200	2.26243500
C	-3.38772600	-2.22964000	-2.66121700	C	1.48524100	-2.65026600	1.30647000
C	-3.14604300	-1.91688300	-4.00128900	C	2.19087600	-0.99163400	3.08042000
C	-3.23589200	-3.56111600	-2.24390900	H	0.26810200	-1.95297800	2.95433100
C	-2.73506000	-2.90576300	-4.90071600	C	2.23440400	-3.76026500	2.05590400
H	-3.26877100	-0.89852600	-4.35109000	H	2.14072400	-2.19814800	0.55462100
C	-2.82575100	-4.54725700	-3.13783900	H	0.62973300	-3.06956600	0.76491600
H	-3.44431100	-3.82180600	-1.21034700	C	2.93002500	-2.10513900	3.83283700
C	-2.56620200	-4.22091300	-4.47268200	H	2.88666300	-0.49760600	2.38830900
H	-2.54276900	-2.63961300	-5.93660400	H	1.82432900	-0.22594800	3.77538800
H	-2.71094600	-5.57220800	-2.79502900	C	3.40571500	-3.19992000	2.87147600
H	-2.24128300	-4.98780400	-5.17036400	H	2.59240500	-4.50666600	1.33672600
C	-4.02954200	0.20566800	-2.17907600	H	1.53849600	-4.28141300	2.73040600
C	-5.33449100	0.69254700	-2.30781600	H	3.77828400	-1.67820300	4.38115100
C	-2.96133600	1.00394400	-2.61312100	H	2.25662800	-2.54399400	4.58378000
C	-5.57736800	1.94910100	-2.86717500	H	3.89975800	-4.00564400	3.42835100
H	-6.16831200	0.07968100	-1.97373400	H	4.15420200	-2.78105600	2.18556600
C	-3.20270900	2.26094400	-3.16694200	C	-1.86706500	2.46502800	1.83771600
H	-1.94339800	0.64298800	-2.50807700	C	-1.39222700	3.87847000	2.18742400
C	-4.51018000	2.73629100	-3.30164100	C	-2.52736600	2.40683400	0.45750600
H	-6.59793900	2.31023900	-2.96106900	H	-2.59709100	2.16566400	2.58990400
H	-2.36549100	2.87179700	-3.49413900	C	-2.54566600	4.88362300	2.08409300
H	-4.69411600	3.71451300	-3.73774800	H	-0.59429600	4.16612600	1.49228600
H	-4.76109800	-1.52722400	-1.19392300	H	-0.96217100	3.88336600	3.19695700
C	-2.79838200	-1.55650100	4.14902100	C	-3.68237000	3.41056700	0.37157600
H	-2.03685300	-1.65344100	4.92787800	H	-1.77189500	2.62899200	-0.30497500
N	-0.71269700	1.55264600	1.93057900	H	-2.88302200	1.39181400	0.26283900
N	0.37826300	-0.44357200	1.52175800	C	-3.20982200	4.83107800	0.70221200
N	-1.83891300	-0.47318200	2.25884500	H	-2.17163300	5.89265400	2.29511000
C	-0.72847300	0.21509600	1.91019500	H	-3.29622200	4.65792600	2.85551600
C	-2.12041200	-1.83603500	1.77344800	H	-4.12470100	3.37254700	-0.62826900
H	-1.22802500	-2.24839900	1.30840600	H	-4.47319300	3.11725200	1.07783700
				H	-4.05084900	5.53415500	0.66019200
				H	-2.48515900	5.15438100	-0.05879800



C	3.52734500	-1.16918400	-0.26993200	H	5.30281000	-2.50802900	-4.28875100
N	2.90069500	-0.41165200	0.66178800	H	4.47295300	-1.36870100	-5.35721900
H	1.88608600	-0.41771600	0.71434200	C	3.84840700	0.38412800	-3.22085100
C	2.63548900	-0.59384400	-3.32751400	H	3.74012700	1.17237100	-3.97366900
H	1.93722100	-0.24416200	-4.08835100	H	3.88205000	0.87526900	-2.24492900
C	3.33471800	-2.71706600	-2.31262200	C	5.11618800	-0.45396000	-3.48986200
H	2.87217000	-3.70531800	-2.37716000	H	5.89496000	0.11420000	-4.00967400
H	4.36680600	-2.84962400	-1.98326900	H	5.53403700	-0.80066200	-2.54029100
H	-0.84055900	0.85172100	-2.38043200	H	-2.04082800	-1.02110300	0.04676200
C	-0.32110800	-2.83659800	-1.78538900	C	-5.40021100	1.01541600	-0.47999000
C	-0.47971700	-3.52907000	-0.41955000	C	-6.36393100	0.34487000	-1.23142700
C	-1.40266500	-3.36520000	-2.74747600	C	-5.97470900	-0.52673100	-2.25102400
H	0.64663600	-3.13695100	-2.21337500	C	-4.61774300	-0.72777900	-2.50999300
C	-0.40714600	-5.05554100	-0.54074900	C	-3.64988500	-0.07390000	-1.74675200
H	-1.45268100	-3.24785300	0.00195900	C	-4.03655600	0.80032900	-0.72257200
H	0.27864800	-3.16170900	0.28170400	C	-3.02571500	1.48047100	0.14892900
C	-1.34711300	-4.89218100	-2.88448900	C	-2.98311200	2.96911500	0.12661500
H	-2.38666400	-3.06033100	-2.36439300	C	-2.35508000	3.66828300	1.17056500
H	-1.28083200	-2.88382500	-3.72592700	C	-2.23552500	5.05299100	1.12207500
C	-1.46434100	-5.58226900	-1.51935900	C	-2.73568900	5.76417900	0.02563900
H	-0.53645400	-5.51741900	0.44630200	C	-3.36885500	5.07975700	-1.01212000
H	0.59260800	-5.34689100	-0.89541900	C	-3.50006500	3.69119800	-0.95906000
H	-2.14175400	-5.23955400	-3.55714400	N	-2.20087400	0.88372000	0.93129500
H	-0.39360800	-5.17840900	-3.35235000	H	-5.70185500	1.69153700	0.31447700
H	-1.37341000	-6.67009800	-1.63202200	H	-7.41790700	0.50411000	-1.02159700
H	-2.46401900	-5.38989400	-1.10299100	H	-4.30638900	-1.40163200	-3.30353900
C	0.94948300	1.91486600	-2.09385300	H	-2.59809000	-0.27967400	-1.92517100
C	1.11101200	2.73870800	-3.38030700	H	-1.95637000	3.10423000	2.00628100
C	0.31146400	2.76403400	-0.98737100	H	-1.75020500	5.58189400	1.93774700
H	1.93098100	1.58328500	-1.75038800	H	-3.76077000	5.62471700	-1.86629000
C	1.89555700	4.03401300	-3.13848100	H	-3.98522900	3.16457200	-1.77404300
H	0.10807000	2.98424000	-3.76053500	H	-2.63550700	6.84520300	-0.01449500
H	1.59816800	2.12751800	-4.14828200	H	-6.72580900	-1.04537700	-2.84044400
C	1.10631800	4.05146600	-0.74165400	C	-0.96895100	-0.99310300	1.80342800
H	-0.70967400	3.02684000	-1.29159700	O	-1.17145300	-2.01252700	2.64102600
H	0.22735900	2.17412800	-0.06933500	O	0.12420100	-0.48829300	1.62199600
C	1.25360100	4.87299900	-2.02667300	C	0.00220500	-2.49979900	3.32678000
H	1.96312900	4.61118800	-4.06949000	H	0.71030100	-2.92128700	2.61159200
H	2.92613500	3.78262600	-2.84844900	H	-0.35947400	-3.27273400	4.00481100
H	0.61351800	4.64348200	0.03724400	H	0.48066100	-1.69183300	3.88210300
H	2.10188400	3.79450800	-0.35720900	C	-4.17970600	-2.17445600	0.98504900
H	1.85059700	5.77461600	-1.83739600	C	-3.51575500	-1.11674600	1.61085800
H	0.25941900	5.21219700	-2.35367400	C	-4.07628100	-0.54178600	2.75764000
C	4.61290700	-1.65679100	-4.30655500	C	-5.28574100	-1.01454900	3.26391200

C	-5.94759000	-2.07027200	2.63062200	N	-2.71542800	-1.40574600	0.52783700
C	-5.38991800	-2.65081100	1.49091800	H	-2.10692100	-0.72867400	0.07680800
H	-3.75651300	-2.61332100	0.08662900	C	-3.59973300	1.84663800	2.13670600
H	-3.56620900	0.28394600	3.24602300	H	-3.43127600	2.90980300	1.98062900
H	-5.71391900	-0.55925400	4.15304700	C	-2.98328200	0.23957200	3.89896800
H	-6.89302300	-2.43517500	3.02276600	H	-2.22326500	0.44685500	4.65726300
H	-5.90025800	-3.46744900	0.98744900	H	-3.57305900	-0.61326500	4.24014300
C	-2.22108000	-0.57733700	1.03527900	H	-0.66747500	3.38882700	0.24976400

**IM6-S**

C	-2.96878200	-2.66855600	-0.15593200	C	0.48401700	1.14346600	2.95845200
C	-1.83139900	-3.66512000	0.06285000	C	1.21244900	-0.19421200	2.72351500
C	-0.49534900	-3.25018700	0.11614600	C	1.44458800	2.14539600	3.62840900
C	-2.11967200	-5.02568700	0.21330100	H	-0.32880200	0.97895400	3.68067700
C	0.53174400	-4.17617800	0.30128100	C	1.81410000	-0.76099400	4.01455700
H	-0.25306800	-2.19896400	0.03023800	H	2.00846000	-0.02643300	1.99016100
C	-1.09442500	-5.95695200	0.39162700	H	0.53912300	-0.92855500	2.26477700
H	-3.15522300	-5.35707400	0.19691100	C	2.04751300	1.58833500	4.92382300
C	0.23558900	-5.53468300	0.43360200	H	2.24196200	2.38988300	2.91448300
H	1.56046900	-3.82968200	0.34607800	H	0.90188100	3.07863100	3.82423100
H	-1.33739900	-7.00961700	0.50963200	C	2.75553400	0.24907800	4.68286400
H	1.03407900	-6.25718200	0.57919300	H	2.34719800	-1.69504700	3.79748200
C	-3.31790700	-2.43583200	-1.62623900	H	1.00354600	-1.01733900	4.71257000
C	-3.13259300	-3.44311600	-2.58105700	H	2.74454300	2.31671900	5.35786900
C	-3.88776300	-1.22491500	-2.03857800	H	1.24665200	1.44293800	5.66379600
C	-3.49348900	-3.24089300	-3.91437600	H	3.13942200	-0.15540000	5.62811300
H	-2.69137200	-4.38953000	-2.28731700	H	3.62812500	0.41348300	4.03368000
C	-4.24891700	-1.01972400	-3.37057800	C	-2.36598000	2.69610800	-0.75559000
H	-4.04838900	-0.43519400	-1.31329200	C	-3.48551400	3.74909300	-0.79629800
C	-4.04849000	-2.02582100	-4.31778800	C	-1.53539700	2.80030200	-2.04421400
H	-3.33465500	-4.03583500	-4.63811700	H	-2.81189500	1.69835900	-0.70412800
H	-4.68780500	-0.07093700	-3.66672300	C	-4.38150400	3.56063600	-2.02807100
H	-4.32570700	-1.86577800	-5.35603000	H	-3.02141000	4.74582800	-0.82451100
H	-3.85380300	-3.08892100	0.33321800	H	-4.08416100	3.70820100	0.11727800
C	-3.84990100	1.49731900	3.63843500	C	-2.40539900	2.61122900	-3.29281600
H	-3.52436600	2.31536000	4.28704500	H	-1.06206000	3.79329300	-2.07470900
N	-1.50843200	2.85197000	0.43110300	H	-0.73259100	2.06492600	-2.02724900
N	0.01826800	1.72994700	1.71069300	C	-3.56865600	3.60937000	-3.32797600
N	-2.35430800	1.13842900	1.76909400	H	-5.16862200	4.32491400	-2.04109600
C	-1.22201800	1.85294500	1.35755200	H	-4.89070200	2.58835900	-1.95375200
C	-2.30149900	-0.09314700	2.55969000	H	-1.78758800	2.71217800	-4.19407400
H	-1.27222000	-0.40995000	2.69548500	H	-2.80064000	1.58611300	-3.29736700
O	-3.54037000	-2.17451700	2.50056200	H	-4.21690400	3.41073100	-4.19108400
C	-2.94312900	-1.30731400	1.85969300	H	-3.16710800	4.62438600	-3.46118600
				C	-5.36346800	1.25411000	3.74550100
				H	-5.63072700	0.64518800	4.61586400

H	-5.88744600	2.21483100	3.84007300	H	2.52354400	0.51358900	-3.58214900
C	-4.87937200	1.37649100	1.38427400	H	1.68229100	2.89340500	-0.11621000
H	-5.43588600	2.25890900	1.04947500	H	2.40876500	4.93625200	-1.33612200
H	-4.63196900	0.79287500	0.49504700	H	3.18039800	4.76192800	-3.69577200
C	-5.72488500	0.59369200	2.40623700	H	3.22637800	2.54297300	-4.81679200
H	-6.79660200	0.63512700	2.18454100	C	1.63256900	0.34372500	-0.97584500
H	-5.43468600	-0.46178500	2.42156900	H	1.24873100	0.68614100	-0.00763400
C	4.30915000	1.51778600	0.98011400				
C	4.88209300	2.77624300	1.16569700	<b>N<sub>2</sub></b>			
C	5.63131000	3.35944200	0.14355500	N	0.00000000	0.00000000	0.55254500
C	5.82571200	2.66835000	-1.05521900	N	0.00000000	0.00000000	-0.55254500
C	5.26898200	1.40339000	-1.23381700				
C	4.48262200	0.83240900	-0.22612800	<b>P-R</b>			
C	3.83854500	-0.50715400	-0.43154400	H	-1.69110300	0.79055700	0.96304400
C	4.69357000	-1.71234500	-0.22494100	C	-5.30766600	1.43031500	-0.02464200
C	4.24701700	-2.97102200	-0.66449200	C	-6.06680600	1.94316800	1.02540800
C	5.01640300	-4.10884800	-0.44795200	C	-5.88148200	1.46340400	2.32414100
C	6.24780700	-4.01070300	0.20974800	C	-4.93700300	0.46472400	2.56804200
C	6.70308700	-2.76529900	0.64223900	C	-4.16802900	-0.04247200	1.51946300
C	5.93438200	-1.62108600	0.42173800	C	-4.34221500	0.44501500	0.21892400
N	2.61564400	-0.71418100	-0.75200100	C	-3.46770900	-0.03669600	-0.89866600
H	3.72141900	1.06773300	1.77098400	C	-4.07920800	-0.90900600	-1.93734700
H	4.73597300	3.30073700	2.10603200	C	-3.37571700	-1.19126400	-3.12119000
H	6.41030800	3.11627600	-1.85373800	C	-3.93535200	-2.00907900	-4.09632200
H	5.41672700	0.86856200	-2.16673500	C	-5.20582400	-2.56399800	-3.90577600
H	3.29344900	-3.03229100	-1.17707900	C	-5.91097000	-2.29191100	-2.73353000
H	4.66076600	-5.07475200	-0.79625100	C	-5.35296700	-1.46796600	-1.75526400
H	7.65810100	-2.68056300	1.15324200	N	-2.22882800	0.27692900	-1.02582300
H	6.29342900	-0.65693100	0.76540200	H	-5.44116700	1.81140700	-1.03235100
H	6.84735600	-4.90067600	0.37995800	H	-6.80067300	2.71985400	0.83023000
H	6.06709300	4.34527900	0.27999300	H	-4.79644900	0.07985700	3.57420300
C	0.43928600	-0.32052000	-1.66025100	H	-3.43114100	-0.81800400	1.70895800
O	0.79199600	-1.01409400	-2.74378400	H	-2.39173400	-0.75555000	-3.25621500
O	-0.71449900	-0.22416700	-1.27464100	H	-3.38334000	-2.21569000	-5.00915000
C	-0.27266600	-1.68710600	-3.44923500	H	-6.89721700	-2.71994900	-2.57721000
H	-0.64151100	-2.51799900	-2.84869500	H	-5.90702300	-1.26216500	-0.84589600
H	0.17834300	-2.05331400	-4.37170700	H	-5.64169400	-3.20226500	-4.66944100
H	-1.08849000	-0.99559600	-3.66399800	H	-6.47370700	1.86419400	3.14199400
C	2.49146900	1.48247000	-3.09554200	C	-0.10695400	1.28488100	-0.32257000
C	2.06010500	1.57608300	-1.76696200	O	0.17849500	1.38772300	-1.62846300
C	2.02103000	2.82884300	-1.14556400	O	0.72613900	1.33283200	0.56085200
C	2.42796900	3.97086000	-1.83456000	C	1.56709000	1.59271100	-1.94829400
C	2.86370000	3.87267800	-3.15753200	H	1.92175700	2.53614200	-1.52406200
C	2.89052700	2.62602900	-3.78653500	H	1.61391900	1.62457500	-3.03725100

H	2.17565100	0.76927300	-1.56541600	H	-3.36017200	0.25088900	5.28638000
C	-2.50531300	3.23627400	1.11677200	H	-3.77416900	-1.44622700	4.87889000
C	-2.19269600	2.58749500	-0.08020300	H	-4.71058800	-0.09388600	4.16789800
C	-2.42935000	3.23649700	-1.29797800	C	0.17191400	2.27728400	2.32034900
C	-2.99140500	4.51223100	-1.31360500	C	-0.21002100	0.93419200	2.23458300
C	-3.31410200	5.15338900	-0.11455800	C	0.63318000	-0.05430500	2.75034000
C	-3.06628900	4.51374400	1.10092400	C	1.85329200	0.29202800	3.33355100
H	-2.33281000	2.72827200	2.06107200	C	2.23488700	1.63270700	3.40999800
H	-2.18346200	2.73506800	-2.22837700	C	1.39086800	2.62389000	2.90230900
H	-3.17822200	5.00684600	-2.26298600	H	-0.48885400	3.04169900	1.92522700
H	-3.75642800	6.14570800	-0.12889100	H	0.33365100	-1.09783900	2.69209900
H	-3.31827800	5.00332000	2.03756100	H	2.50529000	-0.48443200	3.72432400
C	-1.60768400	1.17745600	-0.05615500	H	3.18494900	1.90453400	3.86185300

H	1.68202700	3.66917800	2.96158600
C	-1.56433800	0.55549100	1.65390600

**P-S**

H	-1.54504200	-0.50245000	1.37839100
C	-5.17931700	0.51628600	0.90588400
C	-6.07739700	-0.47044800	1.31265100
C	-5.80738500	-1.81557100	1.05069800
C	-4.63858200	-2.17125000	0.37511200
C	-3.73446500	-1.18718000	-0.02490200
C	-3.99548700	0.16203200	0.24527000
C	-2.99593300	1.21853600	-0.12140100
C	-3.31260500	2.10979100	-1.26863300
C	-2.52306900	3.24522200	-1.51998400
C	-2.80686500	4.07819900	-2.59624900
C	-3.88370800	3.79247600	-3.44290700
C	-4.67314300	2.66799900	-3.20274700
C	-4.39236200	1.83279300	-2.12092500
N	-1.88976000	1.39841900	0.50576800
H	-5.38250100	1.56184200	1.11466600
H	-6.98870700	-0.18793500	1.83227400
H	-4.42870000	-3.21529700	0.16048100
H	-2.82422900	-1.46299400	-0.54997500
H	-1.69169500	3.45794000	-0.85733800
H	-2.19138500	4.95527400	-2.77629400
H	-5.50969600	2.43816000	-3.85663200
H	-5.01038800	0.95946500	-1.94244800
H	-4.10426600	4.44530400	-4.28295600
H	-6.50811400	-2.58298700	1.36735800
C	-2.59586700	0.71331500	2.78053500
O	-2.80472500	-0.45980100	3.39905600
O	-3.11729200	1.75935000	3.10324000
C	-3.72530900	-0.42262100	4.50679100

**Rh<sub>2</sub>(esp)<sub>2</sub>**

Rh	-0.59591100	-1.03330100	-0.10063400
C	1.93160500	-1.00074700	-1.50948800
C	3.07141500	-1.56853600	-2.35913300
C	4.34017900	-1.59075000	-1.48236900
H	4.60035200	-0.58657000	-1.13532000
H	5.18238400	-1.98890800	-2.05933200
H	4.19617200	-2.23394200	-0.60623000
C	2.74570000	-2.98953200	-2.83318200
H	2.61677200	-3.66585400	-1.98263900
H	3.57182800	-3.36659600	-3.44668300
H	1.83098600	-3.01940600	-3.42993800
O	0.92421700	-1.74477600	-1.28215000
O	-0.43633700	1.68970400	-1.56063400
C	-0.23442200	0.04674400	-5.94256700
H	-1.13268700	0.21013200	-6.53214800
C	0.02822200	0.86842800	-4.83872700
C	-0.94143500	1.94341100	-4.40448700
H	-1.49550100	2.32509500	-5.26978600
H	-0.38908100	2.78383300	-3.97306300
C	-2.00078300	1.47328200	-3.35885300
C	-2.94184800	0.42368000	-3.96135900
H	-2.40161700	-0.47079900	-4.28061600
H	-3.45172900	0.84927600	-4.83318700
H	-3.70276900	0.11846100	-3.23676400
C	-2.81481200	2.69782700	-2.89312700
H	-3.55770900	2.40733500	-2.14092100
H	-3.34788000	3.13455700	-3.74521500

H	-2.16601300	3.46440400	-2.45953800	C	-1.93160500	1.00074700	1.50948800
C	-1.26777900	0.91372400	-2.13700700	C	-3.07141500	1.56853600	2.35913300
O	-1.53314700	-0.27350600	-1.76401500	C	-4.34017900	1.59075000	1.48236900
O	2.07426600	0.18794400	-1.07062700	H	-4.60035200	0.58657000	1.13532000
C	3.31576600	-0.61697500	-3.57189700	H	-5.18238400	1.98890800	2.05933200
H	3.68558400	0.33774300	-3.18517600	H	-4.19617200	2.23394200	0.60623000
H	4.11952200	-1.06295900	-4.16887400	C	-2.74570000	2.98953200	2.83318200
C	2.09737400	-0.37730900	-4.43425800	H	-2.61677200	3.66585400	1.98263900
C	1.81083400	-1.18659500	-5.54155100	H	-3.57182800	3.36659600	3.44668300
H	2.49870200	-1.98100400	-5.81922700	H	-1.83098600	3.01940600	3.42993800
C	0.65529700	-0.96965000	-6.29402000	Rh	0.59591100	1.03330100	0.10063400
H	0.44834800	-1.59328800	-7.15976700				
C	1.20495200	0.65227700	-4.11133100				
H	1.42726900	1.29625300	-3.26767400	<b>Rh<sub>2</sub>(OAc)<sub>4</sub></b>			
O	-2.07426600	-0.18794400	1.07062700	Rh	-0.58200000	-1.04257600	-0.09915900
C	-3.31576600	0.61697500	3.57189700	C	1.92816300	-0.94294800	-1.54194200
H	-3.68558400	-0.33774300	3.18517600	C	3.05978000	-1.50101500	-2.36236300
H	-4.11952200	1.06295900	4.16887400	O	0.94234500	-1.71672800	-1.30475800
C	-2.09737400	0.37730900	4.43425800	O	-0.44383100	1.68785100	-1.56681000
C	-1.81083400	1.18659500	5.54155100	C	-1.98357000	1.43065300	-3.35129200
H	-2.49870200	1.98100400	5.81922700	C	-1.27219700	0.90257800	-2.13439400
C	-0.65529700	0.96965000	6.29402000	O	-1.54096800	-0.28379800	-1.75491200
H	-0.44834800	1.59328800	7.15976700	O	2.04790800	0.25211600	-1.11527200
C	-1.20495200	-0.65227700	4.11133100	O	-2.04790800	-0.25211600	1.11527200
H	-1.42726900	-1.29625300	3.26767400	O	1.54096800	0.28379800	1.75491200
O	1.53314700	0.27350600	1.76401500	O	0.44383100	-1.68785100	1.56681000
O	0.43633700	-1.68970400	1.56063400	C	1.98357000	-1.43065300	3.35129200
C	0.23442200	-0.04674400	5.94256700	C	1.27219700	-0.90257800	2.13439400
H	1.13268700	-0.21013200	6.53214800	O	-0.94234500	1.71672800	1.30475800
C	-0.02822200	-0.86842800	4.83872700	C	-1.92816300	0.94294800	1.54194200
C	0.94143500	-1.94341100	4.40448700	C	-3.05978000	1.50101500	2.36236300
H	1.49550100	-2.32509500	5.26978600	Rh	0.58200000	1.04257600	0.09915900
H	0.38908100	-2.78383300	3.97306300	H	-1.24487800	1.71134600	-4.10953500
C	2.00078300	-1.47328200	3.35885300	H	-2.66638300	0.68424400	-3.76025000
C	2.94184800	-0.42368000	3.96135900	H	-2.54116200	2.33442700	-3.08317100
H	2.40161700	0.47079900	4.28061600	H	3.60141000	-0.69819800	-2.86706600
H	3.45172900	-0.84927600	4.83318700	H	2.68457700	-2.22471500	-3.08963400
H	3.70276900	-0.11846100	3.23676400	H	3.75526500	-2.01928500	-1.69064700
C	2.81481200	-2.69782700	2.89312700	H	2.66638300	-0.68424400	3.76025000
H	3.55770900	-2.40733500	2.14092100	H	2.54116200	-2.33442700	3.08317100
H	3.34788000	-3.13455700	3.74521500	H	1.24487800	-1.71134600	4.10953500
H	2.16601300	-3.46440400	2.45953800	H	-2.68457700	2.22471500	3.08963400
C	1.26777900	-0.91372400	2.13700700	H	-3.60141000	0.69819800	2.86706600
O	-0.92421700	1.74477600	1.28215000	H	-3.75526500	2.01928500	1.69064700



**Rh-IM-R**

				C	5.72854600	-0.00301700	-0.76153500
C	-5.39730400	1.49071300	-0.41321000	C	6.74556600	0.56730700	0.21667500
C	-6.73867300	1.23826600	-0.68084100	C	7.77738000	1.40558600	-0.22822600
C	-7.68897400	2.25114600	-0.52321400	C	6.59589600	0.34310300	1.58841000
C	-7.28384900	3.51186000	-0.07929100	C	8.64391900	2.00688900	0.68392900
C	-5.94168200	3.75659000	0.20915200	H	7.90417500	1.58296100	-1.29335500
C	-4.97296500	2.75016500	0.04311300	C	7.46604900	0.94057200	2.50399400
C	-3.55243400	3.00262700	0.39450500	H	5.78658300	-0.29005600	1.93560200
C	-3.31914500	3.98608600	1.49028900	C	8.48995500	1.77517000	2.05456300
C	-3.93545600	3.84709600	2.74499000	H	9.44055700	2.65419100	0.32726400
C	-3.73094000	4.79635300	3.74542700	H	7.33662700	0.75894000	3.56744600
C	-2.93495300	5.91979200	3.49717600	H	9.16472700	2.24413100	2.76533300
C	-2.33023400	6.07572500	2.24879100	C	6.30975300	-0.80445900	-1.91608100
C	-2.51167400	5.10920200	1.25757800	C	5.57027500	-0.98080800	-3.09277500
N	-2.49137500	2.46869800	-0.14659500	C	7.54382300	-1.45542400	-1.79341600
H	-4.66648700	0.70673200	-0.54618900	C	6.05349300	-1.78795800	-4.12383200
H	-7.03796900	0.24933100	-1.01513300	H	4.60472200	-0.49582500	-3.19263100
H	-8.01377000	4.30778000	0.04306100	C	8.02502800	-2.26899200	-2.82051100
H	-5.63847800	4.73901200	0.55642000	H	8.13100200	-1.32793200	-0.89030000
H	-4.57180400	2.98716000	2.93161900	C	7.28236100	-2.43799100	-3.99077400
H	-4.20085000	4.66625000	4.71649600	H	5.46568400	-1.91282000	-5.02911700
H	-1.71289200	6.94696000	2.04658600	H	8.98305800	-2.76839400	-2.70497100
H	-2.04350700	5.22832800	0.28500200	H	7.65803400	-3.06875600	-4.79158100
H	-2.79031900	6.66744000	4.27208700	H	5.05734400	-0.66043300	-0.20176800
H	-8.73533600	2.05854900	-0.74421300	C	4.12715400	5.10401200	-0.03152300
C	-1.46302500	0.80498300	-1.52787000	H	3.75544100	6.04347700	-0.44905800
O	-1.28233200	0.39974600	-2.82647900	N	0.24218300	3.12648600	0.90503200
O	-0.69554200	0.37616400	-0.61223900	N	0.49301200	3.13811400	-1.37369600
C	-0.16539500	-0.44005100	-3.11648200	N	2.37913900	3.49356100	-0.04634300
H	0.72103000	-0.12748500	-2.56098000	C	1.04498400	3.25857900	-0.14409500
H	0.00503400	-0.33787000	-4.19180400	C	3.33626600	2.95643000	-1.00722200
H	-0.38801900	-1.47753900	-2.87140200	H	2.84918200	2.71595900	-1.95094700
C	-3.70849400	3.53172100	-2.67171500	O	3.52682000	1.09919200	0.55694700
C	-3.35465200	2.17971900	-2.48685400	C	3.92128000	1.63019900	-0.47633700
C	-3.88436500	1.24930800	-3.40111500	N	4.88364800	1.08618500	-1.26696600
C	-4.69983500	1.64964200	-4.45775900	H	5.26313900	1.64500400	-2.02171200
C	-5.02622200	2.99653600	-4.63187500	C	3.04561200	4.43372000	0.86892400
C	-4.52428400	3.93505800	-3.72604400	H	2.29861700	5.15003800	1.20914400
H	-3.35007600	4.27603800	-1.96850600	C	4.38330000	4.08752600	-1.17683200
H	-3.64817700	0.20018200	-3.27401700	H	4.26253800	4.56400200	-2.15298200
H	-5.09448500	0.90055700	-5.14019500	H	5.40210500	3.69366400	-1.12885900
H	-5.66768300	3.30882900	-5.45145500	H	-0.75487200	2.98967400	0.65611600
H	-4.77176500	4.98794300	-3.83798000	C	0.75440400	4.01482200	-2.52491200
C	-2.48153400	1.77132200	-1.36210100	C	0.68899000	3.18107700	-3.81151800

C	-0.25784400	5.17135000	-2.55635000	C	1.26973600	-5.08868100	-3.13661300
H	1.75597300	4.43848700	-2.41095400	H	0.77250900	-5.94768600	-2.67584100
C	0.84550100	4.05377200	-5.06293500	H	1.98553300	-5.45918100	-3.87955000
H	-0.27838300	2.66346500	-3.83756000	H	0.51213800	-4.49510600	-3.66214300
H	1.46005600	2.40119400	-3.78084400	C	2.71119100	-3.05915400	-2.76399700
C	-0.08669400	6.03966600	-3.80963100	H	2.00691300	-2.45548100	-3.34460200
H	-1.26773000	4.74458900	-2.54814800	H	3.48001400	-3.43910700	-3.44578400
H	-0.15204700	5.77784200	-1.64827400	H	3.19472100	-2.40609400	-2.03505200
C	-0.18257100	5.19185500	-5.08383800	O	0.71349900	-2.48707900	-1.05598300
H	0.74598100	3.43115900	-5.96004300	O	0.37843600	-3.55323900	2.37621300
H	1.85923300	4.48107700	-5.08653800	C	5.06040300	-3.08928300	1.88020300
H	-0.84664100	6.83040500	-3.81572000	H	5.56480200	-2.56820400	2.68968400
H	0.89189200	6.54122200	-3.77711300	C	3.77629700	-3.61009800	2.08527700
H	-0.03548100	5.81989500	-5.97111300	C	3.03799700	-3.40217900	3.38625200
H	-1.19266100	4.76510700	-5.15647300	H	3.75670100	-3.23402900	4.19724500
C	0.59230200	2.78715500	2.29271600	H	2.46598400	-4.30043200	3.63714100
C	0.46217000	4.02588200	3.19487400	C	2.06121600	-2.18734200	3.38946700
C	-0.34070700	1.66275400	2.76698200	C	2.81831400	-0.88739900	3.10009700
H	1.61859000	2.41760900	2.29189000	H	3.26157800	-0.88626300	2.10394800
C	0.67442500	3.69602900	4.67591300	H	3.61593600	-0.75536400	3.84186500
H	-0.54359900	4.43453800	3.06278100	H	2.15590200	-0.02311300	3.15382300
H	1.16277500	4.80298100	2.87321000	C	1.38209100	-2.12258800	4.77431800
C	-0.12762700	1.35567400	4.25465300	H	0.62069000	-1.33753300	4.80161400
H	-1.38028800	1.97909700	2.61213500	H	2.12773300	-1.90103100	5.54689300
H	-0.18048200	0.77381500	2.15319300	H	0.90075200	-3.07465600	5.01969300
C	-0.29460500	2.60034000	5.13075600	C	0.94230800	-2.40929600	2.36089300
H	0.54140900	4.60607500	5.27434000	O	0.62640200	-1.44471700	1.59575700
H	1.70820100	3.35714500	4.83824200	O	0.34929600	-4.61473400	-0.38436800
H	-0.82268900	0.56856700	4.56329500	C	3.03391900	-5.13534200	-1.33774100
H	0.88317700	0.95773900	4.40623100	H	2.50183900	-6.00665900	-0.94252500
H	-0.12369900	2.35003100	6.18560000	H	3.74515900	-5.49858800	-2.08847900
H	-1.32590900	2.97279900	5.05101900	C	3.77425400	-4.44031500	-0.21798100
C	5.33631400	5.30895900	0.89018700	C	5.05141900	-3.89567100	-0.40448200
H	6.27170300	5.43902400	0.33499100	H	5.54569400	-3.98672200	-1.36795300
H	5.18664700	6.20744300	1.50289000	C	5.69462800	-3.23841800	0.64628100
C	3.82739500	3.83068800	2.07699700	H	6.69104600	-2.83353100	0.49818900
H	3.53490100	4.36966500	2.98457100	C	3.16498900	-4.30361000	1.03558100
H	3.59797400	2.77558200	2.21677200	H	2.18445400	-4.73553900	1.19386200
C	5.32142600	4.05616600	1.77798100	Rh	-0.80720200	-1.74244600	0.12999100
H	5.92314900	4.16636400	2.68521200	Rh	-1.07300100	-3.99534900	0.98277500
H	5.72748800	3.20006000	1.22769800	O	-2.32287900	-1.16974400	1.41880500
H	-0.43986800	2.73082500	-1.38501500	C	-5.08267700	-0.87173500	2.24306200
C	0.94497000	-3.73466200	-1.08888800	H	-4.64565400	0.01758700	1.78159100
C	2.00259600	-4.23472200	-2.08197400	H	-5.86585800	-0.53005400	2.93004800

C	-5.69102500	-1.74109400	1.16756300	C	-3.41558800	3.08724300	0.59650400
C	-6.88911700	-2.43764700	1.37126100	C	-3.61456400	3.51416100	2.01152800
H	-7.40304800	-2.35518900	2.32564800	C	-4.60110200	2.91301600	2.80841500
C	-7.43365900	-3.22054700	0.35144900	C	-4.73826400	3.26754400	4.15002300
H	-8.36757900	-3.75146700	0.51746500	C	-3.91439400	4.25072300	4.70378400
C	-5.06212200	-1.84996100	-0.07792800	C	-2.94845500	4.87451900	3.90925900
H	-4.14022900	-1.30906400	-0.24892100	C	-2.79483000	4.50315200	2.57443900
O	-2.50014300	-4.31066700	-0.46934700	N	-2.20031200	3.00133700	0.18459900
O	-2.17503000	-2.25032100	-1.34008600	H	-3.95946000	0.96585700	-1.03616300
C	-6.79249700	-3.31384000	-0.88572700	H	-6.02909500	0.56303400	-2.33690000
H	-7.22893100	-3.91328900	-1.68085700	H	-7.68087400	4.24315200	-0.84738000
C	-5.59390900	-2.62550400	-1.11409100	H	-5.62634400	4.61895700	0.48364500
C	-4.86848900	-2.70131600	-2.43735800	H	-5.24478300	2.15280200	2.37934400
H	-5.56733200	-2.99184800	-3.23051300	H	-5.49034100	2.77752500	4.76194800
H	-4.48420700	-1.71043100	-2.69727400	H	-2.31445700	5.64963300	4.33041600
C	-3.68664300	-3.71673900	-2.47862800	H	-2.04134000	4.97783700	1.95505600
C	-4.21422900	-5.15241200	-2.37200300	H	-4.02892000	4.53485800	5.74612500
H	-4.76591300	-5.31110300	-1.44176800	H	-7.88794600	2.20480200	-2.26172800
H	-4.88914300	-5.35577600	-3.21173900	C	-1.34989200	1.37026500	-1.41143600
H	-3.39566600	-5.87794300	-2.40642900	O	-1.06155100	1.10892000	-2.70264500
C	-2.92627600	-3.53250400	-3.80680600	O	-1.05085100	0.59613300	-0.48539300
H	-2.07839900	-4.22479100	-3.87333000	C	-0.17218700	0.01921000	-2.99670000
H	-3.59559000	-3.73696400	-4.65054900	H	0.67969600	0.02586300	-2.31621900
H	-2.54628900	-2.51181600	-3.90465700	H	0.15486900	0.18881500	-4.02449700
C	-2.71402800	-3.40573800	-1.33408200	H	-0.69473300	-0.93156300	-2.91669500
O	-2.52090300	-3.26376700	2.25102300	C	-2.78333700	4.89485400	-1.95715500
C	-2.85380000	-2.03822800	2.18441400	C	-2.52549500	3.54025100	-2.25184700
C	-3.98244100	-1.55610000	3.10570100	C	-2.90322000	3.07757500	-3.52442400
C	-3.39230700	-0.50252700	4.06193100	C	-3.49721500	3.93179700	-4.45577500
H	-2.97771800	0.34233900	3.50662600	C	-3.74242100	5.26983200	-4.14674500
H	-4.17400500	-0.12924500	4.73390300	C	-3.38392000	5.74410300	-2.88262800
H	-2.59700500	-0.93943600	4.67643700	H	-2.50505500	5.28494800	-0.98341600
C	-4.56851700	-2.72036700	3.91275100	H	-2.73888500	2.04220200	-3.78886200
H	-3.80582700	-3.18565000	4.54476500	H	-3.78098800	3.53770600	-5.42873600
H	-5.36919000	-2.34750100	4.56261600	H	-4.20830200	5.92957100	-4.87350000
H	-4.98555000	-3.49390900	3.26283200	H	-3.56570600	6.78227700	-2.61599300

### Rh-TS-R

C	-4.77166200	1.68108900	-0.99976900	C	5.65889800	-0.44061500	-0.60813000
C	-5.93640800	1.45851600	-1.73217400	C	6.66626900	-0.06562400	0.47144500
C	-6.98421000	2.37956900	-1.68448900	C	7.80351400	0.69330700	0.16113300
C	-6.86967100	3.52160500	-0.88866900	C	6.41198900	-0.39257000	1.80649500
C	-5.71378000	3.73520900	-0.14054000	C	8.67185200	1.11259200	1.16859100
C	-4.64890300	2.82263100	-0.19776700	H	8.01297000	0.95001400	-0.87433600
				C	7.28240100	0.02309600	2.81724000

H	5.52389900	-0.96437900	2.05015100	H	0.80908100	6.27383500	-1.42944300
C	8.41331400	0.77696000	2.50131600	C	1.12252100	5.54163500	-4.82355200
H	9.55110000	1.69884200	0.91537900	H	1.69979700	3.56523200	-5.52514100
H	7.07083100	-0.23735600	3.85073800	H	2.89932100	4.35358500	-4.50233800
H	9.08931000	1.10415400	3.28645500	H	0.71686400	7.35595600	-3.69489600
C	6.25108200	-1.14133400	-1.82207100	H	2.30347800	6.65049600	-3.39170500
C	5.62763200	-1.05132100	-3.07298900	H	1.54516900	6.06795000	-5.68889300
C	7.38280300	-1.95786300	-1.69454100	H	0.05820100	5.37077400	-5.04025300
C	6.12088400	-1.76155100	-4.16931800	C	0.78363600	2.73336500	2.55910800
H	4.74076400	-0.43633700	-3.18521600	C	0.82050500	3.81814200	3.65204200
C	7.87195800	-2.67531000	-2.78663900	C	-0.30193100	1.68600700	2.86641200
H	7.88433700	-2.03340700	-0.73578100	H	1.74994300	2.23049800	2.49400800
C	7.24288800	-2.58011000	-4.03011500	C	0.95714300	3.23230900	5.06136800
H	5.62138900	-1.67801900	-5.13075700	H	-0.11518900	4.38800600	3.59060600
H	8.74845900	-3.30572200	-2.66480600	H	1.63285300	4.52321900	3.44799600
H	7.62553200	-3.13581000	-4.88158600	C	-0.17301300	1.12630000	4.28873500
H	4.91832100	-1.10980000	-0.16020000	H	-1.28470300	2.15906900	2.76022100
C	4.61471000	4.73609300	0.45658100	H	-0.25583900	0.88199700	2.12738600
H	4.35680500	5.72680700	0.07222200	C	-0.16920600	2.23297500	5.34772900
N	0.51087900	3.35681000	1.25932800	H	0.95678800	4.04259200	5.80203200
N	0.74624400	3.60871200	-1.00234800	H	1.92641500	2.72029600	5.15326500
N	2.68363300	3.33978800	0.36674100	H	-0.98869800	0.41734800	4.47169500
C	1.31679600	3.43586500	0.17707800	H	0.76101700	0.55861000	4.37760900
C	3.57392100	2.74696200	-0.61402400	H	-0.05203600	1.80100900	6.35018700
H	3.07023400	2.62226800	-1.57147200	H	-1.13459500	2.75825500	5.33536000
O	3.52344000	0.73587600	0.77581100	C	5.82734100	4.76379600	1.39652100
C	3.99711200	1.32393300	-0.19103000	H	6.78055500	4.81748800	0.85847500
N	4.91966500	0.75750200	-1.01986800	H	5.76816900	5.64180800	2.05304600
H	5.37969800	1.35786300	-1.69341900	C	4.14835000	3.40232300	2.49442900
C	3.45178400	4.15472000	1.31664100	H	3.90790500	3.91353400	3.43329700
H	2.79274400	4.93622300	1.69561900	H	3.79857700	2.37311000	2.56938600
C	4.76833800	3.73806800	-0.72179100	C	5.66231300	3.47735700	2.21950700
H	4.74061800	4.25911700	-1.68253300	H	6.26142900	3.47334700	3.13538300
H	5.72691400	3.21502200	-0.66168100	H	5.98024400	2.61171800	1.62826700
H	-0.48857600	3.42467300	1.02685700	H	-0.56233400	3.21560000	-1.17126500
C	1.36442400	4.30164700	-2.12693500	C	0.66318600	-3.53240700	-1.42332600
C	1.26429300	3.45158900	-3.40470600	C	1.76565900	-3.94645000	-2.40375200
C	0.68468200	5.66807200	-2.33595900	C	1.05866400	-4.55059600	-3.63590100
H	2.42099100	4.50947600	-1.91970500	H	0.47129300	-5.43252800	-3.36208700
C	1.81849300	4.18866200	-4.63001200	H	1.80291200	-4.84617600	-4.38425800
H	0.20956800	3.20253600	-3.57103500	H	0.38500900	-3.81868000	-4.09773100
H	1.78683800	2.49756500	-3.25679400	C	2.60588300	-2.73721100	-2.82763000
C	1.24440000	6.40316600	-3.56057100	H	1.99454200	-1.99251900	-3.34596800
H	-0.39030700	5.50797800	-2.46968400	H	3.39830900	-3.06423000	-3.50838800

H	3.07371400	-2.25018700	-1.96913800	O	-2.80184200	-4.06174700	-1.04403500
O	0.44403800	-2.29181600	-1.26460600	O	-2.43848200	-1.89619400	-1.57651300
O	-0.05839700	-3.78325100	2.00304600	C	-6.98064700	-3.12731700	-1.29443100
C	4.67440400	-3.68905600	1.82117100	H	-7.38105100	-3.65115200	-2.15878800
H	5.17539900	-3.33380300	2.71806500	C	-5.83904700	-2.32821200	-1.43440000
C	3.32755500	-4.06941700	1.88289400	C	-5.11861700	-2.17599000	-2.75469400
C	2.52488000	-3.92390500	3.15523000	H	-5.81599000	-2.32606700	-3.58717400
H	3.20229900	-3.89140300	4.01664900	H	-4.72763700	-1.15691000	-2.83623700
H	1.86945900	-4.78997700	3.28809000	C	-3.92664200	-3.15798400	-2.96653700
C	1.65381200	-2.63303000	3.22090800	C	-4.43112500	-4.59762100	-3.11801900
C	2.53008200	-1.38699800	3.05690600	H	-4.97829800	-4.92917500	-2.23223800
H	3.03167700	-1.36530700	2.08892000	H	-5.10082100	-4.66078800	-3.98365300
H	3.29051800	-1.36924300	3.84726900	H	-3.59895300	-5.29012900	-3.27882900
H	1.93776100	-0.47523000	3.12746500	C	-3.15369100	-2.73528200	-4.23072300
C	0.92560400	-2.60485600	4.58241100	H	-2.28679600	-3.38680000	-4.39405500
H	0.25584200	-1.74173300	4.64946600	H	-3.80489800	-2.81395700	-5.10874900
H	1.65831600	-2.53160900	5.39450000	H	-2.79954800	-1.70301500	-4.15308100
H	0.33355800	-3.51389600	4.73130900	C	-2.98326800	-3.03401000	-1.76659900
C	0.55909200	-2.67523800	2.14537400	O	-2.92725900	-3.37848700	1.80970500
O	0.30956000	-1.60998000	1.49759500	C	-3.18378000	-2.13837700	1.93517200
O	0.01111000	-4.46991900	-0.85768500	C	-4.29277300	-1.72612900	2.91003400
C	2.66582500	-5.04118300	-1.75662100	C	-3.68870300	-0.74313400	3.93197900
H	2.03781300	-5.90894500	-1.53125200	H	-3.26375000	0.13171600	3.43451700
H	3.39094000	-5.35088300	-2.51808600	H	-4.46577000	-0.40543600	4.62760300
C	3.39532600	-4.59819300	-0.50758600	H	-2.89820700	-1.22757900	4.51666300
C	4.73732400	-4.19885200	-0.54672700	C	-4.86869200	-2.94812800	3.63366000
H	5.28481600	-4.22921200	-1.48461500	H	-4.09308100	-3.46872300	4.20402000
C	5.37513900	-3.76393400	0.61661500	H	-5.64754300	-2.62376600	4.33393300
H	6.41979300	-3.47030300	0.58084500	H	-5.30896700	-3.66326500	2.93441100
C	2.71932000	-4.54995900	0.71812400				
H	1.69039800	-4.88126500	0.76496200				
Rh	-1.08707900	-1.65668900	-0.02674400	<b>TS1</b>			
Rh	-1.45628600	-3.97919100	0.50535900	C	-1.77383200	1.33590900	-1.53196200
O	-2.59226600	-1.19922700	1.31141500	C	-2.84275900	2.36302000	-1.92233200
C	-5.40594200	-0.98130800	2.11008400	C	-2.21270000	3.76451500	-1.78836600
H	-4.98461600	-0.04023900	1.74466300	H	-1.89152800	3.95646300	-0.76065300
H	-6.19937800	-0.73056400	2.82424900	H	-2.94447000	4.52966800	-2.07165600
H	-6.19937800	-0.73056400	2.82424900	H	-1.34362200	3.86779300	-2.44936500
C	-5.98083700	-1.74579300	0.94058000	C	-3.31486900	2.14132100	-3.36346700
C	-7.12100400	-2.55121900	1.05679800	H	-2.48601800	2.25299200	-4.06905100
H	-7.63009100	-2.62985500	2.01407200	H	-4.08075300	2.88406300	-3.61565900
C	-7.61476500	-3.23781500	-0.05467500	H	-3.74111900	1.14475400	-3.50140300
H	-8.50575700	-3.85261500	0.04295700	O	-1.37080600	0.51265000	-2.40907800
C	-5.35864800	-1.65155400	-0.30809500	O	-1.35508500	-1.33081800	0.83095900
H	-4.48070400	-1.02732200	-0.40459300	C	-5.74791400	-1.70093300	-0.71151400

H	-6.16970600	-2.70171400	-0.66724700	H	-0.14108600	5.38289500	0.96089200
C	-4.66842900	-1.36773600	0.11706800	C	0.10211400	0.94233700	2.31134500
C	-4.02933600	-2.39038200	1.02884200	Rh	0.06912700	-0.87793100	-1.90259900
H	-4.76823900	-3.14148900	1.33164800	Rh	0.08144500	0.07882100	0.34636000
H	-3.66955400	-1.89738100	1.93544800	O	1.47240300	-2.24045600	-1.21402500
C	-2.83223200	-3.15861000	0.38749800	C	4.18472900	-3.06641100	-0.39129400
C	-3.30160500	-4.01417800	-0.79477900	H	3.95734900	-3.35518700	-1.42235000
H	-3.74349800	-3.40376900	-1.58590000	H	4.91479200	-3.78566300	-0.00223100
H	-4.05451800	-4.73266600	-0.45007800	C	4.76286600	-1.67014100	-0.37844900
H	-2.46758000	-4.57446600	-1.22755800	C	5.67875800	-1.25770200	0.59823800
C	-2.18227100	-4.06172500	1.45457100	H	6.02309600	-1.96702500	1.34601200
H	-1.34066900	-4.62073500	1.02860800	C	6.16043100	0.05240300	0.60582700
H	-2.91499100	-4.78555700	1.82956800	H	6.87948800	0.35979300	1.36065200
H	-1.80757100	-3.47582600	2.29820800	C	4.35560500	-0.74261200	-1.34488400
C	-1.77879000	-2.13956000	-0.06139500	H	3.65561100	-1.05565200	-2.11260800
O	-1.39564800	-2.17198000	-1.26982100	O	1.54836300	1.36119500	-0.30880500
O	-1.35116100	1.40393700	-0.32979100	O	1.54030000	0.50010200	-2.39691300
C	-4.03259400	2.25867100	-0.91758500	C	5.73166700	0.96726800	-0.35735900
H	-3.66681300	2.55467200	0.07021500	H	6.11683700	1.98355500	-0.34997500
H	-4.77869000	2.99939700	-1.22844000	C	4.81647100	0.57907100	-1.34469200
C	-4.66640400	0.88894100	-0.83215300	C	4.29570600	1.55325300	-2.37595700
C	-5.74529400	0.53011500	-1.65104500	H	5.06171300	2.29926800	-2.61791300
H	-6.16754400	1.26188200	-2.33495300	H	4.06089700	1.01372500	-3.29885800
C	-6.28618900	-0.75485500	-1.58508100	C	3.01867600	2.33533700	-1.93623100
H	-7.13093200	-1.01944700	-2.21577300	C	3.33853400	3.30009500	-0.78761600
C	-4.15574200	-0.06555900	0.05650800	H	3.70010900	2.77293700	0.09786100
H	-3.33209100	0.20585800	0.70725200	H	4.11123100	4.00736200	-1.11001200
C	-0.37826200	-0.07118300	3.30551700	H	2.45327700	3.87481700	-0.49768000
O	-1.71073500	0.03491700	3.42810700	C	2.47934900	3.12536700	-3.14422700
O	0.30109600	-0.90695800	3.87011200	H	1.57481000	3.68376300	-2.87445900
C	-2.34080900	-0.95123700	4.26793500	H	3.23199700	3.84589400	-3.48410500
H	-3.40594900	-0.72447800	4.23052500	H	2.23566200	2.45890300	-3.97625600
H	-1.96966000	-0.86624800	5.29296900	C	1.95212500	1.31678200	-1.51824100
H	-2.14698600	-1.95619200	3.89045200	O	1.50693500	-1.30620400	0.84377200
C	-0.00727900	3.31745600	1.53659900	C	1.87321200	-2.17736100	-0.01002900
C	-0.19945200	2.36938500	2.55944800	C	2.88358200	-3.23092400	0.45557500
C	-0.66694000	2.80997800	3.81476800	C	2.28291400	-4.62318200	0.18382800
C	-0.96477000	4.15184200	4.02777700	H	2.05400000	-4.75653400	-0.87723300
C	-0.77895600	5.08092600	2.99961800	H	2.99249900	-5.40095100	0.48839000
C	-0.29301600	4.66182500	1.75869800	H	1.35862100	-4.76504000	0.75645300
H	0.36948500	2.98951200	0.57900000	C	3.18135000	-3.07914600	1.95220200
H	-0.80305000	2.10032200	4.62338000	H	2.27077900	-3.19928500	2.54670400
H	-1.33218100	4.47583700	4.99691900	H	3.89881000	-3.84838100	2.26106100
H	-1.00832700	6.12931100	3.16834000	H	3.60335000	-2.09891100	2.18485600

N	1.83297800	0.83585900	2.60659700	H	2.59061200	-0.14183700	0.11163300
N	2.90071200	0.91724600	2.31503400	C	3.46170100	3.35097100	1.47903300
				C	3.68794300	4.69603500	1.75964500
<b>TS2</b>				C	4.63880200	5.41714100	1.02975000
C	-2.77542500	-0.76580600	-1.90141200	C	5.36549600	4.78334200	0.01932400
C	-3.54882000	-0.56720200	-3.20989400	C	5.14467200	3.43466900	-0.26021500
C	-2.54849400	-0.71535100	-4.37399500	C	4.18497900	2.70814300	0.46214800
H	-1.75048300	0.02971300	-4.30674100	C	3.87462300	1.29676900	0.11797300
H	-3.06701200	-0.58363200	-5.33049900	C	4.92546400	0.49027000	-0.56839500
H	-2.09323600	-1.71300600	-4.37230200	C	4.62769500	-0.14388000	-1.78037400
C	-4.66418100	-1.60925500	-3.34787500	C	5.58455000	-0.93640800	-2.41473100
H	-4.25370700	-2.62366400	-3.36055100	C	6.84441900	-1.10913100	-1.83683500
H	-5.20209800	-1.44686500	-4.28919100	C	7.15109400	-0.46881500	-0.63216400
H	-5.38051100	-1.54799100	-2.52523400	C	6.20144000	0.33875300	-0.00697100
O	-3.10972700	-1.71379000	-1.13185600	N	2.70538400	0.83724500	0.38364300
O	-2.10018500	1.03090900	1.10281900	H	2.71211400	2.78779500	2.02006100
C	-6.58258200	1.78286600	0.20729700	H	3.12250400	5.18322400	2.54936100
H	-7.19702300	2.00014600	1.07709900	H	6.10342600	5.33867700	-0.55289900
C	-5.20073800	2.00727200	0.26272300	H	5.70231900	2.95007400	-1.05477600
C	-4.52959200	2.48650100	1.52975900	H	3.65046600	0.00328400	-2.22772600
H	-5.22263900	3.10232800	2.11495100	H	5.34470600	-1.42009700	-3.35743100
H	-3.67170400	3.11233600	1.27122300	H	8.13119000	-0.59662200	-0.18124300
C	-4.02828400	1.34464100	2.46777700	H	6.43987900	0.84100000	0.92588600
C	-5.20383100	0.53917800	3.03178400	H	7.58758900	-1.73282900	-2.32556100
H	-5.78364300	0.06029800	2.23891400	H	4.81437800	6.46657100	1.25026900
H	-5.86910100	1.20554200	3.59337300	C	0.03149000	2.73982100	0.59055400
H	-4.85154900	-0.24246000	3.71141800	O	-0.83586900	3.61406500	0.02989000
C	-3.21893900	1.96961000	3.62213400	O	0.43447700	2.83619200	1.73058500
H	-2.86125100	1.19500300	4.31064500	C	-1.29424800	4.67149100	0.89320800
H	-3.85075500	2.66192900	4.19051100	H	-2.04622500	5.21180400	0.31807200
H	-2.34976900	2.51579400	3.24519100	H	-0.46334400	5.33518200	1.14948400
C	-3.07720400	0.44005800	1.67622200	H	-1.72973200	4.26366300	1.80714300
O	-3.30434000	-0.80472900	1.64960000	C	0.97693000	1.12008400	-2.71463300
O	-1.82220400	0.06053700	-1.69342800	C	0.97390700	2.00802700	-1.61064800
C	-4.12793100	0.88258700	-3.23156500	C	1.66849000	3.24035800	-1.73299200
H	-3.28712500	1.58175800	-3.27813200	C	2.35410900	3.55425700	-2.89663400
H	-4.69451700	0.98766500	-4.16439400	C	2.33893400	2.66449100	-3.97808200
C	-5.00538200	1.22576700	-2.04926400	C	1.64321900	1.45425200	-3.88751700
C	-6.38918900	1.00788100	-2.07799200	H	0.45325200	0.17999400	-2.62840100
H	-6.85411400	0.62335100	-2.98210200	H	1.69198400	3.92988700	-0.89672500
C	-7.17262700	1.29178300	-0.95829800	H	2.90217200	4.48873400	-2.96568700
H	-8.24699800	1.13114900	-0.99460200	H	2.87190200	2.91557700	-4.89083200
C	-4.43427400	1.74325100	-0.87976000	H	1.63101300	0.76986500	-4.73065800
H	-3.36721800	1.93412600	-0.85222400	C	0.30657900	1.64585700	-0.38999300

Rh	-2.03000100	-2.04389000	0.60204300	C	2.45143600	0.65195700	1.80979600
Rh	-0.69890300	-0.04813100	0.03766400	C	3.38097000	1.68989600	2.45043800
O	-0.87809500	-2.22634700	2.31495900	C	2.48494500	2.68270500	3.21841200
C	1.63374000	-2.82318900	3.76514800	H	1.78194000	3.17671500	2.54461700
H	0.92119000	-3.65042600	3.84415600	H	3.10510300	3.44876100	3.69845400
H	2.27600800	-2.85897200	4.65304500	H	1.91526500	2.16737700	4.00110100
C	2.45986600	-2.99907200	2.51161800	C	4.35733800	1.01973500	3.42519100
C	3.76962100	-2.51059500	2.40969400	H	3.81934700	0.52947700	4.24153100
H	4.22786700	-2.01644100	3.26218800	H	5.01963000	1.77797200	3.85933600
C	4.49234500	-2.66897600	1.22618400	H	4.97574100	0.26753300	2.92905300
H	5.50808500	-2.29259800	1.15552800	O	2.42205600	-0.51450800	2.31600200
C	1.90313500	-3.64768700	1.40289800	O	1.99962800	-0.88748800	-1.39801900
H	0.89095800	-4.03335100	1.47313700	C	6.65995800	-0.16942300	-0.99409400
O	0.59033900	-1.32948400	-0.96359600	H	7.28628300	-0.85390800	-1.56074900
O	-0.69220000	-3.14241100	-0.52234400	C	5.30894000	-0.02450600	-1.33543800
C	3.91649800	-3.30953600	0.12771000	C	4.68615100	-0.85379300	-2.43587800
H	4.48927400	-3.42858400	-0.78739700	H	5.45667300	-1.16746700	-3.14985700
C	2.60820100	-3.80479600	0.20339700	H	3.95693200	-0.25287000	-2.98340400
C	1.92942400	-4.45515900	-0.97951300	C	3.97275700	-2.14657900	-1.93723600
H	2.65673600	-5.00939600	-1.58449600	C	4.96977600	-3.08349900	-1.24358400
H	1.18583500	-5.17355800	-0.62039600	H	5.40290600	-2.62685600	-0.35053200
C	1.20730700	-3.44997600	-1.93370500	H	5.78415000	-3.32429700	-1.93692200
C	2.23010600	-2.60751500	-2.69897200	H	4.48713400	-4.01878200	-0.94561400
H	2.86699900	-2.04557600	-2.01847600	C	3.34509000	-2.87680400	-3.14211000
H	2.86491200	-3.26325200	-3.30622800	H	2.82676600	-3.78610300	-2.81648000
H	1.73559200	-1.89662600	-3.36876700	H	4.12957900	-3.16863200	-3.84977600
C	0.33571700	-4.24019000	-2.92640500	H	2.62478500	-2.24329500	-3.66606100
H	-0.19403400	-3.56184300	-3.60602200	C	2.83080100	-1.76254400	-0.98743400
H	0.96824000	-4.89859300	-3.53296700	O	2.77694600	-2.35594000	0.13441600
H	-0.40657600	-4.85122400	-2.40624400	O	1.74620500	1.04340300	0.82524600
C	0.29332800	-2.56760600	-1.07437000	C	4.14133300	2.46164200	1.32960800
O	0.30396800	-0.37015300	1.79086000	H	3.40175600	2.95996300	0.69679300
C	0.01468200	-1.35140800	2.54506600	H	4.73347500	3.24202200	1.82210900
C	0.83136600	-1.48582700	3.83547200	C	5.04381800	1.58795800	0.48735900
C	-0.14453800	-1.55466400	5.02493700	C	6.39908700	1.42739700	0.80550600
H	-0.84478700	-2.38812000	4.91844600	H	6.82427100	1.98401900	1.63695000
H	0.41551700	-1.68720000	5.95790200	C	7.20344900	0.56138200	0.06342100
H	-0.72331000	-0.62707500	5.10729400	H	8.25546400	0.45133300	0.31392600
C	1.77537400	-0.28951100	4.00767200	C	4.52478500	0.87498100	-0.60128800
H	1.21340300	0.64808200	4.05421900	H	3.48474700	1.01105500	-0.87133100
H	2.33929800	-0.40249900	4.94133100	H	-1.58103600	0.45105700	-2.61975500
H	2.48091700	-0.20574800	3.17864500	C	-2.39704900	4.40668000	-1.56860800
				C	-2.46899100	5.72730700	-1.13247400
				C	-3.14289800	6.03791800	0.05118400

**TS3'**



C	-3.77287000	5.02608000	0.77980600	H	-1.60467600	-5.27173000	0.48457300
C	-3.71594400	3.70636300	0.33481900	H	-2.87263400	-5.54878400	-0.71207000
C	-2.99899900	3.37996100	-0.82544700	C	-3.25362200	-3.90722900	0.62296000
C	-2.91289100	1.97302000	-1.29140400	C	-4.60658100	-3.78554400	0.28243800
C	-4.17206900	1.22607900	-1.49202100	H	-5.00252400	-4.35482000	-0.55514200
C	-4.17351100	-0.17948100	-1.46056200	C	-5.44705000	-2.94453900	1.01449100
C	-5.34380800	-0.88583700	-1.72477400	H	-6.49613100	-2.86019900	0.74414800
C	-6.53310000	-0.20595300	-2.00067900	C	-2.77766900	-3.18513000	1.72544600
C	-6.54623400	1.19064100	-2.01095500	H	-1.74195000	-3.29840900	2.02034400
C	-5.37617300	1.90317600	-1.75784800	O	-1.05338300	0.17208600	1.18286500
N	-1.81287900	1.36311000	-1.62280100	O	-0.33393500	-1.39724500	2.64321200
H	-1.86471900	4.16457400	-2.48170700	C	-4.94533600	-2.20322600	2.08462800
H	-1.98857500	6.51157600	-1.70982900	H	-5.60342000	-1.54298200	2.64385900
H	-4.31150900	5.26430100	1.69265300	C	-3.59848200	-2.31569300	2.45452600
H	-4.21219800	2.92026600	0.89302800	C	-3.02696600	-1.51631100	3.60498500
H	-3.25548600	-0.70138500	-1.21393900	H	-3.82851700	-1.24954700	4.30354900
H	-5.33150000	-1.96923900	-1.69500500	H	-2.30641600	-2.12911500	4.15512800
H	-7.46648600	1.72714800	-2.22468600	C	-2.32054900	-0.18724300	3.19884100
H	-5.38797000	2.98703100	-1.78912800	C	-3.31022500	0.77874300	2.54003400
H	-7.44519400	-0.76193000	-2.19955700	H	-3.71526200	0.37313800	1.60970200
H	-3.18583900	7.06635000	0.39844000	H	-4.14398700	0.97330000	3.22492500
C	0.10817800	1.06603200	-2.71889600	H	-2.82750000	1.73235600	2.31369900
O	1.33012100	1.30488800	-3.14554000	C	-1.72254200	0.46221800	4.46476200
O	-0.67688800	0.26195600	-3.35955100	H	-1.18952800	1.38700800	4.21365200
C	1.74224200	0.63737900	-4.35653400	H	-2.52327600	0.71290900	5.16997400
H	2.76451100	0.96994300	-4.52997200	H	-1.02021500	-0.21425500	4.96111700
H	1.09984500	0.93990300	-5.18768600	C	-1.14956200	-0.49793300	2.26057200
H	1.70387400	-0.44286900	-4.22444000	O	-0.75567700	-1.70523500	-0.99484800
C	-0.30835200	3.21702800	0.41496800	C	-0.66858200	-2.89947200	-0.56455900
C	0.11007000	2.90432300	-0.89088900	C	-1.48347700	-3.99638900	-1.26025300
C	1.01029500	3.77426100	-1.52633100	C	-0.47334300	-4.96749900	-1.90690600
C	1.46070300	4.92900100	-0.88302400	H	0.19927600	-5.39784800	-1.15921500
C	1.00809200	5.24675400	0.39771000	H	-1.00824600	-5.78380000	-2.40565500
C	0.11892300	4.38102900	1.04252300	H	0.13302500	-4.45006800	-2.65993700
H	-0.97332500	2.53587800	0.92981400	C	-2.39900000	-3.41800500	-2.34256300
H	1.34675700	3.55920300	-2.53327100	H	-1.82662300	-2.85929000	-3.08854700
H	2.15353700	5.59019600	-1.39702300	H	-2.92445500	-4.23457000	-2.85157300
H	1.34590500	6.15412700	0.89052300	H	-3.14625200	-2.74626100	-1.91953500
H	-0.24027700	4.61301800	2.04126500				
C	-0.44605300	1.71477300	-1.56749400				
Rh	1.23811500	-1.93248900	1.41811900	<b>TS3-G2-R</b>			
Rh	0.45995700	-0.25008500	-0.15029900	C	3.91354400	0.48658800	3.06799300
O	0.06693800	-3.28451200	0.40172700	H	4.94547200	0.72973200	2.79740100
C	-2.30923300	-4.76968300	-0.18551000	C	4.11459300	-1.25416200	-2.45513300
				H	3.57428200	-1.74480200	-3.27006600

N	0.69618100	1.02153900	-1.00043700	H	2.19573500	5.09464500	-2.57797300
N	0.24098500	-1.20547700	-0.68858200	H	3.26000800	4.26328500	-1.44676300
N	2.50393200	-0.43922700	-0.89947500	H	1.03178400	4.85142300	1.57890900
C	1.13868500	-0.24977800	-0.85873900	H	2.55311500	4.11575200	1.08186600
C	3.21395700	-1.48453300	-0.15757500	H	2.12051900	6.14147500	-0.29028700
H	2.50096600	-2.17175700	0.29426500	H	0.54258400	5.50753200	-0.76396500
O	5.21958000	-1.11923700	1.18579600	C	5.50059600	-0.76314700	-2.88932000
C	4.01930900	-0.87830500	1.02424300	H	6.24479500	-1.56654900	-2.91751800
N	3.30741800	-0.09724400	1.86582500	H	5.44034900	-0.33370900	-3.89814400
H	2.29368200	-0.03127200	1.78584700	C	4.48795700	1.04667300	-1.61270500
C	3.36595600	0.03004200	-1.99557400	H	4.39395800	1.93696200	-2.24333500
H	2.72650800	0.44314900	-2.77582000	H	4.39365500	1.37602600	-0.57547400
C	4.12092600	-2.16929600	-1.19956500	C	5.83389100	0.33352100	-1.86455500
H	3.73782900	-3.16334600	-1.44313400	H	6.61275200	1.01830300	-2.21525500
H	5.12263100	-2.28828200	-0.78322500	H	6.18767900	-0.12244700	-0.93493500
H	-0.31358500	1.11132300	-1.02188400	H	-0.77845000	-0.92570000	0.10936500
C	0.46526200	-2.59340700	-1.09324800	C	-4.99135500	0.37647400	-0.67551000
C	0.28482800	-3.57411100	0.07867600	C	-5.76803700	-0.45126100	-1.48443800
C	-0.47873700	-2.95061100	-2.25702300	C	-5.17498300	-1.17753300	-2.52027100
H	1.48480200	-2.70269500	-1.47958600	C	-3.80058100	-1.07281500	-2.73979900
C	0.45238900	-5.03031300	-0.37319400	C	-3.02041400	-0.26192900	-1.91506700
H	-0.70957800	-3.43645400	0.51447400	C	-3.60655200	0.46085800	-0.86896400
H	0.99861500	-3.34295400	0.87805000	C	-2.75944800	1.32575400	0.01429900
C	-0.30617300	-4.40852500	-2.70023600	C	-2.94501700	2.79679400	-0.10774100
H	-1.51594400	-2.77928900	-1.94835500	C	-2.59413000	3.64360700	0.95883900
H	-0.28548200	-2.26953100	-3.09515900	C	-2.71703200	5.02517400	0.84147400
C	-0.49932900	-5.37417800	-1.52519200	C	-3.19889000	5.59092100	-0.34340100
H	0.28223500	-5.70202300	0.47707600	C	-3.56479800	4.76003500	-1.40402100
H	1.48972000	-5.19512800	-0.70050500	C	-3.44630100	3.37492500	-1.28557500
H	-1.01276400	-4.63803000	-3.50755000	N	-1.87084900	0.90764100	0.85228000
H	0.70272900	-4.54487500	-3.11706800	H	-5.45261600	0.94047500	0.12963700
H	-0.34279900	-6.40966000	-1.85238000	H	-6.83722900	-0.52876000	-1.30720800
H	-1.53729600	-5.30714400	-1.16818300	H	-3.33221500	-1.62813500	-3.54795000
C	1.42784300	2.25709600	-0.70224400	H	-1.94767500	-0.20517000	-2.06931200
C	1.48193000	3.14589300	-1.95348100	H	-2.21875700	3.19484000	1.87215900
C	0.79204000	3.00924200	0.47355200	H	-2.44169400	5.66324300	1.67704900
H	2.43790100	1.96515400	-0.41691000	H	-3.94283200	5.18994100	-2.32772800
C	2.20445700	4.46978300	-1.67638400	H	-3.72996100	2.73689800	-2.11655700
H	0.44986000	3.35083600	-2.27363000	H	-3.29642600	6.66928100	-0.43419900
H	1.96726200	2.60373700	-2.77334700	H	-5.78197800	-1.81791200	-3.15440100
C	1.52525000	4.32625900	0.75168700	C	-0.58054000	-0.62025400	2.16568400
H	-0.25038800	3.22869900	0.22450800	O	-0.65334200	-1.81490500	2.80842100
H	0.77193900	2.35882700	1.35099300	O	0.37545700	0.13738300	2.33551300
C	1.56853300	5.21570400	-0.49662200	C	0.46356400	-2.14745500	3.64026200

H	1.39149700	-2.17309500	3.06265900	H	0.62887900	1.62540900	-1.32328200
H	0.24604200	-3.13915900	4.04033600	C	-0.19112300	-2.04277700	-1.26838200
H	0.56902800	-1.42925900	4.45817800	C	-0.72996100	-2.86770000	-0.08615000
C	-3.23780000	-2.39129700	0.58034600	C	-1.27531200	-1.93507900	-2.35815900
C	-2.88185700	-1.30330800	1.38219700	H	0.66955400	-2.56181500	-1.71045600
C	-3.75236500	-0.93882300	2.42221900	C	-1.21013000	-4.25298300	-0.53635700
C	-4.94094600	-1.63164700	2.64553200	H	-1.56045500	-2.31587900	0.36485700
C	-5.28465500	-2.71259800	1.82941700	H	0.03273700	-2.96674100	0.69563300
C	-4.42598000	-3.09059200	0.79695400	C	-1.76129200	-3.31527700	-2.81725900
H	-2.59503000	-2.67810400	-0.24115700	H	-2.11923300	-1.36542900	-1.94591900
H	-3.49166600	-0.09373600	3.05464100	H	-0.88147800	-1.35979700	-3.20506900
H	-5.59917400	-1.32878700	3.45611700	C	-2.27460200	-4.14583600	-1.63515500
H	-6.21305200	-3.25222900	1.99688300	H	-1.60801200	-4.80337600	0.32539900
H	-4.68422100	-3.92434400	0.14908900	H	-0.35534500	-4.83466300	-0.91337400
C	-1.64163800	-0.46556600	1.15425500	H	-2.54635900	-3.20101900	-3.57520400
C	3.16480500	1.76396800	3.44279500	H	-0.93056400	-3.84872200	-3.30279100
H	3.20095300	2.49552600	2.62863200	H	-2.57479400	-5.14559000	-1.97378900
H	2.11396900	1.54757600	3.66253300	H	-3.17198700	-3.66743100	-1.21920200
H	3.61485000	2.21901300	4.33187100	C	2.60757100	2.02379800	-0.73264600
C	3.94116500	-0.52466900	4.21892200	C	3.19710300	2.81969400	-1.90562700
H	4.46913000	-0.10768300	5.08465000	C	2.11068600	2.96849900	0.37114200
H	2.92350600	-0.78354500	4.53188200	H	3.37614900	1.37266500	-0.31367000
H	4.45773300	-1.43982500	3.91215900	C	4.31056900	3.76556300	-1.43812600

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C	4.03600800	-0.60015700	3.03887300	C	3.22428100	3.91354600	0.83845100
H	5.09341900	-0.67624600	2.76440900	H	1.27698400	3.56299200	-0.02398300
C	3.85368400	-2.25263100	-2.47733900	H	1.71421700	2.37627900	1.19918200
H	3.23698400	-2.48094400	-3.35139800	C	3.81797000	4.70693300	-0.33177300
N	1.51867300	1.15604600	-1.19492300	H	4.69440100	4.34038800	-2.28997200
N	0.19465500	-0.69037800	-0.86670800	H	5.15217800	3.16944600	-1.05641000
N	2.58037200	-0.89765400	-0.98502300	H	2.83141900	4.59348300	1.60454000
C	1.40389300	-0.18452300	-1.00904800	H	4.02314500	3.32966800	1.31822400
C	2.77388200	-2.14824600	-0.24841400	H	4.63892800	5.34642300	0.01623500
H	1.82193400	-2.50374400	0.13882200	H	3.04709900	5.37512000	-0.74257700
O	4.69424700	-2.59372700	1.19437700	C	5.35285200	-2.33679400	-2.78991300
C	3.68244200	-1.91688900	0.98910800	H	5.72685400	-3.36639000	-2.79267400
N	3.27680100	-0.93786600	1.82804500	H	5.54607200	-1.91288100	-3.78427400
H	2.38487700	-0.46720500	1.68975700	C	5.02326600	-0.27934000	-1.53449400
C	3.62588200	-0.78414600	-2.01394600	H	5.32797500	0.56807500	-2.15752300
H	3.24132600	-0.14601000	-2.80970200	H	4.99007100	0.07652500	-0.50198100
C	3.39687900	-3.11880500	-1.27024400	C	6.00130700	-1.46073000	-1.70540400
H	2.65590800	-3.85801700	-1.58475300	H	7.01141900	-1.13361400	-1.97305300
H	4.23001700	-3.65102000	-0.80780300	H	6.06956900	-2.02064500	-0.76810400

C	3.76580600	-1.59811300	4.16963900	C	-1.27252700	4.29514900	1.27801800
H	4.41382000	-1.38513100	5.02812500	H	-1.24160000	2.63220600	2.64184900
H	2.72517000	-1.53781100	4.50637600	H	-1.55263400	1.64438400	-1.52113200
H	3.96901600	-2.61951700	3.83421300	H	-1.50439500	4.04205100	-2.10491400
C	3.71539400	0.83558000	3.44692200	H	-1.33107600	5.75978000	-0.30708800
H	3.98332000	1.53978100	2.65233100	H	-1.19962400	5.03622200	2.06992300
H	2.64718200	0.95171000	3.65753100	C	-1.46069500	0.48956900	0.93451600
H	4.27739100	1.10625200	4.34712100	H	-0.68794500	-0.08075300	-0.04603700
C	-4.37849700	1.25963900	-1.70363900				
C	-4.76274900	2.42409700	-2.36869300				
C	-5.02659400	3.58796200	-1.64367600				
C	-4.91130200	3.57818300	-0.25178800				
C	-4.52601500	2.41355400	0.41112700				
C	-4.23749600	1.24875500	-0.30967800				
C	-3.80920100	-0.00523400	0.39513800				
C	-4.83498300	-1.08759500	0.50526200				
C	-4.50696300	-2.31768600	1.10791300				
C	-5.44677100	-3.33752500	1.21151800				
C	-6.74495500	-3.15645600	0.72119100				
C	-7.08786800	-1.93910200	0.13440600				
C	-6.14484400	-0.91491800	0.02808800				
N	-2.65984100	-0.24442600	0.91838100				
H	-4.17257900	0.35311000	-2.26705400				
H	-4.85595700	2.42270500	-3.45153700				
H	-5.11477600	4.48034700	0.31843400				
H	-4.42605400	2.40927900	1.49196700				
H	-3.50524700	-2.44762400	1.49974300				
H	-5.16780600	-4.27894600	1.67798200				
H	-8.09453800	-1.78018800	-0.24343000				
H	-6.43260100	0.02555600	-0.42807500				
H	-7.47839200	-3.95429100	0.80045400				
H	-5.32222600	4.49717800	-2.16007500				
C	-0.53779100	0.05493800	2.00707900				
O	-0.97525100	-0.99161100	2.73890000				
O	0.59858200	0.51276500	2.16018900				
C	-0.01603500	-1.57038100	3.63340300				
H	0.85115900	-1.94779900	3.08606800				
H	-0.53613900	-2.39453400	4.12428100				
H	0.31515600	-0.83993900	4.37661300				
C	-1.29884900	2.93833900	1.60116900				
C	-1.39596900	1.96040000	0.60251400				
C	-1.45803800	2.38543000	-0.73366600				
C	-1.43826700	3.74019500	-1.06325300				
C	-1.34492600	4.70275000	-0.05577900				
				<b>TS3-G3-R</b>			
				C	-4.35445900	-0.33691800	-0.37430500
				C	-4.50606200	-1.36691000	-1.49983500
				C	-4.64168300	-1.02373100	-2.84759600
				C	-4.51664900	-2.72666400	-1.15094400
				C	-4.75720300	-2.01489900	-3.82772900
				H	-4.65195600	0.01883800	-3.14294100
				C	-4.63224800	-3.71569800	-2.12474700
				H	-4.43777800	-3.00973300	-0.10518900
				C	-4.74501000	-3.36258700	-3.47300800
				H	-4.85242300	-1.72605700	-4.87104600
				H	-4.63652600	-4.76248800	-1.83256400
				H	-4.82978400	-4.13194700	-4.23551400
				C	-4.36156500	1.11128300	-0.82704100
				C	-5.42610900	1.93958200	-0.45676200
				C	-3.34629400	1.63609400	-1.63958800
				C	-5.48596200	3.26556400	-0.89208200
				H	-6.21760200	1.54138300	0.17348600
				C	-3.40783100	2.95797100	-2.07942900
				H	-2.50792300	1.00979000	-1.92428400
				C	-4.47823100	3.77660900	-1.71027600
				H	-6.32057500	3.89452200	-0.59412200
				H	-2.61297900	3.34983500	-2.70829200
				H	-4.52200600	4.80688000	-2.05290500
				H	-5.19406300	-0.47477300	0.31097400
				C	-1.62094100	-1.54853000	4.70889900
				H	-0.65253500	-1.93745000	5.04086800
				N	0.32393600	1.01373800	1.84571100
				N	0.85390600	-1.17162800	1.34775000
				N	-1.10701200	-0.64101400	2.60968400
				C	0.03643900	-0.30557500	1.92072000
				C	-1.98483500	-1.76767400	2.28485500
				H	-1.51589800	-2.41289200	1.54406700
				O	-4.39504500	-1.39926700	2.21157500
				C	-3.30613600	-1.25118500	1.65086200

N	-3.17247900	-0.66988500	0.43483700	C	6.33990400	0.38727900	-0.71052300
H	-2.26648900	-0.63805700	-0.03462500	C	6.39989700	-0.27830400	0.51646100
C	-1.40666800	-0.21193900	3.98128900	C	5.26892700	-0.32633200	1.33273400
H	-0.58346300	0.38020000	4.38131200	C	4.07920900	0.27138700	0.91572900
C	-2.23932900	-2.47692900	3.63602100	C	4.00900600	0.93147800	-0.31740700
H	-1.77680100	-3.46714100	3.64670700	C	2.72659800	1.56792700	-0.76203700
H	-3.31377100	-2.59805800	3.77737000	C	2.68733700	3.05480100	-0.79168200
H	1.20146800	1.22802500	1.38524000	C	1.77273500	3.71967000	-1.62748500
C	0.99355600	-2.55133400	1.81575000	C	1.68169900	5.10838700	-1.62054700
C	0.74406000	-3.56850400	0.69027700	C	2.50546200	5.86370800	-0.77940900
C	2.38721500	-2.74744000	2.44122100	C	3.42707800	5.21551200	0.04504900
H	0.26933200	-2.74427400	2.61537800	C	3.52425200	3.82364000	0.03330800
C	0.95231800	-5.00709200	1.17877100	N	1.64703200	0.94354900	-1.09532000
H	1.42159200	-3.36279800	-0.14387500	H	5.11201900	1.51927400	-2.07034000
H	-0.27036900	-3.44414600	0.29386900	H	7.21617000	0.42759800	-1.35164600
C	2.59165400	-4.19021700	2.92014500	H	5.30889200	-0.83485100	2.29228000
H	3.15594900	-2.49014600	1.70363500	H	3.19492200	0.20534000	1.54115400
H	2.50394500	-2.04329900	3.27467800	H	1.13002000	3.12383300	-2.26647500
C	2.34786500	-5.19413400	1.78669300	H	0.96895900	5.60505700	-2.27361000
H	0.79998900	-5.70586800	0.34721800	H	4.07251900	5.79367000	0.70089900
H	0.19295200	-5.24969300	1.93708500	H	4.24088800	3.32786900	0.68043800
H	3.60358600	-4.30782400	3.32737600	H	2.43454800	6.94790300	-0.77404800
H	1.89447700	-4.40122500	3.74455200	H	7.32381200	-0.75335900	0.83465700
H	2.46841300	-6.22059900	2.15479800	C	0.19468200	-0.88020400	-1.61000400
H	3.10486300	-5.04694200	1.00267600	O	0.15994500	-2.08049000	-2.23591300
C	-0.62274400	2.13081400	1.95399100	O	-0.84267600	-0.29183900	-1.29645300
C	-0.17906800	3.08974100	3.06916300	C	-1.14585200	-2.63909500	-2.44646700
C	-0.73951400	2.87535300	0.61960900	H	-1.66132600	-2.79632800	-1.49695800
H	-1.59624200	1.70170800	2.20331600	H	-0.97774500	-3.59638400	-2.94208000
C	-1.12290000	4.29339500	3.18305300	H	-1.75377000	-1.98840700	-3.07860400
H	0.83655600	3.44151600	2.83501800	C	3.52901900	-2.09794000	-1.31651300
H	-0.11857900	2.55351700	4.02321500	C	2.68803100	-1.16171800	-1.92486300
C	-1.68644200	4.07501600	0.73018800	C	2.95070000	-0.80708400	-3.25816300
H	0.25596200	3.23037600	0.33538400	C	4.02155300	-1.36397400	-3.95519000
H	-1.06217100	2.18020300	-0.15881300	C	4.85654100	-2.29346500	-3.32921500
C	-1.24793500	5.03174000	1.84495800	C	4.60405400	-2.65952100	-2.00708000
H	-0.76642300	4.97245600	3.96759200	H	3.36041600	-2.36835400	-0.28262400
H	-2.11709000	3.94270500	3.49691600	H	2.30720900	-0.07873900	-3.74540600
H	-1.72161500	4.60080100	-0.23062100	H	4.20564900	-1.07353700	-4.98654900
H	-2.70737200	3.72095400	0.92775400	H	5.69587400	-2.72593700	-3.86732600
H	-1.95712700	5.86423000	1.93602600	H	5.25067200	-3.37422200	-1.50445600
H	-0.27411300	5.46925900	1.58071400	C	1.55023300	-0.47453900	-1.20269500
H	1.33245500	-0.88454800	0.14919400	H	-2.26056300	-1.43794300	5.58920800
C	5.15749500	1.00316000	-1.11630500	H	-2.31761600	0.39990000	4.00264100

**TS3-G3-S**

			H	-1.74776500	2.12205800	-0.46449300
			C	-3.39262700	4.81829400	1.02638400
C	-4.23632300	-1.30906100	H	-3.51642700	5.02925200	3.18973500
H	-5.08430400	-1.60927900	H	-4.26691700	3.56619500	2.55590600
N	-0.63508500	1.63298100	H	-3.12058100	4.15182000	-1.02483500
N	0.65443400	-0.25681600	H	-4.02224300	3.03305500	-0.01585600
N	-1.51449900	-0.37196800	H	-4.33519000	5.34433200	0.82821600
C	-0.47391500	0.29586700	H	-2.58944600	5.56602500	0.94897100
C	-1.92594800	-1.73980500	C	5.09446200	1.87078600	0.33270300
H	-1.14985200	-2.25109600	C	5.53688700	3.18982000	0.43481800
O	-4.25273600	-2.27409800	C	5.39961300	4.05831800	-0.65001500
C	-3.21625300	-1.75222400	C	4.82634300	3.59832700	-1.83766400
N	-3.12166300	-1.19167800	C	4.38466000	2.27985500	-1.93789400
H	-2.22629400	-0.85620200	C	4.49793800	1.40915000	-0.84800200
C	-2.16988100	-2.34944200	C	4.00618400	-0.00482100	-0.94268700
H	-1.20600600	-2.64447700	C	5.05045200	-1.06945600	-1.05286300
H	-2.82227600	-3.22186200	C	4.67568400	-2.42554400	-1.12103200
H	0.19776000	2.10994200	C	5.63314600	-3.42910800	-1.22187600
C	1.22870200	-1.46195100	C	6.99459200	-3.10744700	-1.26206700
C	1.40749600	-2.59304800	C	7.37983300	-1.76871600	-1.20902400
C	2.59546800	-1.09973700	C	6.41957400	-0.76005900	-1.10766400
H	0.58528300	-1.81578800	N	2.78197700	-0.39624600	-0.95041500
C	2.07651600	-3.82121000	H	5.19791000	1.19307300	1.17615500
H	2.02456000	-2.21590600	H	5.98633300	3.53951200	1.36050900
H	0.44245200	-2.87049600	H	4.71593200	4.26928500	-2.68495100
C	3.27834600	-2.32015300	H	3.92958800	1.92455400	-2.85694500
H	3.23147100	-0.69199700	H	3.61999200	-2.66916300	-1.10521600
H	2.45942800	-0.30358600	H	5.31823300	-4.46844700	-1.27076400
C	3.42928800	-3.45933900	H	8.43283400	-1.50198200	-1.24775100
H	2.20513400	-4.60224000	H	6.74089800	0.27470300	-1.07348500
H	1.41828700	-4.24101500	H	7.74237400	-3.89217500	-1.33805800
H	4.25814400	-2.03295600	H	5.73910200	5.08751400	-0.57154300
H	2.67875800	-2.67097700	C	0.41399500	-0.45816400	-1.33347900
H	3.87510100	-4.34018800	O	0.71385700	-1.65067200	-1.88058200
H	4.11944500	-3.14568400	O	-0.75708700	-0.08761800	-1.19578000
C	-1.89308900	2.34059000	C	-0.40307000	-2.48756100	-2.21853700
C	-2.11635400	3.44111700	H	-1.00709300	-2.70983500	-1.33741600
C	-1.88238800	2.92970900	H	0.03252200	-3.40671400	-2.61243800
H	-2.69831100	1.60331800	H	-1.03215400	-2.01596100	-2.97627100
C	-3.39938900	4.23312800	C	0.91038300	2.41757300	-2.03184900
H	-1.25234400	4.12088800	C	1.44821900	1.79445700	-0.89794400
H	-2.14039000	3.00273700	C	1.90599500	2.61006600	0.14876800
C	-3.16609300	3.71987700	C	1.85183900	4.00043600	0.05817000
H	-1.01531400	3.59526600	C	1.32044800	4.60657100	-1.08235100

C	0.84518000	3.80809700	-2.12485700	C	-4.16147500	-3.27182000	-3.45407500
H	0.54136300	1.80634200	-2.85058900	H	-4.30990800	-2.84287200	-1.35334500
H	2.33832800	2.14623400	1.03002400	C	-4.02340900	-2.74229500	-4.74091100
H	2.23065100	4.60880000	0.87476900	H	-3.83522400	-0.93497100	-5.89982000
H	1.27738800	5.68963100	-1.15768100	H	-4.24870500	-4.34579400	-3.31238700
H	0.42667000	4.26884200	-3.01602400	H	-3.99550200	-3.40115100	-5.60438600
C	1.56677100	0.29354400	-0.79246800	C	-4.01215900	1.32716400	-1.48631100
H	1.18622400	0.06340100	0.50508600	C	-5.11981200	2.12903300	-1.19225500
C	-3.96453900	-2.45484500	-1.64109300	C	-2.87155600	1.92537700	-2.04191400
C	-3.62870500	-3.71391000	-1.11778700	C	-5.09971600	3.50096700	-1.45419000
C	-4.04140500	-2.31056900	-3.02920800	H	-6.00789000	1.67395000	-0.76037900
C	-3.34321600	-4.78656200	-1.95910300	C	-2.85352800	3.29335400	-2.31115800
H	-3.59793000	-3.85430300	-0.04183900	H	-1.99918600	1.32051800	-2.26419200
C	-3.75435200	-3.38616300	-3.87587800	C	-3.96718400	4.08574500	-2.02124900
H	-4.31818000	-1.35604600	-3.46093000	H	-5.96957300	4.10824900	-1.21857200
C	-3.39497600	-4.62419200	-3.34683100	H	-1.96310500	3.74154700	-2.74347800
H	-3.08135400	-5.75088300	-1.53179300	H	-3.94848300	5.15197500	-2.22991200
H	-3.80955900	-3.24774800	-4.95232000	H	-5.02508300	-0.37151700	-0.71030200
H	-3.16629600	-5.45773300	-4.00511700	C	-2.22686900	-1.94373300	4.01601300
C	-4.58764900	0.01292300	-1.31326600	H	-1.38898100	-2.37871300	4.56875600
C	-3.66481800	0.71554200	-2.10146400	N	0.21738400	0.85809300	1.74928100
C	-5.88638200	0.51669700	-1.18526300	N	0.80914700	-1.28259800	1.16942800
C	-4.04393900	1.88465200	-2.75962600	N	-1.35631400	-0.81457400	2.09882700
H	-2.65027200	0.34606400	-2.19760900	C	-0.09504200	-0.45434800	1.66383700
C	-6.26595300	1.69123500	-1.83954300	C	-2.11517400	-1.93672300	1.54013900
H	-6.60933300	-0.02095900	-0.57676500	H	-1.49839700	-2.48125000	0.82732000
C	-5.34646800	2.37445600	-2.63560000	O	-4.49245900	-1.78174900	1.00911800
H	-3.31669700	2.41644800	-3.36712500	C	-3.34084600	-1.42999500	0.73386500
H	-7.27997600	2.06627600	-1.73049400	N	-3.04427900	-0.61992300	-0.30759700
H	-5.63888600	3.28573000	-3.15008200	H	-2.07407900	-0.47371400	-0.58990900
C	-2.78972300	-1.18238500	4.56169400	C	-1.84759100	-0.54054800	3.46007600
H	-2.56426600	-1.23456900	5.63004100	H	-1.03651500	-0.07762700	4.02230800
H	-3.87566000	-1.19792500	4.44315600	C	-2.52561200	-2.79612600	2.75294900
C	-2.20805200	0.10246000	3.92137700	H	-1.95336600	-3.72701300	2.76785300
H	-3.00646400	0.81251800	3.68672800	H	-3.58305500	-3.05355600	2.67538200
H	-1.48784400	0.61112600	4.56803300	H	1.17503300	1.07972200	1.50162100

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C	-4.08989800	-0.16712700	-1.23700300	C	0.89592300	-2.68859500	1.56679800
C	-4.07858200	-1.03393500	-2.50204900	C	0.84382600	-3.63994100	0.35952400
C	-3.96419100	-0.51277100	-3.79356000	C	2.18231100	-2.90593900	2.38696400
C	-4.19148600	-2.42506800	-2.34858600	H	0.06146900	-2.93434400	2.23245400
C	-3.93311700	-1.36137500	-4.90509200	C	1.01812100	-5.10267600	0.78759900
H	-3.89312800	0.55846500	-3.94164800	H	1.63030300	-3.36878700	-0.35090500
				H	-0.10402600	-3.51469500	-0.17670100
				C	2.34867100	-4.37170400	2.80558800

H	3.04705500	-2.59233100	1.79092200	C	2.17630500	3.80843200	-1.32236800
H	2.15557100	-2.25316000	3.26844000	C	2.10189100	5.19605600	-1.25152200
C	2.30992300	-5.30412800	1.58932300	C	2.85938600	5.89506200	-0.30564300
H	1.01136900	-5.74977300	-0.09785000	C	3.69938700	5.19110400	0.55881800
H	0.16050000	-5.40714500	1.40571500	C	3.77869500	3.79990500	0.48481900
H	3.28874800	-4.49732800	3.35719700	N	1.98362600	1.01215400	-0.97744900
H	1.53881100	-4.64745800	3.49707100	H	5.55960300	1.60382600	-1.49047400
H	2.40105200	-6.35020800	1.90736700	H	7.54554800	0.42776200	-0.59111200
H	3.17364800	-5.09194700	0.94281100	H	5.17844200	-1.05217100	2.68315200
C	-0.70565100	1.99492700	1.80885400	H	3.18867000	0.07668200	1.74746300
C	-0.52769400	2.76173100	3.12928400	H	1.58499300	3.25658800	-2.04493200
C	-0.48859200	2.92819700	0.61405200	H	1.45413500	5.73648400	-1.93682900
H	-1.71495000	1.58539200	1.75255900	H	4.29372300	5.72450500	1.29589900
C	-1.45195500	3.98331800	3.20029800	H	4.43044900	3.26136200	1.16548000
H	0.52001300	3.08958200	3.19610400	H	2.80112500	6.97863500	-0.25047700
H	-0.70599400	2.09347200	3.97872800	H	7.36416200	-0.90452500	1.50144200
C	-1.42092900	4.14190400	0.68175000	C	0.58273400	-0.72909400	-1.80153500
H	0.55055700	3.27341000	0.62472100	O	0.60655000	-1.88413200	-2.50695200
H	-0.62855400	2.36738800	-0.31319800	O	-0.47286900	-0.12658800	-1.59453400
C	-1.24520700	4.91014500	1.99626200	C	-0.66920200	-2.37322500	-2.94854200
H	-1.28087000	4.52462800	4.13930600	H	-1.30644700	-2.62152500	-2.09712100
H	-2.49743800	3.64301000	3.21818100	H	-0.45340600	-3.27342400	-3.52573600
H	-1.22655300	4.79933200	-0.17350700	H	-1.17794700	-1.63598300	-3.57254100
H	-2.46272700	3.80836100	0.58803700	C	3.83910700	-2.04345200	-1.14494600
H	-1.94500700	5.75413100	2.04312800	C	3.08898400	-1.06303000	-1.80086200
H	-0.23092500	5.33400300	2.03368900	C	3.51812200	-0.64417500	-3.07084300
C	-3.44523000	-1.69138300	4.91292400	C	4.66298600	-1.17958100	-3.65839600
H	-4.03104300	-2.59898600	5.09518400	C	5.40601700	-2.15259300	-2.98451300
H	-3.11320200	-1.31175700	5.88838800	C	4.98758100	-2.58363100	-1.72567900
C	-3.14612400	0.31660000	3.56782300	H	3.54246900	-2.36437000	-0.15533500
H	-2.95679100	1.16876200	4.22911300	H	2.94644600	0.11785200	-3.59493700
H	-3.44070900	0.72244200	2.59683200	H	4.97673800	-0.83844200	-4.64187800
C	-4.23282800	-0.60516900	4.16032300	H	6.30264800	-2.56826600	-3.43673400
H	-4.93376800	-0.06705900	4.80660800	H	5.56002400	-3.33358800	-1.18582100
H	-4.80911100	-1.06015100	3.34968800	C	1.87869000	-0.39317900	-1.18747000
H	1.46760800	-0.90242400	0.08693500				
C	5.47887100	1.02234000	-0.57700800	<b>TS3-R-1b</b>			
C	6.59468100	0.35853900	-0.06991500	C	-4.12588300	-0.16632300	-1.07788600
C	6.49234800	-0.39213600	1.10396400	C	-4.21051500	-1.26909600	-2.14037700
C	5.26627200	-0.47698900	1.76532300	C	-4.21027700	-1.01173300	-3.51424800
C	4.14552500	0.16986000	1.24495900	C	-4.31657000	-2.60112600	-1.70918100
C	4.23750600	0.91609200	0.06357600	C	-4.28609300	-2.05980600	-4.43706000
C	3.02403300	1.59969600	-0.49038700	H	-4.14864000	0.00852900	-3.87414400
C	3.00643100	3.08654700	-0.44604300	C	-4.39746600	-3.64615100	-2.62666200



H	-4.34779600	-2.81692200	-0.64565200	H	2.17899100	-1.75734000	3.56694100
C	-4.37430900	-3.37974300	-3.99926500	C	2.05010500	-5.02131900	2.34963700
H	-4.27508700	-1.83677100	-5.50060100	H	0.65330000	-5.61134700	0.79073300
H	-4.48038600	-4.66986700	-2.27123100	H	-0.10858200	-4.99587600	2.25512700
H	-4.43181800	-4.19355100	-4.71689500	H	3.16033700	-4.03771700	3.94088200
C	-3.98018200	1.24045800	-1.62755400	H	1.41299100	-4.03817200	4.16456900
C	-5.00771500	2.16703000	-1.42298400	H	2.08653700	-6.01319700	2.81692400
C	-2.85282300	1.63130900	-2.36430200	H	2.89491100	-4.96907900	1.64773600
C	-4.92293600	3.45763200	-1.95093700	C	-0.58847200	2.38850600	1.46114800
H	-5.88457600	1.87302200	-0.85132500	C	-0.29918800	3.39792000	2.58303900
C	-2.76866400	2.91792000	-2.89501200	C	-0.42232400	3.04455200	0.08739800
H	-2.04041100	0.92956600	-2.51618700	H	-1.61115100	2.02123000	1.54930000
C	-3.80434000	3.83419500	-2.69476600	C	-1.16817900	4.65491300	2.45009600
H	-5.73142600	4.16396900	-1.78309000	H	0.76293700	3.67850600	2.52579400
H	-1.88765100	3.20539300	-3.46236500	H	-0.45051900	2.92479200	3.55992800
H	-3.73535800	4.83626500	-3.10922000	C	-1.29900700	4.29469500	-0.04344200
H	-5.05092400	-0.20412700	-0.49715400	H	0.62666400	3.33079500	-0.03681000
C	-2.16877800	-1.00332300	4.39548000	H	-0.64770100	2.31349500	-0.69249200
H	-1.32809600	-1.37985600	4.98568200	C	-1.00166700	5.30381700	1.07115100
N	0.29450300	1.22492500	1.59102800	H	-0.91673700	5.36634700	3.24646000
N	0.78962400	-1.00790800	1.38782700	H	-2.22305700	4.37960900	2.59354900
N	-1.32254600	-0.29083200	2.28090900	H	-1.13707600	4.75253100	-1.02627100
C	-0.06847200	-0.06809700	1.74657200	H	-2.35865000	4.00780400	-0.00572100
C	-2.15450900	-1.45179100	1.95659500	H	-1.65847300	6.17845000	0.98134500
H	-1.59134900	-2.15364900	1.34447600	H	0.03070400	5.66776400	0.96294300
O	-4.53646000	-1.24501600	1.46569100	C	-3.33029200	-0.52639700	5.27592600
C	-3.37693200	-1.03617300	1.09523200	H	-3.94758100	-1.35258000	5.64534000
N	-3.07292800	-0.48161000	-0.10096200	H	-2.93515600	0.00698400	6.15053400
H	-2.10547100	-0.43596900	-0.42480200	C	-3.00353700	1.17970400	3.56791300
C	-1.74798500	0.25260600	3.58130700	H	-2.74858500	2.13265500	4.04326800
H	-0.89672000	0.77039400	4.02331900	H	-3.32434700	1.40560000	2.54781700
C	-2.56943200	-2.04718000	3.31776300	C	-4.10156900	0.44476900	4.36584500
H	-2.05826700	-2.99802700	3.48770400	H	-4.74266800	1.13146100	4.92824000
H	-3.64368200	-2.23801900	3.31811200	H	-4.73982200	-0.11791600	3.67798000
H	1.24261000	1.35792800	1.25830600	H	1.45147500	-0.83662800	0.25262500
C	0.81233300	-2.33997300	1.99281400	C	5.52825300	0.71337700	-0.68634100
C	0.64928400	-3.45119300	0.94087900	C	6.60597900	0.06013500	-0.09132300
C	2.11893900	-2.52708000	2.78770400	C	6.47153400	-0.50300600	1.18016500
H	-0.00348900	-2.42831800	2.71864000	C	5.25115800	-0.41114400	1.85082200
C	0.74046100	-4.84591000	1.57171200	C	4.16625300	0.22293100	1.24475800
H	1.42625700	-3.34279600	0.17821200	C	4.29062100	0.78170100	-0.03323200
H	-0.30557300	-3.33448000	0.41536400	C	3.11599300	1.45704000	-0.67640400
C	2.20635500	-3.92604100	3.41067900	C	3.18944000	2.93480900	-0.82974700
H	2.97369400	-2.36519000	2.12141400	C	2.40344900	3.58533900	-1.79778200

C	2.41849300	4.97208000	-1.91295800	H	-3.06048100	-0.08553500	-3.65581800
C	3.22352800	5.74045700	-1.06545100	C	-5.11259100	-3.24776400	-2.76824100
C	4.02013900	5.10550400	-0.11101600	H	-5.38831000	-2.33319400	-0.83604100
C	4.01014500	3.71484300	0.00130400	C	-4.53363700	-3.12668400	-4.03460600
N	2.03911800	0.87058900	-1.08190800	H	-3.34022900	-1.87925800	-5.32676500
H	5.63439400	1.14817900	-1.67553400	H	-5.69768800	-4.12876400	-2.51789100
H	7.55268000	-0.00899000	-0.62008700	H	-4.66477000	-3.91181100	-4.77430600
H	5.13976000	-0.83877700	2.84360500	C	-3.83905800	1.38142700	-1.56297900
H	3.21191800	0.26663900	1.75878700	C	-4.96162200	2.21581200	-1.63130700
H	1.77494600	2.98077300	-2.44263100	C	-2.61139800	1.86167900	-2.03933600
H	1.80335500	5.45676200	-2.66653000	C	-4.86887600	3.49993800	-2.16941400
H	4.65079000	5.69323300	0.55075100	H	-5.91784600	1.85160100	-1.26340000
H	4.62954900	3.23086300	0.74966300	C	-2.51983600	3.14442000	-2.58269000
H	3.23516000	6.82320500	-1.15536200	H	-1.72504900	1.23880400	-1.99121500
H	7.31425500	-1.00667700	1.64571300	C	-3.64496100	3.96768900	-2.65114000
C	0.54370100	-0.91664300	-1.62240600	H	-5.75104800	4.13321700	-2.21014500
O	0.51774600	-2.16060100	-2.15160500	H	-1.56005400	3.50180400	-2.94521800
O	-0.48805200	-0.25595700	-1.47835100	H	-3.56782400	4.96706100	-3.07071200
C	-0.78349300	-2.70009700	-2.46950300	H	-4.92565800	-0.04264100	-0.42477500
H	-1.41262000	-2.66463500	-1.57650400	C	-2.08116800	-1.37988000	4.34706400
H	-1.25707700	-2.07693900	-3.23348700	H	-1.22862200	-1.78866800	4.89775800
C	3.72210700	-2.29716000	-0.86015100	N	0.30793800	1.23747600	1.78112800
C	3.03158500	-1.34783600	-1.61824700	N	0.89757900	-0.96456400	1.46501800
C	3.47952500	-1.09554000	-2.92533400	N	-1.25931400	-0.38113000	2.33889500
C	4.58486000	-1.76182400	-3.45091300	C	-0.00125200	-0.07416700	1.85549800
C	5.26873400	-2.70245900	-2.67576400	C	-2.02180900	-1.54529600	1.87248900
C	4.83080000	-2.96817200	-1.37836300	H	-1.40239600	-2.13958300	1.20197300
H	3.41039400	-2.49194700	0.15746900	O	-4.40897200	-1.29234800	1.42131000
H	2.95420600	-0.35899500	-3.52820200	C	-3.25171600	-1.08175600	1.04566800
H	4.91312100	-1.54799600	-4.46509600	N	-2.95348300	-0.43716100	-0.10724400
H	6.13500500	-3.21962400	-3.07986400	H	-1.99692200	-0.44618300	-0.46465900
H	5.35845200	-3.69016100	-0.76044300	C	-1.70739400	-0.01756700	3.69324200
C	1.86450100	-0.54449000	-1.08732800	H	-0.87419200	0.47080400	4.20004000
C	-0.57500600	-4.11930700	-2.95309800	C	-2.42829300	-2.30700900	3.14995700
H	-1.54140700	-4.56155300	-3.21568300	H	-1.88404300	-3.25218400	3.21749400
H	0.06664300	-4.13965400	-3.84052200	H	-3.49453200	-2.53536100	3.11251600
H	-0.10832100	-4.73561100	-2.17690000	H	1.26920500	1.43502700	1.52947400
				C	1.00563600	-2.27744800	2.10775000
				C	0.94918600	-3.43401700	1.09977800
<b>TS3-R-1c</b>				C	2.30440600	-2.33055300	2.93474700
C	-4.02005900	-0.02999000	-1.03309200	H	0.17848400	-2.40442700	2.81549500
C	-4.20202200	-1.08627000	-2.12695200	C	1.12803000	-4.79001000	1.79316800
C	-3.63029300	-0.97123100	-3.39766000	H	1.73051600	-3.30255300	0.34445300
C	-4.94609600	-2.23601300	-1.82339200	H	-0.00060400	-3.41054500	0.55992400
C	-3.79263900	-1.98565000	-4.34438900				

C	2.48687000	-3.69173800	3.61780000	C	2.83888900	3.02937100	-0.95902700
H	3.15719300	-2.12913400	2.27542600	C	1.98123200	3.53867300	-1.94978300
H	2.28617200	-1.52497700	3.67959200	C	1.82123400	4.91073600	-2.11572000
C	2.42951700	-4.83906700	2.60183100	C	2.51791800	5.80498200	-1.29576600
H	1.11068500	-5.59236400	1.04538200	C	3.38820800	5.31120600	-0.32214800
H	0.27738200	-4.97035100	2.46753600	C	3.55624500	3.93494000	-0.16132800
H	3.43746400	-3.70980700	4.16526700	N	1.91033500	0.85608000	-1.09827800
H	1.69133300	-3.83163800	4.36465800	H	5.43361100	1.51203300	-1.80342100
H	2.52511900	-5.80486400	3.11351000	H	7.50515600	0.62370600	-0.77471000
H	3.28395100	-4.75829800	1.91438500	H	5.30086000	-0.37653400	2.78215400
C	-0.61632800	2.37286500	1.72815600	H	3.22753900	0.45020600	1.72344100
C	-0.46519900	3.25707100	2.97581600	H	1.43764000	2.83495400	-2.57077800
C	-0.37518300	3.19674400	0.45978900	H	1.15484400	5.28689300	-2.88765100
H	-1.62424100	1.95499100	1.69058100	H	3.93739600	5.99838900	0.31606400
C	-1.40372600	4.46864000	2.91692900	H	4.22987600	3.55876700	0.60235500
H	0.57765300	3.60215400	3.02938400	H	2.39080800	6.87651600	-1.42310000
H	-0.65153000	2.66776200	3.87984400	H	7.44823500	-0.32173300	1.52499000
C	-1.32224600	4.39883800	0.39260100	C	0.59525500	-1.04929000	-1.63675300
H	0.66035200	3.55527000	0.46464300	O	0.67912300	-2.30008700	-2.14208400
H	-0.48353500	2.55099500	-0.41465100	O	-0.47598800	-0.43945700	-1.59051300
C	-1.18542100	5.28455100	1.63643100	C	-0.50122000	-2.84356500	-2.80087200
H	-1.25592800	5.09618900	3.80447800	H	-1.04702400	-2.00462000	-3.23583300
H	-2.44526000	4.11799400	2.94839400	C	3.91224900	-2.08736000	-0.75469400
H	-1.11284400	4.97745900	-0.51443700	C	3.10607000	-1.27730100	-1.55901400
H	-2.35768500	4.04387600	0.30567300	C	3.50698200	-1.06369300	-2.88851700
H	-1.89746400	6.11822000	1.59210300	C	4.67705700	-1.62913200	-3.39099800
H	-0.17807800	5.72573100	1.65435000	C	5.47653900	-2.42836300	-2.56905800
C	-3.26598800	-1.05810900	5.26651700	C	5.08709900	-2.65650600	-1.24956900
H	-3.85559900	-1.94541100	5.52214000	H	3.63765800	-2.25104400	0.27909400
H	-2.89645900	-0.62657100	6.20635200	H	2.89166100	-0.43604700	-3.52846200
C	-2.99244000	0.86001500	3.78885700	H	4.96667100	-1.44625600	-4.42289400
H	-2.77289100	1.75139300	4.38594600	H	6.39365500	-2.86594800	-2.95457300
H	-3.31448700	1.20413200	2.80299500	H	5.70289100	-3.26928700	-0.59623400
C	-4.06722200	-0.00768900	4.47745700	C	1.86492600	-0.56754500	-1.05914300
H	-4.73537100	0.57975100	5.11560400	C	0.02511700	-3.75913100	-3.89355600
H	-4.67886200	-0.50206200	3.71788700	H	-0.81107800	-4.17279000	-4.46775000
H	1.49131600	-0.81342500	0.30595500	H	0.67932100	-3.20905300	-4.57785300
C	5.40756900	1.09838200	-0.79984300	H	0.59569500	-4.59101900	-3.46493100
C	6.57153800	0.59756500	-0.21947400	C	-1.39551200	-3.56180000	-1.80206400
C	6.53938600	0.06417200	1.07143900	H	-1.74662000	-2.87774100	-1.02598900
C	5.33487300	0.03204300	1.77565100	H	-2.27580800	-3.95893900	-2.31689800
C	4.16668200	0.51354300	1.18461000	H	-0.86286100	-4.39610100	-1.33259500
C	4.18847300	1.04232800	-0.11212700				
C	2.93115900	1.56084100	-0.74391900				

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C	-3.69949300	1.08732600	-0.21776600	C	2.18975300	-3.82273900	1.29734700
C	-4.40666000	0.48747300	-1.43807400	H	0.15481300	-3.32223400	1.71699500
C	-4.13267700	0.88077900	-2.75134100	C	0.12005900	-5.38856900	-0.10919300
C	-5.35863600	-0.52023600	-1.22105800	H	0.98433400	-3.73018400	-1.19149700
C	-4.78854200	0.27492600	-3.82648500	H	-0.65591500	-3.43485300	-0.65060300
H	-3.41175200	1.66801400	-2.94131600	C	2.02637900	-5.32736500	1.54992700
C	-6.01668100	-1.12290700	-2.29188700	H	2.91994600	-3.65973000	0.49393400
H	-5.57205800	-0.83123800	-0.20274300	H	2.58173900	-3.32443800	2.19241500
C	-5.73258800	-0.72742900	-3.60219300	C	1.43875400	-6.03974000	0.32577900
H	-4.56177500	0.59371900	-4.84042100	H	-0.26409100	-5.86986700	-1.01719200
H	-6.75538300	-1.89770100	-2.10395600	H	-0.63721900	-5.54490700	0.67335200
H	-6.24698300	-1.19256200	-4.43873900	H	2.99401800	-5.76738800	1.82120600
C	-3.18878600	2.50045800	-0.43149100	H	1.35958900	-5.47905000	2.41155100
C	-3.96359400	3.56765700	0.03928600	H	1.28631100	-7.10465000	0.54115700
C	-2.01094700	2.78217700	-1.13745800	H	2.15846500	-5.98317300	-0.50362300
C	-3.57970400	4.88938700	-0.19209400	C	0.69769400	1.63802000	2.03554100
H	-4.87917100	3.35966500	0.58789700	C	1.33882400	2.08177500	3.36003700
C	-1.63004400	4.10407300	-1.37377700	C	0.93944500	2.68598300	0.94542400
H	-1.38919500	1.97427500	-1.50751500	H	-0.37828400	1.51046600	2.16901200
C	-2.41126300	5.16181400	-0.90538500	C	0.83159800	3.46348700	3.79116800
H	-4.19331200	5.70333500	0.18474800	H	2.42901700	2.11826300	3.21959200
H	-0.71275200	4.30332600	-1.92077000	H	1.14433500	1.33830800	4.14056900
H	-2.10881600	6.18928800	-1.08871200	C	0.42151700	4.06256600	1.37328700
H	-4.43441000	1.11956900	0.58799100	H	2.01633000	2.75169700	0.75538800
C	-1.37922600	-2.19697700	4.03797600	H	0.47344800	2.35275900	0.01516900
H	-0.61184600	-2.94314000	4.26478500	C	1.05922300	4.51006700	2.69344800
N	1.22577100	0.33867700	1.61382400	H	1.32529900	3.76593800	4.72300800
N	1.05120100	-1.74126200	0.65876600	H	-0.24402300	3.39906600	4.01032200
N	-0.64200300	-0.93041200	2.15517700	H	0.62804500	4.79142200	0.58170600
C	0.54464000	-0.81660000	1.45934800	H	-0.66997000	4.02466100	1.48737100
C	-1.79544100	-1.68013300	1.64767500	H	0.65365000	5.48094900	3.00518600
H	-1.51985900	-2.20214400	0.73210700	H	2.13966000	4.64943600	2.54191400
O	-4.03871200	-0.74164900	1.84674200	C	-2.23273500	-1.85202900	5.26482700
C	-2.94563100	-0.70626000	1.27291900	H	-3.01067800	-2.59762500	5.46230500
N	-2.66212200	0.16946100	0.27942200	H	-1.59195100	-1.80056400	6.15506600
H	-1.81735900	0.05590000	-0.28209200	C	-1.64941100	0.26399600	4.20450900
C	-0.72457500	-0.84832600	3.62220500	H	-1.07206100	0.88118200	4.90065000
H	0.29003600	-0.74208200	4.00761600	H	-2.01918900	0.92662600	3.41826000
C	-2.19102900	-2.63891800	2.78939900	C	-2.79964400	-0.45957500	4.93730200
H	-1.95626100	-3.67069600	2.51685500	H	-3.13375400	0.07990400	5.82948900
H	-3.26620300	-2.57264200	2.96196900	H	-3.65687200	-0.55697500	4.26556800
H	2.14506900	0.34752000	1.18731000	H	1.40093100	-1.37520200	-0.54963400
C	0.85408300	-3.17408800	0.88575000	C	5.72561200	-0.04503500	-1.82730600
C	0.29443800	-3.88493000	-0.35416900	C	6.81202300	-0.88710500	-1.59256500

C	6.73027000	-1.88179400	-0.61479500	C	1.39915500	3.33116500	-1.02369800
C	5.55419000	-2.02789300	0.12346800	C	3.47214400	4.50903700	-1.37360900
C	4.46451700	-1.19179200	-0.12037100	C	0.69838000	4.53386500	-1.10954200
C	4.53187600	-0.19549800	-1.10554000	H	0.85906600	2.40873100	-0.84261500
C	3.37377600	0.72348300	-1.34436700	C	2.77298200	5.71477000	-1.46695000
C	3.64434900	2.18516500	-1.21157600	H	4.55584600	4.50122600	-1.46168900
C	2.81528300	3.11249200	-1.86742800	C	1.38352900	5.73023600	-1.33560800
C	2.98986000	4.48095800	-1.68482500	H	-0.38287900	4.53340900	-1.00033600
C	4.00000700	4.95702600	-0.84210900	H	3.31604500	6.64162600	-1.63088900
C	4.84056500	4.04771100	-0.19792300	H	0.83899600	6.66810000	-1.40155400
C	4.67072600	2.67521800	-0.38759000	C	3.63351100	1.21741600	-2.37464300
N	2.15052500	0.39635100	-1.59886600	C	3.58458300	1.88727300	-3.60288200
H	5.79525700	0.73272400	-2.58257600	C	3.79895600	-0.17294500	-2.37723700
H	7.72379500	-0.76542700	-2.17125300	C	3.68688900	1.18469200	-4.80451400
H	5.48296800	-2.79403400	0.89107600	H	3.45462500	2.96403900	-3.62388100
H	3.54785000	-1.32233700	0.44524200	C	3.89718300	-0.87767900	-3.57659400
H	2.02212600	2.73336200	-2.50272400	H	3.83713100	-0.70992900	-1.43517400
H	2.33884000	5.18146700	-2.20173100	C	3.83947100	-0.20228100	-4.79707900
H	5.62967200	4.40537600	0.45835700	H	3.64091900	1.72451900	-5.74658200
H	5.32452800	1.97874100	0.12773100	H	4.01500400	-1.95702800	-3.55580800
H	4.13418600	6.02538500	-0.69654800	H	3.91282800	-0.75154300	-5.73171700
H	7.57848100	-2.53439000	-0.42704800	H	4.58740200	2.24157100	-0.75913700
C	0.21712600	-0.79867300	-2.23343900	C	3.09160600	-0.31320400	4.26888400
O	-0.20830800	-1.77746200	-3.06784400	H	2.41011500	-0.62127000	5.06646200
O	-0.57086500	0.02961200	-1.76796800	N	0.87515400	-2.19434800	1.09567600
C	-1.60689700	-1.75740400	-3.47526800	N	-0.31291000	-0.27649600	1.48327200
H	-1.92784400	-0.71491000	-3.49127800	N	1.97624200	-0.43118700	2.15479100
C	1.64175100	-0.89329100	-1.85536700	C	0.82822900	-0.93126800	1.59309400
C	-1.63988700	-2.34536800	-4.87622500	C	2.25061800	0.99323700	2.34165800
H	-2.66519600	-2.32983800	-5.26161500	H	1.35230200	1.57890200	2.16767900
H	-1.00627600	-1.76607200	-5.55589400	O	4.11871600	2.35603600	1.61337600
H	-1.28813400	-3.38360100	-4.87425200	C	3.24654400	1.54620900	1.30254000
C	-2.46077700	-2.53384200	-2.48443700	N	3.02313000	1.16293300	0.01567000
H	-2.39824700	-2.09328800	-1.48671400	H	2.19503000	0.61533500	-0.20831500
H	-3.50904200	-2.50434300	-2.79665600	C	2.90008500	-1.20115500	3.00442600
H	-2.14292600	-3.58129200	-2.43397700	H	2.42754400	-2.15487100	3.23368100
C	2.50191300	-1.90504900	-2.61042200	C	2.73873000	1.12145100	3.79459900
H	3.07754600	-1.41259000	-3.40676300	H	1.94598300	1.54894200	4.41383200
H	3.22148800	-2.41176700	-1.96247000	H	3.59525500	1.79691000	3.83604700
H	1.87420900	-2.66584700	-3.07647000	H	-0.03669800	-2.54632800	0.82122600
				C	-0.85000000	0.69060400	2.43905500
				C	-1.11303200	2.05250200	1.77083200
				C	-2.16344600	0.12334700	3.01037900
				H	-0.15702600	0.81780600	3.28149100
<b>TS3-S</b>							
C	3.56511100	1.99316500	-1.06152400				
C	2.79321900	3.30696900	-1.15832400				

C	-1.80470900	3.03867400	2.71961500	C	-4.66142300	-0.99709800	-0.43417400
H	-1.74684500	1.87665200	0.89503900	C	-3.94788900	0.31525200	-0.56185100
H	-0.17806600	2.48478700	1.39488100	C	-4.76045800	1.55535800	-0.39451800
C	-2.84855100	1.10654500	3.96701900	C	-4.14695700	2.82127100	-0.47972400
H	-2.83322800	-0.09671000	2.16991900	C	-4.87958200	3.98850600	-0.29822300
H	-1.95330200	-0.82963600	3.51204200	C	-6.25174700	3.92883700	-0.02858600
C	-3.10517400	2.45540900	3.28464500	C	-6.87706800	2.68461100	0.04070700
H	-2.00828400	3.97644100	2.18802500	C	-6.14258500	1.51132900	-0.14361400
H	-1.12588300	3.28832200	3.54900700	N	-2.69396300	0.47445100	-0.81521900
H	-3.78967100	0.67549400	4.33169600	H	-5.01152700	-0.81658700	1.68336500
H	-2.21071800	1.26102000	4.85011300	H	-6.13046500	-3.01843700	1.88859200
H	-3.56277500	3.15929400	3.99122300	H	-5.61867300	-3.65964800	-2.33527900
H	-3.82176500	2.31619700	2.46416900	H	-4.49528600	-1.45996900	-2.52751600
C	2.00508000	-2.89618800	0.47511000	H	-3.08635900	2.86280600	-0.69847200
C	2.29613800	-4.21091900	1.21525900	H	-4.37990900	4.95170500	-0.36624300
C	1.71614200	-3.17142900	-1.00776700	H	-7.94400600	2.62090100	0.23870600
H	2.87305100	-2.23893900	0.54116200	H	-6.65021300	0.55465300	-0.09132400
C	3.44152300	-4.99126600	0.55753200	H	-6.82298200	4.84121400	0.11963600
H	1.38018600	-4.81925600	1.20378700	H	-6.42980500	-4.45382000	-0.12124500
H	2.52615700	-4.00952100	2.26693900	C	-0.52183700	0.10141800	-1.73065800
C	2.86758200	-3.94301100	-1.66401700	O	-0.93377800	0.84553100	-2.77791700
H	0.79488200	-3.76447400	-1.08056200	O	0.67245800	-0.10807000	-1.52431100
H	1.52999700	-2.22580600	-1.52069200	C	0.09646000	1.31512500	-3.66819400
C	3.16158500	-5.25404300	-0.92679700	H	0.72542100	2.05906700	-3.17892000
H	3.60381500	-5.93503000	1.09258100	H	-0.43371000	1.76753100	-4.50800900
H	4.37225100	-4.41259200	0.65171000	H	0.71649400	0.48357000	-4.00965800
H	2.62653000	-4.13755500	-2.71627500	C	-1.58605000	-2.56379000	-2.27919600
H	3.77252000	-3.31835200	-1.65951400	C	-1.80229700	-1.92860100	-1.04713600
H	4.01209600	-5.77143500	-1.38804000	C	-2.16483500	-2.72860100	0.05088600
H	2.29399600	-5.92331900	-1.01900400	C	-2.31823500	-4.10783600	-0.08068600
C	4.56326500	-0.49818500	4.66116600	C	-2.09887800	-4.72411800	-1.31560900
H	4.93167200	0.30819200	5.30426500	C	-1.73116000	-3.94520000	-2.41437900
H	4.68577300	-1.44202000	5.20884800	H	-1.31278800	-1.96710500	-3.14577300
C	4.33553400	-1.41066900	2.42730700	H	-2.34578300	-2.25684100	1.01077900
H	4.59190100	-2.47378300	2.48900600	H	-2.61324800	-4.70083500	0.78079600
H	4.39150700	-1.12277700	1.37487000	H	-2.21710700	-5.79914100	-1.42012600
C	5.28748200	-0.57679300	3.30856700	H	-1.56088100	-4.41299200	-3.38070800
H	6.28573300	-1.01970700	3.38334400	C	-1.62900300	-0.43718300	-0.88356500
H	5.40469900	0.42831500	2.88969400	H	-0.98408500	-0.36368300	0.37598700
C	-5.14264000	-1.44185800	0.80457800				
C	-5.77345900	-2.68124500	0.91897300				
C	-5.94261300	-3.48649500	-0.20906400				
C	-5.48859400	-3.04009400	-1.45231000				
C	-4.85808600	-1.80208400	-1.56356900				
				<b>TS3-S-1b</b>			
				C	3.56930700	2.04466300	-0.78656200
				C	2.80671400	3.36686600	-0.75605500
				C	1.41638600	3.39196200	-0.59088600

C	3.49050600	4.57708500	-0.90159200	H	-1.73284000	1.71218400	1.12770700
C	0.72193300	4.60155700	-0.58601100	H	-0.15066400	2.25675500	1.65754600
H	0.87287500	2.46389000	-0.45708900	C	-2.82325100	0.70508300	4.13018900
C	2.79864600	5.79044600	-0.90145100	H	-2.83071400	-0.33652200	2.23457000
H	4.57217300	4.56829700	-1.01211600	H	-1.96199600	-1.19740900	3.50679800
C	1.41139800	5.80583300	-0.74630800	C	-3.05855100	2.11392100	3.57236200
H	-0.35696200	4.59945000	-0.45488900	H	-1.94590500	3.70322300	2.59561900
H	3.34538900	6.72287000	-1.01321300	H	-1.06186400	2.88699000	3.88297800
H	0.87274100	6.74933900	-0.74142600	H	-3.77110700	0.25956700	4.45812800
C	3.64106600	1.40467100	-2.17193400	H	-2.18162500	0.76854700	5.02160100
C	3.53993800	2.18405600	-3.33036800	H	-3.49229300	2.76102600	4.34524900
C	3.85775400	0.02789700	-2.30891600	H	-3.78832300	2.06361500	2.75355600
C	3.63815400	1.60134200	-4.59499900	C	2.00705800	-2.98646500	0.24417000
H	3.37012900	3.25218000	-3.24793100	C	2.36922700	-4.35217500	0.84897300
C	3.95354000	-0.55652200	-3.57118400	C	1.66611200	-3.13803600	-1.24570200
H	3.93812100	-0.59236500	-1.42198200	H	2.85783000	-2.30904100	0.33674000
C	3.84127900	0.22707000	-4.72123800	C	3.51641500	-5.02163500	0.08177800
H	3.54905600	2.22481000	-5.48060500	H	1.47607500	-4.99222700	0.80918000
H	4.11079000	-1.62767600	-3.65536900	H	2.63066200	-4.24188400	1.90657600
H	3.91064300	-0.23023000	-5.70437400	C	2.81263000	-3.80739200	-2.01291300
H	4.59129200	2.25425500	-0.45489700	H	0.76084900	-3.75307300	-1.33673600
C	3.09475500	-0.79320500	4.29063000	H	1.43270900	-2.15696300	-1.66375800
H	2.41228400	-1.17783800	5.05344500	C	3.18405900	-5.16572000	-1.40780600
N	0.88256900	-2.37575500	0.96495500	H	3.73890900	-6.00025700	0.52439100
N	-0.30834600	-0.50234600	1.53324300	H	4.42609200	-4.41290000	0.19088000
N	1.98831600	-0.71384800	2.16870100	H	2.53322600	-3.91714600	-3.06807300
C	0.83439700	-1.16300900	1.57662800	H	3.69505200	-3.15217500	-1.98833200
C	2.25562300	0.68732100	2.49256200	H	4.03203300	-5.60741100	-1.94628200
H	1.35483100	1.28129100	2.37178100	H	2.33756300	-5.85796800	-1.52363700
O	4.13276600	2.10662900	1.90977700	C	4.56633700	-1.00867700	4.66841800
C	3.25135300	1.34403600	1.51593000	H	4.93063800	-0.26337600	5.38356400
N	3.01733200	1.11024000	0.19592700	H	4.69086600	-1.99792700	5.12870300
H	2.19078000	0.58736800	-0.08679600	C	4.34732900	-1.71246500	2.35933200
C	2.90991600	-1.55871100	2.94742400	H	4.60392200	-2.77692400	2.32637500
H	2.43817100	-2.53047300	3.08209300	H	4.40802400	-1.33207700	1.33694200
C	2.73657600	0.67838900	3.95299800	C	5.29413600	-0.96056400	3.31636500
H	1.93791400	1.04017400	4.60587100	H	6.29401800	-1.40464800	3.35283300
H	3.58839700	1.35195200	4.06333300	H	5.40737100	0.07944300	2.99252900
H	-0.03094200	-2.70762400	0.67253000	C	-5.07971200	-1.62707200	0.79139000
C	-0.83660500	0.39288700	2.56315800	C	-5.70047500	-2.87681700	0.79552200
C	-1.08724000	1.80711700	2.00724900	C	-5.90759100	-3.55802800	-0.40533900
C	-2.15654300	-0.20185500	3.08874500	C	-5.49837900	-2.97893900	-1.60887600
H	-0.14336000	0.44827800	3.41291500	C	-4.87723400	-1.73102700	-1.61001800
C	-1.75342600	2.72046900	3.04348000	C	-4.64526400	-1.04842400	-0.40871500

C	-3.94556400	0.27825900	-0.41596400	C	2.80003800	3.37142200	-0.53338900
C	-4.76521800	1.48941500	-0.11722000	C	1.40599200	3.39261400	-0.40634900
C	-4.17213500	2.76794600	-0.14442000	C	3.49277500	4.58459900	-0.57338100
C	-4.90833200	3.90775700	0.15688400	C	0.71843700	4.60321400	-0.32259900
C	-6.26329900	3.80784100	0.49356100	H	0.85450900	2.46085400	-0.36186200
C	-6.86852500	2.55203100	0.50883100	C	2.80689500	5.79930000	-0.50188900
C	-6.13090400	1.40613800	0.20332000	H	4.57705300	4.57714800	-0.65424000
N	-2.69665400	0.47676000	-0.66153100	C	1.41699700	5.81196300	-0.37466700
H	-4.92222500	-1.09641600	1.72611800	H	-0.36266200	4.59866800	-0.21237500
H	-6.02237300	-3.31722900	1.73562000	H	3.36056400	6.73383200	-0.53149200
H	-5.65648800	-3.50325800	-2.54731000	H	0.88274700	6.75565800	-0.30836800
H	-4.54888600	-1.28738700	-2.54449600	C	3.66811100	1.47059900	-2.01749800
H	-3.12564200	2.84186000	-0.41653200	C	3.63931800	2.30838800	-3.13891000
H	-4.42511800	4.88130500	0.12956300	C	3.87047400	0.09886600	-2.21166400
H	-7.92218700	2.45760800	0.75893300	C	3.81295000	1.78879700	-4.42265300
H	-6.62372500	0.44044900	0.21640800	H	3.47656400	3.37339700	-3.01139600
H	-6.83732600	4.69864800	0.73371600	C	4.03775000	-0.42296800	-3.49411100
H	-6.38774800	-4.53282200	-0.40439200	H	3.89145100	-0.56512500	-1.35374500
C	-0.51844000	0.24890600	-1.60968000	C	4.01077400	0.42012900	-4.60641900
O	-0.93074500	1.17872800	-2.49411400	H	3.78689500	2.45737800	-5.27896200
O	0.67406600	-0.02602800	-1.47359300	H	4.18628400	-1.49092100	-3.62308000
C	0.08817500	1.76409000	-3.34061700	H	4.13880400	0.01338600	-5.60568900
H	0.91137700	2.12087600	-2.72559700	H	4.57682200	2.24669600	-0.25213200
H	0.47994800	0.98182200	-3.99918600	C	3.07396300	-1.01426800	4.33846300
C	-1.59150100	-2.31095600	-2.51371700	H	2.38105600	-1.42408800	5.07840700
C	-1.78275100	-1.86063900	-1.19925300	N	0.85744800	-2.42835700	0.94482900
C	-2.12345500	-2.81017500	-0.22125200	N	-0.31881400	-0.56630200	1.57203500
C	-2.27788400	-4.15725800	-0.54695600	N	1.96765100	-0.82778800	2.22615000
C	-2.08230300	-4.58890700	-1.86144200	C	0.81677700	-1.24052800	1.60344200
C	-1.73713700	-3.65869100	-2.84381000	C	2.24787400	0.55559600	2.61034800
H	-1.33764300	-1.59428100	-3.29047500	H	1.35143300	1.16203100	2.52466600
H	-2.29146300	-2.48222000	0.79945900	O	4.13657100	1.97915700	2.08081200
H	-2.55780300	-4.86839300	0.22555000	C	3.24284400	1.24715700	1.65748400
H	-2.20202600	-5.63806700	-2.11756600	N	2.99763700	1.07904800	0.32887100
H	-1.58645000	-3.98070700	-3.87105000	H	2.16168300	0.58337500	0.02528700
C	-1.61930300	-0.40249300	-0.83933500	C	2.88696500	-1.71304200	2.96077900
H	-0.97684400	-0.47641900	0.42128200	H	2.41417600	-2.68978600	3.04957400
C	-0.55677600	2.89233000	-4.11489600	C	2.73844400	0.47616600	4.06641500
H	-0.92622900	3.66775900	-3.43517800	H	1.95075600	0.82329800	4.74012700
H	0.18320400	3.34574400	-4.78409400	H	3.60281300	1.12951100	4.19872000
H	-1.39592400	2.53259400	-4.72014100	H	-0.05625100	-2.73816200	0.62996400
				C	-0.85072700	0.29959300	2.62439600
				C	-1.07527600	1.73519900	2.11410200
				C	-2.18524500	-0.29473800	3.11242200
<b>TS3-S-1c</b>							
C	3.56111700	2.05041000	-0.60996600				



H	-0.16993500	0.31665200	3.48592500	C	-4.88037100	-1.69106200	-1.62929600
C	-1.74033900	2.62218000	3.17362300	C	-4.65901800	-1.05925800	-0.39864800
H	-1.71351400	1.67967300	1.22552400	C	-3.96363200	0.26866900	-0.34682600
H	-0.12867500	2.18206800	1.78895300	C	-4.78917000	1.46526900	-0.00719200
C	-2.85156600	0.58569700	4.17666600	C	-4.20333700	2.74740700	-0.00162800
H	-2.85065700	-0.39132600	2.24617400	C	-4.94465300	3.87431100	0.33371400
H	-2.00924800	-1.30650000	3.49867400	C	-6.29730900	3.75712200	0.67419300
C	-3.06021000	2.01652600	3.66616600	C	-6.89493400	2.49762400	0.65946600
H	-1.91322800	3.62269300	2.75802000	C	-6.15238600	1.36490100	0.31848500
H	-1.05660600	2.74967000	4.02640800	N	-2.71499500	0.48169300	-0.58009800
H	-3.80963900	0.14318000	4.47783300	H	-4.94523100	-1.20125700	1.73089300
H	-2.21995300	0.60838200	5.07725100	H	-6.03086500	-3.42725200	1.63870600
H	-3.49429800	2.64249400	4.45609600	H	-5.64005800	-3.42772400	-2.64590500
H	-3.78068100	2.00476400	2.83769900	H	-4.55010400	-1.20453900	-2.54156200
C	1.98345100	-3.03574400	0.22594700	H	-3.15823000	2.83423000	-0.27519400
C	2.25154600	-4.45683300	0.74436500	H	-4.46739700	4.85116600	0.33002200
C	1.71117300	-3.06022100	-1.28487600	H	-7.94652900	2.39018300	0.91295900
H	2.85907400	-2.41211500	0.40721200	H	-6.63941600	0.39629300	0.30790100
C	3.40241000	-5.12724700	-0.01698200	H	-6.87550100	4.63770300	0.94060600
H	1.33185600	-5.04608800	0.61711600	H	-6.37505800	-4.55337500	-0.55294300
H	2.46493100	-4.43282300	1.81884600	C	-0.53998000	0.31064400	-1.54416700
C	2.86820400	-3.72118300	-2.04396600	O	-0.97218500	1.27068300	-2.38521300
H	0.78859100	-3.62699000	-1.46604900	O	0.65547900	0.04220900	-1.41799100
H	1.53542900	-2.04195500	-1.63734200	C	0.01013900	1.91351700	-3.25170800
C	3.14472900	-5.13817000	-1.52847200	H	0.93813500	2.02193300	-2.69152600
H	3.55081200	-6.14805000	0.35599300	C	-1.57661500	-2.24379900	-2.52444400
H	4.33472800	-4.57990100	0.18557000	C	-1.78450900	-1.82826500	-1.20114000
H	2.64101900	-3.73923100	-3.11700100	C	-2.13262200	-2.80484600	-0.25226200
H	3.77621900	-3.11225600	-1.92467700	C	-2.27510600	-4.14384900	-0.61355900
H	3.99959500	-5.57929500	-2.05634600	C	-2.06110100	-4.54108700	-1.93607600
H	2.27491000	-5.77579400	-1.74259100	C	-1.71043400	-3.58391800	-2.89008500
C	4.53977400	-1.26884300	4.71225400	H	-1.31798400	-1.50753800	-3.28048500
H	4.91024500	-0.56869700	5.46868700	H	-2.31417500	-2.50380300	0.77422600
H	4.64801300	-2.28325900	5.11844900	H	-2.56030900	-4.87576300	0.13733500
C	4.32474900	-1.84099000	2.36529200	H	-2.17121400	-5.58415700	-2.21976100
H	4.57386800	-2.90277100	2.26287400	H	-1.54551100	-3.87908300	-3.92325900
H	4.38922200	-1.39433600	1.37010900	C	-1.63141600	-0.38161700	-0.79494600
C	5.27629500	-1.15786500	3.36850500	H	-0.98403300	-0.49873400	0.45760800
H	6.26899000	-1.61882100	3.38617200	C	0.24654000	1.02346400	-4.46432800
H	5.40764700	-0.10378500	3.10177500	H	0.95258700	1.50217700	-5.14994700
C	-5.09610700	-1.69134100	0.77319500	H	0.67144300	0.06314500	-4.15999100
C	-5.70771900	-2.94442600	0.72013000	H	-0.69343400	0.84895000	-5.00098900
C	-5.90273000	-3.57572900	-0.50975900	C	-0.56515400	3.27339500	-3.60270500
C	-5.49187600	-2.94245400	-1.68514200	H	-0.74708900	3.86365600	-2.69985500

H	0.14155400	3.82360200	-4.23368700	H	-2.88672400	0.18864000	-4.29490200
H	-1.51017600	3.17031400	-4.14818000	H	0.66684000	-2.56450300	0.24706000
<b>TS3-S-1d</b>				C	1.44658100	0.09269200	-2.27363000
C	-3.74168200	1.58096700	0.30621100	C	1.55065700	1.61444400	-2.07436500
C	-3.50069000	3.07275600	0.55093600	C	2.84279100	-0.47632000	-2.59120600
C	-2.84673400	3.84745800	-0.41546500	H	0.81083200	-0.11517000	-3.14401000
C	-3.99106200	3.70968600	1.69691000	C	2.14475500	2.29971000	-3.30999300
C	-2.67653500	5.22036800	-0.23777000	H	2.19470200	1.80606000	-1.21112400
H	-2.46311100	3.37066500	-1.31169800	H	0.56968800	2.04044400	-1.83237800
C	-3.82107800	5.08351300	1.87792600	C	3.45881300	0.20201000	-3.82192900
H	-4.50548000	3.13104200	2.45666500	H	3.49035500	-0.31707200	-1.72028200
C	-3.16194900	5.84539300	0.91278200	H	2.76757400	-1.55962200	-2.74745700
H	-2.16198800	5.80106600	-0.99896100	C	3.52582000	1.72426000	-3.64731100
H	-4.20487400	5.55632800	2.77798000	H	2.21351200	3.38114100	-3.13767900
H	-3.02773600	6.91423800	1.05477700	H	1.47091100	2.16016900	-4.16858200
C	-3.96948200	0.77013500	1.57223800	H	4.46028800	-0.20530900	-4.00696700
C	-3.00581900	0.72569500	2.58955700	H	2.85303000	-0.03484700	-4.70930800
C	-5.16421000	0.06327600	1.73816700	H	3.92583300	2.19467900	-4.55446400
C	-3.24001800	-0.01191100	3.74958100	H	4.22203200	1.96107900	-2.83043700
H	-2.07438700	1.26721300	2.46312000	C	-1.39533900	-3.03984500	0.33046000
C	-5.40143300	-0.67350100	2.90154800	C	-1.37904100	-4.54474700	0.02321100
H	-5.91648500	0.09382000	0.95367500	C	-1.48786600	-2.79033400	1.84199400
C	-4.43988500	-0.71080800	3.91167200	H	-2.26311500	-2.57914400	-0.14276000
H	-2.48360000	-0.03986000	4.52955400	C	-2.59073700	-5.25854500	0.63524700
H	-6.33719400	-1.21380600	3.01731500	H	-0.45348000	-4.97254400	0.43559200
H	-4.62202700	-1.28150400	4.81820900	H	-1.34473200	-4.70143300	-1.06056600
H	-4.63943100	1.48934600	-0.31212700	C	-2.69818600	-3.50850100	2.45123500
C	-1.78757600	-1.71873900	-4.23635200	H	-0.56453000	-3.14886400	2.31969300
H	-0.85314100	-1.95410000	-4.75453000	H	-1.55465500	-1.71503000	2.02677000
N	-0.21039800	-2.38788300	-0.23094000	C	-2.67972600	-5.00984300	2.14579500
N	0.89984100	-0.58364100	-1.09533800	H	-2.53576900	-6.33336500	0.42298900
N	-1.23209300	-1.22570100	-1.97442900	H	-3.50736600	-4.88817600	0.15398900
C	-0.16085200	-1.36992500	-1.12442200	H	-2.72125900	-3.33510800	3.53330400
C	-1.65056100	0.07208500	-2.52263300	H	-3.61736300	-3.06391900	2.04698500
H	-0.87551800	0.81367300	-2.35181600	H	-3.57404200	-5.49338800	2.55821300
O	-4.02715400	0.58824800	-2.30061100	H	-1.81235000	-5.47151100	2.64014900
C	-2.91036400	0.57426900	-1.77679400	C	-3.00694500	-2.35348200	-4.91566900
N	-2.67610300	1.00284000	-0.51400200	H	-3.34157900	-1.79140100	-5.79435200
H	-1.72923200	1.04782900	-0.13484000	H	-2.75521200	-3.36859500	-5.24999400
C	-1.78186100	-2.31191100	-2.80158400	C	-3.25655000	-2.73686300	-2.51933400
H	-1.11545300	-3.17006700	-2.70999800	H	-3.28485400	-3.81027100	-2.30470800
C	-1.89836300	-0.18471600	-4.02173700	H	-3.66267500	-2.22098800	-1.64624500
H	-1.15729400	0.34723900	-4.62368400	C	-4.06045300	-2.40708100	-3.79563200
				H	-4.85104300	-3.13782100	-3.99451800

H	-4.53182200	-1.42704800	-3.68147300	<b>DP-TS</b>			
C	3.25075200	-2.56485900	0.61536100	C	-3.85477000	2.04753900	-0.74528500
C	2.96430800	-3.88302100	0.97683900	C	-3.07149100	3.35146400	-0.75759400
C	3.18145200	-4.31305700	2.28839200	C	-2.20082400	3.68755800	0.28517600
C	3.70829300	-3.42380400	3.22754900	C	-3.21592000	4.23460700	-1.83249800
C	3.99830400	-2.10789900	2.86293800	C	-1.48141300	4.88096300	0.24792000
C	3.74918000	-1.65693300	1.56083300	H	-2.08711700	3.01537200	1.12918700
C	3.97754500	-0.22204500	1.17350800	C	-2.50369500	5.43504700	-1.86897000
C	5.36095700	0.17586500	0.80006100	H	-3.89057100	3.97853400	-2.64566500
C	5.63564000	1.50275300	0.41350500	C	-1.63248500	5.76014400	-0.82787100
C	6.91745200	1.88386500	0.03402800	H	-0.80408800	5.12581100	1.06139300
C	7.96438400	0.95421200	0.03735200	H	-2.62944200	6.11338700	-2.70842200
C	7.70769600	-0.36057100	0.42484500	H	-1.07586100	6.69291500	-0.85258300
C	6.42005800	-0.74722300	0.80172600	C	-4.60749900	1.84540300	0.56512500
N	3.05155400	0.66954900	1.07578800	C	-5.85919700	2.44632500	0.73663100
H	3.07325200	-2.22842000	-0.40018100	C	-4.06566100	1.10124100	1.61556800
H	2.57486500	-4.57383200	0.23319800	C	-6.55976000	2.30008400	1.93355700
H	3.89045000	-3.75318600	4.24702600	H	-6.28927700	3.02633300	-0.07654300
H	4.39773200	-1.41595600	3.59910800	C	-4.76654100	0.94683600	2.81328500
H	4.82133500	2.21901100	0.42152500	H	-3.09777600	0.63161800	1.48745100
H	7.10610700	2.91282000	-0.26210600	C	-6.01604600	1.54633600	2.97677300
H	8.51021400	-1.09380000	0.43247600	H	-7.53405100	2.76753900	2.04901300
H	6.23614900	-1.77607400	1.09267400	H	-4.33625100	0.35438400	3.61625900
H	8.96612500	1.25479300	-0.25743000	H	-6.56422700	1.42392100	3.90685900
H	2.95279400	-5.33644500	2.57287400	H	-4.60528700	2.09780400	-1.53925200
C	0.87971600	1.71661500	1.14629900	C	-3.41243500	-3.52856000	-1.24030400
O	1.57663600	2.85858700	0.97969800	H	-3.03769800	-4.53241100	-1.46012500
O	-0.35899500	1.71008700	1.11362500	N	0.05863800	-1.24634000	0.66414400
C	0.81515700	4.07303500	0.72839300	N	0.28953700	-1.35311400	-1.62116400
H	-0.04407200	3.80823800	0.10851000	N	-1.82077000	-1.79525100	-0.69879900
C	1.67696200	0.48262300	1.26971300	C	-0.48743900	-1.49745700	-0.49488300
H	1.29175400	-0.12206800	0.05379500	C	-2.52324200	-1.34464600	-1.91096500
C	1.13724200	-0.43409500	2.37294800	H	-1.80052300	-0.91783400	-2.60501000
H	1.27881600	-1.49538900	2.17074600	O	-4.73841800	-0.33515400	-1.76053900
H	1.62987100	-0.21920300	3.33195400	C	-3.52555200	-0.21776600	-1.56891800
H	0.06793000	-0.25403800	2.49278500	N	-2.97814800	0.92045600	-1.07575900
C	1.75047200	5.00530900	-0.02308100	H	-1.96990800	1.01745800	-0.93058800
H	2.09753300	4.54434100	-0.95373800	C	-2.56532900	-2.90151000	-0.07137000
H	1.22831800	5.93570700	-0.27294600	H	-1.84197800	-3.61599000	0.32846400
H	2.62694000	5.25538700	0.58562900	C	-3.20594200	-2.60412000	-2.46047200
C	0.32656400	4.64773500	2.05075500	H	-2.55251900	-3.07263800	-3.20139000
H	-0.22311400	5.57874200	1.87790200	H	-4.14861700	-2.35414600	-2.94976100
H	-0.34611800	3.94522400	2.54882100	H	1.16025500	-0.85687400	-1.46372100
H	1.17422600	4.86153800	2.71231200	H	1.19271300	-0.60701800	0.56670400

C	4.12647500	2.17426700	1.63713200	C	0.54135000	-1.63781100	-4.04517400
C	5.17298400	3.03040300	1.96166300	C	1.57776800	-3.30339900	-2.44840600
C	6.44570400	2.51875500	2.23346500	H	-0.52398900	-2.93757400	-2.69195600
C	6.65720000	1.13984200	2.19199900	C	0.71485700	-2.63657900	-5.19623900
C	5.60603500	0.27939000	1.88083400	H	1.41436900	-0.97134600	-3.99333700
C	4.32546400	0.78222500	1.59295700	H	-0.33152800	-0.99789200	-4.22048100
C	3.20734300	-0.13332600	1.30118900	C	1.74317600	-4.30493700	-3.59933800
C	3.13620200	-1.41720400	2.02710000	H	2.49473100	-2.70374300	-2.35091700
C	3.41399100	-1.49567200	3.40480800	H	1.43511200	-3.83108600	-1.49767200
C	3.33247400	-2.71211500	4.07754200	C	1.89261400	-3.58642400	-4.94572500
C	2.99031500	-3.87927400	3.38659900	H	0.85268800	-2.09550100	-6.14008400
C	2.72776700	-3.81767500	2.01680400	H	-0.20751700	-3.22631500	-5.30373100
C	2.79915500	-2.59950100	1.34437800	H	2.60928100	-4.95033400	-3.40885200
N	2.24544500	0.11582700	0.42680300	H	0.86191200	-4.96196600	-3.63429800
H	3.14276500	2.57687000	1.42020000	H	1.97052000	-4.31744800	-5.75990600
H	4.99779800	4.10207100	1.99772100	H	2.82880400	-3.00982200	-4.94520500
H	7.64310100	0.73218200	2.39830600	C	-0.69639900	-1.01691000	1.89337300
H	5.77687800	-0.79189300	1.84724400	C	-0.55053600	-2.21249900	2.84990700
H	3.67809500	-0.59290500	3.94657800	C	-0.20503300	0.26994300	2.58233000
H	3.53569500	-2.75080700	5.14425500	H	-1.75496100	-0.89013300	1.64595900
H	2.47214300	-4.72054700	1.46854800	C	-1.28445000	-1.97280500	4.17453400
H	2.60917700	-2.55663000	0.27755100	H	0.51535300	-2.36837600	3.04679400
H	2.93507000	-4.82835500	3.91238300	H	-0.91775700	-3.12418100	2.36450100
H	7.26446700	3.19096100	2.47444300	C	-0.94293700	0.51617800	3.90300600
C	1.00372500	1.51417600	-1.07670500	H	0.86681200	0.16840000	2.79114200
O	1.07080500	2.10120000	-2.31146200	H	-0.31607400	1.11078700	1.89238400
O	-0.08610900	1.40801300	-0.48564100	C	-0.80690000	-0.68175800	4.85052000
C	-0.13914400	2.69908400	-2.78148200	H	-1.13627300	-2.83169000	4.84098000
H	-0.49374400	3.46373400	-2.08899900	H	-2.36636000	-1.90237600	3.98971800
H	-0.92394000	1.95079900	-2.92703000	H	-0.55084400	1.42419400	4.37819200
H	0.11517300	3.15401300	-3.74133100	H	-2.00617500	0.70558500	3.70340700
C	4.55325900	0.46155100	-1.47441800	H	-1.36945900	-0.50456400	5.77615400
C	3.54133600	1.41891800	-1.26190900	H	0.24884300	-0.79659900	5.13550300
C	3.79583900	2.73507200	-1.68985500	C	-4.86273000	-3.60885400	-0.71250600
C	4.99390300	3.07313500	-2.31630200	H	-5.41924800	-2.72963100	-1.05337700
C	5.98378000	2.10983600	-2.51983300	H	-5.38812000	-4.49980600	-1.07208700
C	5.75302600	0.79916100	-2.09256200	C	-3.60054000	-2.53353200	1.01503100
H	4.39449600	-0.56154500	-1.14533300	H	-3.18003300	-2.54896700	2.02220600
H	3.04115300	3.49685900	-1.52760500	H	-3.98748600	-1.52739200	0.82794800
H	5.16000300	4.09973700	-2.63363200	C	-4.72436800	-3.55626600	0.81522000
H	6.92179400	2.37539800	-2.99958500	H	-4.42048100	-4.53572000	1.20964900
H	6.51147200	0.03496000	-2.24347700	H	-5.65176000	-3.26927300	1.32200800
C	2.27393400	1.03988600	-0.61020400				
C	0.39645800	-2.34873900	-2.69340300				

**DP-IM**

C	-3.57477400	2.27115100	-1.11558800	C	5.29851800	3.26946700	1.04782900
C	-2.59958400	3.42493900	-1.29453800	C	6.55518900	2.83574500	1.48173300
C	-1.63952800	3.71104800	-0.31695500	C	6.73435300	1.50380400	1.85828400
C	-2.63243400	4.19573700	-2.46061600	C	5.66710100	0.61062600	1.80009600
C	-0.71430000	4.73446300	-0.51329200	C	4.40178700	1.03172900	1.35309200
H	-1.61292900	3.12755500	0.59747000	C	3.27554700	0.09365000	1.32378300
C	-1.71515900	5.23130900	-2.65488400	C	3.14898200	-0.95162000	2.34777900
H	-3.37599900	3.97800900	-3.22333500	C	3.45697700	-0.68480400	3.69659900
C	-0.74870600	5.49775900	-1.68360600	C	3.31228700	-1.67377400	4.66448300
H	0.03361500	4.93653500	0.24856000	C	2.87163600	-2.95243800	4.30648700
H	-1.75274600	5.82314800	-3.56540400	C	2.57688500	-3.23264500	2.97103900
H	-0.02921900	6.29800400	-1.83402200	C	2.71354500	-2.24341600	2.00007600
C	-4.34609000	2.38604600	0.19544400	N	2.34026300	0.12884900	0.37215000
C	-5.42279700	3.27609500	0.27793900	H	3.26395400	2.71937200	0.63266300
C	-3.98454500	1.65468700	1.32805800	H	5.15015900	4.30623100	0.75953000
C	-6.12593900	3.43102500	1.47182700	H	7.70790800	1.15715000	2.19322800
H	-5.71018900	3.85016100	-0.59999600	H	5.81303700	-0.42502500	2.08858600
C	-4.68989700	1.80279800	2.52446500	H	3.78957500	0.30815300	3.98098200
H	-3.15796600	0.95749200	1.26477400	H	3.54063000	-1.44702900	5.70208700
C	-5.76208100	2.69220600	2.60113600	H	2.24311600	-4.22497200	2.68098500
H	-6.96241500	4.12323300	1.51971000	H	2.49893300	-2.47274100	0.96311000
H	-4.40156700	1.21821100	3.39400200	H	2.76490400	-3.72415500	5.06352900
H	-6.31301700	2.80734600	3.53052100	H	7.38728900	3.53280000	1.52404600
H	-4.30862600	2.31397600	-1.92598000	C	1.11240300	1.07295200	-1.43694200
C	-3.81888200	-3.37025200	-0.83329400	O	1.15328200	1.30596500	-2.77736800
H	-3.52309700	-4.42096000	-0.90934500	O	0.05846500	1.16501500	-0.78949200
N	-0.13839800	-1.31934300	0.91311400	C	-0.04459900	1.83329500	-3.35604200
N	0.09880600	-1.84897400	-1.32275600	H	-0.32726500	2.77346900	-2.88006400
N	-2.07910900	-1.73663600	-0.42864800	H	-0.87070300	1.12177000	-3.27417600
C	-0.70347700	-1.65084000	-0.19937200	H	0.19193100	2.00353300	-4.40828200
C	-2.66681800	-1.39543700	-1.73174300	C	4.67051000	-0.11844500	-1.50633000
H	-1.86234500	-1.16830200	-2.43308800	C	3.66083400	0.86026700	-1.59956900
O	-4.75371000	-0.12561900	-1.82204600	C	3.93069800	2.00517400	-2.37271100
C	-3.53889600	-0.12403600	-1.60598900	C	5.14704600	2.15644800	-3.03493000
N	-2.86561900	0.99872800	-1.25529900	C	6.13657600	1.17738900	-2.93010600
H	-1.85431800	0.97972800	-1.10783200	C	5.88732000	0.03653700	-2.16187700
C	-2.96454200	-2.66747500	0.28585400	H	4.49577500	-1.01068300	-0.91202700
H	-2.34172500	-3.38680400	0.82413100	H	3.17715100	2.78108700	-2.44840700
C	-3.48636600	-2.62795900	-2.14700900	H	5.32806600	3.05276500	-3.62269700
H	-2.88713700	-3.25409000	-2.81302100	H	7.08909200	1.30018500	-3.43799000
H	-4.38728600	-2.32942700	-2.68563200	H	6.64549800	-0.73738400	-2.07390200
H	1.04876800	-1.53248000	-1.16099900	C	2.38531300	0.69419300	-0.89420500
H	1.45213400	-0.37542800	0.60743900	C	0.08430400	-3.12277200	-2.05355100
C	4.23516900	2.37789100	0.97421200	C	0.49817600	-2.88293400	-3.50929900

C	0.98916500	-4.17370900	-1.38892500	C	-2.30831900	2.06670200	3.26452000
H	-0.94242600	-3.49771500	-2.03442800	C	-3.28547500	1.23729800	4.11833200
C	0.53285800	-4.19011700	-4.31142300	H	-4.20868200	1.02463400	3.57559700
H	1.49453300	-2.41667900	-3.51606200	H	-3.53440100	1.78518200	5.03495700
H	-0.18832800	-2.16117700	-3.96778900	H	-2.83104500	0.28251000	4.40927200
C	1.01494300	-5.48285900	-2.18898500	C	-1.01334300	2.29499900	4.04591300
H	2.00887500	-3.76411900	-1.32578800	H	-0.55947000	1.34348900	4.33134600
H	0.65207000	-4.35253400	-0.36055000	H	-1.22987400	2.86130500	4.95969800
C	1.43503200	-5.23615500	-3.64369900	H	-0.28049200	2.84713100	3.45902700
H	0.87021400	-3.99175000	-5.33602000	O	-0.83641200	1.04822000	1.64307500
H	-0.48788700	-4.59237900	-4.38940700	O	-2.63696700	1.64478900	-1.58708100
H	1.69065800	-6.20285900	-1.71083100	C	-0.82789200	5.62143800	-0.13705000
H	0.01208700	-5.93413100	-2.17324300	H	-0.27927200	6.16403200	-0.90211900
H	1.41169700	-6.17534400	-4.21036100	C	-1.87101900	4.76188600	-0.50741000
H	2.47533200	-4.88012300	-3.66269500	C	-2.23134600	4.52184000	-1.95586500
C	-0.90222700	-0.78497400	2.03232800	H	-2.08002400	5.43499100	-2.54350500
C	-0.95760100	-1.80203300	3.18490100	H	-3.29151700	4.26006300	-2.02335000
C	-0.25063800	0.52286100	2.51791200	C	-1.40536600	3.38904100	-2.64528600
H	-1.93057000	-0.55710000	1.72571100	C	0.04321900	3.82586900	-2.86448200
C	-1.67310300	-1.23139500	4.41541100	H	0.53721600	4.08875300	-1.92978200
H	0.06978900	-2.07756200	3.45219100	H	0.07214500	4.70028600	-3.52480300
H	-1.45205900	-2.71977400	2.84407900	H	0.62333500	3.02736400	-3.33343100
C	-0.96412900	1.10047100	3.74514700	C	-2.05024900	3.04854500	-4.00205100
H	0.79182300	0.31071600	2.78500200	H	-1.46998900	2.27824100	-4.52373900
H	-0.23158600	1.23985600	1.69123000	H	-2.07486700	3.94116900	-4.63792600
C	-1.02164800	0.07562700	4.88445100	H	-3.06993300	2.67579500	-3.87973900
H	-1.67117300	-1.97186700	5.22569400	C	-1.47912100	2.14648700	-1.75212600
H	-2.72806500	-1.03940700	4.16962800	O	-0.40564200	1.70462100	-1.23072400
H	-0.44981900	2.01129300	4.07771800	O	-3.06781700	0.99696700	1.27613300
H	-1.98431900	1.40242100	3.47288100	C	-2.98723900	3.42421600	2.89499900
H	-1.56611600	0.48682000	5.74435200	H	-3.99629100	3.20779100	2.53151200
H	0.00159500	-0.13764300	5.22643900	H	-3.08762000	3.99725600	3.82454600
C	-5.28936500	-3.26577200	-0.36656200	C	-2.24340600	4.23078000	1.85514000
H	-5.76068300	-2.40339600	-0.85029900	C	-1.20057700	5.10114500	2.19979100
H	-5.87479300	-4.15525000	-0.62289300	H	-0.94296500	5.24563300	3.24548100
C	-4.00517200	-2.05593600	1.25022000	C	-0.49846300	5.79011100	1.20901800
H	-3.62634500	-1.94591600	2.26910200	H	0.30727600	6.46401200	1.48795100
H	-4.29802200	-1.06436800	0.89146600	C	-2.56789500	4.08441600	0.50080200
C	-5.20175200	-3.00696200	1.14474800	H	-3.37513500	3.41502400	0.22271200
H	-4.99291500	-3.94092800	1.68485600	C	-5.56414800	0.66205000	-1.91673700
H	-6.12109600	-2.58258600	1.56243500	O	-5.84076200	1.88848400	-1.45168900
				O	-5.42913800	0.39196400	-3.09814300
				C	-5.98474900	2.91674500	-2.44883200
				H	-6.16161200	3.83451000	-1.88769500
<b>G-IMI</b>							
C	-2.04008100	1.30742100	1.96026800				

H	-6.83594300	2.69923000	-3.09941500	N	4.99968000	-1.65594000	2.51195300
H	-5.07571000	3.00076400	-3.04509400	N	6.34888700	-0.77633700	0.87198900
C	-6.28238800	-1.50897100	1.22819400	N	4.30927300	-1.95639300	0.30222900
C	-5.99140800	-0.30844100	0.55578100	C	5.26512600	-1.41084800	1.17834500
C	-6.20967800	0.90528700	1.22971700	C	3.80167300	-1.22299200	-0.85430900
C	-6.72219700	0.90880200	2.52602700	H	4.61254700	-0.80542100	-1.45929100
C	-7.00767500	-0.28644900	3.18736600	O	1.85625600	-0.26339000	0.25153800
C	-6.77938600	-1.49598200	2.52936500	C	2.88599300	-0.06907300	-0.41582400
H	-6.12074000	-2.46521000	0.74229900	N	3.31304800	1.14476200	-0.80394000
H	-5.97274000	1.83992300	0.74459600	H	4.22663300	1.18966000	-1.23521600
H	-6.88624000	1.86019300	3.02477600	C	4.06123200	-3.39889900	0.19769000
H	-7.40054800	-0.27604100	4.19981100	H	4.95751200	-3.94480000	0.51032900
H	-6.99564300	-2.43873900	3.02406900	C	3.04410000	-2.29018600	-1.66519700
C	-5.44726500	-0.34170400	-0.82885900	H	3.06811400	-2.06801500	-2.73586300
N	-5.24578700	-1.55856700	-1.34779100	H	1.99797600	-2.30949300	-1.35147900
N	-5.04651900	-2.58691600	-1.76615500	H	5.74754700	-1.30038400	3.10022000
Rh	-0.46550400	-0.02069000	-0.08471800	C	3.66648900	-1.55497100	3.11331300
Rh	-2.84899700	-0.06462700	-0.46825900	C	3.56284000	-2.52111700	4.29842800
C	2.72254200	2.41850400	-0.39274700	C	3.32356300	-0.12388000	3.54595800
C	3.12110200	3.50343000	-1.39167000	H	2.95286500	-1.85063700	2.34318600
C	3.13854200	4.84860400	-1.00021400	C	2.16827900	-2.47065000	4.93283700
C	3.40522700	3.19057100	-2.72710500	H	4.32075200	-2.24608500	5.04821100
C	3.42617000	5.85508500	-1.92212500	H	3.80322800	-3.53802800	3.96579800
H	2.91841100	5.11054700	0.02890900	C	1.92948700	-0.06012200	4.18071000
C	3.70360100	4.19627800	-3.64847700	H	4.08025100	0.22385300	4.26516300
H	3.37044200	2.15812900	-3.06081800	H	3.37016200	0.54145100	2.68102900
C	3.71349200	5.53347200	-3.25044700	C	1.79000700	-1.04328900	5.35026700
H	3.43125500	6.89246900	-1.59874600	H	2.11885500	-3.14872700	5.79439900
H	3.92091100	3.93130100	-4.67967200	H	1.43682000	-2.83768600	4.20069800
H	3.94280800	6.31723900	-3.96696800	H	1.72691300	0.96340200	4.51356600
C	3.11371400	2.77124200	1.03384400	H	1.18093800	-0.28779300	3.40982400
C	2.13206300	3.13716000	1.95650400	H	0.76481200	-1.02560800	5.74305900
C	4.45944300	2.77523800	1.42235000	H	2.44829000	-0.72388700	6.17226600
C	2.49290700	3.51710000	3.25249800	C	6.95950600	-0.90472400	-0.44037500
H	1.08818500	3.11676100	1.66033100	C	7.12330100	0.46962600	-1.11111300
C	4.81877800	3.14150400	2.71757600	C	8.34578200	-1.56072100	-0.27865000
H	5.22883300	2.47776200	0.71562300	H	6.38146000	-1.55694600	-1.11372900
C	3.83440200	3.51982800	3.63577000	C	7.85396200	0.37259400	-2.45608900
H	1.72419200	3.80184100	3.96476300	H	7.68385000	1.12000500	-0.42560000
H	5.86491300	3.12978300	3.01063500	H	6.14168900	0.93982600	-1.24842500
H	4.11272000	3.80815800	4.64576100	C	9.08382000	-1.67332800	-1.61876200
H	1.63724100	2.29451200	-0.43758400	H	8.93423100	-0.95566100	0.42496700
C	3.74614200	-3.61212900	-1.30097400	H	8.22715900	-2.55122000	0.17772000
H	4.67041400	-3.70664300	-1.88091400	C	9.22131600	-0.30516700	-2.29864200

H	7.96997900	1.37192200	-2.89432300	O	-2.48642700	-1.14246100	-2.17267100
H	7.24094300	-0.21040900	-3.15963300	C	-1.29251400	-1.41402500	-2.50748500
H	10.07237600	-2.12509600	-1.46714100	C	-1.08180900	-2.19605400	-3.80726700
H	8.52785600	-2.35173200	-2.28297900	C	-0.21556800	-1.33374300	-4.74591900
H	9.70922500	-0.41022900	-3.27601500	H	0.73914200	-1.07635400	-4.27804300
H	9.87135200	0.33700700	-1.68686800	H	-0.01337000	-1.88055100	-5.67406600
C	2.86435300	-4.87893300	-1.38417600	H	-0.73279400	-0.40298100	-5.00737400
H	1.94027100	-4.67367200	-1.93119700	C	-2.42382900	-2.51061300	-4.47879100
H	3.37289400	-5.69072600	-1.91388600	H	-2.96738600	-1.59241200	-4.72028600
C	2.82851700	-3.99780000	0.90463500	H	-2.24546700	-3.06133400	-5.41006300
H	1.99033100	-3.29610300	0.82796700	H	-3.06391700	-3.11842400	-3.83488400
H	2.99877700	-4.20188200	1.96509200				
C	2.55707200	-5.26954600	0.08672500				
H	3.24076200	-6.06450300	0.41045000	<b>G-TS1</b>			
H	1.53835500	-5.64686900	0.21308400	C	-2.07982200	1.79145500	1.43349100
O	-0.25215400	-1.08627100	-1.84915600	C	-2.37896800	2.93235000	2.41598000
C	-0.30673800	-3.50657800	-3.47405100	C	-2.95336400	2.28490500	3.69378800
H	0.69565200	-3.22793300	-3.13912300	H	-3.87005200	1.72825800	3.47882200
H	-0.19466100	-4.06194300	-4.41271000	H	-3.18373700	3.06116000	4.43264900
C	-0.96189700	-4.38210800	-2.42973000	H	-2.22589500	1.59814600	4.14338300
C	-1.84604400	-5.40793700	-2.78749900	C	-1.11791900	3.72861100	2.76170000
H	-2.04626000	-5.60171000	-3.83808900	H	-0.36401300	3.09282000	3.23043000
C	-2.45967800	-6.18696800	-1.80538600	H	-1.37511600	4.52721100	3.46775700
H	-3.13507400	-6.98798100	-2.09441500	H	-0.67104400	4.18301900	1.87707400
C	-0.70782400	-4.16448100	-1.06926300	O	-0.87596900	1.49860600	1.16406400
H	-0.01740900	-3.38084800	-0.78035000	O	-2.80395800	0.98264100	-1.97022400
O	-2.94080200	-1.79287600	0.62367300	C	-2.23528500	5.64579000	-1.94302000
O	-0.71789200	-1.74668900	1.02875100	H	-1.91222100	6.08805300	-2.88231600
C	-2.20376400	-5.94723900	-0.45425900	C	-2.80130800	4.36423300	-1.93859800
H	-2.68020600	-6.56117400	0.30576000	C	-2.92564400	3.55295700	-3.20886400
C	-1.32603000	-4.92555700	-0.06865000	H	-2.95781400	4.22100100	-4.07752600
C	-1.06390000	-4.61477800	1.38786400	H	-3.86231200	2.99136700	-3.19141300
H	-1.18552200	-5.52007600	1.99401900	C	-1.76558900	2.54082400	-3.45335600
H	-0.03215600	-4.27460400	1.51089600	C	-0.42793500	3.27022600	-3.61907700
C	-2.00431800	-3.52751700	1.99166500	H	-0.16361400	3.83028100	-2.71927000
C	-3.45644300	-4.01765300	2.03162000	H	-0.49313300	3.97466600	-4.45661000
H	-3.83734700	-4.23427800	1.03066000	H	0.38211600	2.56505000	-3.82710000
H	-3.51576000	-4.93359500	2.63141100	C	-2.07753100	1.72418400	-4.72470200
H	-4.10880500	-3.26699900	2.48659000	H	-1.28305000	0.99530800	-4.92390400
C	-1.52911200	-3.18949600	3.41724300	H	-2.15228600	2.39187200	-5.59076200
H	-2.17246000	-2.42609400	3.87050700	H	-3.02119400	1.18014800	-4.62205500
H	-1.56550500	-4.08463900	4.04873200	C	-1.70554100	1.54857400	-2.28576200
H	-0.50450200	-2.81106100	3.40786200	O	-0.58212900	1.34331100	-1.73319000
C	-1.87908900	-2.25623500	1.14707300	O	-3.10205000	1.18654600	0.97260800
				C	-3.46718600	3.86269700	1.79674100



H	-4.37707400	3.27296200	1.65084600	C	3.75446700	1.70510200	3.55459500
H	-3.68977400	4.63348600	2.54379800	C	1.61747500	0.72943500	5.05994000
C	-3.06506600	4.51412600	0.49183200	H	0.47750900	0.88981500	3.23335200
C	-2.49054500	5.79158700	0.46036300	C	3.93732200	1.38405900	4.90091500
H	-2.35780500	6.34422600	1.38684200	H	4.59458100	2.07064100	2.96993000
C	-2.09260600	6.35818300	-0.75115400	C	2.86720700	0.90180100	5.65934500
H	-1.66009100	7.35526900	-0.76514500	H	0.78422400	0.33668900	5.63652700
C	-3.23425100	3.82868800	-0.71827400	H	4.91562200	1.50881500	5.35692500
H	-3.70218700	2.85186300	-0.70999000	H	3.01039300	0.65260400	6.70717300
C	-5.49795800	-0.35789500	-1.88260100	H	1.34978900	1.39142800	1.18946200
O	-5.75444800	0.95297600	-2.03471700	C	4.07955200	-1.16515500	-3.26857800
O	-5.58186100	-1.17868600	-2.77731000	H	4.38845800	-1.12318200	-4.31730500
C	-6.10472700	1.36489300	-3.36966100	N	5.93006600	-2.07026900	0.72059700
H	-6.25536400	2.44242400	-3.30998800	N	7.04951000	-0.19690300	0.00235000
H	-7.02628600	0.87004200	-3.68790600	N	5.00633600	-0.93373700	-1.11126400
H	-5.30014200	1.12633400	-4.06757900	C	6.03860900	-0.98408500	-0.12894800
C	-5.41337600	-0.35728100	1.96246000	C	4.26855500	0.31601700	-1.30667600
C	-5.90039500	-0.24994200	0.64471700	H	4.91027500	1.19418200	-1.19431600
C	-7.22298600	0.19678500	0.44672900	O	2.13584300	-0.28701200	-0.29944700
C	-8.01697800	0.56048400	1.53043800	C	3.12812500	0.45369700	-0.28880200
C	-7.51810000	0.45320800	2.83156500	N	3.29632200	1.46677400	0.59031200
C	-6.21897200	-0.01596400	3.04432400	H	4.11345800	2.05450200	0.48442000
H	-4.40569700	-0.71456000	2.12087800	C	5.25489000	-1.63536400	-2.39064100
H	-7.62562200	0.27422800	-0.55662500	H	6.23466300	-1.35459700	-2.80421000
H	-9.02947300	0.91509200	1.36171100	C	3.73928200	0.24645000	-2.76016000
H	-8.14191300	0.73002600	3.67683000	H	4.25507900	1.00429100	-3.35788600
H	-5.83090700	-0.10745900	4.05462200	H	2.66708400	0.45303800	-2.80991000
C	-5.02191500	-0.60864100	-0.48763700	H	6.70470500	-2.09166900	1.37853500
Rh	-0.45450500	-0.02679000	-0.20306400	C	4.65584600	-2.50614600	1.30461400
Rh	-2.87871800	-0.34408300	-0.37920500	C	4.67076000	-4.02222400	1.53174500
C	2.24651500	1.91974100	1.50409900	C	4.35809600	-1.74768900	2.60544700
C	2.00518800	3.40394100	1.25306100	H	3.88053600	-2.26147200	0.57589700
C	2.39320200	4.40744500	2.14279900	C	3.37635700	-4.50520500	2.20083700
C	1.36463700	3.76117800	0.05669000	H	5.52978600	-4.27659600	2.17149500
C	2.14760200	5.75164000	1.84311300	H	4.82492200	-4.53244100	0.57373100
H	2.87388500	4.14580000	3.07967100	C	3.06706100	-2.23827800	3.27094200
C	1.12275000	5.09893100	-0.24306400	H	5.20322700	-1.88513100	3.29809900
H	1.02871500	2.98294000	-0.62283100	H	4.29233800	-0.67693600	2.39324600
C	1.51333500	6.10077500	0.65182800	C	3.11222200	-3.75221600	3.51039900
H	2.45062500	6.52235400	2.54690300	H	3.42861200	-5.58646800	2.38068800
H	0.60433800	5.35966600	-1.15939400	H	2.53417500	-4.34120800	1.51397900
H	1.31480800	7.14425900	0.42282100	H	2.90834000	-1.70120000	4.21191300
C	2.50212300	1.54463300	2.95046500	H	2.21541300	-1.99470300	2.62168100
C	1.43957600	1.04284600	3.71155300	H	2.17566100	-4.09686400	3.96481700

H	3.91413000	-3.98242300	4.22783100	H	-0.47671800	-4.72490900	3.36281600
C	7.40524600	0.77481100	-1.01705700	H	0.48922700	-3.56582500	2.44712500
C	7.33354700	2.19677700	-0.43240500	C	-1.51894400	-2.90500700	2.87685700
C	8.83395800	0.48861400	-1.51466400	C	-2.90260900	-3.49318500	3.17314700
H	6.74817000	0.72984600	-1.89849300	H	-3.31303400	-4.01834200	2.30729000
C	7.79102900	3.25418700	-1.44408500	H	-2.82739500	-4.20400600	4.00427700
H	7.97146500	2.23032400	0.46145600	H	-3.61213000	-2.71057900	3.46004600
H	6.31078800	2.40849800	-0.09194100	C	-0.99339600	-2.14315800	4.11050300
C	9.29945200	1.53704100	-2.53320600	H	-1.66824500	-1.32123400	4.37982100
H	9.50879300	0.48027100	-0.64752600	H	-0.92862200	-2.82251000	4.96820200
H	8.86941000	-0.51664300	-1.95285900	H	-0.00075700	-1.72664500	3.92237200
C	9.20604600	2.95649200	-1.95782000	C	-1.57319400	-1.91473600	1.70978900
H	7.75191000	4.25216500	-0.98962300	O	-2.52825700	-1.85460600	-1.70680900
H	7.09279100	3.26899800	-2.29417000	C	-1.33388400	-2.12281100	-2.05490900
H	10.32718700	1.32127200	-2.85163000	C	-1.15246800	-3.24198100	-3.08638000
H	8.67159200	1.47116400	-3.43425900	C	-0.55182800	-2.60959000	-4.35782000
H	9.50007600	3.69548300	-2.71408900	H	0.38846700	-2.09835800	-4.14317700
H	9.91780600	3.05416700	-1.12513600	H	-0.36291000	-3.38616500	-5.10825800
C	2.97099700	-2.24154200	-3.08360900	H	-1.24911200	-1.88254200	-4.79132700
H	2.07491800	-1.81409600	-2.62888400	C	-2.49843000	-3.89278100	-3.43003600
H	2.68444300	-2.64453000	-4.06102200	H	-3.18920400	-3.16022600	-3.85657200
C	5.09185000	-3.15279700	-2.28027300	H	-2.34192900	-4.68982600	-4.16675000
H	5.64479200	-3.57251400	-1.43592400	H	-2.97753800	-4.32737900	-2.54975700
H	5.48556800	-3.60701700	-3.19969400	N	-5.06639600	-2.38911300	-0.50283000
C	3.57068500	-3.35494700	-2.19092400	N	-4.69227100	-3.38763600	-0.19311100
H	3.26477700	-4.35873100	-2.50385900				
H	3.23603500	-3.22099500	-1.15926400				
O	-0.29332000	-1.53606400	-1.62520500	<b>TS3-R'</b>			
C	-0.15554200	-4.29004500	-2.50472100	C	-3.41343600	-0.68720300	1.61898500
H	0.80874200	-3.79849700	-2.36163300	C	-3.20102400	-0.22888800	3.06671400
H	-0.02080700	-5.06847600	-3.26499100	C	-2.77389400	-1.08065600	4.08897300
C	-0.60927600	-4.90749700	-1.20123800	C	-3.46232900	1.11469100	3.38048800
C	-1.36171200	-6.08938100	-1.17651400	C	-2.57847100	-0.59654900	5.38627700
H	-1.58185500	-6.60510200	-2.10778600	H	-2.58204600	-2.12624800	3.87923200
C	-1.82590300	-6.60832200	0.03305200	C	-3.27018300	1.59841400	4.67228300
H	-2.40162300	-7.53028000	0.04102900	H	-3.82414100	1.78259400	2.60483900
C	-0.31937400	-4.27487100	0.01465900	C	-2.81692100	0.74414600	5.68215800
H	0.27819600	-3.36998700	0.00942900	H	-2.23462800	-1.27430400	6.16308800
O	-2.70822100	-1.69552300	1.16952100	H	-3.47537700	2.64279500	4.89212400
O	-0.48177900	-1.37302700	1.36281800	H	-2.66123600	1.12058200	6.68943800
C	-1.55021400	-5.95027700	1.23259500	C	-3.12567600	-2.15448900	1.36526400
H	-1.91345100	-6.35904400	2.17212900	C	-4.18032500	-3.00077700	1.00698700
C	-0.79351400	-4.77146500	1.23642100	C	-1.84324000	-2.69948800	1.52645500
C	-0.49768500	-4.02722700	2.51748900	C	-3.97086500	-4.36944000	0.82395100
				H	-5.17672900	-2.58486400	0.87920600

C	-1.63660900	-4.06793100	1.35358700	C	-0.10892200	-2.35926900	-1.66926400
H	-1.01047300	-2.05536300	1.78953800	H	-1.64348100	-0.97931100	-2.22121700
C	-2.69733900	-4.90792600	1.00591900	C	-1.35971900	-2.82446900	-4.31051300
H	-4.80279500	-5.01108400	0.54654700	H	0.47119900	-1.66894500	-4.31352500
H	-0.64191800	-4.48124500	1.48808100	H	-0.97405500	-0.70107600	-4.59914400
H	-2.52885900	-5.97291700	0.87140300	C	-0.90220000	-3.63739400	-1.96530200
H	-4.46342700	-0.50914900	1.37603800	H	0.94495700	-2.53619000	-1.90377800
C	-3.13287400	2.81757800	-3.07471500	H	-0.16655000	-2.08798300	-0.61271600
H	-2.52426200	3.55841300	-3.60110300	C	-0.85349400	-3.99198300	-3.45568100
N	0.15168100	0.03390800	-2.26251700	H	-1.28761300	-3.06663600	-5.37820400
N	0.54321400	1.99107000	-1.14624400	H	-2.42505900	-2.65666700	-4.09584500
N	-1.68328800	1.40165700	-1.81054400	H	-0.50485300	-4.46402600	-1.36514400
C	-0.32047600	1.18577500	-1.72649700	H	-1.94637400	-3.50250700	-1.65268600
C	-2.43354200	2.13965000	-0.79378700	H	-1.44652800	-4.89377300	-3.65412300
H	-1.74810000	2.58816900	-0.07728900	H	0.18434900	-4.22348800	-3.73728400
O	-4.54981900	1.36592000	0.13286300	C	-4.48185800	2.57731100	-3.76439700
C	-3.33173500	1.18816100	0.03731400	H	-5.21710200	3.35691500	-3.53698000
N	-2.68346400	0.19192300	0.69122800	H	-4.34288200	2.56172400	-4.85360200
H	-1.66535400	0.13280300	0.68376800	C	-3.58321000	0.38359200	-3.22181900
C	-2.43170600	1.42770000	-3.07694300	H	-3.44157200	-0.17718900	-4.15189100
H	-1.71560600	1.32337400	-3.89248200	H	-3.57441200	-0.34151600	-2.40420300
C	-3.24453600	3.19513600	-1.57223400	C	-4.90042400	1.18541200	-3.26325300
H	-2.83442800	4.19186700	-1.39117600	H	-5.65886300	0.71585900	-3.89811500
H	-4.27935500	3.18945600	-1.22643500	H	-5.31415500	1.26463700	-2.25332500
H	1.16119400	-0.07078900	-2.17837000	H	1.48662200	1.43067000	-0.40373100
C	0.38902000	3.43523100	-1.00521800	C	1.92334000	-2.99145900	1.64529800
C	0.48596600	3.86823300	0.46825700	C	1.74185700	-3.35101000	2.97941000
C	1.48059500	4.13658300	-1.83597100	C	2.48860700	-2.72489900	3.98065200
H	-0.57971500	3.75479300	-1.40801200	C	3.42121300	-1.74404200	3.63846700
C	0.41973800	5.39251700	0.61820600	C	3.59784000	-1.37957200	2.30333200
H	1.43702500	3.50933100	0.87550600	C	2.84462600	-1.99572600	1.29620000
H	-0.30389300	3.38983700	1.06045400	C	2.96928800	-1.53890000	-0.12402000
C	1.42229500	5.66164400	-1.68277300	C	3.41321400	-2.52673900	-1.15102800
H	2.45919500	3.76828900	-1.50352200	C	3.44134900	-2.16871500	-2.51197400
H	1.36992000	3.84768000	-2.88864200	C	3.83870700	-3.08080800	-3.48272900
C	1.51506900	6.07563000	-0.20943400	C	4.22502400	-4.37517400	-3.11725500
H	0.51444800	5.66385900	1.67701300	C	4.21987600	-4.73780400	-1.77136000
H	-0.56539700	5.75448100	0.28734000	C	3.81982300	-3.82206200	-0.79634700
H	2.23075400	6.12403000	-2.26277100	N	2.73194100	-0.33631900	-0.51380300
H	0.47777900	6.03641900	-2.10491800	H	1.33048200	-3.46195500	0.86809300
H	1.44311600	7.16639100	-0.11305400	H	1.01211500	-4.11291700	3.23904300
H	2.49826000	5.78200500	0.18535400	H	4.00923200	-1.25612000	4.41083700
C	-0.61573000	-1.18813200	-2.51788800	H	4.31141900	-0.60507600	2.04112200
C	-0.57866200	-1.53880500	-4.01340600	H	3.14121000	-1.16580800	-2.79293700

H	3.84647600	-2.78484800	-4.52826200
H	4.52771300	-5.73637000	-1.47373200
H	3.82707000	-4.11829100	0.24614500
H	4.53058700	-5.08971300	-3.87644800
H	2.34523900	-3.00197400	5.02143900
C	1.28648400	0.42602400	1.37259500
O	1.28094700	1.20968500	2.47711700
O	0.33924900	-0.33295500	1.13479700
C	0.11678200	1.11964700	3.31230900
H	-0.78212800	1.39585300	2.76039200
H	0.28877400	1.82690700	4.12488800
H	0.00338200	0.10909200	3.70901200
C	4.30349900	1.95017000	-0.50192700
C	3.47008700	1.68412200	0.60825400
C	3.73931600	2.39619200	1.79307800
C	4.76860300	3.33946400	1.85101600
C	5.56737000	3.60202000	0.73928100
C	5.32699300	2.89121900	-0.43977200
H	4.13094500	1.40722600	-1.42405600
H	3.14256000	2.21264900	2.67424600
H	4.94541200	3.86794100	2.78494400
H	6.36583500	4.33718000	0.79051300
H	5.93945000	3.07094000	-1.32012000
C	2.34332700	0.72016300	0.40281900