

*Supporting Information*

**DFT Study of Manganese Complex-Catalyzed Alcohol  
Cross-Coupling Reactions**

**Junjie Xiao, Lina Geng, Yanlong Kang, Yan Li\*, Zhiqiang Zhang**

*School of Chemical Engineering, University of Science and Technology Liaoning,  
Qianshan Road 185, Anshan 114051, China*

***Corresponding person: Yan Li***

***E-mail: yanli@ustl.edu.cn***

***Telephone: +86-412-5929627***

***Fax: +86-412-5929627***

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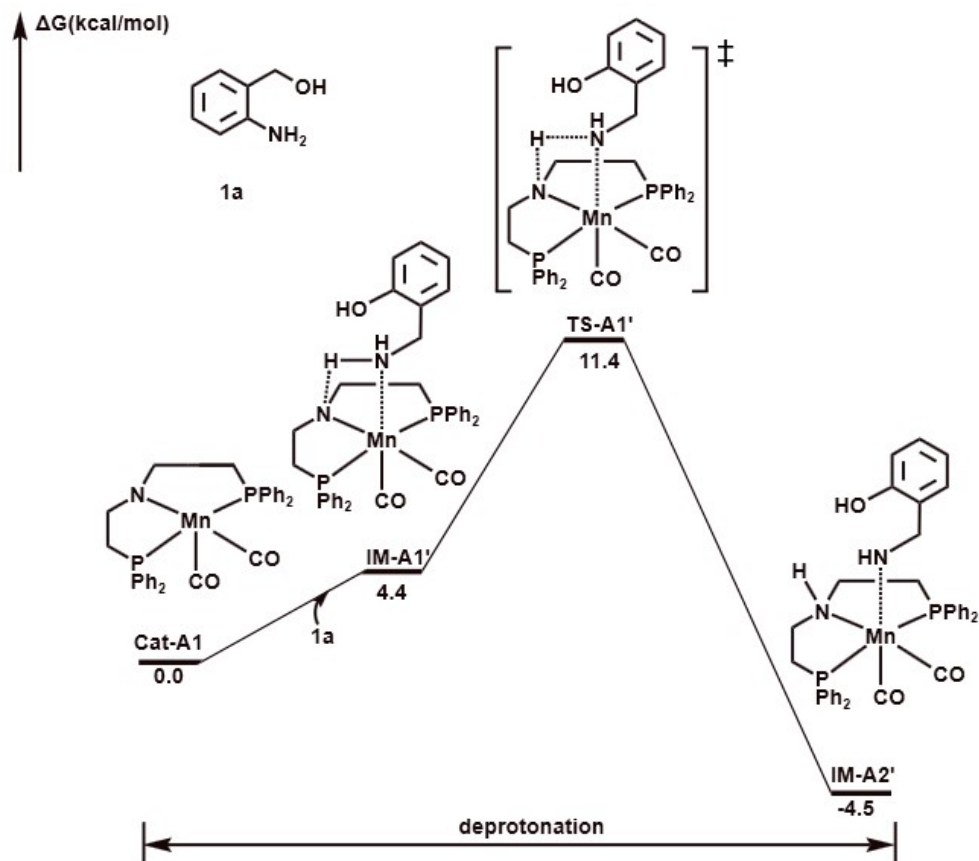
## 1. Test results of different functionals

**Table S1.** The relative Gibbs free energies (in kcal/mol) of rate-controlling step with different DFT functionals.

species	M06L	M06	B3LYP-D3(BJ)	M06-2X-D3	$\omega$ B97X-D
<b>2a</b>	0.0	0.0	0.0	0.0	0.0
<b>IM-C7</b>	-27.0	-24.7	-25.2	-27.7	-21.3
<b>TS-C7</b>	-3.0	-6.8	-8.6	-15.4	-10.4

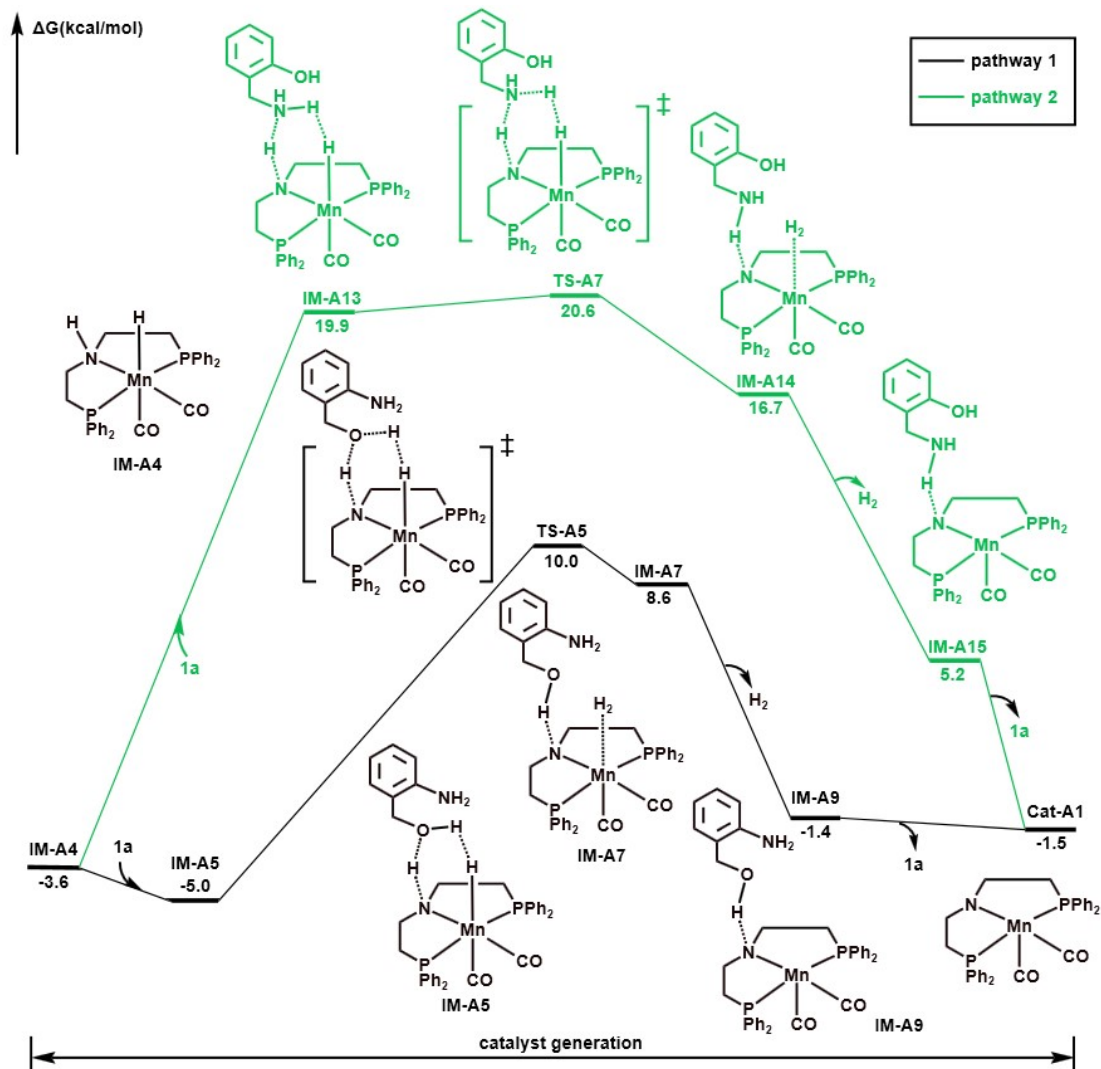
## 2. Free energy profiles of processes 1

**Fig. S1.** The Gibbs free energy profiles of the coordination of amines with manganese center in process 1, the relative energies are given in kcal/mol.



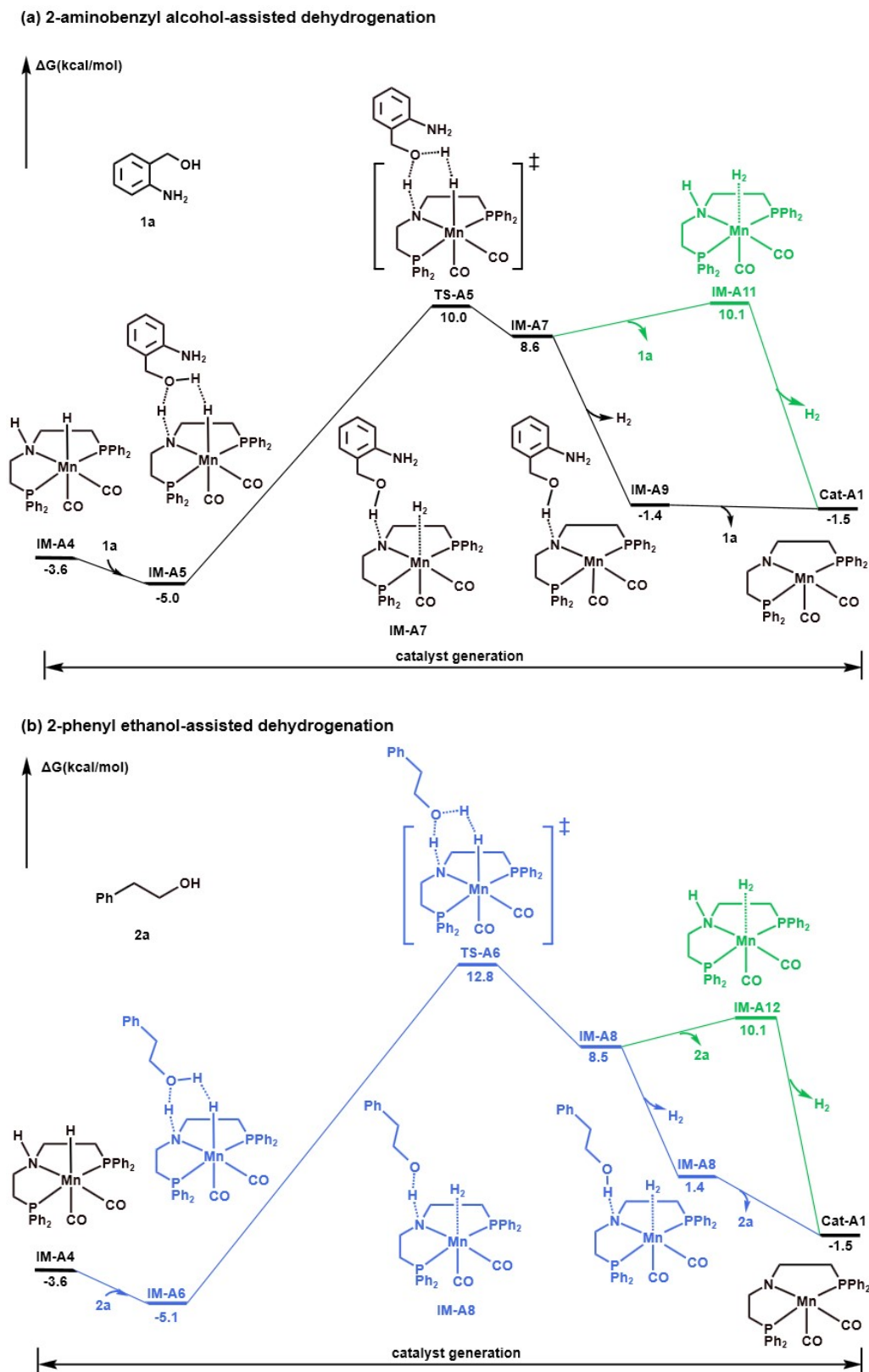
### 3. Possible reaction pathways of process 1

**Fig. S2.** The Gibbs free energy profiles of the coordination of amines and alcohol with manganese in processes 1, the relative energies are given in kcal/mol.



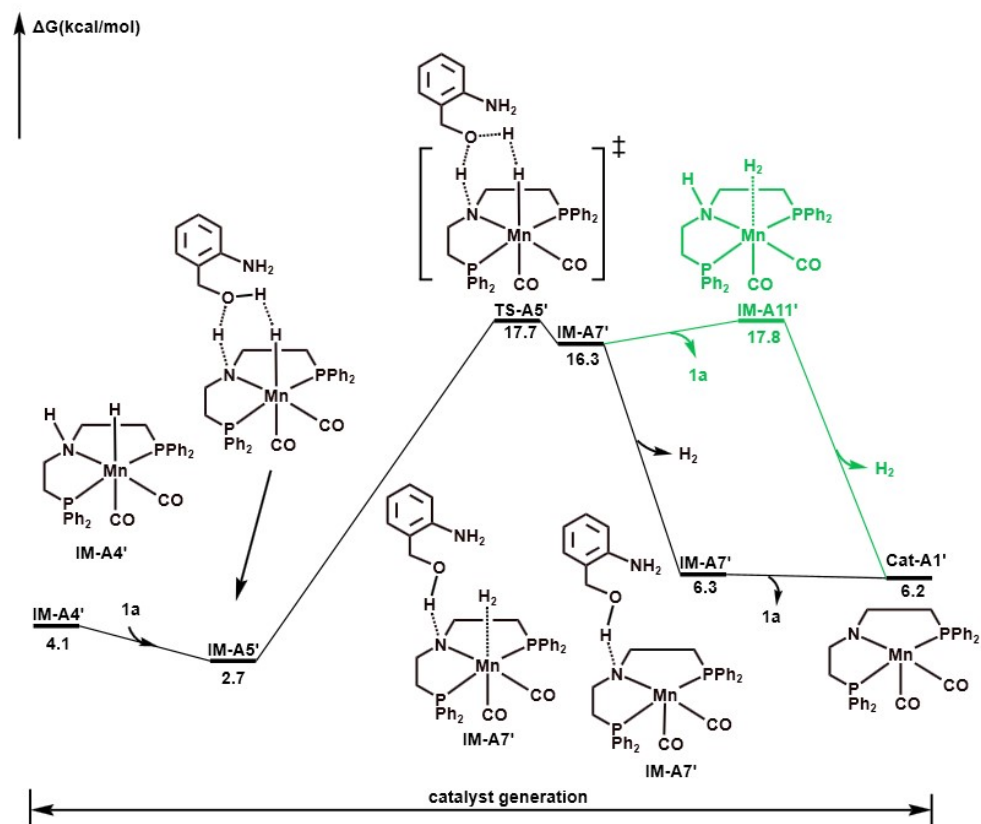
## 4. Hydrogen and alcohol release sequence in processes 1 and 2

**Fig. S3.** Possible pathways for catalyst regeneration in process 1, the relative energies are given in kcal/mol.

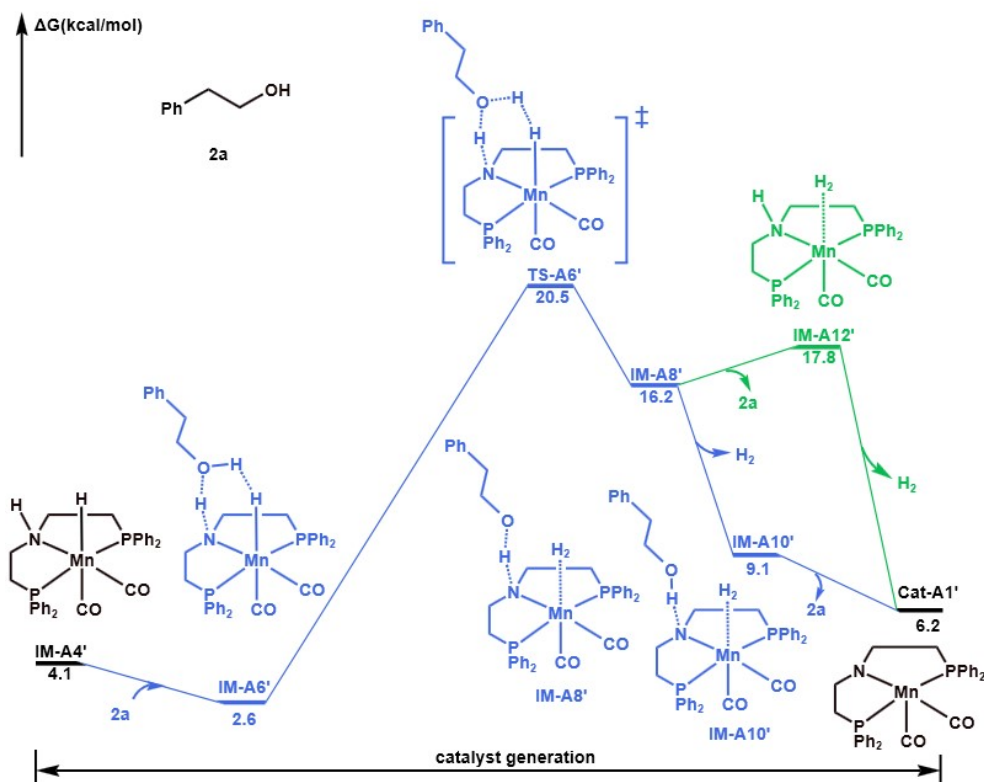


**Fig. S4** Possible pathways for catalyst regeneration in process 2, the relative energies are given in kcal/mol.

**(a) 2-aminobenzyl alcohol-assisted dehydrogenation**



**(b) 2-phenyl ethanol-assisted dehydrogenation**



## 5. Energies of all the structures

**Table S2.** Calculated thermodynamic corrections ( $G_{cor}$ , in a.u.), single-point energies ( $E$ , in a.u.), Gibbs free energies ( $G$ , in a.u.), and relative Gibbs energies ( $\Delta G$ , in kcal/mol) (Calculated at 298.15 K and 1 atm).

<i>species</i>	<i>G<sub>cor</sub></i>	<i>E</i>	<i>G</i>	$\Delta G$
<b>Cat-A1</b>	0.440757	-3199.211173	-3198.770416	0.0
<b>IM-A1</b>	0.582843	-3601.425489	-3600.842646	-0.6
<b>IM-A2</b>	0.583695	-3601.441869	-3600.858174	-10.3
<b>IM-A3</b>	0.586921	-3601.419258	-3600.832337	5.9
<b>IM-A4</b>	0.461656	-3200.408498	-3199.946842	-3.6
<b>IM-A5</b>	0.607427	-3602.627840	-3602.020413	-5.0
<b>IM-A6</b>	0.613881	-3586.569604	-3585.955723	-5.1
<b>IM-A7</b>	0.604048	-3602.602797	-3601.998749	8.6
<b>IM-A8</b>	0.609661	-3586.543735	-3585.934074	8.5
<b>IM-A9</b>	0.582190	-3601.423730	-3600.841540	-1.4
<b>IM-A10</b>	0.593991	-3585.366245	-3584.772254	1.4
<b>IM-A11/12</b>	0.455083	-3200.380148	-3199.925065	10.1
<b>TS-A1</b>	0.578299	-3601.423667	-3600.845368	-2.3
<b>TS-A2</b>	0.580780	-3601.402815	-3600.822035	12.0
<b>TS-A3</b>	0.454271	-3200.371954	-3199.917683	7.9
<b>TS-A4</b>	0.454271	-3200.371954	-3199.917683	14.7
<b>TS-A5</b>	0.599861	-3602.596465	-3601.996604	10.0
<b>TS-A6</b>	0.610663	-3586.538007	-3585.927344	12.8
<b>IM-B1</b>	0.594918	-3585.371399	-3584.776481	0.3
<b>IM-B2</b>	0.604380	-3585.383912	-3584.788039	-1.6
<b>IM-B3</b>	0.595398	-3585.361835	-3584.766437	6.6
<b>TS-B1</b>	0.592500	-3585.369299	-3584.776799	0.1
<b>TS-B2</b>	0.597073	-3585.347715	-3584.750642	16.5
<b>TS-B3</b>	0.590302	-3585.357465	-3584.767163	6.1
<b>1b</b>	0.095055	-400.995597	-400.900542	0.0
<b>IM-C1</b>	0.206377	-634.141931	-633.935554	-20.2
<b>IM-C2</b>	0.082207	-400.417778	-400.335571	-20.3
<b>IM-C3</b>	0.211101	-785.364580	-785.153479	-16.8
<b>IM-C4</b>	0.344159	-1019.102101	-1018.757942	-19.5
<b>IM-C5</b>	0.338912	-1019.089431	-1018.750519	-14.9
<b>IM-C6</b>	0.310704	-942.640764	-942.33006	-25.7
<b>IM-C7</b>	0.183803	-708.915775	-708.731972	-27.0
<b>IM-C8</b>	0.184568	-708.908833	-708.724265	-22.2
<b>IM-C9</b>	0.187738	-708.891624	-708.703886	-9.4
<b>IM-C10</b>	0.317953	-942.633310	-942.315357	-16.5
<b>IM-C11</b>	0.317694	-942.607285	-942.289591	-3.0

<b>IM-C12</b>	0.317786	-942.654023	-942.336237	-29.6
<b>IM-C13</b>	0.314275	-942.652261	-942.337986	-30.7
<b>3a</b>	0.179325	-633.052891	-632.873566	-15.7
<b>TS-C1</b>	0.206477	-634.141912	-633.935435	-20.2
<b>TS-C2</b>	0.209302	-785.361076	-785.151774	-15.7
<b>TS-C3</b>	0.338099	-1019.083013	-1018.744914	-11.3
<b>TS-C4</b>	0.332363	-1019.056257	-1018.723894	1.8
<b>TS-C5</b>	0.183503	-708.901677	-708.718174	-18.0
<b>TS-C6</b>	0.185538	-708.888474	-708.702936	-8.8
<b>TS-C7</b>	0.313529	-942.607561	-942.294032	-3.1
<b>TS-C8</b>	0.314799	-942.645843	-942.331044	-26.4
<b>1a</b>	0.119538	-402.190832	-402.071294	/
<b>2a</b>	0.128786	-386.135283	-386.006497	/
<b>2b</b>	0.10321	-384.92674	-384.82353	/
<b><sup>t</sup>BuOH</b>	0.107622	-233.707777	-233.600155	/
<b><sup>t</sup>BuO<sup>-</sup></b>	0.091839	-233.094603	-233.002764	/
<b>H<sub>2</sub></b>	-0.001581	-1.171556	-1.173137	/
<b>H<sub>2</sub>O</b>	0.00325	-76.44104	-76.43779	/

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## 6. Cartesian coordinates of all the structures

### Cat-A1

N	0.00634100	-0.99942300	-0.95527400
C	2.44918400	-1.00007300	-1.18599200
H	2.53727100	-0.35960400	-2.07324100
H	3.34536000	-1.62986300	-1.11459100
C	-2.34321100	-0.68031400	-1.56082200
C	0.20451300	2.25498400	-0.28488100
O	0.34755600	3.37097900	-0.62350600
P	-2.21644900	0.41823700	-0.09510100
P	2.20935500	0.10338500	0.26233800
C	2.68915900	-0.97053500	1.66797700
C	3.97215700	-0.96696600	2.22564600
C	1.72674400	-1.85210100	2.17932000
C	4.28718700	-1.82956400	3.27166900
H	4.72718500	-0.27815400	1.84746500
C	2.04793200	-2.72078300	3.21713200
H	0.71661100	-1.83597500	1.76244000
C	3.32792000	-2.70909800	3.76678600
H	5.28626100	-1.81083800	3.70455800
H	1.29187400	-3.40006800	3.60716800
H	3.57521700	-3.37961400	4.58821100
C	3.53603000	1.34439700	0.18088000
C	4.70826600	1.12791700	-0.55329600
C	3.38505300	2.54560600	0.88439100
C	5.70969600	2.09417600	-0.58435600
H	4.84324900	0.19562700	-1.10202800
C	4.38897800	3.50806000	0.85538300
H	2.47148300	2.72578100	1.45138600
C	5.55102100	3.28464800	0.12043100
H	6.61604100	1.91586700	-1.16070200
H	4.25865500	4.44020700	1.40202900
H	6.33266300	4.04194400	0.09282600
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C	-3.16306000	0.13945000	2.51138200
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C	-3.78010800	-0.51324700	3.57218100
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C	-4.21795000	-2.40986100	2.15490700
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H	-3.84360200	-0.02277500	4.54180400
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H	-4.78661800	-2.30402300	4.23012300
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H	-6.33346500	3.24686000	0.17394900
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H	-3.32197700	-1.16377000	-1.67532600
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H	-0.99213000	-2.10474000	-2.45404800
H	-1.46925700	-2.51520000	-0.80940500
Mn	0.02216800	0.56283200	0.13926300
C	-0.04371500	1.00443100	1.83981100
O	-0.05872200	1.26165000	2.98680300
<b>1a</b>			
O	2.40259500	0.79940700	0.79653300
C	0.25043500	0.00515200	-0.06228800
C	-0.43354500	1.24056400	-0.12832400
C	-0.48089900	-1.17051100	0.09002600
C	-1.83278600	1.24447700	-0.05031900
C	-1.87128500	-1.16292400	0.16558600
H	0.06305800	-2.11532600	0.14327000
C	-2.53977000	0.05650600	0.09016700
H	-2.36496500	2.19463200	-0.10708700
H	-2.42289500	-2.09318500	0.28171500
H	-3.62675500	0.08822400	0.14937700
C	1.74283900	-0.01580900	-0.17943200
H	2.06832100	0.40707100	-1.13936800
H	2.11390300	-1.05285100	-0.13522300
H	2.07426300	0.51188700	1.66104100
N	0.28772100	2.40858600	-0.33225300
H	-0.21637900	3.25824200	-0.11810800
H	1.21286100	2.39055500	0.08527600
<b>IM-A1</b>			
N	0.06526200	-1.27467200	-1.21929100

C	2.48406900	-1.42306700	-1.24209200
H	2.56110100	-0.81017400	-2.15272000
H	3.36942000	-2.07081900	-1.20726100
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C	0.22366400	1.57800400	1.36416600
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P	-2.10266600	0.24154400	-0.09407200
P	2.35815600	-0.24865400	0.16688400
C	3.00656800	-1.13308100	1.62766400
C	3.05097100	-0.43588300	2.84226100
C	3.36214000	-2.48400300	1.60892000
C	3.46096900	-1.07201100	4.00693300
H	2.74060600	0.60996400	2.87481500
C	3.76343200	-3.12298200	2.78037400
H	3.31725800	-3.05448800	0.68227300
C	3.81730700	-2.41961900	3.97864100
H	3.49049800	-0.51737200	4.94311700
H	4.03211100	-4.17759500	2.75312100
H	4.12852000	-2.92162800	4.89309300
C	3.65534600	1.00597500	-0.14443600
C	4.77338800	0.72402800	-0.93863000
C	3.52492100	2.28321900	0.41525600
C	5.73616000	1.70107900	-1.17481800
H	4.89354800	-0.26630300	-1.37725700
C	4.49550700	3.25446100	0.18886000
H	2.64713800	2.52241700	1.01550700
C	5.59970900	2.96702800	-0.60992700
H	6.59805900	1.47099400	-1.79897200
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H	6.35331000	3.73045000	-0.79469700
C	-3.21079100	-0.26727000	1.26033500
C	-3.44944900	0.64803800	2.29388700
C	-3.73931500	-1.55740500	1.36105100
C	-4.21804900	0.28579200	3.39325500
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C	-4.50661000	-1.91924200	2.46610800
H	-3.54368000	-2.29404800	0.58210700
C	-4.75028000	-0.99946200	3.48094900
H	-4.39835000	1.00847400	4.18706100
H	-4.91138900	-2.92766100	2.53363800
H	-5.34885100	-1.28478400	4.34404300
C	-2.90146400	1.76024000	-0.73227200
C	-2.28715400	3.00276500	-0.54243500
C	-4.11615400	1.70233200	-1.42815100

C	-2.87430000	4.16437300	-1.03851000
H	-1.33507500	3.05104800	-0.01543100
C	-4.69817800	2.86240400	-1.92996700
H	-4.61109800	0.74151800	-1.57536900
C	-4.07718100	4.09566300	-1.73542000
H	-2.38301900	5.12416700	-0.89003800
H	-5.64149600	2.80508400	-2.47112200
H	-4.53160900	5.00293700	-2.12990600
H	-3.32143300	-1.46480500	-1.44187900
H	-2.24394100	-0.42596800	-2.39155700
C	1.17765900	-2.20238800	-1.26592300
H	1.15804600	-2.92073700	-0.41715900
H	1.13134000	-2.82013000	-2.18319100
C	-1.19063300	-1.98887600	-1.34759500
H	-1.18133300	-2.63156900	-2.24896700
H	-1.36760700	-2.67613800	-0.49144900
Mn	0.13302200	0.19756600	0.26266600
C	-0.06140400	-0.94836500	1.56800800
O	-0.20816100	-1.76230900	2.39735400
O	0.10610400	1.22618000	-1.69721100
C	1.05179500	1.91020000	-3.82031100
C	-0.13492100	2.18763400	-4.53731900
C	2.18650000	1.49018500	-4.51184600
C	-0.12908500	2.04273100	-5.93171900
C	2.18724200	1.34924700	-5.89690200
H	3.09273900	1.28260600	-3.93823600
C	1.01829400	1.63269300	-6.59958900
H	-1.03900900	2.26195800	-6.49127500
H	3.08451400	1.02550000	-6.41949900
H	0.99342900	1.52743200	-7.68335400
C	1.07824500	2.07243700	-2.33584900
H	0.80684600	3.09392000	-2.02926800
H	2.08453700	1.86699100	-1.94380600
H	0.18905800	0.25793600	-2.00828100
N	-1.24908400	2.66251100	-3.86413900
H	-2.11706100	2.62146100	-4.38059700
H	-1.35447100	2.32339800	-2.91369800
<b>TS-A1</b>			
N	0.07247600	-1.20396100	-1.22220400
C	2.49598700	-1.31103700	-1.24596900
H	2.57330000	-0.66326500	-2.13236400
H	3.38625400	-1.95240900	-1.23351400
C	-2.32386400	-0.90106700	-1.45850000
C	0.19952100	1.59917000	1.43511100

O	0.24212900	2.48513300	2.20801500
P	-2.10398100	0.28485300	-0.05746100
P	2.36204100	-0.18869500	0.20782400
C	3.02339700	-1.12089500	1.63253500
C	3.08028100	-0.46300500	2.86851800
C	3.37518000	-2.47152500	1.56860900
C	3.49431400	-1.13789500	4.00956800
H	2.77814700	0.58357200	2.93689500
C	3.78118400	-3.14933200	2.71628400
H	3.32439500	-3.01239400	0.62449500
C	3.84414200	-2.48551400	3.93638500
H	3.53311700	-0.61341300	4.96267000
H	4.04634500	-4.20339300	2.65329100
H	4.15770900	-3.01803100	4.83245700
C	3.65314600	1.08009700	-0.06937700
C	4.80225300	0.79751400	-0.81782800
C	3.49113900	2.36184900	0.46984300
C	5.76554800	1.77913600	-1.02939500
H	4.94606200	-0.19677100	-1.24060000
C	4.46260800	3.33827000	0.26821400
H	2.59010600	2.59956200	1.03521200
C	5.59817700	3.05036700	-0.48462400
H	6.65143300	1.54922500	-1.61897100
H	4.32505000	4.33130800	0.69223700
H	6.35232500	3.81765900	-0.65002600
C	-3.23106600	-0.27034200	1.26142600
C	-3.50866300	0.61920000	2.30796000
C	-3.73204800	-1.57365200	1.32888400
C	-4.28725500	0.21843300	3.38670300
H	-3.10610900	1.63290200	2.27575400
C	-4.50959400	-1.97406700	2.41311500
H	-3.50794500	-2.29103600	0.53954700
C	-4.79091200	-1.07993200	3.44113200
H	-4.49785600	0.92131600	4.19077100
H	-4.89259000	-2.99238300	2.45407300
H	-5.39717500	-1.39520300	4.28832000
C	-2.88814200	1.82383000	-0.65866100
C	-2.20395500	3.03886600	-0.55112300
C	-4.15877600	1.80669400	-1.24944100
C	-2.77540700	4.21472500	-1.03093600
H	-1.20974100	3.05151600	-0.10729200
C	-4.72544700	2.98109500	-1.73459900
H	-4.70892300	0.86763300	-1.32450200
C	-4.03280700	4.18676200	-1.62667600

H	-2.22987400	5.15302100	-0.94945000
H	-5.71212100	2.95673400	-2.19479500
H	-4.47577100	5.10494600	-2.00864000
H	-3.31211900	-1.37817800	-1.46526900
H	-2.23765900	-0.30569200	-2.37819900
C	1.20315000	-2.10932200	-1.31199300
H	1.17914500	-2.85642300	-0.49263700
H	1.16783800	-2.68561400	-2.25518100
C	-1.18611200	-1.90888500	-1.39470700
H	-1.17010600	-2.51133600	-2.32220300
H	-1.35512500	-2.62696200	-0.56643700
Mn	0.12913500	0.23395100	0.31614500
C	-0.06024000	-0.92894000	1.61166700
O	-0.20472600	-1.75296900	2.43151800
O	0.09201000	1.17968700	-1.64486500
C	1.03383100	1.73957900	-3.79384600
C	-0.16055800	1.97007600	-4.51457700
C	2.16600900	1.29783300	-4.47440500
C	-0.16602100	1.75208600	-5.89930700
C	2.15727300	1.08532600	-5.85117500
H	3.08044500	1.13180700	-3.89901200
C	0.97945100	1.31851200	-6.55652300
H	-1.08310000	1.93417700	-6.46093700
H	3.05407500	0.74485900	-6.36427200
H	0.94582700	1.15611200	-7.63311900
C	1.06844700	1.97126600	-2.31496600
H	0.84112800	3.02228200	-2.06838300
H	2.07991000	1.76620800	-1.93028200
H	0.16140800	0.07432000	-1.85312000
N	-1.27277800	2.47281000	-3.85648800
H	-2.14591600	2.39076100	-4.35936000
H	-1.35636300	2.18681400	-2.88582400

### IM-A2

N	-0.28964300	-1.46169100	-1.08401300
C	2.11841700	-1.51449600	-1.35611800
H	2.07921400	-0.90789800	-2.27311500
H	3.01499700	-2.14426000	-1.39847700
C	-2.68792700	-1.11397100	-1.12488500
C	0.11488900	1.57548800	1.34959600
O	0.25491500	2.56213200	1.97022700
P	-2.34721700	0.24263600	0.11096200
P	2.16007800	-0.30962700	0.05731300
C	3.13251400	-1.21039400	1.33127900
C	4.38023700	-0.76249100	1.78321100

C	2.61065400	-2.39137300	1.87784500
C	5.08426600	-1.47807100	2.74851300
H	4.81031500	0.15225000	1.37970600
C	3.32069400	-3.11163600	2.83186200
H	1.62696000	-2.74343600	1.57475400
C	4.56068800	-2.65578800	3.27242900
H	6.05020600	-1.10964900	3.08989400
H	2.89473200	-4.02546600	3.24212000
H	5.11274500	-3.21349100	4.02679500
C	3.36993400	0.93931700	-0.50225100
C	4.34227000	0.64922600	-1.46641300
C	3.37729100	2.19972600	0.10843800
C	5.29442200	1.60085200	-1.82093000
H	4.36277500	-0.32718100	-1.94804600
C	4.33372400	3.14900500	-0.24216300
H	2.62527800	2.44003800	0.85981200
C	5.29198300	2.85206500	-1.20906600
H	6.03796400	1.36411500	-2.58007100
H	4.32375500	4.12610700	0.23689900
H	6.03478000	3.59724900	-1.48796400
C	-3.52067800	-0.13488500	1.46257300
C	-4.39154500	0.83151300	1.97856300
C	-3.51433600	-1.41260100	2.03788500
C	-5.24157400	0.52246600	3.03725300
H	-4.41021000	1.83097700	1.54604000
C	-4.36930700	-1.72189400	3.08949800
H	-2.82180600	-2.17050600	1.67220600
C	-5.23593000	-0.75384800	3.59240300
H	-5.91392800	1.28486600	3.42693900
H	-4.35147300	-2.71993000	3.52357000
H	-5.90170700	-0.99374300	4.41945100
C	-3.09145500	1.70557900	-0.68181600
C	-2.55694000	2.97300200	-0.43010800
C	-4.22231200	1.59599400	-1.50288400
C	-3.13050400	4.10609800	-1.00134200
H	-1.68154600	3.06890500	0.20979700
C	-4.78811400	2.72794100	-2.08009800
H	-4.66958600	0.61890200	-1.68794500
C	-4.24039700	3.98502800	-1.83198100
H	-2.69760600	5.08511700	-0.80511200
H	-5.66123200	2.62909500	-2.72296500
H	-4.68003900	4.87016800	-2.28784400
H	-3.67348000	-1.56953500	-0.97284400
H	-2.68946600	-0.64290800	-2.11830000

C	0.86052700	-2.35463600	-1.25284900
H	0.89815300	-3.03358400	-0.38955600
H	0.73738900	-2.98476800	-2.15020100
C	-1.58213000	-2.15070800	-1.06633000
H	-1.66609300	-2.85694800	-1.91038500
H	-1.63316300	-2.74596400	-0.14296400
Mn	-0.07972900	0.12435500	0.37763400
C	-0.21849300	-0.88675200	1.81056400
O	-0.35484900	-1.55956500	2.76555400
O	-0.12408600	1.04105800	-1.46034900
C	0.85768000	2.27353500	-3.23998300
C	-0.07568500	1.98280700	-4.26012900
C	2.18292100	2.51356700	-3.58512300
C	0.35954100	1.93603700	-5.59065900
C	2.61717300	2.46713100	-4.91030400
H	2.88804000	2.74711400	-2.78555400
C	1.69336900	2.17508100	-5.90989200
H	-0.36127500	1.71767100	-6.38021200
H	3.66110300	2.65742100	-5.15481900
H	2.00814900	2.13015900	-6.95206000
C	0.39130600	2.29090800	-1.80948000
H	-0.38117900	3.08347200	-1.69423300
H	1.23180700	2.59548300	-1.16055500
H	-0.27430900	-0.76392600	-1.84586900
N	-1.41568300	1.82503800	-3.92219500
H	-1.97710600	1.34421000	-4.61193000
H	-1.54644100	1.46037800	-2.98170700

### TS-A2

N	-0.55316900	-1.64518700	-1.28757200
C	1.83411700	-2.08530600	-1.54583400
H	1.89015600	-1.67685200	-2.56068800
H	2.63146700	-2.82787800	-1.42008400
C	-2.88628700	-0.98073800	-1.33731400
C	0.27619200	1.28279800	1.16789400
O	0.54234600	2.14041200	1.92192300
P	-2.40393600	0.22452400	-0.02193800
P	2.03197000	-0.64090400	-0.41409500
C	2.99079600	-1.28724200	1.00693400
C	3.69986400	-0.39189700	1.81811900
C	2.94252600	-2.63535900	1.37866200
C	4.35568600	-0.83718700	2.96056700
H	3.74510700	0.66323300	1.54609400
C	3.59953600	-3.08103100	2.52221000
H	2.38045000	-3.35073300	0.77815500

C	4.30909600	-2.18385300	3.31501800
H	4.90761900	-0.12859600	3.57563400
H	3.55316700	-4.13401800	2.79467400
H	4.82236400	-2.53237600	4.20935800
C	3.20271600	0.49188700	-1.21749100
C	4.14396200	0.02475800	-2.14157300
C	3.18538100	1.85049800	-0.88800000
C	5.03721300	0.90845700	-2.73951700
H	4.18003000	-1.03343200	-2.39993400
C	4.08536000	2.73072100	-1.48008600
H	2.44153100	2.23086000	-0.18810500
C	5.00662200	2.26250400	-2.41215000
H	5.76047200	0.53641500	-3.46374700
H	4.03323700	3.79087800	-1.24111000
H	5.69665900	2.95555500	-2.89060800
C	-3.39951700	-0.20274300	1.44999400
C	-4.68906000	-0.73971900	1.36095700
C	-2.86776300	0.07904200	2.71387600
C	-5.42202800	-1.00894200	2.51225400
H	-5.13524300	-0.94258100	0.38756400
C	-3.60565800	-0.18125600	3.86436500
H	-1.86614400	0.50179700	2.79195700
C	-4.88060200	-0.73165500	3.76562200
H	-6.42119300	-1.43306200	2.42987900
H	-3.17797300	0.03959200	4.84021100
H	-5.45468900	-0.94401000	4.66563300
C	-3.12787200	1.80480100	-0.57845100
C	-2.54669900	2.99829600	-0.13589400
C	-4.23192100	1.86085000	-1.43669600
C	-3.05267500	4.22513800	-0.55299300
H	-1.68258400	2.96252900	0.52845600
C	-4.73589300	3.08915000	-1.85367400
H	-4.70075600	0.94214900	-1.78940200
C	-4.14466500	4.27191900	-1.41575700
H	-2.58047800	5.14587300	-0.21557100
H	-5.58949800	3.12200000	-2.52829700
H	-4.53271700	5.23133400	-1.75231700
H	-3.92861300	-1.31600300	-1.27971300
H	-2.76236400	-0.45739200	-2.29638000
C	0.46343600	-2.70365700	-1.31546700
H	0.42321600	-3.24704900	-0.35869100
H	0.23442500	-3.43377800	-2.11049200
C	-1.92440600	-2.15367900	-1.26783600
H	-2.09697300	-2.84832800	-2.10699600

H	-2.07472900	-2.72514100	-0.33805300
Mn	-0.12317700	-0.05294500	0.08197300
C	-0.20618700	-1.15545000	1.41959900
O	-0.26237000	-1.94112600	2.28808000
O	0.53925000	0.29817000	-2.59297000
C	0.71739200	2.74368700	-2.68736700
C	1.47458200	2.78869900	-3.88031600
C	0.70496700	3.86318700	-1.85869200
C	2.18876000	3.95884100	-4.18456000
C	1.40753200	5.02682400	-2.16644800
H	0.14200100	3.80321900	-0.92304400
C	2.15394500	5.06347300	-3.34322700
H	2.78056200	3.98694100	-5.10113700
H	1.37964700	5.88440300	-1.49652300
H	2.72118100	5.95599300	-3.60663600
C	-0.06808000	1.49818800	-2.31617100
H	-1.08784800	1.58031900	-2.78061400
H	-0.28920900	1.64423600	-1.21253700
H	-0.35868500	-0.98704000	-2.10054300
N	1.46094500	1.70693100	-4.74754200
H	2.28481400	1.64161100	-5.33143000
H	1.24778100	0.84310600	-4.23835900

**IM-A3**

N	-0.40692100	-1.08122600	-1.18925900
C	1.98865600	-0.96687600	-1.60459100
H	1.86745600	-0.19406300	-2.37902500
H	2.90484400	-1.52684400	-1.82898400
C	-2.82142100	-0.93602100	-1.00983800
C	0.02494400	1.55553100	1.58948800
O	0.12211400	2.45316700	2.33752400
P	-2.44960700	0.33973500	0.28463600
P	2.06071000	-0.13675400	0.04560200
C	3.07556900	-1.31430500	1.02636200
C	4.41811000	-1.06191400	1.33833000
C	2.51393400	-2.53426100	1.42732600
C	5.17280300	-2.00349100	2.03224400
H	4.88014100	-0.12328300	1.03820600
C	3.27215300	-3.47634500	2.11431000
H	1.46841000	-2.74648900	1.21724100
C	4.60419900	-3.21235000	2.42184200
H	6.21314800	-1.78708700	2.26936800
H	2.81409200	-4.41506900	2.42083300
H	5.19534400	-3.94531700	2.96825300
C	3.18665300	1.27671800	-0.14624200

C	3.95840200	1.48193700	-1.29419600
C	3.34020500	2.14252500	0.94558900
C	4.87979900	2.52392800	-1.33888400
H	3.84429000	0.83416700	-2.16248200
C	4.26462700	3.17974600	0.89683700
H	2.74013100	1.99557300	1.84316000
C	5.04033800	3.36843000	-0.24458400
H	5.46439400	2.68281800	-2.24336400
H	4.37637900	3.84345900	1.75238100
H	5.76112600	4.18354600	-0.28695300
C	-3.40721200	-0.17246700	1.75972700
C	-4.69878900	-0.70133400	1.63727300
C	-2.89485000	0.06107600	3.04024900
C	-5.44526400	-1.01987900	2.76617500
H	-5.13896900	-0.84227400	0.65027200
C	-3.64571000	-0.24904300	4.17094200
H	-1.90282100	0.49487100	3.15424500
C	-4.91744300	-0.79773200	4.03663700
H	-6.44530000	-1.43526000	2.65375000
H	-3.23001200	-0.06439500	5.15960000
H	-5.50160100	-1.04685900	4.92071400
C	-3.41548800	1.80650800	-0.25409900
C	-4.12290200	2.56614300	0.68822400
C	-3.41897200	2.21544300	-1.59580400
C	-4.83987500	3.69166600	0.29497100
H	-4.12642500	2.27155500	1.73659600
C	-4.14437000	3.33954800	-1.98150000
H	-2.82324700	1.67563600	-2.33575100
C	-4.85977000	4.07730600	-1.04256000
H	-5.38929300	4.26524100	1.03964700
H	-4.14042300	3.64278800	-3.02711400
H	-5.42565600	4.95514800	-1.35002600
H	-3.75373300	-1.47541500	-0.80971700
H	-2.93594300	-0.40330500	-1.96104600
C	0.76848100	-1.86934200	-1.59945300
H	0.89127700	-2.70979100	-0.90154800
H	0.60141400	-2.30237800	-2.59958700
C	-1.63983700	-1.88307900	-1.10829200
H	-1.73812700	-2.52807900	-1.99727900
H	-1.57411500	-2.53900500	-0.22879200
Mn	-0.15265400	0.21550800	0.45344000
C	-0.28288500	-0.97827200	1.72646400
O	-0.37945800	-1.78366900	2.57598300
O	-0.81292400	1.00377500	-2.80347800

C	0.95283600	2.67071300	-2.45397200
C	1.66591200	2.36315200	-3.63354200
C	1.32543100	3.79738000	-1.71689900
C	2.68035300	3.23854100	-4.05817100
C	2.34364700	4.64595500	-2.12803600
H	0.77595100	4.01062300	-0.79603700
C	3.00894100	4.36674500	-3.32256900
H	3.21401500	3.00974900	-4.98236700
H	2.61229300	5.51618000	-1.53256800
H	3.79931100	5.02773200	-3.67799800
C	-0.26431000	1.89481900	-1.99381500
H	-0.98315700	2.62767500	-1.55763200
H	0.10532900	1.38518700	-0.95022000
H	-0.57155600	-0.36216700	-1.95067600
N	1.41107400	1.18772100	-4.33525500
H	1.62958800	1.24888700	-5.32225800
H	0.46019200	0.85860300	-4.14404100

**TS-A3**

N	-0.42075300	-1.11787400	-1.24988500
C	1.98385300	-1.03121100	-1.59339100
H	1.88758200	-0.28181600	-2.39382500
H	2.90035300	-1.60543600	-1.77683000
C	-2.83419200	-0.92544900	-1.07992600
C	-0.03724100	1.44351300	1.62702500
O	0.02382900	2.33115300	2.39422200
P	-2.42759000	0.29383800	0.25953800
P	2.02084900	-0.13291400	0.02952400
C	3.10008700	-1.22458600	1.05063900
C	4.39443100	-0.85651900	1.44132000
C	2.62314600	-2.48443300	1.43831500
C	5.18268400	-1.72130600	2.19612900
H	4.79693900	0.11399500	1.15860400
C	3.41610100	-3.35177400	2.18244400
H	1.61105700	-2.78582200	1.17864500
C	4.69917500	-2.97129400	2.56746500
H	6.18311600	-1.41132100	2.49439700
H	3.02102800	-4.32325900	2.47475400
H	5.31591500	-3.64459300	3.16039400
C	3.12768600	1.28851600	-0.24349300
C	3.99890900	1.35057100	-1.33540900
C	3.20438700	2.27994500	0.74443400
C	4.93937600	2.37160500	-1.42910800
H	3.95154100	0.59775400	-2.12157800
C	4.15188500	3.29434100	0.65196800

H	2.52604600	2.24823100	1.59655200
C	5.02436900	3.33940000	-0.43313200
H	5.60262800	2.41383500	-2.29193300
H	4.20554500	4.05433800	1.42976800
H	5.76424900	4.13509500	-0.50746800
C	-3.45656000	-0.22777500	1.68712400
C	-4.78586700	-0.63440200	1.51050500
C	-2.94674600	-0.14373900	2.98622300
C	-5.57398800	-0.97917900	2.60263400
H	-5.21872400	-0.66422700	0.50989000
C	-3.73898400	-0.47971400	4.08138900
H	-1.92261000	0.19177900	3.14110800
C	-5.04967700	-0.90549800	3.89181000
H	-6.60320700	-1.29926600	2.44761100
H	-3.32500000	-0.41040700	5.08557700
H	-5.66638500	-1.17499700	4.74743600
C	-3.31866700	1.82988500	-0.21071600
C	-3.73533600	2.69469400	0.81153400
C	-3.53094000	2.21126200	-1.54113100
C	-4.36681400	3.89637800	0.51201600
H	-3.57148700	2.41910500	1.85366000
C	-4.17247200	3.41185800	-1.83672400
H	-3.15141800	1.59616900	-2.35591600
C	-4.59615700	4.25503000	-0.81435500
H	-4.68527900	4.55256500	1.32031200
H	-4.33284200	3.69032000	-2.87721100
H	-5.09693100	5.19290900	-1.04914000
H	-3.77645500	-1.45269200	-0.89380300
H	-2.93711000	-0.37236500	-2.02051600
C	0.75893700	-1.92660100	-1.59533700
H	0.84793500	-2.73350800	-0.85448900
H	0.62300200	-2.40396600	-2.58055700
C	-1.67132100	-1.89494400	-1.20106100
H	-1.77757900	-2.51671400	-2.10593400
H	-1.61891600	-2.57086400	-0.33641700
Mn	-0.17635400	0.14847200	0.44530800
C	-0.30688000	-1.14566900	1.63866400
O	-0.40524700	-2.01167800	2.42805300
O	-0.91336700	1.05172700	-2.91625600
C	0.86552600	2.65289500	-2.56790200
C	1.62836600	2.29884800	-3.70661000
C	1.23624900	3.78056500	-1.82458700
C	2.69204100	3.13337100	-4.09009300
C	2.30349200	4.58134300	-2.19372800

H	0.64932400	4.01769400	-0.93435000
C	3.01922100	4.25715800	-3.34954700
H	3.26764700	2.87372600	-4.97957200
H	2.57893800	5.44743600	-1.59613500
H	3.85470200	4.88119900	-3.66600000
C	-0.39498300	1.96765900	-2.20433000
H	-1.07273700	2.62283000	-1.62035400
H	0.03579100	1.33282400	-0.77922800
H	-0.54218700	-0.41399500	-2.00088200
N	1.36441100	1.13295000	-4.40837100
H	1.65495400	1.15237500	-5.37745000
H	0.40897700	0.80677800	-4.26436700
<b>1b</b>			
O	2.47711300	0.92633400	0.05348800
C	0.25266500	0.04141500	0.05080300
C	-0.44605200	1.28007300	-0.05275200
C	-0.47517500	-1.15706800	0.13867000
C	-1.85551800	1.24972600	-0.04312700
C	-1.85593500	-1.17240900	0.13661900
H	0.08980200	-2.08767300	0.21545800
C	-2.53666900	0.05028300	0.04838700
H	-2.40353100	2.18877700	-0.11675800
H	-2.40553800	-2.10764600	0.20564300
H	-3.62581100	0.06246500	0.05098700
C	1.69880600	-0.02326600	0.09628700
H	2.10071800	-1.06232200	0.18875700
N	0.23284800	2.44764800	-0.18307500
H	-0.25649100	3.32232400	-0.08389600
H	1.24059500	2.42085500	-0.07129300
<b>IM-A4</b>			
N	-0.13210700	-1.11984700	-1.25139100
C	2.29160900	-1.36067100	-1.12353800
H	2.52215300	-0.73500200	-1.99697400
H	3.11899400	-2.07127200	-1.00573900
C	-2.51726500	-0.64104500	-1.38628400
C	0.01691600	1.22852300	1.87467200
O	0.06105300	2.06162000	2.70037500
P	-2.20975300	0.34807600	0.16370200
P	2.12431000	-0.22161500	0.35052600
C	3.08696900	-1.09250200	1.64481100
C	3.94283700	-0.40218500	2.51041900
C	2.89695500	-2.46571400	1.84380500
C	4.60668700	-1.07296300	3.53415100
H	4.09653300	0.66847000	2.37950300

C	3.56607800	-3.13716300	2.86107400
H	2.20615200	-3.01786000	1.20501600
C	4.42569400	-2.44194700	3.70868300
H	5.27011800	-0.52014500	4.19736200
H	3.40920700	-4.20593000	2.99697400
H	4.94675200	-2.96573500	4.50806000
C	3.25834000	1.15210500	-0.07399300
C	4.57611700	0.89832900	-0.47917200
C	2.81911900	2.47524100	0.01511900
C	5.42954500	1.94615700	-0.80601100
H	4.93953800	-0.12932600	-0.52735000
C	3.67908700	3.52562900	-0.29983600
H	1.79323600	2.66960600	0.32547100
C	4.98078200	3.26329500	-0.71551800
H	6.44900000	1.73642800	-1.12617900
H	3.32746300	4.55309800	-0.22206100
H	5.64994800	4.08486000	-0.96663400
C	-3.44497900	-0.30784500	1.34490700
C	-3.93394100	0.51530000	2.36726400
C	-3.82626500	-1.65378800	1.32787100
C	-4.79830800	0.00865100	3.33192500
H	-3.63804800	1.56416800	2.40267300
C	-4.69371800	-2.16019000	2.29091000
H	-3.43922400	-2.32237400	0.55780900
C	-5.18422300	-1.32926100	3.29425200
H	-5.17280000	0.66366300	4.11694900
H	-4.98345500	-3.20910100	2.25900200
H	-5.86215500	-1.72471700	4.04856100
C	-2.94199600	1.97890600	-0.23451200
C	-2.14935900	3.12925700	-0.21118400
C	-4.30098500	2.09302300	-0.55948700
C	-2.70372700	4.37137300	-0.51386700
H	-1.09417900	3.03578500	0.04322800
C	-4.85056600	3.33134900	-0.87077300
H	-4.93333800	1.20406700	-0.55278500
C	-4.05086100	4.47367400	-0.84689800
H	-2.07922000	5.26267600	-0.48657900
H	-5.90616800	3.40803400	-1.12695100
H	-4.48286400	5.44497900	-1.08332000
H	-3.52834600	-1.06600800	-1.42575800
H	-2.42724200	0.05407400	-2.23271600
C	0.97469000	-2.08500900	-1.33114400
H	0.80230800	-2.82452700	-0.53686900
H	0.96209800	-2.62507200	-2.29379400

C	-1.45485900	-1.72153500	-1.48483800
H	-1.49045700	-2.23307400	-2.46206200
H	-1.59334800	-2.48639000	-0.70729500
Mn	-0.06047300	0.05277700	0.57049200
C	-0.30960300	-1.36306700	1.62251900
O	-0.48730200	-2.30742000	2.29801800
H	0.15182800	1.29203000	-0.47416900
H	0.01796900	-0.39785300	-1.95590700
<b>TS-A4</b>			
N	-0.14860400	-1.07708600	-1.26123300
C	2.26447700	-1.33368700	-1.18916100
H	2.44763100	-0.69137500	-2.06062500
H	3.10341900	-2.03735600	-1.11359300
C	-2.50878000	-0.56908500	-1.48070700
C	0.06679300	1.57306000	1.56421400
O	0.12619900	2.47039900	2.31661700
P	-2.25482000	0.39073700	0.07426200
P	2.15178500	-0.20242300	0.27206400
C	2.95331900	-1.09679900	1.64416700
C	3.50319000	-0.37342800	2.71029900
C	2.94150400	-2.49367900	1.70934200
C	4.04705800	-1.03515500	3.80548400
H	3.50912500	0.71672400	2.67683700
C	3.48708500	-3.15440400	2.80622400
H	2.49326200	-3.07349300	0.90192700
C	4.04358600	-2.42747300	3.85454600
H	4.47634600	-0.46046900	4.62443600
H	3.47338900	-4.24237400	2.84176300
H	4.47062500	-2.94485400	4.71188400
C	3.37222600	1.10670200	-0.09753000
C	4.73017500	0.79023300	-0.24308100
C	2.96125900	2.43176500	-0.26335300
C	5.65443100	1.77895500	-0.55839500
H	5.06351500	-0.23822100	-0.09870200
C	3.88996000	3.42339000	-0.57427000
H	1.90667000	2.68027100	-0.14500300
C	5.23463500	3.09803100	-0.72404000
H	6.70650700	1.52210000	-0.67133500
H	3.56001000	4.45376700	-0.69522000
H	5.95986000	3.87364400	-0.96490100
C	-3.34098800	-0.37579800	1.32138800
C	-3.53114400	0.29197700	2.53920000
C	-3.88884500	-1.65130200	1.15799400
C	-4.26601100	-0.29818800	3.56011900

H	-3.09473800	1.28102700	2.68702300
C	-4.62107500	-2.24332000	2.18454300
H	-3.73700000	-2.19894800	0.22823600
C	-4.81307800	-1.56859600	3.38534300
H	-4.40690700	0.23255400	4.50017000
H	-5.03988800	-3.23821200	2.04297700
H	-5.38164200	-2.03373100	4.18857400
C	-3.06853400	1.99465700	-0.24497800
C	-2.28765600	3.12218900	-0.51939600
C	-4.46465200	2.11293400	-0.25211800
C	-2.89150000	4.34348100	-0.80701500
H	-1.20104400	3.03458600	-0.50012800
C	-5.06554900	3.33398600	-0.53725000
H	-5.07990800	1.24271700	-0.02091500
C	-4.27917300	4.45064400	-0.81649400
H	-2.27510800	5.21600700	-1.01604400
H	-6.15119000	3.41638400	-0.53886800
H	-4.75103500	5.40751000	-1.03405500
H	-3.52833700	-0.96197600	-1.58523800
H	-2.34252400	0.13882300	-2.30390800
C	0.92330200	-2.03541600	-1.33841100
H	0.81859800	-2.81401400	-0.54910400
H	0.89475700	-2.57740800	-2.30375600
C	-1.44412400	-1.65604000	-1.51371500
H	-1.46037300	-2.16560900	-2.49665800
H	-1.68661400	-2.43861400	-0.75938700
Mn	-0.04435400	0.23240400	0.41391300
C	-0.27027100	-0.98496000	1.67654900
O	-0.42727600	-1.82696000	2.47195900
H	0.17106400	1.23904500	-1.05267900
H	0.07216400	0.35572500	-1.39146900
<b>H<sub>2</sub></b>			
H	-3.30014700	0.35849100	0.00000000
H	-4.04324900	0.35849100	0.00000000
<b>IM-A5</b>			
N	0.16793600	-0.32942600	2.43486000
C	-2.26878900	-0.22379900	2.48660500
H	-2.31384100	0.73486900	3.01972400
H	-3.19178900	-0.77472500	2.70623100
C	2.59977300	-0.25141200	2.27990900
C	-0.00993200	0.37816400	-1.42363400
O	-0.08596900	0.71292700	-2.54588900
P	2.29186000	0.06879100	0.46608200
P	-2.08961900	0.15872900	0.67005900

C	-3.25820400	-1.00093700	-0.12789400
C	-4.02353700	-0.61656500	-1.23447400
C	-3.31568500	-2.33210100	0.30264500
C	-4.84012100	-1.53910400	-1.88222200
H	-3.98314600	0.41376300	-1.58773100
C	-4.13747300	-3.25086000	-0.33998900
H	-2.70008500	-2.66055800	1.14104000
C	-4.90360500	-2.85571200	-1.43426500
H	-5.43101100	-1.22578800	-2.74121700
H	-4.17329500	-4.28102400	0.01018500
H	-5.54436900	-3.57549900	-1.94065200
C	-2.96743000	1.75440600	0.46604700
C	-4.24293600	1.95160300	1.01425400
C	-2.38838300	2.77608600	-0.29260300
C	-4.92063300	3.14906600	0.81188700
H	-4.71489900	1.15378700	1.58922200
C	-3.07737000	3.96674900	-0.51537600
H	-1.38902900	2.63353600	-0.70377500
C	-4.33994600	4.15663000	0.03979500
H	-5.90931500	3.29306300	1.24507000
H	-2.61433600	4.75265400	-1.10882800
H	-4.87729500	5.08904200	-0.13229500
C	3.37903100	-1.15370300	-0.35977500
C	4.16648100	-0.80852800	-1.46357200
C	3.36170200	-2.48873900	0.06329400
C	4.92776300	-1.77309900	-2.11818100
H	4.18965100	0.22390900	-1.81068400
C	4.12999400	-3.44940500	-0.58425200
H	2.73070300	-2.78476600	0.90217300
C	4.91597100	-3.09334900	-1.67812300
H	5.53497200	-1.48849200	-2.97584100
H	4.10778900	-4.48157700	-0.23896100
H	5.51283300	-3.84639900	-2.18978600
C	3.19654600	1.62599900	0.14326600
C	2.66771500	2.56419500	-0.74813000
C	4.44766500	1.87002000	0.72485200
C	3.38338400	3.71705100	-1.06420800
H	1.68602000	2.39125900	-1.18702900
C	5.14854200	3.03527700	0.43107400
H	4.88380500	1.13564900	1.40324700
C	4.61946800	3.95766000	-0.47112900
H	2.96188400	4.43565700	-1.76467600
H	6.11538600	3.21901200	0.89699900
H	5.17331400	4.86427400	-0.71039900

H	3.53366100	-0.80098000	2.45273200
H	2.69920500	0.72514100	2.77517800
C	-1.04333800	-1.00077200	2.93694900
H	-1.04154900	-2.02046900	2.52571500
H	-1.01481500	-1.08799700	4.03638200
C	1.40885000	-1.00106000	2.84870500
H	1.47191800	-1.06884000	3.94824200
H	1.36487100	-2.02883400	2.46104600
Mn	0.08540500	-0.04536100	0.27894400
C	0.01549600	-1.79854800	-0.00750300
O	-0.02689000	-2.95879100	-0.18617800
H	0.21294000	1.56976700	0.54977500
H	0.16803200	0.61893300	2.82955100
O	-0.43854200	2.49870000	2.80568200
C	0.22131700	4.73170600	2.06107400
C	-1.05794500	5.30952000	1.90314100
C	1.28844900	5.21472900	1.30848700
C	-1.21019300	6.37350900	1.00312500
C	1.13135600	6.26891900	0.41240900
H	2.26591400	4.74566000	1.43419200
C	-0.12790700	6.84792800	0.27109600
H	-2.19662700	6.82316400	0.88002400
H	1.98016700	6.63318400	-0.16338600
H	-0.27566300	7.67323700	-0.42449800
C	0.41936200	3.62152800	3.04444900
H	0.17242500	3.94668900	4.06486500
H	1.47733100	3.30729600	3.04130600
H	-0.29685800	2.23812100	1.85617900
N	-2.11870700	4.85544600	2.67799900
H	-3.02674300	5.09259900	2.29665700
H	-2.06088000	3.85941500	2.86931100
<b>TS-A5</b>			
N	-0.07790000	0.14565100	2.46649100
C	-2.52029700	-0.04519000	2.43252300
H	-2.67909500	0.97574300	2.80013200
H	-3.38481700	-0.65105000	2.72790100
C	2.37974200	0.29490300	2.48990000
C	-0.03065200	0.45006800	-1.40846400
O	0.02635800	0.53187200	-2.57585800
P	2.16420700	0.47109800	0.66830500
P	-2.32812400	0.07053700	0.60186000
C	-3.13466000	-1.40781300	-0.10765500
C	-2.60290800	-1.98788900	-1.26425300
C	-4.31036600	-1.94109900	0.43611800

C	-3.22175500	-3.08453700	-1.85661800
H	-1.69469600	-1.57712100	-1.70275000
C	-4.92360400	-3.04320500	-0.15054700
H	-4.76120000	-1.48310200	1.31652800
C	-4.37876800	-3.61793100	-1.29708900
H	-2.79316800	-3.52520800	-2.75472300
H	-5.83334400	-3.45171400	0.28625200
H	-4.85989600	-4.48045000	-1.75514100
C	-3.44792600	1.43269500	0.11507700
C	-4.39824500	1.28922500	-0.90179100
C	-3.30366400	2.67403400	0.75250000
C	-5.20287800	2.36603800	-1.26653800
H	-4.51720200	0.33200700	-1.40802800
C	-4.11536800	3.74192200	0.38533600
H	-2.55380400	2.79689000	1.54082800
C	-5.06591800	3.59223100	-0.62300600
H	-5.94181700	2.24164700	-2.05640600
H	-4.00219100	4.69984200	0.89086300
H	-5.69725600	4.43215000	-0.90835200
C	3.22188200	-0.80614100	-0.09180300
C	3.74372200	-0.61223600	-1.37638000
C	3.44257400	-2.02775100	0.55337700
C	4.48194000	-1.61551000	-1.99507100
H	3.57283500	0.33313700	-1.89288800
C	4.18158100	-3.02991700	-0.06763500
H	3.02581700	-2.20577100	1.54506000
C	4.70437200	-2.82561900	-1.34147100
H	4.88629700	-1.45039800	-2.99221700
H	4.34567400	-3.97563000	0.44601800
H	5.28111700	-3.61054000	-1.82730000
C	3.04923200	2.01560400	0.25627300
C	2.49906400	2.94694100	-0.62907800
C	4.29713300	2.27868400	0.83524100
C	3.18035600	4.12633900	-0.92489100
H	1.53320300	2.74511800	-1.09408200
C	4.97542800	3.45547200	0.54089200
H	4.73462600	1.56138000	1.52999700
C	4.41619700	4.38226300	-0.33773600
H	2.74287800	4.84477300	-1.61548000
H	5.94152500	3.65326400	1.00266800
H	4.94697400	5.30506400	-0.56590000
H	3.30301200	-0.23796200	2.75075500
H	2.46843500	1.31270400	2.88749100
C	-1.22522400	-0.59694600	3.00100600

H	-1.12667200	-1.67181600	2.76134000
H	-1.23535000	-0.51379000	4.10220800
C	1.15026000	-0.38795000	3.06202500
H	1.12236500	-0.24673100	4.15583800
H	1.19991400	-1.47867200	2.88138300
Mn	-0.06768100	0.26772900	0.35624500
C	0.11137900	-1.48083400	0.26469900
O	0.23088900	-2.64337400	0.25283000
H	0.02172300	2.06652300	0.36381300
H	-0.33767600	1.36080300	2.76432000
O	-0.88451300	2.47019100	2.93605800
C	1.27177000	3.33742700	3.72549200
C	1.26196700	2.65171300	4.96367800
C	2.47881000	3.85987000	3.26006200
C	2.46237100	2.53152100	5.68223800
C	3.66637200	3.74164500	3.97872300
H	2.47986500	4.36788400	2.29245800
C	3.64706700	3.07393700	5.20088500
H	2.45285100	1.98979500	6.62916700
H	4.59194200	4.15655000	3.58310800
H	4.56171100	2.96308300	5.78232000
C	0.00395200	3.53797700	2.92214900
H	0.31464800	3.81338300	1.88506200
H	-0.51871900	4.43709000	3.30827400
H	-0.57027900	1.95245500	0.89721500
N	0.10900300	2.03810700	5.44282200
H	-0.00712800	2.06076100	6.44607800
H	-0.72510100	2.25133600	4.90199300

**IM-A6**

N	-0.17121400	0.01813700	2.50072800
C	-2.59409600	-0.12725800	2.28574500
H	-2.78260300	0.86770600	2.71090500
H	-3.48680400	-0.73827500	2.47037400
C	2.24582100	0.32526500	2.59522000
C	0.05969100	0.49582300	-1.38905300
O	0.13806100	0.77699100	-2.52537700
P	2.11477000	0.44067700	0.74191100
P	-2.25771400	0.10355700	0.46714200
C	-3.18229800	-1.25894300	-0.32901700
C	-3.73666000	-1.07970400	-1.60230900
C	-3.25910000	-2.52285400	0.26628000
C	-4.36898500	-2.13374300	-2.25363600
H	-3.67717800	-0.10378600	-2.08442400
C	-3.89705200	-3.57529600	-0.38289700

H	-2.80678600	-2.69433000	1.24377800
C	-4.45605500	-3.38264400	-1.64371100
H	-4.79765100	-1.97717200	-3.24206600
H	-3.95323600	-4.55090300	0.09710000
H	-4.95370100	-4.20634800	-2.15219200
C	-3.30808900	1.54118100	0.03300500
C	-4.67684900	1.54335700	0.33609700
C	-2.75596800	2.64722700	-0.61861500
C	-5.47037000	2.63742800	0.01085600
H	-5.12539900	0.67501500	0.82101600
C	-3.55449700	3.73935600	-0.95378100
H	-1.69320300	2.64185100	-0.85926300
C	-4.90885100	3.73809000	-0.63559100
H	-6.53071300	2.63110600	0.25778800
H	-3.11413200	4.59285900	-1.46662100
H	-5.53106100	4.59309600	-0.89472400
C	3.30306400	-0.81047600	0.13418800
C	3.86077800	-0.65676500	-1.14170600
C	3.59083200	-1.97139700	0.85833100
C	4.70339600	-1.62948200	-1.66777200
H	3.63431600	0.23714100	-1.72434000
C	4.43639500	-2.94435900	0.33263800
H	3.14848300	-2.12605300	1.84297600
C	4.99766900	-2.77398900	-0.92979900
H	5.13281300	-1.49274000	-2.65874400
H	4.65528000	-3.83966200	0.91217400
H	5.65937100	-3.53456600	-1.34040000
C	3.03692400	1.98667600	0.39077500
C	2.39720900	3.08107100	-0.19701800
C	4.38922900	2.09844600	0.74680300
C	3.08744900	4.27430000	-0.40233400
H	1.34727800	2.98868000	-0.47501000
C	5.07686300	3.28918400	0.54112500
H	4.90498200	1.24147500	1.18245300
C	4.42356200	4.38169800	-0.02892700
H	2.57843500	5.12171400	-0.85824500
H	6.12560100	3.36613100	0.82545900
H	4.96000600	5.31659900	-0.18436000
H	3.20526400	-0.09135300	2.92839200
H	2.19381500	1.35470800	2.98119800
C	-1.36145200	-0.73457700	2.93076400
H	-1.21770100	-1.77777000	2.61443300
H	-1.45032900	-0.73106700	4.03048000
C	1.06962700	-0.48283400	3.11139900

H	1.00995400	-0.44043200	4.21265700
H	1.16467400	-1.54103500	2.82831300
Mn	-0.04063900	0.15483300	0.33298800
C	0.11532100	-1.60834500	0.15507000
O	0.23026100	-2.77210900	0.05408100
H	-0.16219600	1.77846800	0.52746600
H	-0.30823700	0.99476000	2.79370000
C	1.99039500	4.54811800	4.33652300
C	2.05423700	5.59707600	5.25754600
C	3.11725700	4.29202800	3.54545000
C	3.20893900	6.36290000	5.39557300
C	4.27241800	5.05451500	3.68016500
H	3.09427800	3.48943300	2.80486700
C	4.32427300	6.09230400	4.60778500
H	3.23574100	7.17536200	6.12028800
H	5.13498900	4.83381200	3.05268200
H	5.22850300	6.68951100	4.71328300
C	0.74478000	3.71739600	4.19085900
H	0.93154600	2.68019400	4.51844900
H	-0.04876100	4.09932000	4.84720100
C	0.23268200	3.67729100	2.76360300
H	1.00689900	3.26567500	2.09239400
H	0.02135000	4.70141100	2.41079700
O	-0.93606900	2.87408100	2.70687600
H	-0.99500100	2.57311900	1.77228100
H	1.18216700	5.81420700	5.87521500

### TS-A6

N	0.01372700	-0.45542300	2.43050400
C	-2.41821300	-0.38346300	2.46235600
H	-2.42940200	0.58173400	2.98474000
H	-3.34524900	-0.91479700	2.70833300
C	2.46344200	-0.40982800	2.42965400
C	-0.00201400	0.38695600	-1.36879900
O	0.00925900	0.62613600	-2.51563100
P	2.25297100	0.02811300	0.64254100
P	-2.26454500	-0.02284400	0.65866800
C	-3.26201200	-1.28270800	-0.20654600
C	-2.81843800	-1.78187100	-1.43588500
C	-4.49569500	-1.71822600	0.29459900
C	-3.58323200	-2.70429900	-2.14382900
H	-1.86798700	-1.44119500	-1.84284700
C	-5.25591500	-2.64629300	-0.40899800
H	-4.87500900	-1.31675100	1.23439200
C	-4.79931600	-3.14242800	-1.62912000

H	-3.22270800	-3.08376800	-3.09786100
H	-6.21032800	-2.98060900	-0.00601000
H	-5.39519600	-3.86932600	-2.17846600
C	-3.21794700	1.51872500	0.42021900
C	-4.20035300	1.63926500	-0.56946300
C	-2.90208800	2.63064000	1.21625900
C	-4.86796100	2.84777500	-0.75189300
H	-4.45087600	0.78612900	-1.19882700
C	-3.57910700	3.83106500	1.02982800
H	-2.11787800	2.55780300	1.97696000
C	-4.56150000	3.94463100	0.04799400
H	-5.63153200	2.92970900	-1.52368800
H	-3.33168900	4.68677000	1.65608700
H	-5.08486600	4.88865600	-0.09592600
C	3.29217000	-1.16825500	-0.26036500
C	4.00147700	-0.78287500	-1.40324400
C	3.32855000	-2.50861900	0.14276400
C	4.74163500	-1.71830600	-2.11991800
H	3.98310300	0.25812900	-1.72547700
C	4.07190700	-3.44062200	-0.57330100
H	2.76567000	-2.83106100	1.01919500
C	4.78076200	-3.04722600	-1.70579800
H	5.29439800	-1.40535700	-3.00392800
H	4.09332200	-4.47874700	-0.24696500
H	5.36141300	-3.77734000	-2.26674500
C	3.14030500	1.61040200	0.44113300
C	2.66097600	2.55598300	-0.47209200
C	4.26098000	1.92191000	1.22103800
C	3.28134500	3.79581800	-0.59343900
H	1.78773100	2.32381800	-1.08165800
C	4.87069600	3.16666200	1.10841000
H	4.64978800	1.19769600	1.93711800
C	4.37792200	4.10668200	0.20590500
H	2.89515300	4.52509400	-1.30309800
H	5.72184600	3.40805500	1.74172100
H	4.85028700	5.08452300	0.12800800
H	3.37312200	-0.99838300	2.60553800
H	2.57183000	0.53758800	2.97529200
C	-1.18702300	-1.16641700	2.88054400
H	-1.20679500	-2.18618300	2.45674900
H	-1.16958600	-1.27670500	3.97920000
C	1.21650400	-1.14177000	2.89576700
H	1.21353000	-1.21203800	3.99891000
H	1.21668800	-2.18108900	2.51988500

Mn	-0.00035800	-0.02760400	0.35440700
C	0.04097600	-1.75181500	0.00897200
O	0.07506400	-2.90582100	-0.18081200
H	0.10406200	1.76032900	0.52826300
H	-0.09627800	0.68055800	2.88126200
C	2.86135600	3.07511000	4.58722400
C	3.05626900	4.43394200	4.30594800
C	3.99348400	2.28863900	4.82785500
C	4.33269000	4.98504600	4.27210700
C	5.27463900	2.83572600	4.80152800
H	3.86109200	1.22779000	5.05141600
C	5.44873500	4.18896900	4.52442800
H	4.45826100	6.04507100	4.05397700
H	6.13837700	2.20364200	5.00523500
H	6.44788500	4.62243400	4.50724500
C	1.48424300	2.48122000	4.57512100
H	1.53748800	1.40622100	4.81038600
H	0.84847300	2.92677900	5.35424000
C	0.77184700	2.64408200	3.22051900
H	1.50559100	2.37008100	2.42338700
H	0.57711100	3.72307500	3.05346200
O	-0.39320100	1.91440700	3.13738800
H	-0.23638100	1.65651900	1.25520100
H	2.18971800	5.06732200	4.11469700

**IM-A7**

N	0.33499600	-0.21854400	2.37605800
C	-2.09812700	-0.09202500	2.51727300
H	-2.12693600	0.84650800	3.08420900
H	-3.02365100	-0.64549600	2.72043100
C	2.76965600	-0.30757800	2.27421900
C	0.16220000	0.59238300	-1.40509400
O	0.07594600	0.82813700	-2.55097000
P	2.50629400	-0.01438500	0.47489500
P	-1.94182400	0.35781600	0.73471700
C	-3.06339700	-0.77377600	-0.15350400
C	-3.73285100	-0.35449800	-1.30902100
C	-3.18945800	-2.10538200	0.25969700
C	-4.52415000	-1.24620100	-2.02614000
H	-3.63964500	0.67862700	-1.64448800
C	-3.98329600	-2.99393700	-0.45804500
H	-2.65362200	-2.45618900	1.14256800
C	-4.65357000	-2.56602400	-1.60114200
H	-5.04337600	-0.90678500	-2.92077200
H	-4.07398100	-4.02603800	-0.12411800

H	-5.27338500	-3.26206900	-2.16353200
C	-2.78984400	1.96530600	0.55674300
C	-4.05265100	2.16558200	1.13324200
C	-2.20513000	3.00065700	-0.17702100
C	-4.70899100	3.38165000	0.98546900
H	-4.52510100	1.35817000	1.69351000
C	-2.87219000	4.21301800	-0.34063100
H	-1.21968400	2.86372200	-0.62425900
C	-4.11977500	4.40686900	0.24387400
H	-5.68699000	3.52874200	1.44077100
H	-2.40253900	5.00969300	-0.91352000
H	-4.63837700	5.35656500	0.11979100
C	3.33640200	-1.39115800	-0.38718000
C	3.75617300	-1.22846000	-1.71249600
C	3.48277200	-2.64175000	0.22260500
C	4.32991100	-2.28903700	-2.40488600
H	3.64052600	-0.26122900	-2.20287100
C	4.05642700	-3.70189600	-0.47314000
H	3.14017900	-2.79553200	1.24603800
C	4.48393900	-3.52769200	-1.78588000
H	4.65918200	-2.14622900	-3.43265900
H	4.16691500	-4.66886200	0.01443000
H	4.93418400	-4.35706500	-2.32819600
C	3.54899900	1.42646800	0.05773900
C	3.18257800	2.24944600	-1.01372600
C	4.69786500	1.74139600	0.79441500
C	3.95488400	3.35761100	-1.34947900
H	2.27876900	2.02887500	-1.58126500
C	5.45474000	2.86439400	0.47261700
H	5.00064200	1.10871600	1.62871500
C	5.08601400	3.67227500	-0.60140300
H	3.65823500	3.98727800	-2.18645200
H	6.33699600	3.10842200	1.06163800
H	5.67965200	4.54968600	-0.85147200
H	3.67171600	-0.89755200	2.48287900
H	2.90119600	0.68192900	2.73472000
C	-0.85276700	-0.88183000	2.89190700
H	-0.93847800	-1.92549800	2.51619600
H	-0.79406600	-0.96543700	3.99408900
C	1.50519500	-0.95600800	2.81334200
H	1.55194700	-0.98641400	3.91891400
H	1.46580700	-2.02054200	2.48920900
Mn	0.26483100	0.17567600	0.31650500
C	0.10920600	-1.54904400	-0.02015900

O	0.02131500	-2.69956400	-0.19704400
H	0.84739200	1.81940100	0.72921700
H	0.12293700	1.34363300	3.05747300
O	-0.15430200	2.23016600	3.45733700
C	0.73122000	4.19341100	2.29525800
C	-0.46182600	4.94994400	2.26179100
C	1.72787300	4.46120700	1.35993000
C	-0.58895200	5.97147100	1.30893100
C	1.58727000	5.45937500	0.39759500
H	2.64366300	3.86540800	1.39197100
C	0.42062100	6.22034700	0.38721800
H	-1.50451700	6.56491900	1.29367800
H	2.38278200	5.64509500	-0.32151500
H	0.28965800	7.01406900	-0.34781100
C	0.92466800	3.14018400	3.35404600
H	1.04349200	3.62645300	4.33791900
H	1.87266200	2.60549800	3.15589300
H	0.05881800	1.87634600	0.88457300
N	-1.45759600	4.71712700	3.20029300
H	-2.37441900	5.03612600	2.91456900
H	-1.47456100	3.75447000	3.52484000

**IM-A8**

N	-0.02399900	-0.37031300	2.40315500
C	-2.45320400	-0.26801300	2.37431500
H	-2.47964500	0.69571400	2.89855500
H	-3.39967500	-0.78747500	2.57258200
C	2.40440200	-0.37675200	2.47603200
C	0.08267700	0.66844000	-1.33052400
O	0.12108900	0.97762600	-2.46145200
P	2.25705800	0.00486700	0.68178400
P	-2.21121200	0.11453000	0.59315200
C	-3.10926500	-1.17360900	-0.33511300
C	-3.34066200	-0.97089200	-1.70214100
C	-3.49220300	-2.38664300	0.24450300
C	-3.95749200	-1.95370300	-2.46647800
H	-3.03696700	-0.03226900	-2.16806400
C	-4.10947800	-3.37071500	-0.52400700
H	-3.30040800	-2.57585200	1.30042700
C	-4.34524700	-3.15632400	-1.87810500
H	-4.13528800	-1.78079100	-3.52646800
H	-4.40372700	-4.31052200	-0.05982700
H	-4.82684300	-3.92715500	-2.47710000
C	-3.22002600	1.59869000	0.25894400
C	-4.58317900	1.61753100	0.58345100

C	-2.64507200	2.72718400	-0.33044800
C	-5.34874400	2.75074800	0.33653700
H	-5.04603400	0.73493700	1.02668800
C	-3.41468700	3.86032600	-0.58421800
H	-1.58952100	2.71081800	-0.60138500
C	-4.76451400	3.87413200	-0.24759100
H	-6.40552200	2.75801400	0.59733700
H	-2.95701500	4.73266800	-1.04729700
H	-5.36610200	4.75968700	-0.44492800
C	3.14493800	-1.32745700	-0.19097100
C	3.47701300	-1.14165500	-1.53940300
C	3.42030900	-2.55815500	0.41240300
C	4.09173400	-2.15880300	-2.25995600
H	3.25230900	-0.19091400	-2.02525700
C	4.03419900	-3.57661800	-0.31245300
H	3.14523600	-2.73359200	1.45201100
C	4.37354300	-3.37858300	-1.64674900
H	4.34930700	-1.99950300	-3.30556400
H	4.24295900	-4.53012400	0.16966400
H	4.85330300	-4.17562600	-2.21176700
C	3.37440000	1.43121100	0.43611700
C	2.89274400	2.64648700	-0.05700200
C	4.72913300	1.32500300	0.78236700
C	3.74133500	3.74480100	-0.18202300
H	1.84715200	2.72964700	-0.35441200
C	5.57527400	2.42040300	0.65687100
H	5.11913200	0.37454800	1.14865600
C	5.07996600	3.63387600	0.17879700
H	3.35389600	4.68720500	-0.56378500
H	6.62474100	2.32964400	0.93331500
H	5.74237600	4.49301100	0.08692100
H	3.32055000	-0.92830100	2.72514100
H	2.45791200	0.59586100	2.98541100
C	-1.23289900	-1.06346300	2.81624600
H	-1.28492400	-2.09808000	2.40745400
H	-1.25058000	-1.17686100	3.91752000
C	1.13233900	-1.10233000	2.88251000
H	1.09878300	-1.19704700	3.98580900
H	1.15850000	-2.14667200	2.49607400
Mn	0.03399600	0.13954200	0.36435600
C	0.00234900	-1.56559800	-0.08997000
O	-0.02283600	-2.70321600	-0.34629300
H	0.43190500	1.80350700	0.89385700
H	-0.28380800	1.22084200	3.13856300

C	2.68334800	3.43775700	4.83971200
C	2.85612500	4.41075800	5.82828300
C	3.69877200	3.27720700	3.88802900
C	4.00689900	5.19380000	5.87455600
C	4.84986000	4.05683500	3.92986700
H	3.58693900	2.53408300	3.09454200
C	5.00902300	5.01931700	4.92420300
H	4.12027100	5.94343800	6.65639200
H	5.62545000	3.91039800	3.17906200
H	5.90976200	5.63001900	4.95779800
C	1.42670300	2.61971200	4.76027200
H	1.66104400	1.54284600	4.78540200
H	0.78343000	2.81040900	5.62928400
C	0.62367700	2.90618600	3.48748100
H	1.28845200	2.74181500	2.60988400
H	0.34670700	3.97000500	3.46565400
O	-0.55197800	2.15627000	3.39409700
H	-0.35952300	1.76867000	1.04904300
H	2.07303500	4.55202400	6.57409600

**IM-A9**

N	0.20977500	-0.13789600	2.02717800
C	-2.21031900	0.06782400	2.33254200
H	-2.22777500	0.99510200	2.92005600
H	-3.13039900	-0.49083500	2.54302100
C	2.61928600	0.20026200	2.25133600
C	0.23846500	1.91001000	-0.90708400
O	0.28772500	2.77363700	-1.70275300
P	2.44109100	0.34964200	0.43537800
P	-2.07200200	0.55084900	0.55369000
C	-3.06199300	-0.73541700	-0.29398700
C	-4.29330800	-0.48237100	-0.90680900
C	-2.55439900	-2.04212400	-0.30417900
C	-5.00442700	-1.51718500	-1.51053800
H	-4.70025300	0.52776100	-0.91507400
C	-3.27193000	-3.07484600	-0.89579900
H	-1.57827300	-2.24293800	0.13920800
C	-4.49933900	-2.81384400	-1.50204000
H	-5.95887300	-1.30586000	-1.98983300
H	-2.86454600	-4.08415600	-0.89588500
H	-5.05701700	-3.62042400	-1.97467500
C	-3.13165500	2.03944500	0.44870300
C	-4.20580200	2.21751200	1.33287000
C	-2.87514700	3.02842800	-0.50777700
C	-4.99093100	3.36521200	1.27566900

H	-4.43164300	1.45229000	2.07487100
C	-3.66457000	4.17577100	-0.56642600
H	-2.04358700	2.91532600	-1.19867400
C	-4.71821400	4.35039700	0.32776000
H	-5.81572000	3.49173000	1.97463500
H	-3.44626000	4.93982600	-1.31064100
H	-5.32672900	5.25190000	0.28710000
C	3.15793200	-1.19320200	-0.24512100
C	3.19560600	-1.34382400	-1.63788100
C	3.64389900	-2.23220600	0.55583800
C	3.71263900	-2.49740200	-2.21394400
H	2.80865300	-0.55087000	-2.27796200
C	4.15519100	-3.39214200	-0.02263300
H	3.63039400	-2.14564900	1.64100400
C	4.19241100	-3.52711900	-1.40674300
H	3.73365500	-2.59554200	-3.29760700
H	4.52889900	-4.19126800	0.61542200
H	4.59278000	-4.43353200	-1.85713900
C	3.66987500	1.59879000	-0.08062700
C	3.53960400	2.22574600	-1.32493300
C	4.75669700	1.93136100	0.73623700
C	4.47785000	3.16471200	-1.74310400
H	2.68846000	1.99501400	-1.96271600
C	5.68883400	2.87787600	0.32131700
H	4.87787900	1.45210600	1.70730900
C	5.55195200	3.49524300	-0.92027900
H	4.36068800	3.64820100	-2.71121300
H	6.52597900	3.13217600	0.96927300
H	6.28089200	4.23596500	-1.24429200
H	3.56980000	-0.23721200	2.58250200
H	2.56601300	1.22760100	2.63984600
C	-0.96486300	-0.71969400	2.68475000
H	-1.07940400	-1.78231200	2.40163800
H	-0.82842700	-0.71023400	3.78015600
C	1.41380700	-0.58939300	2.72545300
H	1.28587400	-0.45908000	3.81529500
H	1.57393100	-1.67311500	2.56499700
Mn	0.18577700	0.55262400	0.22624400
C	0.09375000	-0.49595500	-1.16281600
O	0.02672700	-1.22600000	-2.07975000
H	0.01953200	1.48157900	3.16607300
O	-0.21331100	1.99501000	3.97272500
C	0.91231400	3.77822400	2.73795600
C	-0.20174600	4.28775500	2.03017600

C	2.18973400	3.95230900	2.20891900
C	0.01559600	4.94556300	0.81235700
C	2.40237600	4.61731800	1.00412200
H	3.04162300	3.55755400	2.76867100
C	1.30096800	5.10792100	0.30913800
H	-0.84360300	5.32315900	0.25627700
H	3.40906900	4.72641200	0.60536600
H	1.43799100	5.60143600	-0.65210200
C	0.70613500	3.08176100	4.04896900
H	0.27589200	3.76510700	4.79582800
H	1.68025900	2.74249900	4.44726000
N	-1.47211000	4.19560700	2.58387500
H	-2.22720900	4.31465400	1.91943300
H	-1.59938600	3.37423500	3.16686900

**IM-A10**

N	-0.03923900	-0.67108500	2.18459700
C	-2.46942300	-0.40514600	2.40254500
H	-2.48940300	0.54674600	2.94887100
H	-3.41669200	-0.91893500	2.60931500
C	2.38467500	-0.42996100	2.51745300
C	-0.07117700	1.94098600	0.05340000
O	-0.15927900	3.08960500	-0.17790800
P	2.23812700	-0.01771900	0.73255200
P	-2.25609700	0.04745200	0.63673200
C	-2.98415700	-1.31003000	-0.33691400
C	-3.01448800	-1.19418400	-1.73498400
C	-3.43430800	-2.49913700	0.24792300
C	-3.49759000	-2.23229700	-2.52199800
H	-2.65032600	-0.28323100	-2.20911400
C	-3.90745100	-3.54283200	-0.54328300
H	-3.41605400	-2.62076500	1.32978100
C	-3.94294800	-3.41167100	-1.92794800
H	-3.51599000	-2.12333500	-3.60472000
H	-4.25200000	-4.46206400	-0.07235200
H	-4.31233000	-4.22884400	-2.54503900
C	-3.37833400	1.47095800	0.42494700
C	-4.52518700	1.45528200	-0.37505600
C	-3.05414900	2.63360800	1.13994000
C	-5.33540500	2.58510900	-0.45884100
H	-4.79397800	0.55734800	-0.92946300
C	-3.87226400	3.75380200	1.05842300
H	-2.15988300	2.65338500	1.76751300
C	-5.01211800	3.73416700	0.25684100
H	-6.22651800	2.56279300	-1.08394000

H	-3.61314200	4.64979700	1.61962100
H	-5.64813100	4.61530200	0.19020400
C	2.92746500	-1.46616000	-0.14506600
C	3.16252100	-1.35958200	-1.52320600
C	3.17501800	-2.68963600	0.48686900
C	3.63747200	-2.44650000	-2.24629800
H	2.96716600	-0.41605200	-2.03274900
C	3.64730200	-3.77977900	-0.24047600
H	3.00128300	-2.80155800	1.55607000
C	3.87957200	-3.66118000	-1.60692300
H	3.81517000	-2.34594100	-3.31543700
H	3.83571700	-4.72470900	0.26675700
H	4.24745900	-4.51390300	-2.17478500
C	3.55654800	1.22964300	0.49831100
C	3.25068500	2.55611700	0.18071000
C	4.89670100	0.86759800	0.70101900
C	4.26528600	3.50525900	0.07170400
H	2.21720400	2.85223900	0.01915500
C	5.90667700	1.81715900	0.59459800
H	5.14731100	-0.16830000	0.93305800
C	5.59087900	3.13814300	0.27742600
H	4.01347000	4.53579200	-0.17028200
H	6.94363500	1.52572500	0.75437400
H	6.38201600	3.88143500	0.19055700
H	3.30317400	-0.97831700	2.76578200
H	2.43769500	0.53751700	3.03725500
C	-1.25111700	-1.20755900	2.81407000
H	-1.37365300	-2.27397000	2.54767300
H	-1.14650600	-1.18132300	3.91369000
C	1.12335100	-1.16848300	2.92226000
H	0.95574400	-1.05246300	4.00955700
H	1.23864600	-2.25623900	2.75631200
Mn	0.00138000	0.24469800	0.49154400
C	0.05210600	-0.16813100	-1.21440900
O	0.09218900	-0.47684500	-2.34642700
H	-0.23053200	1.18804800	2.87193200
C	2.67838500	3.72619200	4.52310100
C	2.66605000	4.93559200	5.22360000
C	3.81268600	3.40930800	3.76680800
C	3.75654000	5.79976800	5.18283700
C	4.90555700	4.26922200	3.72312500
H	3.84111300	2.47305600	3.20340600
C	4.88171500	5.46748800	4.43309600
H	3.72885500	6.73393000	5.74206700

H	5.77992100	3.99752500	3.13382000
H	5.73854100	6.13869800	4.40381000
C	1.48646600	2.81446700	4.53848300
H	1.79551100	1.77308200	4.72392000
H	0.80508200	3.07995100	5.35768100
C	0.70042300	2.86158900	3.22909700
H	1.35676100	2.56609500	2.38756400
H	0.38271800	3.89347200	3.02091300
O	-0.45574300	2.05324100	3.28051100
H	1.78703900	5.19673100	5.81397100

**IM-A11**

N	-0.28043700	-0.25390800	-1.82064900
C	-2.25732200	-1.64620900	-1.97814100
H	-1.69199000	-2.58055100	-1.86828400
H	-3.18720800	-1.87245000	-2.51672200
C	1.79808200	0.98206100	-1.66815400
C	-1.12786300	0.62927300	1.83200900
O	-1.39450800	0.89852900	2.94364200
P	1.12367500	1.49405400	-0.03857400
P	-2.55748800	-1.02104200	-0.27414500
C	-4.18836500	-0.20320400	-0.32074000
C	-4.87576400	0.01264100	0.88060500
C	-4.72839000	0.29466800	-1.51028900
C	-6.08741900	0.69366600	0.88643200
H	-4.45782600	-0.35993400	1.81683200
C	-5.94146800	0.97807000	-1.50164600
H	-4.19432900	0.16132900	-2.45109300
C	-6.62432600	1.17629700	-0.30571600
H	-6.61345300	0.85028200	1.82670600
H	-6.35062000	1.36002000	-2.43526000
H	-7.57198900	1.71214400	-0.30012100
C	-2.93356500	-2.50800300	0.72223000
C	-3.97666000	-3.35928800	0.33337700
C	-2.20101000	-2.81234800	1.87218000
C	-4.26898500	-4.49940400	1.07159200
H	-4.56907000	-3.11621900	-0.54947400
C	-2.49770500	-3.95362100	2.61577400
H	-1.40454700	-2.14018600	2.19414100
C	-3.52768800	-4.79834200	2.21445000
H	-5.08010100	-5.15523900	0.75950600
H	-1.92403400	-4.17930100	3.51295700
H	-3.75991600	-5.68887400	2.79595700
C	0.91317800	3.30463900	-0.12854500
C	0.58058200	3.99443900	1.04545900

C	0.95623600	4.00642900	-1.33640000
C	0.30849500	5.35642000	1.01058300
H	0.52918500	3.45483100	1.99234000
C	0.68011400	5.37138000	-1.36927700
H	1.18882000	3.48761700	-2.26535700
C	0.35646600	6.04854800	-0.19841200
H	0.05174100	5.87954400	1.93013800
H	0.71322600	5.90431700	-2.31812200
H	0.13535000	7.11401800	-0.22661500
C	2.50758900	1.32283500	1.14284800
C	2.39699100	0.47246200	2.24596100
C	3.70148600	2.02940500	0.94367400
C	3.46428600	0.31783700	3.12836600
H	1.46135200	-0.06006000	2.42015300
C	4.76777300	1.87026500	1.82075000
H	3.78820400	2.71417000	0.09900900
C	4.65074100	1.01168700	2.91334700
H	3.36550400	-0.34369700	3.98712900
H	5.69304000	2.41969900	1.65480300
H	5.48526800	0.89085000	3.60199700
H	2.46826900	1.72929600	-2.11340600
H	2.38091500	0.06972700	-1.48676500
C	-1.38997100	-0.60628100	-2.67220200
H	-2.01938100	0.27106000	-2.96361500
H	-1.02049200	-1.02377500	-3.63011800
C	0.59062800	0.65022100	-2.53281300
H	0.93548700	0.18656600	-3.47854500
H	0.08498800	1.59865800	-2.84165400
Mn	-0.76844600	0.28322100	0.12459700
C	-1.67797200	1.68067400	-0.44390900
O	-2.26096700	2.59949700	-0.86387400
H	0.52485000	-0.93388400	0.56357000
H	-0.13510400	-1.38759200	0.51134200
<b>2a</b>			
C	0.28088400	-0.09758200	-0.13302000
C	-0.34603400	1.13563100	0.06881700
C	-0.51676500	-1.24398200	-0.20250800
C	-1.72947100	1.22400700	0.19232500
C	-1.90076900	-1.16169200	-0.07964400
H	-0.04121000	-2.21292700	-0.36140600
C	-2.51163100	0.07411900	0.11819700
H	-2.19929900	2.19467500	0.34327000
H	-2.50475800	-2.06558700	-0.14220800
H	-3.59419000	0.14118800	0.21062700

C	1.77709000	-0.19269900	-0.21388100
H	2.08467600	-1.02087400	-0.86618200
H	2.20478400	0.72324400	-0.64326400
C	2.39993200	-0.40920700	1.15435100
H	1.99477300	-1.33744700	1.59858200
H	2.10576000	0.41915300	1.82541300
O	3.80005500	-0.47605500	0.98663400
H	4.19362600	-0.60973500	1.85820800
H	0.26380200	2.03847600	0.12338000

**IM-B1**

N	-0.06042100	-1.47319600	-1.26494500
C	2.36292700	-1.53823800	-1.40072300
H	2.36849600	-1.04296500	-2.38300200
H	3.27222000	-2.14971000	-1.33969900
C	-2.48426700	-1.30735200	-1.35391400
C	0.10427600	1.72535600	0.88794500
O	0.15751700	2.72292600	1.51089500
P	-2.23003100	0.10682600	-0.19365900
P	2.25885400	-0.21098000	-0.13420700
C	2.97762900	-0.91868400	1.39317400
C	2.92228400	-0.12906700	2.54966200
C	3.52983200	-2.19881900	1.47567000
C	3.42280300	-0.60271800	3.75526600
H	2.46258200	0.85987500	2.50344700
C	4.02167600	-2.67741400	2.68874200
H	3.57106900	-2.84093000	0.59730900
C	3.97395400	-1.88079100	3.82781000
H	3.37212200	0.02310600	4.64426500
H	4.44184700	-3.68056600	2.74059100
H	4.35746500	-2.25776400	4.77409700
C	3.55067000	1.01105300	-0.57577400
C	4.66233800	0.67495000	-1.35869900
C	3.46929300	2.30035300	-0.03277600
C	5.67408900	1.60545700	-1.58449400
H	4.74652700	-0.32478300	-1.78487100
C	4.48716200	3.22433100	-0.24937900
H	2.60286300	2.57997800	0.56685800
C	5.59258400	2.87776800	-1.02263300
H	6.53289900	1.33157800	-2.19535200
H	4.40918100	4.22254600	0.17727800
H	6.38416500	3.60410900	-1.19871800
C	-3.20208700	-0.29878000	1.29456300
C	-3.57224200	0.73327700	2.16646700
C	-3.50408100	-1.61916800	1.64192200

C	-4.24753900	0.45018300	3.34794800
H	-3.33082400	1.76653300	1.91342600
C	-4.17902700	-1.90087200	2.82632700
H	-3.20064100	-2.43890100	0.99070400
C	-4.55530400	-0.86794400	3.67950200
H	-4.53431800	1.26299900	4.01311100
H	-4.40839600	-2.93352000	3.08332500
H	-5.08343200	-1.08927800	4.60538700
C	-3.18265900	1.48696900	-0.91762200
C	-2.57414300	2.73315500	-1.08556600
C	-4.51904200	1.32231900	-1.30255900
C	-3.28475100	3.79646200	-1.63693800
H	-1.53517000	2.85945600	-0.78457200
C	-5.22617600	2.38255000	-1.85955400
H	-5.00986500	0.35896100	-1.15784700
C	-4.60877200	3.62148600	-2.02816300
H	-2.80007800	4.76409700	-1.76125300
H	-6.26388900	2.24418100	-2.15914900
H	-5.16409800	4.45110700	-2.46277800
H	-3.44437500	-1.81690200	-1.19956900
H	-2.49559600	-0.87569400	-2.36375000
C	1.08823400	-2.35786500	-1.25070600
H	1.14331800	-2.95499900	-0.31401000
H	1.02237100	-3.09664800	-2.07260900
C	-1.29030200	-2.24087800	-1.20924800
H	-1.31422800	-2.99623300	-2.01842600
H	-1.37276100	-2.81681300	-0.26187600
Mn	0.02637700	0.19617700	0.00112000
C	-0.07148900	-0.75916100	1.46202800
O	-0.16076700	-1.45477200	2.40012400
C	1.76801200	3.92462400	-3.30482700
C	1.31568000	5.05244500	-3.99479200
C	3.12086000	3.58247300	-3.40840500
C	2.18744000	5.82349900	-4.75897700
C	3.99559400	4.35001300	-4.17028200
H	3.49529300	2.70601700	-2.87953000
C	3.53245100	5.47495800	-4.84872800
H	1.81379900	6.69926800	-5.28762300
H	5.04589800	4.06558000	-4.22934400
H	4.21549600	6.07661100	-5.44608300
C	0.82575400	3.09497300	-2.47831300
H	1.06045600	3.18538500	-1.40417200
H	-0.20290000	3.46023800	-2.60095200
C	0.85839700	1.62542000	-2.84846000

H	1.86659300	1.21216900	-2.66736500
H	0.63996400	1.50257800	-3.92114900
O	-0.11448200	0.92402800	-2.09197100
H	-0.04755700	-0.08648300	-2.23486500
H	0.26216500	5.32759200	-3.92881800
<b>TS-B1</b>			
N	-0.01809700	-1.42179000	-1.28458100
C	2.40850900	-1.47967600	-1.35779500
H	2.45005200	-0.98825400	-2.34045900
H	3.31365800	-2.09314600	-1.26563700
C	-2.42408100	-1.19079600	-1.48889100
C	0.09538400	1.80402800	0.84717300
O	0.13173200	2.82023700	1.43886100
P	-2.21756400	0.15070500	-0.24070400
P	2.27584300	-0.14197000	-0.10025800
C	2.98223700	-0.83537600	1.43904700
C	2.94419000	-0.02501600	2.58180100
C	3.50503600	-2.12600700	1.54448000
C	3.43311000	-0.48942900	3.79574400
H	2.51012600	0.97447100	2.51829700
C	3.98688400	-2.59447500	2.76546400
H	3.53240100	-2.78423400	0.67752200
C	3.95630800	-1.77778500	3.89061500
H	3.39642300	0.15252600	4.67387300
H	4.38582700	-3.60521100	2.83435900
H	4.33190700	-2.14646300	4.84330600
C	3.56584500	1.07963700	-0.54416300
C	4.70736700	0.72540300	-1.27479200
C	3.44838400	2.39003900	-0.06309900
C	5.71012000	1.66150000	-1.51474300
H	4.82009600	-0.29153000	-1.65095000
C	4.45656000	3.32109800	-0.29552500
H	2.56124600	2.68139700	0.49928800
C	5.58902000	2.95850800	-1.02024900
H	6.59107800	1.37474200	-2.08694000
H	4.35012800	4.33659300	0.08138100
H	6.37240600	3.69028300	-1.20975600
C	-3.18582700	-0.36282200	1.21653300
C	-3.32401500	0.56244900	2.26040700
C	-3.72224500	-1.64349000	1.37349400
C	-4.00114900	0.21968100	3.42361800
H	-2.89284100	1.55933700	2.15580600
C	-4.39726300	-1.98745600	2.54296400
H	-3.60991600	-2.38740800	0.58555800

C	-4.54154800	-1.05757100	3.56701500
H	-4.10475000	0.95065700	4.22357700
H	-4.81012800	-2.98896500	2.65215400
H	-5.06988400	-1.32784800	4.47964000
C	-3.19625900	1.54961000	-0.88629300
C	-2.55886200	2.75853100	-1.17322600
C	-4.57653500	1.43489200	-1.09413500
C	-3.28649100	3.83613700	-1.67120400
H	-1.48672800	2.84040000	-1.00406900
C	-5.30164200	2.51073100	-1.59455100
H	-5.08577600	0.50128000	-0.84994700
C	-4.65657500	3.71249600	-1.88451700
H	-2.78017600	4.77569900	-1.88942600
H	-6.37446900	2.41457400	-1.75377400
H	-5.22682200	4.55526900	-2.27210900
H	-3.40593800	-1.67879800	-1.44251300
H	-2.34481700	-0.70139600	-2.46817900
C	1.13335100	-2.30514400	-1.25316300
H	1.15095500	-2.90371000	-0.31974800
H	1.09054000	-3.03439700	-2.08369600
C	-1.26815300	-2.16454500	-1.30687400
H	-1.26719700	-2.90349100	-2.12995500
H	-1.40204400	-2.74505800	-0.37188500
Mn	0.03890400	0.25669700	-0.00264900
C	-0.06853800	-0.66210500	1.48597600
O	-0.15778100	-1.32672100	2.44623100
C	1.83256600	3.79489700	-3.43427000
C	1.39949400	4.89581600	-4.17868700
C	3.18251300	3.43421200	-3.51294200
C	2.28548100	5.62203700	-4.96999200
C	4.07156100	4.15610100	-4.30215700
H	3.54303600	2.57904600	-2.94161100
C	3.62707100	5.25482900	-5.03408400
H	1.92597300	6.47744200	-5.54022800
H	5.11900900	3.85753900	-4.33984100
H	4.32160900	5.82171700	-5.65202200
C	0.87578900	3.01386500	-2.57817600
H	1.10812300	3.14647300	-1.50741400
H	-0.14616900	3.39104000	-2.72077700
C	0.88325800	1.52406700	-2.87686800
H	1.89836200	1.12080900	-2.69495200
H	0.66523400	1.36245600	-3.94658100
O	-0.07891900	0.85499300	-2.10056400
H	0.00911600	-0.27435700	-2.10749200

H	0.34887600	5.18580000	-4.13328100
<b>IM-B2</b>			
N	-0.04194400	-1.49083800	-1.23220300
C	2.38519200	-1.45708200	-1.38571800
H	2.35054000	-0.92764200	-2.34517100
H	3.30321300	-2.05095900	-1.37234500
C	-2.43561900	-1.17965000	-1.48232200
C	0.09383500	1.82731700	0.84961400
O	0.11996200	2.84979900	1.39967300
P	-2.22701300	0.18365900	-0.25105600
P	2.28770500	-0.16036500	-0.07361400
C	3.02782200	-0.93373600	1.42080100
C	2.88788400	-0.24086700	2.62906500
C	3.72080700	-2.14537000	1.41877400
C	3.43613500	-0.74187900	3.80305100
H	2.33368400	0.69430400	2.65240300
C	4.26088700	-2.65494500	2.59760500
H	3.84884500	-2.70990300	0.50058300
C	4.12314800	-1.95372500	3.79056900
H	3.31570600	-0.19234500	4.73162000
H	4.79138400	-3.60249800	2.57978600
H	4.54485400	-2.35195600	4.70853400
C	3.59982000	1.05316100	-0.47784500
C	4.73138600	0.72264200	-1.22950500
C	3.50482200	2.33272800	0.07854200
C	5.74783100	1.65488500	-1.42002000
H	4.82978000	-0.26592400	-1.66869500
C	4.52668900	3.26003500	-0.10197000
H	2.62632700	2.61132300	0.65199300
C	5.65035200	2.92240000	-0.85064100
H	6.61915100	1.38826900	-2.01098600
H	4.43503900	4.25114100	0.33088800
H	6.44267600	3.64941400	-1.00072800
C	-3.21492600	-0.31313900	1.20942800
C	-3.30927200	0.61672100	2.25262500
C	-3.81258900	-1.56397700	1.36654600
C	-3.99902000	0.30692500	3.41732100
H	-2.83541500	1.59021800	2.14978100
C	-4.49933700	-1.87817400	2.53845900
H	-3.74623800	-2.31215600	0.58217200
C	-4.59650900	-0.94408200	3.56333700
H	-4.06539700	1.04060400	4.21502800
H	-4.95787900	-2.85662000	2.64781200
H	-5.13053200	-1.18948000	4.47648500

C	-3.23151600	1.54794700	-0.92942500
C	-2.61288300	2.75603600	-1.24835000
C	-4.61018600	1.40608000	-1.11999800
C	-3.36244000	3.81287900	-1.75855400
H	-1.54343000	2.85015000	-1.10792000
C	-5.35645700	2.45911000	-1.63701900
H	-5.10378200	0.47571500	-0.84948700
C	-4.73189300	3.66416400	-1.95644500
H	-2.87328400	4.75174900	-2.00144700
H	-6.42604900	2.34286000	-1.78499000
H	-5.31646600	4.48801600	-2.35578700
H	-3.42784300	-1.63995400	-1.46339400
H	-2.30599200	-0.70187900	-2.45935000
C	1.14665200	-2.34453000	-1.24644700
H	1.18288800	-2.91114300	-0.30762800
H	1.10585000	-3.06946400	-2.07319300
C	-1.32158800	-2.20484800	-1.26378600
H	-1.33412800	-2.95747200	-2.06641900
H	-1.45158500	-2.73103400	-0.30999400
Mn	0.04056700	0.26114700	0.01575400
C	-0.10790300	-0.64799600	1.54234300
O	-0.23299500	-1.26500500	2.51445900
C	1.83646000	3.87545900	-3.37386200
C	1.34006400	4.80546200	-4.29064100
C	3.20651900	3.59494300	-3.39692300
C	2.18448200	5.44665000	-5.19406800
C	4.05499400	4.23238400	-4.29548300
H	3.61172400	2.86847500	-2.70085600
C	3.54755600	5.16380100	-5.19873700
H	1.77633200	6.16884100	-5.89607200
H	5.11706600	4.00109200	-4.28677400
H	4.20844700	5.66473600	-5.90051100
C	0.92245700	3.15276900	-2.41671100
H	1.25747200	3.29218000	-1.38073500
H	-0.08813700	3.56971900	-2.48985400
C	0.84592500	1.64252200	-2.70833000
H	1.88177700	1.24885100	-2.62801000
H	0.57133200	1.53179600	-3.77413400
O	-0.05179500	0.95370900	-1.92427900
H	-0.00812800	-0.80644000	-2.01241000
H	0.27562000	5.02995600	-4.29520900
<b>TS-B2</b>			
N	-0.02504200	-1.51955700	-1.22280400
C	2.39025300	-1.49676700	-1.44925800

H	2.34034400	-0.93508900	-2.39292300
H	3.31970300	-2.07982700	-1.47013400
C	-2.45869200	-1.30176500	-1.28870600
C	0.19995900	1.58358000	1.15516400
O	0.26922900	2.50826100	1.87231100
P	-2.15638000	0.15291100	-0.19962900
P	2.33863400	-0.23238700	-0.10857700
C	3.09414200	-1.02460000	1.35138200
C	3.16179800	-0.25815600	2.52333500
C	3.52968100	-2.35173000	1.38383300
C	3.66668400	-0.80415500	3.69582800
H	2.80330800	0.77250900	2.51366700
C	4.02804400	-2.90058200	2.56421000
H	3.48096600	-2.97287800	0.49001000
C	4.09847700	-2.12946100	3.71951300
H	3.71253200	-0.19707800	4.59785300
H	4.35976800	-3.93733500	2.57782400
H	4.48479200	-2.56100400	4.64102200
C	3.58372900	1.00482600	-0.59516700
C	4.91264200	0.62305700	-0.82330800
C	3.21528000	2.34284700	-0.75583800
C	5.85056800	1.56504800	-1.22834900
H	5.21301900	-0.41523100	-0.67370400
C	4.15685900	3.28576600	-1.16199500
H	2.18410400	2.64910600	-0.57579400
C	5.47096000	2.89587600	-1.40212500
H	6.88084800	1.26202800	-1.40793800
H	3.84959200	4.32101000	-1.29918200
H	6.20620800	3.63132600	-1.72480400
C	-3.15181400	-0.17533000	1.30409600
C	-3.53723900	0.88312500	2.13664600
C	-3.44512200	-1.48343900	1.70638600
C	-4.21300500	0.63940800	3.32712400
H	-3.31492100	1.90999300	1.84610800
C	-4.12118100	-1.72721400	2.89793400
H	-3.13946300	-2.32852000	1.08965000
C	-4.50977600	-0.66639100	3.71061700
H	-4.51067500	1.47575000	3.95729600
H	-4.34326400	-2.75173200	3.19155900
H	-5.03848400	-0.85641700	4.64300300
C	-2.97952500	1.59150100	-0.94619700
C	-2.59307700	2.87490700	-0.54294700
C	-3.99714400	1.45577900	-1.89602000
C	-3.20488900	4.00135000	-1.08732300

H	-1.79767000	2.99394700	0.19334800
C	-4.60208200	2.58162400	-2.44310300
H	-4.31365800	0.46495600	-2.21900400
C	-4.20648800	3.85685800	-2.04259500
H	-2.88318300	4.99359900	-0.77454500
H	-5.38537300	2.46270800	-3.18973800
H	-4.67785300	4.73639100	-2.47752800
H	-3.41226600	-1.79884400	-1.07290900
H	-2.48092700	-0.90778700	-2.31035700
C	1.15717400	-2.37556200	-1.31068400
H	1.21588000	-2.99058500	-0.39776800
H	1.07433100	-3.07061200	-2.16337300
C	-1.28637600	-2.26416300	-1.13766700
H	-1.32934900	-3.03824000	-1.92279500
H	-1.31851200	-2.78692200	-0.16838600
Mn	0.09983300	0.15990700	0.11214400
C	0.01098900	-0.87979700	1.50006000
O	-0.05720200	-1.61951400	2.40571000
C	0.62810800	4.05486000	-2.84217500
C	1.56613900	4.56216700	-3.74790800
C	0.51722300	4.68678300	-1.59469300
C	2.34436200	5.67453200	-3.43606900
C	1.29837700	5.79231400	-1.27188300
H	-0.20091000	4.30060200	-0.86942200
C	2.21063700	6.29828200	-2.19761500
H	3.05692000	6.05789100	-4.16555300
H	1.18853900	6.26638600	-0.29729900
H	2.81339500	7.17179900	-1.95323200
C	-0.21086300	2.85759800	-3.16070400
H	-1.27544200	3.06544800	-2.98113200
H	-0.11770700	2.58236800	-4.22049500
C	0.13715900	1.59964200	-2.33140700
H	0.10556300	1.96309700	-1.24796000
H	1.22652800	1.38135700	-2.50821600
O	-0.68920300	0.55917200	-2.57380100
H	-0.11448200	-0.83664100	-2.04070400
H	1.67480400	4.07949000	-4.71994200

### IM-B3

N	-0.86315600	0.73743200	2.16594500
C	1.17827000	2.01693000	2.27824600
H	1.70985400	1.13922600	2.67428900
H	1.68361000	2.91620800	2.64916800
C	-2.59366400	-0.93000600	2.12923500
C	-0.45633100	0.30549900	-1.65836300

O	-0.37013900	0.15327500	-2.82035200
P	-2.47857300	-0.77952800	0.30298200
P	1.17835100	1.84840200	0.43761000
C	1.20662000	3.55429000	-0.22787700
C	0.62842300	3.79065900	-1.48041000
C	1.84655900	4.60982200	0.43111600
C	0.68328000	5.05555400	-2.05684200
H	0.12969800	2.97375900	-2.00192800
C	1.89214200	5.87719300	-0.14062000
H	2.32554700	4.44542500	1.39638400
C	1.31036700	6.10201400	-1.38608400
H	0.22853200	5.22390100	-3.03119500
H	2.38832800	6.69048300	0.38604200
H	1.34726900	7.09368700	-1.83375600
C	2.85792600	1.26196300	0.02641200
C	3.96712800	1.63281300	0.79609500
C	3.04517900	0.46182700	-1.10529200
C	5.24261000	1.20718300	0.44103400
H	3.83587100	2.25605100	1.68141000
C	4.32464600	0.04848800	-1.46514700
H	2.18526800	0.14707000	-1.69784600
C	5.42239600	0.41622100	-0.69163000
H	6.09834800	1.49379400	1.05004700
H	4.45498800	-0.58135800	-2.34256600
H	6.42128100	0.08405600	-0.96994900
C	-4.08676800	-0.10306700	-0.25490900
C	-4.13287300	0.60231400	-1.46362400
C	-5.27747600	-0.31217700	0.44945500
C	-5.34039500	1.08530300	-1.95701900
H	-3.20904100	0.78433400	-2.01399500
C	-6.48292000	0.18576800	-0.03613100
H	-5.27265800	-0.87477500	1.38260900
C	-6.51701600	0.88288100	-1.24120600
H	-5.35817400	1.63365000	-2.89706200
H	-7.40018700	0.02266800	0.52734300
H	-7.46085800	1.27024800	-1.62036600
C	-2.55508300	-2.47601500	-0.36839800
C	-2.65211200	-2.62186300	-1.75975200
C	-2.47357700	-3.62157800	0.42893400
C	-2.66466800	-3.88475300	-2.33868800
H	-2.70313800	-1.73668500	-2.39497000
C	-2.48077000	-4.88694500	-0.15514900
H	-2.39349500	-3.53512400	1.51144100
C	-2.57495500	-5.02110000	-1.53645100

H	-2.73514300	-3.98235300	-3.42039500
H	-2.41147300	-5.77041400	0.47686100
H	-2.57552200	-6.01076000	-1.98958000
H	-3.56059700	-1.28487600	2.50405700
H	-1.81225100	-1.64309000	2.43656500
C	-0.26911700	1.95535300	2.73788800
H	-0.83959700	2.83277500	2.39931400
H	-0.32446500	1.92543300	3.83832100
C	-2.20372900	0.42839600	2.68963500
H	-2.18371600	0.40153500	3.79107800
H	-2.90901400	1.21724700	2.38698400
Mn	-0.67164700	0.58216700	0.07221500
C	-1.66310000	2.00454800	-0.17367600
O	-2.31962100	2.97081100	-0.27746300
C	1.74509000	-3.00818600	-0.47617200
C	3.10111300	-3.31819100	-0.62689700
C	0.99979500	-2.72772500	-1.62609500
C	3.68877100	-3.36443700	-1.88762700
C	1.58393200	-2.75920500	-2.88880000
H	-0.05773500	-2.48710800	-1.52105400
C	2.93255600	-3.08315300	-3.02421900
H	4.74446700	-3.61753700	-1.98384600
H	0.98097000	-2.53103500	-3.76690800
H	3.39152200	-3.12132300	-4.01148200
C	1.11732600	-2.91311100	0.87658000
H	0.09223500	-3.30735300	0.87064800
H	1.68225700	-3.50528700	1.60946400
C	1.08041900	-1.47741500	1.44420000
H	0.39492700	-0.88541900	0.61114800
H	2.06923000	-0.98767600	1.24239900
O	0.61209200	-1.35826100	2.65744600
H	-0.24480600	-0.07581100	2.48947800
H	3.69867800	-3.53175700	0.26045000

### TS-B3

N	-0.72348200	0.68607800	2.16131900
C	1.36460900	1.90410400	2.24060300
H	1.91856400	0.98777200	2.48900600
H	1.93112100	2.74895200	2.65165300
C	-2.59440700	-0.83152500	2.04908300
C	-0.47858000	0.62838300	-1.72357100
O	-0.34796500	0.53940700	-2.88963700
P	-2.46660100	-0.59734200	0.22308100
P	1.20977200	1.94290200	0.39791100
C	1.14108600	3.71982600	-0.02952900

C	1.21393000	4.07031600	-1.38508800
C	0.92673200	4.72732400	0.91482700
C	1.08887400	5.39624100	-1.78003600
H	1.36968500	3.29407900	-2.13593800
C	0.79819700	6.05620000	0.51753100
H	0.85232900	4.48453900	1.97433500
C	0.88021400	6.39397100	-0.82894900
H	1.15050600	5.65262400	-2.83623700
H	0.63210700	6.82874900	1.26637400
H	0.77838500	7.43228100	-1.13956100
C	2.87062500	1.48339200	-0.20123300
C	4.00617500	2.19473200	0.20947000
C	3.01377100	0.41599200	-1.08929400
C	5.26564000	1.82567900	-0.24773900
H	3.90010200	3.04782500	0.88129300
C	4.27652700	0.04960000	-1.55111400
H	2.12902700	-0.13176700	-1.41190000
C	5.40096400	0.75165400	-1.12772300
H	6.14459600	2.38073300	0.07623800
H	4.36999700	-0.78818100	-2.24015600
H	6.38874200	0.46559400	-1.48610800
C	-4.10713800	0.03629400	-0.30159400
C	-4.17494500	0.95033100	-1.35796900
C	-5.29945600	-0.42174800	0.27258600
C	-5.40537100	1.41226600	-1.81673600
H	-3.25310500	1.30123200	-1.82094100
C	-6.52839700	0.04751500	-0.17853800
H	-5.27385900	-1.16265700	1.07236300
C	-6.58306100	0.96841800	-1.22284700
H	-5.44123900	2.12570800	-2.63797900
H	-7.44730800	-0.31166100	0.28221700
H	-7.54516400	1.33559800	-1.57584600
C	-2.54165200	-2.29023000	-0.46393100
C	-2.26606700	-2.44875100	-1.82777500
C	-2.85185200	-3.42098800	0.29956400
C	-2.27885300	-3.71109100	-2.41064400
H	-2.02081200	-1.57433800	-2.43249300
C	-2.86231500	-4.68517100	-0.28525500
H	-3.07446500	-3.32445100	1.36158400
C	-2.57043300	-4.83319800	-1.63828700
H	-2.04482900	-3.81967200	-3.46833200
H	-3.09569000	-5.55787300	0.32228500
H	-2.56887100	-5.82319500	-2.09089900
H	-3.60041300	-1.08598100	2.40315300

H	-1.91443800	-1.65634500	2.30839800
C	-0.03851800	1.81195800	2.81477600
H	-0.61740700	2.72639900	2.61718000
H	-0.01124700	1.66498700	3.90722100
C	-2.07131400	0.43694200	2.69671000
H	-2.03817400	0.33201100	3.79374000
H	-2.70496500	1.30451500	2.46181100
Mn	-0.65961800	0.74312500	0.02089500
C	-1.61174700	2.23420500	-0.01797200
O	-2.21246400	3.24165300	-0.00541100
C	1.72049000	-3.04617000	-0.95347900
C	2.97168400	-3.67001400	-0.98142300
C	1.25721300	-2.43943000	-2.12564200
C	3.73145700	-3.70599800	-2.14782400
C	2.01789300	-2.45856400	-3.29139000
H	0.29267200	-1.93476000	-2.11232800
C	3.25502500	-3.10123700	-3.30905800
H	4.69773400	-4.20892600	-2.15019300
H	1.63810300	-1.96894900	-4.18756300
H	3.84582700	-3.12847100	-4.22363000
C	0.91984900	-3.00572400	0.31142400
H	-0.14931900	-3.15524900	0.12084900
H	1.22848300	-3.82765900	0.97452700
C	1.10234800	-1.74270100	1.15715900
H	0.29389100	-0.69708100	0.18550400
H	2.04058200	-1.18225400	0.92923200
O	0.61285400	-1.69788600	2.30856700
H	-0.16531600	-0.16736100	2.36370200
H	3.34862700	-4.14386100	-0.07387100
<b>2b</b>			
C	0.28701200	-0.09480400	-0.35196500
C	-0.28625900	1.12947700	0.00251700
C	-0.53470700	-1.22408500	-0.42693800
C	-1.65026300	1.22715200	0.25915900
C	-1.89822800	-1.13006400	-0.16581600
H	-0.10070800	-2.18546600	-0.70575300
C	-2.46016900	0.09710400	0.17671400
H	-2.08232600	2.19017100	0.52608700
H	-2.52457300	-2.01778700	-0.23443400
H	-3.52737100	0.17278100	0.37697100
C	1.76839300	-0.20729900	-0.57754600
H	1.97300300	-0.91536800	-1.39611700
H	2.22594000	0.74994000	-0.85012100
C	2.47830600	-0.74405000	0.64741300

H	1.97018300	-1.62758700	1.11336600
O	3.49584800	-0.28999500	1.11115200
H	0.34612900	2.01462100	0.07090700
<b><sup>t</sup>BuO-</b>			
O	1.42050600	-0.87614900	-0.40097100
C	2.70029500	-1.09519700	-0.19443100
C	3.62017400	-0.16766100	-1.06453300
C	3.12143100	-0.85043500	1.29781200
C	3.12206200	-2.56839700	-0.53077700
H	3.38248200	-0.32979000	-2.12726200
H	3.38028000	0.88246700	-0.83714700
H	4.71170400	-0.30799300	-0.93098400
H	2.51870200	-1.50435200	1.94667800
H	4.19089100	-1.02336300	1.53297100
H	2.87573000	0.18780200	1.56890000
H	4.19196600	-2.81278900	-0.37427000
H	2.52062700	-3.25641900	0.08308700
H	2.87464300	-2.77495000	-1.58331700
<b>IM-C1</b>			
O	2.64350600	-1.08579500	2.09387700
C	0.82738300	-2.10693000	0.89991400
C	0.43812800	-0.97670400	0.09746600
C	0.12534400	-3.32544000	0.77123200
C	-0.66173800	-1.15376600	-0.80119900
C	-0.92853000	-3.47383600	-0.10033200
H	0.45282100	-4.16059200	1.39755000
C	-1.31043500	-2.35964800	-0.88638700
H	-0.93676300	-0.27822800	-1.39465800
H	-1.45783800	-4.42186000	-0.18689100
H	-2.14568700	-2.46171600	-1.58215200
C	1.91343400	-2.04685300	1.83599300
H	2.08116800	-3.02102300	2.37542300
N	1.04011500	0.21017700	0.14282900
H	0.62621900	1.03187400	-0.50173300
H	1.80692200	0.29200300	0.80096400
O	-0.10303100	1.88944700	-1.43727600
C	-0.81898200	2.86647000	-0.81484600
C	0.10867900	3.82470700	-0.03009900
C	-1.58078700	3.69693700	-1.86800100
C	-1.85438500	2.28752700	0.17810600
H	0.64057600	3.26932400	0.75596800
H	0.86534100	4.23662000	-0.71205700
H	-0.41961900	4.66609700	0.45092400
H	-2.25072100	3.03749000	-2.43671600

H	-2.18217000	4.51544600	-1.43663400
H	-0.86514200	4.13016500	-2.58018000
H	-2.44874900	3.05896100	0.69785000
H	-2.54919400	1.62429500	-0.35639700
H	-1.34467600	1.68081300	0.93959600
<b>TS-C1</b>			
O	1.75272400	1.32505200	1.75307600
C	-0.06165300	0.29365100	0.56496100
C	-0.45761500	1.42082600	-0.23964500
C	-0.75822700	-0.92851300	0.44057300
C	-1.55877500	1.23475500	-1.13574100
C	-1.81301800	-1.08461400	-0.42847900
H	-0.42547200	-1.76053400	1.06837600
C	-2.20175300	0.02573200	-1.21680900
H	-1.83946400	2.10615000	-1.73215400
H	-2.33776700	-2.03547000	-0.51166300
H	-3.03756000	-0.08222300	-1.91107500
C	1.02594100	0.36049100	1.49856100
H	1.19878800	-0.61190200	2.03976000
N	0.13741200	2.61084800	-0.19922400
H	-0.28310600	3.43470900	-0.85351100
H	0.90635500	2.69468900	0.45655800
O	-0.99854500	4.28134400	-1.77735700
C	-1.71449300	5.25820400	-1.15198400
C	-0.78616300	6.21353800	-0.36528800
C	-2.47417200	6.09008200	-2.20462100
C	-2.75036500	4.67712300	-0.16145000
H	-0.25501000	5.65639000	0.41988500
H	-0.02911400	6.62651500	-1.04611100
H	-1.31444100	7.05406100	0.11704700
H	-3.14412900	5.43214900	-2.77495900
H	-3.07512400	6.90807600	-1.77196200
H	-1.75766100	6.52414000	-2.91536300
H	-3.34447200	5.44810200	0.35905000
H	-3.44512100	4.01545700	-0.69784800
H	-2.24164800	4.06879300	0.59926300
<b><sup>t</sup>BuOH</b>			
H	1.15470900	-0.01316800	-0.17619500
O	1.38104900	-0.92704900	-0.40005100
C	2.78473700	-1.08136900	-0.15748500
C	3.57045600	-0.12574800	-1.04992900
C	3.08724600	-0.81659200	1.31404400
C	3.08383600	-2.52617500	-0.51774300
H	3.32389000	-0.29649400	-2.10387000

H	3.33227900	0.92005400	-0.81131200
H	4.65315400	-0.25156100	-0.92336000
H	2.48896700	-1.47625100	1.95249000
H	4.14746400	-0.98093900	1.54499700
H	2.85083000	0.22197800	1.58382900
H	4.14471200	-2.75712400	-0.36725300
H	2.48866600	-3.20507900	0.10291600
H	2.83152200	-2.71822700	-1.56639800

**IM-C2**

O	2.32137600	1.17552500	1.04958100
C	0.17684900	0.20605600	0.52456500
C	-0.32260100	1.22746300	-0.41019300
C	-0.61433200	-0.92354000	0.83317700
C	-1.64550700	0.94746600	-0.94470700
C	-1.86261200	-1.13692200	0.29570000
H	-0.18884500	-1.64920600	1.53682100
C	-2.36770100	-0.16382000	-0.61299000
H	-2.03943300	1.68865000	-1.64228300
H	-2.44981600	-2.01842100	0.55260800
H	-3.35779500	-0.31139300	-1.05451900
C	1.45401800	0.29499800	1.15511200
H	1.65977400	-0.58381800	1.83730000
N	0.29002600	2.32270000	-0.79164100
H	1.19520700	2.33784100	-0.31275800

**TS-C2**

O	2.30497800	-3.25760000	-1.44459200
C	0.93896000	-1.98789100	-2.96462600
C	0.49810000	-0.93989600	-2.05712400
C	0.52029800	-1.97987000	-4.31010300
C	-0.37476000	0.04909000	-2.63601900
C	-0.31591300	-1.01345000	-4.82463800
H	0.88829000	-2.78864200	-4.95004000
C	-0.76116700	0.00701800	-3.95174800
H	-0.72212700	0.85117700	-1.98434500
H	-0.62502300	-1.02826100	-5.86857200
H	-1.42608500	0.78479300	-4.33419700
C	1.80511400	-3.05663200	-2.55365900
H	2.02681100	-3.77928300	-3.39118200
N	0.84628100	-0.83178900	-0.78445400
H	1.38001300	-1.64206200	-0.46761000
C	-0.46362900	1.85976400	2.01516800
C	-1.02303300	3.12055100	1.78191500
C	-0.59289100	1.30971300	3.30008200
C	-1.67774800	3.82041500	2.79370100

C	-1.24953300	2.00354400	4.30975000
H	-0.19427300	0.31052700	3.46651000
C	-1.79204600	3.26542000	4.06551000
H	-2.10082100	4.80409500	2.58657700
H	-1.34306200	1.55507400	5.29945500
H	-2.30199100	3.81007100	4.86021100
C	0.24302800	1.09779000	0.93308300
H	0.26855000	1.67923900	0.00158300
H	1.28473000	0.90809800	1.22152300
C	-0.39211300	-0.28476400	0.68695800
H	-1.25285500	-0.23211900	-0.02709900
O	-0.35629900	-1.14652200	1.57392000
H	-0.93630600	3.55928700	0.78623300

### IM-C3

O	2.27808800	-3.33194200	-1.53097600
C	0.94210100	-1.99753400	-3.01889500
C	0.41967900	-1.04378200	-2.06669300
C	0.58552200	-1.90108900	-4.37677700
C	-0.44967000	-0.03413700	-2.59196400
C	-0.26052600	-0.92222300	-4.85234600
H	1.00974900	-2.64525500	-5.05724600
C	-0.77370100	0.01119400	-3.92794200
H	-0.85537200	0.70427500	-1.90446100
H	-0.52374000	-0.86521200	-5.90706500
H	-1.44327500	0.79866000	-4.27887900
C	1.83201400	-3.06607700	-2.64666800
H	2.12725500	-3.70803100	-3.52385000
N	0.72652900	-1.07152800	-0.76989100
H	1.26304200	-1.87894600	-0.45980600
C	-0.17669300	1.76015000	1.70943700
C	-0.77554500	2.99434400	1.43207600
C	-0.28626400	1.25358100	3.01571100
C	-1.44455500	3.71500500	2.42003400
C	-0.95911300	1.96800200	4.00001700
H	0.12736300	0.26387300	3.20069100
C	-1.53574000	3.20637200	3.71320300
H	-1.89590600	4.67844300	2.17783200
H	-1.03908800	1.55410900	5.00641100
H	-2.05391800	3.76827200	4.49107500
C	0.52610800	0.96783700	0.65843700
H	0.55292600	1.52949000	-0.28970800
H	1.56788100	0.77703600	0.95243500
C	-0.10931000	-0.45792700	0.46246400
H	-1.12335000	-0.29509400	-0.02126700

O	-0.04119700	-1.24646400	1.46208300
H	-0.70764300	3.39634500	0.41869100
<b>TS-C3</b>			
O	2.48286300	-3.28435400	-1.77790200
C	0.90399500	-1.84835800	-2.91537900
C	0.28930600	-1.16183300	-1.80189800
C	0.56525000	-1.49621600	-4.23075400
C	-0.60553100	-0.09851700	-2.15089800
C	-0.32954500	-0.48685800	-4.53395300
H	1.05948600	-2.05029000	-5.03361600
C	-0.90427800	0.21185300	-3.46251800
H	-1.09496500	0.46348800	-1.35965400
H	-0.57121200	-0.23448900	-5.56483300
H	-1.61128500	1.01988500	-3.66090200
C	1.94865900	-2.85316000	-2.78571300
H	2.28510500	-3.22656800	-3.79749200
N	0.55822500	-1.51683500	-0.53283500
H	0.63694100	-2.66956400	-0.22085100
C	-0.18385000	1.51695300	1.63318400
C	-0.69689400	2.71279000	1.11953300
C	-0.45098200	1.20691000	2.97446800
C	-1.44436200	3.58056600	1.91287700
C	-1.19894400	2.07005200	3.76805300
H	-0.08050400	0.26259400	3.36784300
C	-1.69733900	3.26258800	3.24411200
H	-1.83112300	4.50746000	1.48853800
H	-1.39863900	1.80909800	4.80764600
H	-2.28291700	3.93659000	3.86930600
C	0.59992200	0.58150400	0.76169100
H	0.77239000	1.04649200	-0.21768200
H	1.58569100	0.36786200	1.19593500
C	-0.06947900	-0.79208600	0.56577600
H	-1.15200700	-0.62823400	0.34884100
O	0.06663200	-1.50655400	1.75785600
H	-0.50124300	2.96272500	0.07496700
H	0.11214800	-2.48281800	1.50034900
O	0.39458200	-3.76680300	0.51868700
C	-0.73256800	-4.46528300	0.10650000
C	-0.52365400	-5.01593300	-1.31085000
C	-0.94406800	-5.63596800	1.07491200
C	-1.99115600	-3.57756200	0.11629500
H	-0.42969700	-4.19036200	-2.02972800
H	0.40853500	-5.59289400	-1.34915900
H	-1.35513300	-5.65875400	-1.64081900

H	-1.09377500	-5.25525400	2.09409300
H	-1.81319400	-6.25732600	0.80713000
H	-0.05033900	-6.27257700	1.08682500
H	-2.90168500	-4.13691600	-0.14921700
H	-2.13630600	-3.13475700	1.11115300
H	-1.88608800	-2.75264400	-0.60169400

**IM-C4**

O	1.17345000	-3.56601200	-2.18127100
C	0.48708500	-1.51057700	-3.26540000
C	-0.10894900	-0.78529900	-2.14554400
C	0.53978900	-0.92352000	-4.54539900
C	-0.59546700	0.53950200	-2.47963000
C	0.04910100	0.33496000	-4.81852900
H	0.99971200	-1.51640000	-5.34228100
C	-0.52472800	1.05727800	-3.74907400
H	-1.04945700	1.14235400	-1.69489400
H	0.10709500	0.76393700	-5.81766200
H	-0.92084200	2.05946700	-3.93248200
C	1.06354700	-2.81879700	-3.15934000
H	1.47006400	-3.18035200	-4.14576800
N	-0.17251000	-1.34421600	-0.95276500
H	0.58031500	-3.29663900	-0.30614400
C	-0.23858700	1.36424200	1.69264500
C	-0.51618000	2.69455700	1.35399100
C	-0.53685000	0.94513200	2.99674800
C	-1.05796800	3.58164500	2.28034300
C	-1.07682000	1.82840000	3.92565800
H	-0.35680700	-0.09534900	3.25997600
C	-1.33812100	3.15294300	3.57495800
H	-1.25917400	4.61347700	1.99050000
H	-1.29819000	1.48039000	4.93519700
H	-1.75832100	3.84408100	4.30550000
C	0.31077000	0.41905300	0.67338000
H	0.72490200	0.98326600	-0.17430700
H	1.12683700	-0.18821900	1.08898700
C	-0.73333300	-0.59422200	0.12617400
H	-1.64970200	-0.03024400	-0.14724700
O	-1.13239900	-1.46878900	1.16698700
H	-0.29251500	3.03507700	0.34104700
H	-0.54289800	-2.25370600	1.06918200
O	0.41586200	-3.73203200	0.56804800
C	-0.51817600	-4.79049500	0.34378300
C	0.21488400	-5.97910100	-0.27510700
C	-1.05803700	-5.14913100	1.72177300

C	-1.65015800	-4.32147600	-0.56630900
H	0.65829700	-5.68264400	-1.23186900
H	1.02276300	-6.31396900	0.38855400
H	-0.46567600	-6.82637700	-0.44551800
H	-1.59152400	-4.29479600	2.15699500
H	-1.75122600	-5.99908300	1.66689000
H	-0.23459300	-5.41677800	2.39606200
H	-2.40164500	-5.11352800	-0.69877100
H	-2.13193900	-3.43307500	-0.14176300
H	-1.25461200	-4.03964600	-1.54841200

**IM-C5**

O	1.87500900	-2.53874400	-3.15940300
C	0.39037700	-0.85023400	-4.07184400
C	-0.17583600	-0.27098000	-2.86101900
C	-0.01946200	-0.38786800	-5.33238600
C	-1.16918300	0.75384400	-3.08918100
C	-0.96768400	0.60373000	-5.50680100
H	0.44523000	-0.85838300	-6.20490200
C	-1.54293900	1.16112400	-4.34989700
H	-1.65121600	1.21283700	-2.22649400
H	-1.26270800	0.94028300	-6.49955400
H	-2.30433300	1.93907900	-4.44984000
C	1.36596300	-1.92063900	-4.08518500
H	1.65734200	-2.18584300	-5.14745700
N	0.22508000	-0.69017000	-1.67228000
H	1.21080400	-0.84641100	1.82096000
C	-0.54120300	1.90080800	1.00062100
C	-1.73425100	2.58654800	0.73217300
C	-0.11093300	1.82822800	2.33061200
C	-2.46941600	3.18526300	1.75012500
C	-0.84282000	2.42993100	3.35105700
H	0.79629400	1.27019200	2.56738700
C	-2.02360300	3.11308500	3.06841100
H	-3.39175000	3.71632100	1.51287100
H	-0.48602100	2.36232400	4.37958400
H	-2.59266700	3.58572500	3.86882000
C	0.20343900	1.23515800	-0.11396300
H	0.16644100	1.86434200	-1.01496600
H	1.26211500	1.08888700	0.13700700
C	-0.36610100	-0.14567400	-0.51235900
H	-1.47625000	-0.06196700	-0.55048500
O	-0.06739700	-1.09145100	0.54825900
H	-2.08055800	2.65444800	-0.30124000
H	0.38681300	-1.77615300	0.01686800

O	1.83484500	-0.87271400	2.58520800
C	1.27915900	-1.78264800	3.52620700
C	1.16739000	-3.17424100	2.90284300
C	2.25321000	-1.80303600	4.69515200
C	-0.09884100	-1.30355100	3.97935800
H	0.44274300	-3.16799200	2.07956100
H	2.13814800	-3.49092100	2.50322900
H	0.83319200	-3.92119100	3.63664200
H	2.36103000	-0.79636100	5.11699900
H	1.90725900	-2.47749200	5.48913600
H	3.24345500	-2.13600300	4.36151700
H	-0.55076700	-1.99890700	4.70102300
H	-0.02772900	-0.31547800	4.45071100
H	-0.76900800	-1.21555200	3.11542300

**TS-C4**

O	3.18582000	-2.62308200	-5.32577800
C	1.41991600	-1.70308100	-6.68853500
C	1.04782200	-0.58320300	-5.88987900
C	0.67989000	-2.01835300	-7.83747000
C	-0.10493600	0.13344400	-6.28271200
C	-0.43812500	-1.29125100	-8.21157100
H	1.00106900	-2.87996200	-8.42833800
C	-0.82909100	-0.21059700	-7.41191500
H	-0.39477300	0.99213300	-5.67671000
H	-1.00309500	-1.55530200	-9.10389700
H	-1.71001800	0.37296700	-7.68233700
C	2.51951600	-2.59971000	-6.34426100
H	2.71528500	-3.35721100	-7.15597000
N	1.82274700	-0.14509200	-4.85277900
H	2.07846600	-1.81034000	-1.62236400
C	1.06920100	1.42878100	-1.63812900
C	0.30280900	2.54863500	-1.97994800
C	0.88999800	0.84417000	-0.38009500
C	-0.61991500	3.08430300	-1.08503100
C	-0.03412700	1.38131300	0.51342000
H	1.49110300	-0.04322600	-0.13985200
C	-0.79081600	2.49986000	0.16864400
H	-1.20728100	3.95919500	-1.36603500
H	-0.16698400	0.91627300	1.49133400
H	-1.51301600	2.91570800	0.87202900
C	2.02418700	0.82233200	-2.62970700
H	2.59628700	1.60728900	-3.14697700
H	2.74487900	0.17839800	-2.11363800
C	1.29592700	0.02379200	-3.68207400

H	0.22872000	-0.16127800	-3.50293700
O	1.43931100	-1.95230200	-2.64127900
H	0.43414100	3.00417800	-2.96457500
H	2.09880800	-2.21924800	-3.30235900
O	2.69847300	-1.66766400	-0.56940400
C	2.42448600	-2.77106600	0.22299400
C	2.88565100	-4.05711200	-0.48411300
C	3.17799400	-2.61605400	1.54709100
C	0.91490900	-2.88281100	0.50535300
H	2.35191800	-4.15128000	-1.43859800
H	3.95969600	-3.99532400	-0.70482700
H	2.70425100	-4.96640300	0.11154300
H	2.85423600	-1.69670900	2.05460000
H	3.01448500	-3.46391000	2.23125300
H	4.25558600	-2.52687500	1.35596500
H	0.65326600	-3.77796400	1.09284000
H	0.56618000	-2.00032500	1.06070400
H	0.37198500	-2.91538400	-0.44764300
<b>H<sub>2</sub>O</b>			
O	-1.04838706	-0.17473118	0.00000000
H	-0.08838706	-0.17473118	0.00000000
H	-1.36884165	0.73020465	0.00000000
<b>IM-C6</b>			
O	3.85245300	-2.16000500	-5.90989600
C	1.68574900	-1.65560200	-6.88577000
C	1.13456000	-0.70829700	-5.94686500
C	0.93717500	-2.04049000	-8.01100900
C	-0.16436700	-0.20156800	-6.27069400
C	-0.32708200	-1.54945700	-8.27833300
H	1.39746900	-2.76343300	-8.69066500
C	-0.86618500	-0.60898400	-7.38508600
H	-0.58581400	0.57051300	-5.62903400
H	-0.87973700	-1.86401100	-9.16223400
H	-1.84916700	-0.17626800	-7.58316100
C	2.99445500	-2.28311900	-6.76857000
H	3.18502500	-2.98007900	-7.63845100
N	1.84673700	-0.29636400	-4.87921800
C	1.18435200	1.51542700	-1.66492200
C	-0.18173900	1.32879900	-1.33753200
C	1.93714400	2.30330200	-0.76170400
C	-0.74326000	1.90097100	-0.20649700
C	1.37170000	2.87140100	0.36992500
H	2.99703800	2.45707100	-0.97256500
C	0.02059500	2.68290500	0.66289100

H	-1.79985900	1.72890800	0.00573700
H	1.99515200	3.47030200	1.03540600
H	-0.42586300	3.12645000	1.55216500
C	1.82648700	0.95153200	-2.82448500
H	2.89277300	1.15959000	-2.94826000
H	2.74949100	-0.48101100	-1.32735000
C	1.20890700	0.24671100	-3.83668100
H	0.11920200	0.07970100	-3.73596000
H	-0.80652600	0.71446100	-1.98543200
O	3.13942600	-1.13582400	-0.71940500
C	2.88081200	-2.41296600	-1.30518500
C	3.55378200	-2.51464100	-2.66877900
C	3.47362200	-3.41724100	-0.32809500
C	1.37245900	-2.61949600	-1.43553600
H	3.16082900	-1.77775100	-3.38207300
H	4.63391600	-2.34625800	-2.57258700
H	3.40595100	-3.50506400	-3.12131800
H	3.00424900	-3.31831900	0.65887000
H	3.32758200	-4.44533700	-0.68329300
H	4.54993600	-3.24192600	-0.20995500
H	1.13247000	-3.62079500	-1.81974100
H	0.88314600	-2.48958300	-0.46179100
H	0.94822400	-1.88499700	-2.13227200

#### IM-C7

O	3.85235500	-2.16181100	-5.90085700
C	1.69458500	-1.64532000	-6.89176600
C	1.13022600	-0.71085100	-5.94333500
C	0.95222300	-2.02970500	-8.02174200
C	-0.18229300	-0.22892700	-6.26240100
C	-0.31953600	-1.55746400	-8.28585000
H	1.42427200	-2.74017000	-8.70705800
C	-0.87571700	-0.63628800	-7.38083400
H	-0.61799900	0.52815700	-5.61227800
H	-0.86653000	-1.87188000	-9.17357900
H	-1.86650100	-0.21888500	-7.57499300
C	3.00346200	-2.26895200	-6.77128500
H	3.20296600	-2.95246900	-7.65167800
N	1.83851800	-0.29320500	-4.88008700
C	1.18061600	1.52006600	-1.67137800
C	-0.19308300	1.36466600	-1.34889800
C	1.94378100	2.28625900	-0.75455300
C	-0.74463700	1.93029600	-0.21045100
C	1.38716200	2.85073600	0.38309100
H	3.00516000	2.42995800	-0.96545000

C	0.03208300	2.68330600	0.67474200
H	-1.80649600	1.78019900	-0.00569500
H	2.02014900	3.43367400	1.05477500
H	-0.40794800	3.12526700	1.56815100
C	1.81048200	0.96759200	-2.83556200
H	2.88126300	1.14979000	-2.94748600
C	1.19822000	0.24429700	-3.83332300
H	0.11176800	0.06100200	-3.72512100
H	-0.83117600	0.78102900	-2.01200100

### TS-C5

O	3.80039300	-2.83091600	-7.18449400
C	1.54994800	-1.96036900	-7.38343300
C	1.47198400	-1.12082300	-6.21848200
C	0.45286800	-2.05746400	-8.25710300
C	0.23376600	-0.44215300	-6.02674200
C	-0.73486300	-1.38602300	-8.03698500
H	0.56454200	-2.70176100	-9.13451800
C	-0.83024100	-0.57208200	-6.89742700
H	0.15841800	0.19741100	-5.14795900
H	-1.57225900	-1.48390800	-8.72649900
H	-1.75933600	-0.03644500	-6.69164200
C	2.72961600	-2.73374400	-7.75572700
H	2.56271300	-3.29370700	-8.72452500
N	2.50202100	-0.87292700	-5.39041000
C	4.12428900	-1.96612300	-2.20953600
C	3.35839600	-3.06199200	-1.72022500
C	5.22973600	-1.59304100	-1.39641500
C	3.67480900	-3.71337200	-0.54040500
C	5.54057500	-2.24960600	-0.21587100
H	5.84948500	-0.75694100	-1.72792300
C	4.77021300	-3.32403200	0.23742500
H	3.05097900	-4.54922000	-0.21527600
H	6.40444300	-1.91789800	0.36489400
H	5.01457100	-3.84090100	1.16505800
C	3.83861100	-1.25514500	-3.41368000
H	4.49008400	-0.41479900	-3.66220900
C	2.80672500	-1.54133300	-4.29295500
H	2.17031200	-2.40926900	-4.04367600
H	2.49341600	-3.40050100	-2.29053200

### IM-C8

O	1.21348800	1.58290000	1.91919600
C	2.91152200	0.71540000	0.43279100
C	2.34362300	-0.55341700	0.02273500
C	4.24764600	1.01682900	0.09675100

C	3.26206000	-1.46548900	-0.58892800
C	5.07673900	0.13857500	-0.56899300
H	4.62835900	1.99288200	0.41334300
C	4.56225900	-1.13295100	-0.89127800
H	2.85999100	-2.44369700	-0.85201600
H	6.10343700	0.40697600	-0.81443200
H	5.19849900	-1.86356400	-1.39550200
C	2.27558700	1.67130200	1.32046400
H	2.92046300	2.58702300	1.46997300
N	1.09428500	-1.00854700	0.20703400
C	-1.55321200	1.48606600	-0.79331700
C	-2.77653100	0.99775600	-0.26415000
C	-1.65103500	2.66561700	-1.57481200
C	-3.98204300	1.63887300	-0.50032800
C	-2.85932400	3.30444200	-1.80689200
H	-0.73245200	3.07618300	-1.99828700
C	-4.04808800	2.80109100	-1.27462600
H	-4.89570100	1.22475300	-0.06888000
H	-2.87575500	4.21157000	-2.41427000
H	-4.99971600	3.30065600	-1.45384600
C	-0.27455500	0.87388900	-0.58793900
H	0.57600600	1.37779800	-1.05367700
C	-0.02901500	-0.29246300	0.10138600
H	-0.89566600	-0.79783200	0.54943900
H	-2.76796900	0.09822200	0.35052200

**TS-C6**

O	2.41322200	2.23235300	2.21226400
C	2.73300400	0.74916200	0.35663200
C	2.63002800	-0.64447600	0.59974500
C	3.65446000	1.20104700	-0.58355100
C	3.42771300	-1.52210000	-0.15471200
C	4.43256900	0.32136100	-1.33841300
H	3.74072300	2.27890800	-0.74335300
C	4.30846500	-1.05021000	-1.12060500
H	3.33266300	-2.58982300	0.04623100
H	5.12183800	0.70308700	-2.09271500
H	4.90610600	-1.75490300	-1.70154100
C	1.93674500	1.78592900	1.14120800
H	1.43416500	2.49422000	0.41822700
N	1.85125600	-1.17202300	1.62827000
C	-0.69918600	1.50757800	2.01540100
C	-1.79045600	2.07560900	1.33056400
C	-0.57072700	1.80938300	3.38777100
C	-2.72773200	2.86424700	1.98537300

C	-1.51316900	2.59308200	4.04183600
H	0.31390100	1.45335600	3.91437100
C	-2.60504400	3.12140200	3.35217700
H	-3.56827100	3.27986700	1.42664200
H	-1.38566700	2.81159100	5.10348700
H	-3.34229600	3.73670600	3.86831200
C	0.31395300	0.71127700	1.34976800
H	0.16901100	0.57410500	0.27234500
C	0.83809300	-0.45369700	2.01431100
H	0.38411100	-0.74751800	2.97457700
H	-1.89779900	1.87609400	0.26220800

**IM-C9**

O	1.14265800	1.15367000	0.80745600
C	1.53675300	-0.24717800	-1.02850500
C	1.49296000	-1.62959800	-0.74522900
C	2.53852400	0.22700400	-1.87364500
C	2.43413500	-2.49001400	-1.33015400
C	3.45487000	-0.63287900	-2.47514200
H	2.57734000	1.30118100	-2.07120000
C	3.40048500	-2.00231100	-2.20153900
H	2.37651100	-3.55102900	-1.08341800
H	4.20823700	-0.24103800	-3.16076500
H	4.11595700	-2.68462300	-2.66269300
C	0.60956500	0.72539500	-0.29975700
H	0.30144800	1.51591300	-1.06125800
N	0.57447000	-2.18041500	0.16157000
C	-1.78278700	0.63695300	0.64612000
C	-2.97799000	1.10156600	0.08799100
C	-1.50018700	0.95889200	1.98509700
C	-3.88423800	1.84409500	0.84149100
C	-2.40254900	1.70682000	2.73564200
H	-0.53014100	0.65903400	2.37856200
C	-3.60139300	2.14578300	2.17341500
H	-4.81636900	2.18601800	0.38923000
H	-2.16648200	1.95801600	3.77072300
H	-4.31026700	2.72308100	2.76820400
C	-0.77700000	-0.13038300	-0.12120900
H	-1.11754000	-0.31001400	-1.15641800
C	-0.42884800	-1.44097100	0.49004900
H	-1.06815900	-1.81932900	1.30217100
H	-3.19780100	0.86970300	-0.95640700

**IM-C10**

O	1.07437200	1.25830000	0.67520800
C	1.61306400	0.26807900	-1.40094300

C	1.77802400	-1.13088000	-1.34895300
C	2.51908700	1.01948600	-2.14665200
C	2.81924500	-1.73983600	-2.06111900
C	3.53987400	0.41010100	-2.87215000
H	2.41853500	2.10602700	-2.14528800
C	3.68801000	-0.97794300	-2.83291200
H	2.92323400	-2.82258300	-1.98821400
H	4.22495200	1.01704800	-3.46522800
H	4.48980100	-1.46170600	-3.39172900
C	0.56940300	0.94425700	-0.51726700
H	0.15857600	1.81814500	-1.10269400
N	0.97110400	-1.95134500	-0.53967400
C	-1.72454400	0.38580800	0.47128100
C	-2.99273400	0.74606800	0.00874400
C	-1.46005300	0.48752000	1.84568800
C	-3.98057800	1.18835200	0.88621800
C	-2.44397600	0.93373000	2.72228500
H	-0.45265300	0.25526400	2.18541300
C	-3.70889400	1.28146000	2.24943400
H	-4.96549200	1.45974700	0.50418700
H	-2.22095600	1.01676700	3.78649000
H	-4.47897500	1.62588800	2.94034000
C	-0.64480400	-0.07787300	-0.44351900
H	-1.03353600	-0.14885200	-1.47704600
C	-0.11050700	-1.43044300	-0.08272600
H	-0.69156300	-2.04238900	0.62226100
H	-3.20468200	0.67748400	-1.06032900
H	2.46386000	2.19489400	0.59494900
O	3.37013800	2.63049900	0.63071700
C	4.12891600	1.83720500	1.51892000
C	4.13771300	0.37619600	1.06539000
C	5.53958800	2.41220000	1.49955200
C	3.53303200	1.93181700	2.92692100
H	3.10773200	-0.00129900	1.05268400
H	4.53533000	0.29492800	0.04511400
H	4.74680000	-0.25463100	1.73075900
H	5.52554700	3.46868200	1.79793400
H	6.20710300	1.86673700	2.18125000
H	5.95626100	2.35429800	0.48602400
H	4.10263900	1.34168500	3.66124600
H	3.51562700	2.97762500	3.26127100
H	2.50064700	1.56236200	2.90778300
<b>TS-C7</b>			
O	0.17668500	-2.14402100	-1.89136700

C	-1.67870600	-0.90556600	-0.97564200
C	-2.07954600	-1.40934800	0.28385000
C	-2.64356400	-0.52394700	-1.90373300
C	-3.45255400	-1.52745900	0.55180100
C	-4.00419900	-0.63407300	-1.62167700
H	-2.31401500	-0.11142800	-2.86105900
C	-4.40301900	-1.14549500	-0.38560200
H	-3.74357400	-1.90813100	1.53060900
H	-4.74581200	-0.31651000	-2.35447600
H	-5.46410300	-1.23484300	-0.14901800
C	-0.21320500	-0.87932200	-1.30715500
H	-0.00176100	-0.06679700	-2.02427300
N	-1.17959700	-1.76444900	1.28589600
C	2.07436600	-0.72109000	-0.22573700
C	2.77107900	-1.92846200	-0.08416300
C	2.80349600	0.43368400	-0.54590000
C	4.15172500	-1.98676000	-0.25136900
C	4.18339600	0.37250400	-0.72210100
H	2.24913500	1.37316200	-0.61942400
C	4.86548400	-0.83444400	-0.57475500
H	4.67253500	-2.93882200	-0.13787500
H	4.73623200	1.28063700	-0.96754500
H	5.94715000	-0.87747600	-0.70921800
C	0.58714700	-0.65167600	-0.04198200
H	0.33494600	0.55514900	0.11878000
C	0.06121000	-1.41891200	1.07417100
H	0.76081500	-1.66016200	1.88743900
H	2.20587200	-2.83390000	0.13997900
H	-0.48918400	-2.33655300	-2.56753900
O	0.16634400	1.96889000	-0.12144200
C	-0.25107800	2.57337300	1.04085400
C	-0.47063400	4.06867800	0.75631300
C	-1.57677600	1.96797000	1.54342600
C	0.80866900	2.43495600	2.15325300
H	0.46197800	4.51537900	0.38607800
H	-1.22983900	4.18896400	-0.02768000
H	-0.79724900	4.63195800	1.64589200
H	-1.44053900	0.91281600	1.81857500
H	-1.98406000	2.49431900	2.42254000
H	-2.32595100	1.99984100	0.74040700
H	0.51544600	2.92188500	3.09813100
H	0.99502900	1.37294500	2.36649400
H	1.75869300	2.87408100	1.81861500

IM-C11

O	-0.01444400	-2.86015100	-1.42075800
C	-1.64528900	-1.22089700	-0.67281300
C	-2.05291100	-1.29387700	0.68788400
C	-2.59846400	-1.01049200	-1.67174000
C	-3.43836800	-1.21449700	0.96059500
C	-3.95577200	-0.91079200	-1.38085800
H	-2.25488500	-0.92082200	-2.70746100
C	-4.36833200	-1.03090500	-0.04756400
H	-3.74277700	-1.27287100	2.00603700
H	-4.68304100	-0.74483700	-2.17541400
H	-5.42904000	-0.96243600	0.20108400
C	-0.20790700	-1.45954300	-1.02278800
H	0.07100700	-0.84264000	-1.90241900
N	-1.17917800	-1.35790200	1.74358300
C	2.09950300	-0.96468000	-0.07538500
C	2.71060900	-1.32200400	-1.30091700
C	2.94974100	-0.39179600	0.90059100
C	4.06582900	-1.12061700	-1.52723400
C	4.30577100	-0.20789500	0.67498900
H	2.52458600	-0.06243900	1.84836000
C	4.88450700	-0.56546400	-0.54405200
H	4.49460700	-1.41797700	-2.48609800
H	4.91969600	0.24118000	1.45792100
H	5.94865200	-0.41185000	-0.72255700
C	0.67692300	-1.15590900	0.13806700
H	0.18821200	0.99225700	-0.18019800
C	0.10874000	-1.23988800	1.41065800
H	0.78841500	-1.19990100	2.27239500
H	2.10239300	-1.80903000	-2.06139900
H	-0.78197000	-3.06825800	-1.97586900
O	0.10420900	1.92887200	-0.45223100
C	-0.32392700	2.66147500	0.68947400
C	-0.33949400	4.11497800	0.23910100
C	-1.71826100	2.21302600	1.12066600
C	0.66617400	2.46395400	1.83607100
H	0.65939000	4.42179000	-0.09455600
H	-1.03087300	4.24341500	-0.60256200
H	-0.65626200	4.77937300	1.05355700
H	-1.69784600	1.17777600	1.48446700
H	-2.11084000	2.84586800	1.93004000
H	-2.41355900	2.25971600	0.27315200
H	0.40561800	3.07749100	2.71029600
H	0.66494900	1.41222600	2.15304100
H	1.68299100	2.72070300	1.51400700

**IM-C12**

C	-1.08361200	0.83334200	-0.24018700
C	-1.92407500	0.55647600	0.87454900
C	-1.65133200	1.17352000	-1.47065000
C	-3.32285900	0.59448000	0.66540500
C	-3.02827100	1.23208600	-1.64723200
H	-0.98639400	1.37184400	-2.31459700
C	-3.86390100	0.92625800	-0.56345000
H	-3.95818100	0.36893500	1.52237700
H	-3.44996900	1.49443500	-2.61740200
H	-4.94817200	0.95537300	-0.68739800
C	0.39407900	0.67765200	-0.10285400
H	0.93122100	1.39819000	-0.74029500
N	-1.45722900	0.28568000	2.13588300
C	2.20912100	0.98280200	1.64271000
C	3.22905700	0.88562500	0.66429000
C	2.62756300	1.36877600	2.93975300
C	4.55814400	1.15542200	0.96386000
C	3.95893600	1.61873400	3.23709200
H	1.87739800	1.50454400	3.71786600
C	4.94541000	1.51948600	2.25346300
H	5.30941700	1.06301600	0.17738800
H	4.23092100	1.91735600	4.25128800
H	5.98954500	1.72597900	2.48722400
C	0.82082100	0.72979300	1.31477300
C	-0.14078500	0.43511000	2.28503700
H	0.21092900	0.29284900	3.31535800
H	2.95903800	0.55207600	-0.33644700
H	0.68649000	-1.27827700	-0.05400800
H	0.02557400	-1.08852200	-2.34773600
C	-1.07287100	-2.62593700	-2.80702800
C	-0.05362100	-3.70621100	-2.43511400
H	0.53721900	-3.39324500	-1.56450300
H	-0.53654400	-4.66264600	-2.18763600
H	0.64318200	-3.87344100	-3.26601800
C	-2.02868100	-2.37368400	-1.64342900
H	-1.48032200	-2.04159100	-0.75306500
H	-2.73517400	-1.57328800	-1.89210400
H	-2.59319500	-3.27915600	-1.37875200
C	-1.84754800	-3.04452700	-4.04898600
H	-2.56744500	-2.26441200	-4.32318400
H	-1.16289300	-3.18542500	-4.89486100
H	-2.39444800	-3.98193700	-3.88306000
O	-0.39443800	-1.43450100	-3.16864200

O	0.83559500	-0.61649900	-0.74840800
<b>TS-C8</b>			
C	-1.19405600	-1.61644800	-0.99916700
C	-1.90091700	-1.30319200	0.20076800
C	-1.91246200	-1.79159200	-2.19997400
C	-3.30808100	-1.16952100	0.13637100
C	-3.28624400	-1.65121800	-2.23109800
H	-1.36268400	-2.09395700	-3.09359200
C	-3.98763100	-1.33509600	-1.05220300
H	-3.82808500	-0.93049100	1.06383400
H	-3.82817500	-1.80077800	-3.16518900
H	-5.07300100	-1.22747500	-1.07809100
C	0.23284600	-1.76563400	-0.94238000
H	0.80000300	-1.67172900	-1.86463200
N	-1.28661200	-1.10799200	1.40866200
C	2.31600800	-1.47485500	0.41107300
C	3.08896700	-2.32695300	-0.40141700
C	2.99308800	-0.64770000	1.32579200
C	4.47545200	-2.33614700	-0.30245700
C	4.37959100	-0.66854700	1.42681200
H	2.41777800	0.04036700	1.94606000
C	5.13318100	-1.50959700	0.60879800
H	5.05218500	-3.01008400	-0.93717400
H	4.87793100	-0.01025400	2.13979100
H	6.22074300	-1.52113300	0.68293900
C	0.85882500	-1.46521900	0.28697200
C	0.03453400	-1.19559400	1.39578000
H	0.52071500	-1.03688900	2.36625600
H	2.55760200	-3.01764300	-1.05752100
H	-0.22853200	-4.12246700	-0.86461600
H	0.24483700	-3.72830600	-2.98762100
C	-0.43238200	-5.03650200	-4.24751500
C	0.54887400	-6.09699600	-3.74109600
H	0.74025300	-5.92010500	-2.67478400
H	0.16774800	-7.11990700	-3.88007300
H	1.50552500	-6.00835600	-4.27201100
C	-1.77993600	-5.20026600	-3.53902500
H	-1.64557900	-5.04586800	-2.46126500
H	-2.49324800	-4.44553700	-3.89424700
H	-2.21791700	-6.19693600	-3.69881000
C	-0.61328100	-5.14666100	-5.75542400
H	-1.29833500	-4.36788300	-6.11399600
H	0.34909500	-5.00650800	-6.26327100
H	-1.01978500	-6.12624000	-6.04330200

O	0.09336800	-3.75164700	-3.99507300
O	0.51796000	-3.80518200	-1.39238200
<b>IM-C13</b>			
C	-1.40939400	0.93724900	0.28114400
C	-2.12721200	1.66777000	1.27699900
C	-2.10105900	0.42241200	-0.84589600
C	-3.51700400	1.87075500	1.11092600
C	-3.45480000	0.63657300	-0.97368200
H	-1.54497600	-0.13972300	-1.60447900
C	-4.16556100	1.36455700	0.00657600
H	-4.04456400	2.42955600	1.88312100
H	-3.98344400	0.23851900	-1.84041700
H	-5.23794300	1.52363700	-0.11290200
C	-0.02137700	0.74317000	0.45165900
H	0.51989500	0.11921400	-0.29027000
N	-1.51649600	2.16318500	2.39336100
C	2.05118800	1.07541600	1.81323200
C	2.77551100	0.11107200	1.08387500
C	2.74495800	1.85082900	2.75756000
C	4.13475400	-0.06288100	1.32070600
C	4.10455500	1.66645400	2.98642300
H	2.22258300	2.63046600	3.31096000
C	4.80893400	0.70189800	2.27101200
H	4.67391800	-0.81547400	0.74492300
H	4.61547600	2.28741400	3.72305100
H	5.87501500	0.55521900	2.44736800
C	0.60353800	1.25789000	1.57876000
C	-0.22172500	1.94967300	2.51015500
H	0.22322300	2.33523100	3.43270600
H	2.28241300	-0.50590900	0.30953400
H	0.72389600	-1.95590900	-0.47860100
H	0.30979700	-1.31830200	-2.28486700
C	-0.78154300	-2.64566600	-3.26018400
C	0.46426900	-3.52073700	-3.43901400
H	1.12636600	-3.34806100	-2.57954800
H	0.21994000	-4.59136100	-3.51924000
H	1.00715900	-3.22049800	-4.34526400
C	-1.58547700	-3.14546100	-2.05226000
H	-0.97189400	-3.06868100	-1.14586800
H	-2.47914500	-2.52444300	-1.90424500
H	-1.90614000	-4.19275500	-2.16367500
C	-1.65721600	-2.69044700	-4.50756400
H	-2.53472300	-2.04285500	-4.37645000
H	-1.09604100	-2.32097200	-5.37506700

H	-2.00799300	-3.70973300	-4.72663600
O	-0.39568100	-1.30880800	-3.07582100
O	1.24658900	-1.45197800	-1.12136900
<b>3a</b>			
C	1.66785300	-2.64361000	-1.72729500
C	1.18500200	-2.53187600	-3.03966800
C	2.56630900	-1.66968300	-1.26764300
C	1.58171300	-1.48346800	-3.86071400
C	2.96465900	-0.62165900	-2.08961900
H	2.93313700	-1.71821500	-0.24330400
C	2.47428400	-0.52336000	-3.38914000
H	1.19939100	-1.42118200	-4.87822900
H	3.65604300	0.12807100	-1.70899100
H	2.78597100	0.29763600	-4.03221400
C	1.24054900	-3.74851300	-0.85570100
C	2.12124900	-4.28876000	0.12543600
H	3.13412300	-3.88354300	0.20033600
H	0.50982300	-3.29490500	-3.42602900
C	-0.37773100	-5.37688100	-0.08371300
C	0.59334800	-5.82398100	0.86631500
C	-1.64911600	-5.99815100	-0.11384800
C	0.25844700	-6.87806100	1.74695200
C	-1.94547700	-7.02090100	0.75566900
H	-2.38688800	-5.65161200	-0.83769900
C	-0.98508800	-7.46375600	1.69171100
H	1.01522500	-7.20115400	2.45875300
H	-2.92495700	-7.49482200	0.72518300
H	-1.23487600	-8.27519500	2.37303200
C	-0.01458500	-4.31918400	-0.94176000
H	-0.74703700	-3.93931600	-1.65582200
N	1.83557800	-5.26922100	0.95043200