

*Supporting Information for*  
**Insights into the Regioselectivity and Diastereoselectivity of Nazarov  
Cyclization of 3-Alkenyl-2-indolylmethanol with Tryptophol**

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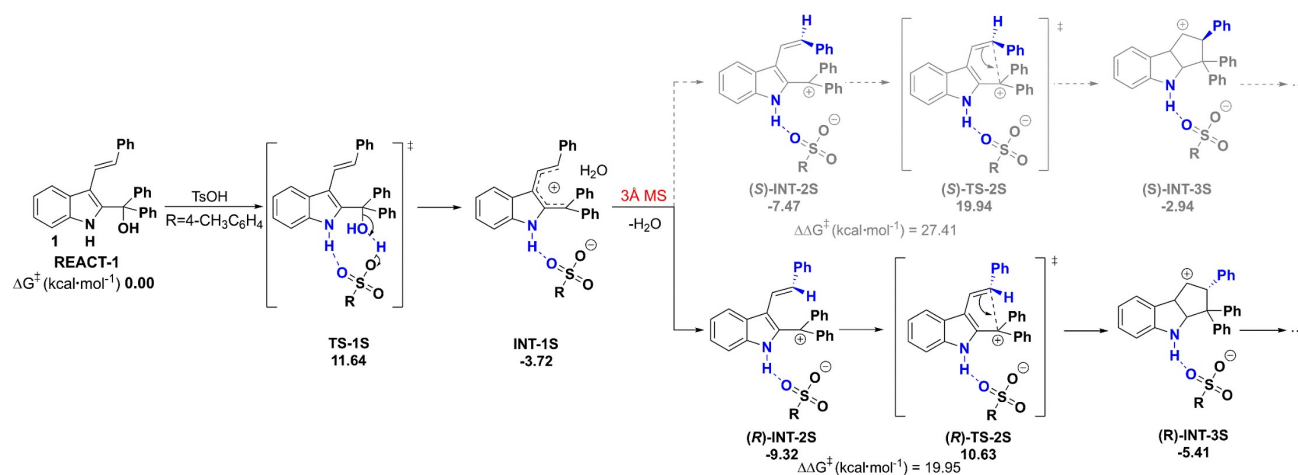
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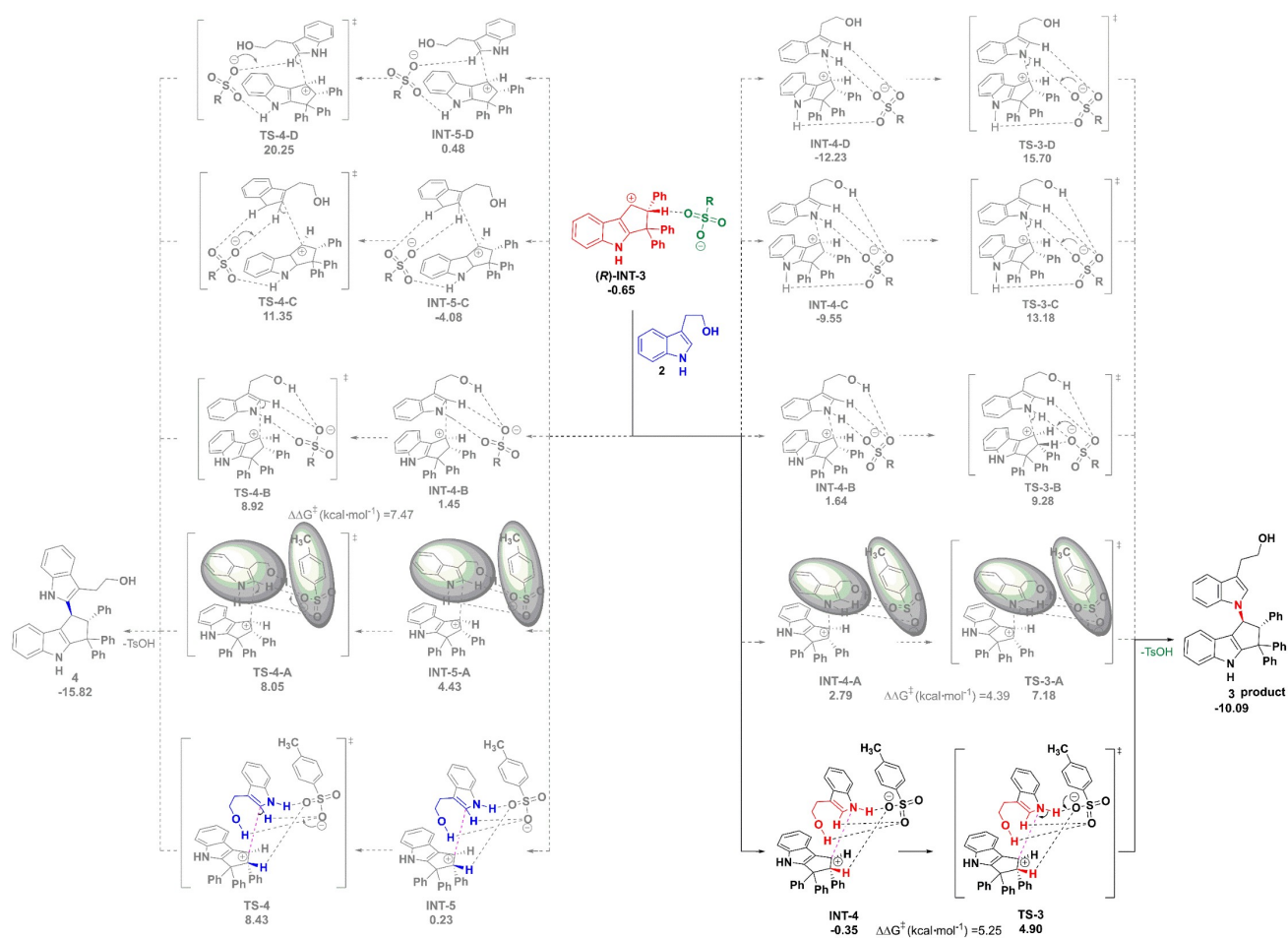
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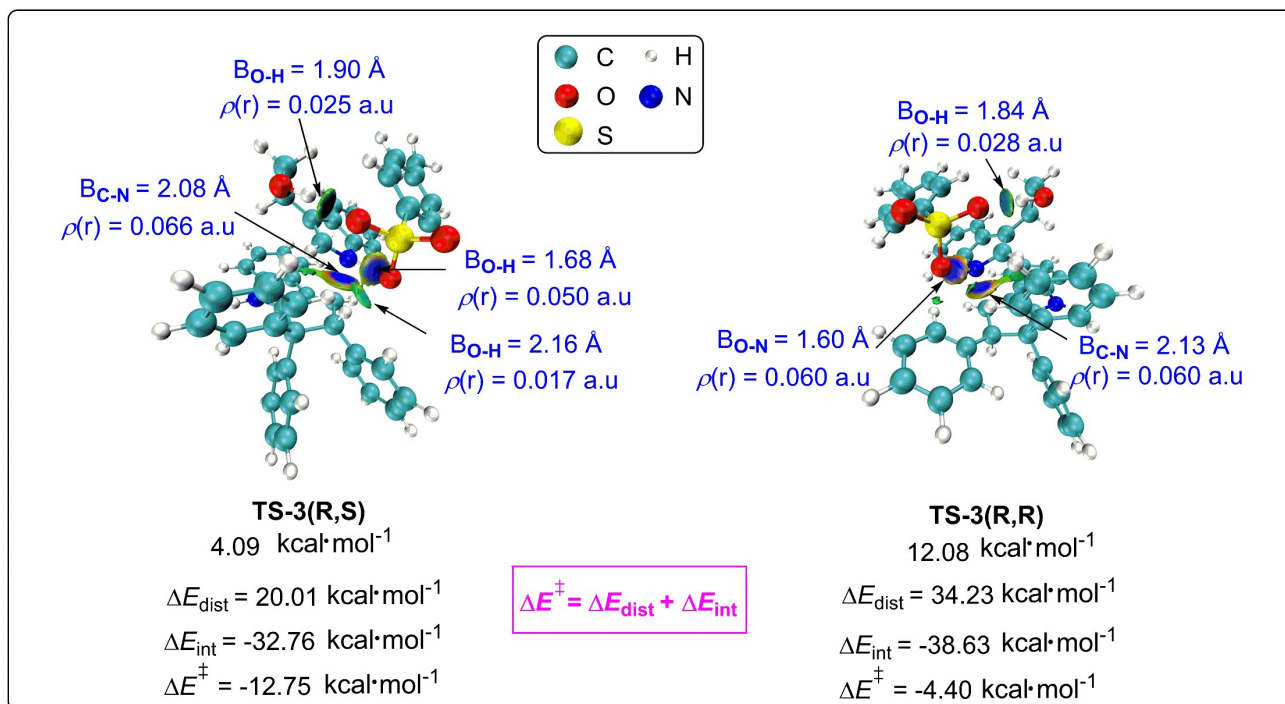
# 1. Different catalytic models



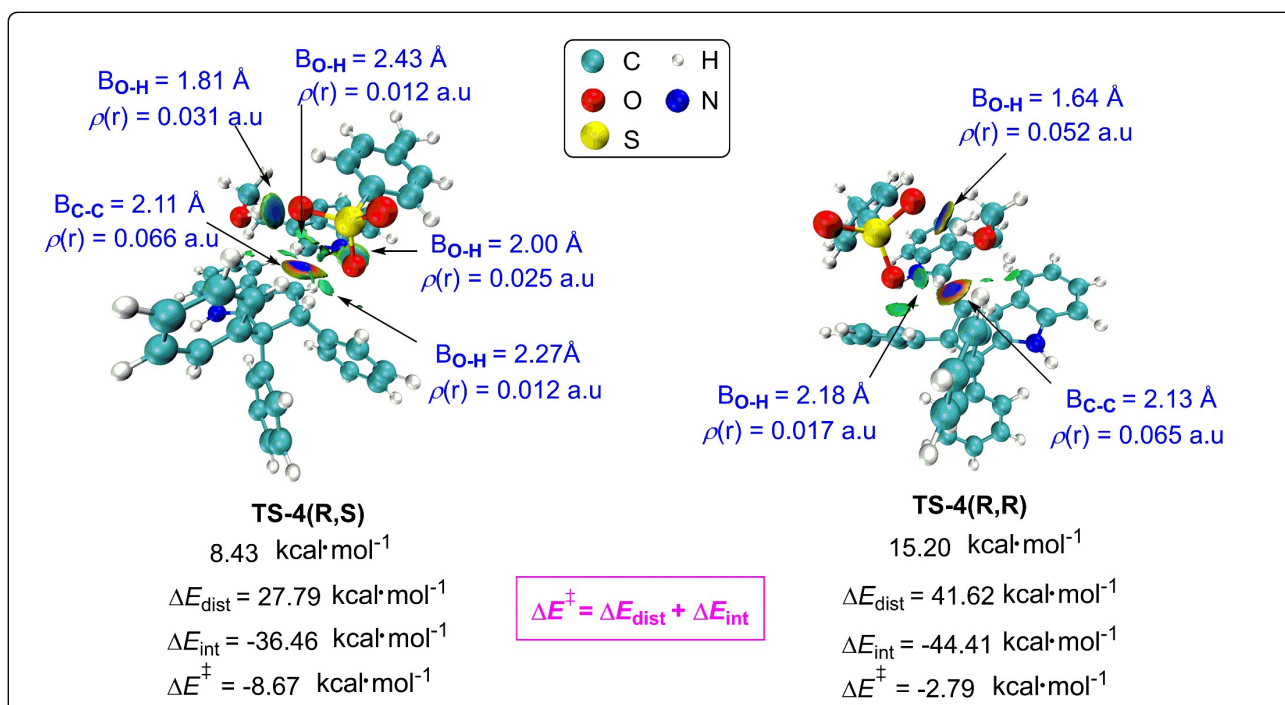
**Fig. S1** The different models of dehydration and cyclization for 3-alkenyl-2-indolylmethanol with TsOH



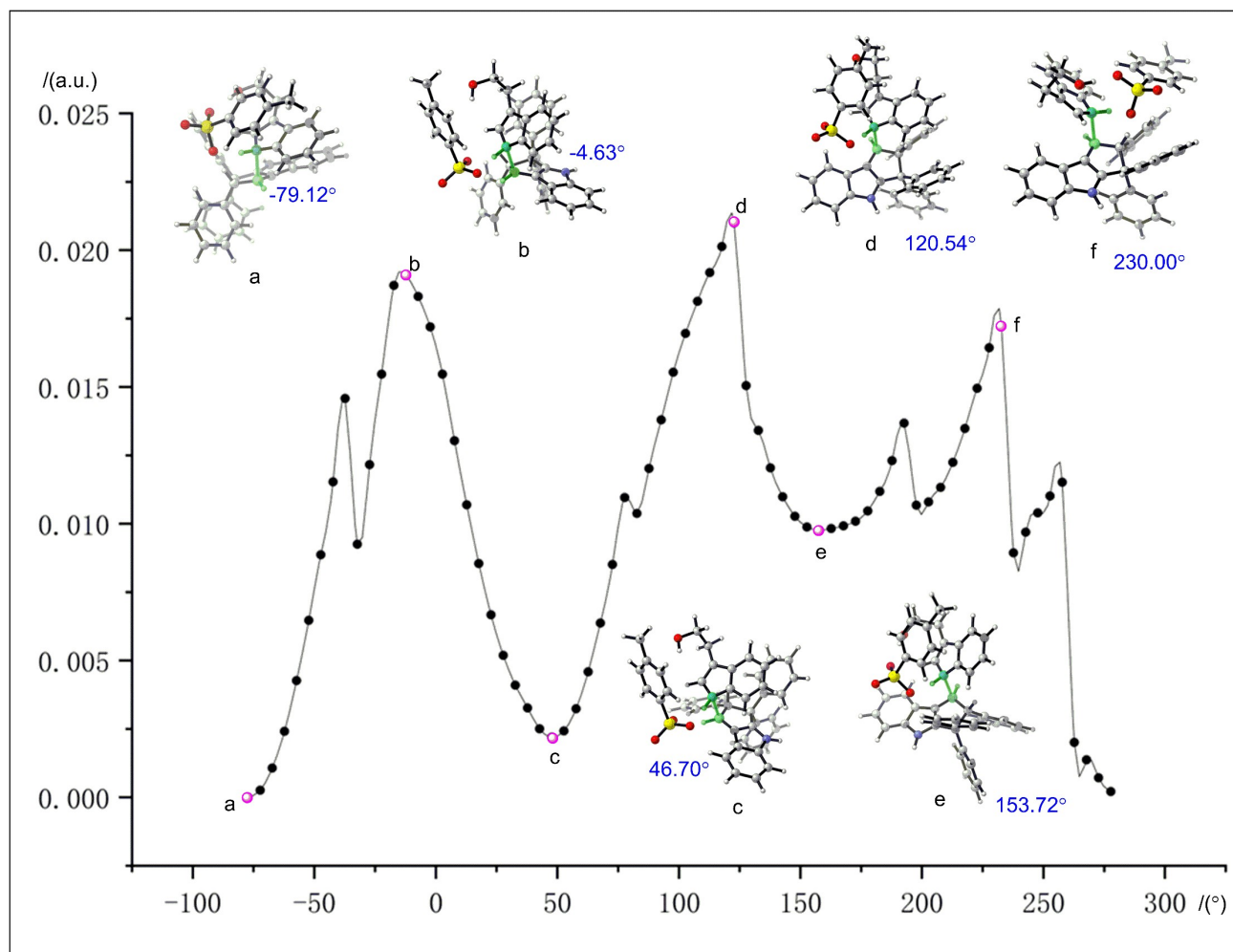
**Fig. S2** The different models of nucleophilic addition reaction at 303.15K with 3Å MS of **REACT-1**



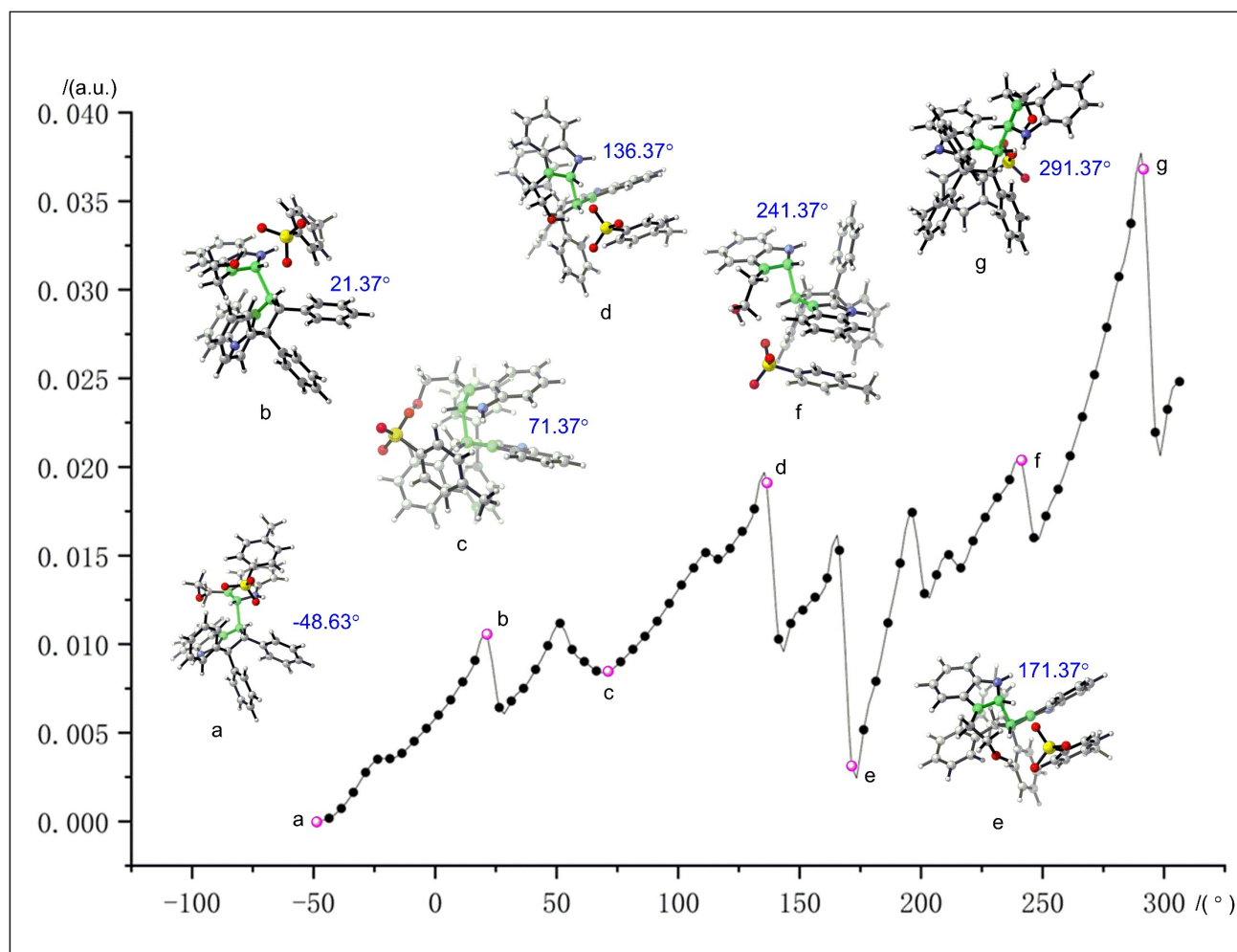
**Fig. S3** The IGMH (isovalue: 0.015), electron density  $\rho(r)$  (AIM theory) and distortion/interaction analysis for **TS-3(R,S)** and **TS-3(R,R)** in **REACT-1**



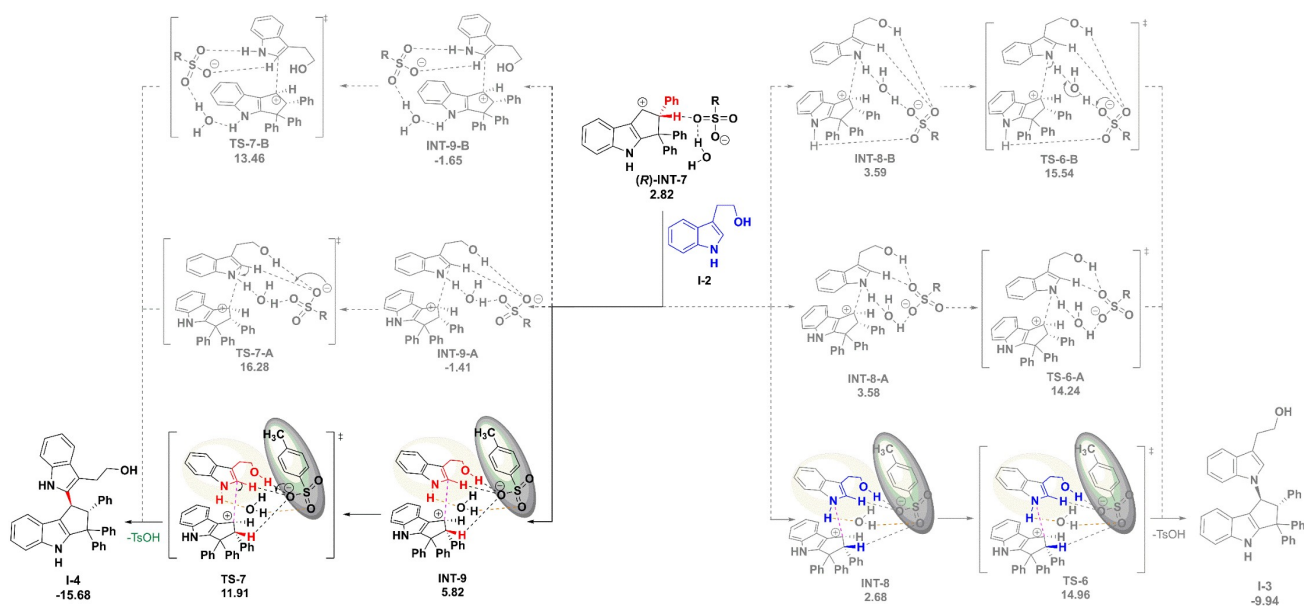
**Fig. S3** The IGMH (isovalue: 0.015), electron density  $\rho(r)$  (AIM theory) and distortion/interaction analysis for **TS-4(R,S)** and **TS-4(R,R)** in **REACT-1**



**Fig. S5** The restrictive optimization curves and structures of TS-3 in REACT-1



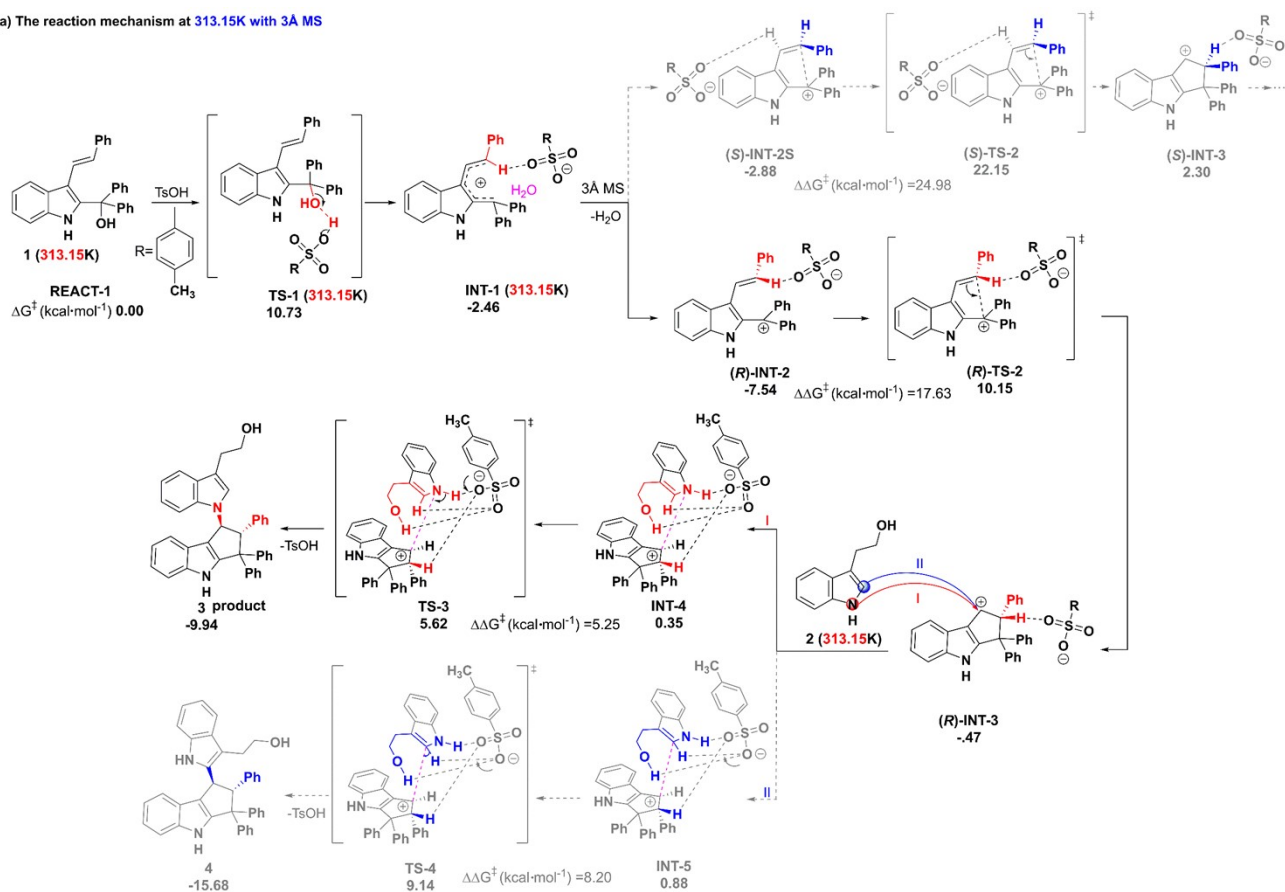
**Fig. S6** The restrictive optimization curves and structures of TS-4 in REACT-1



**Fig. S7** The different models of nucleophilic addition reaction at 313.15K without 3Å MS of REACT-2



(a) The reaction mechanism at 313.15K with 3Å MS



(b) The reaction mechanism at 303.15K without 3Å MS

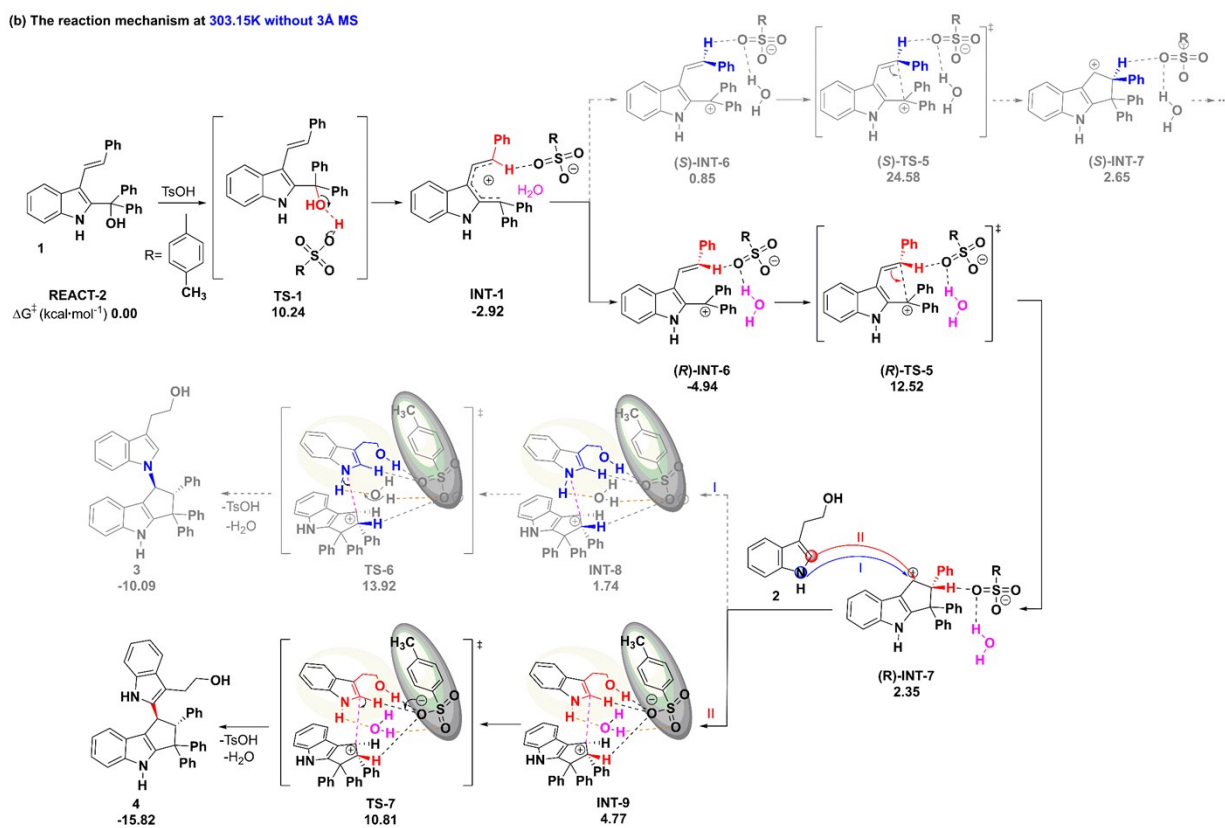


Fig. S8 The exchange conditional reaction mechanism was simulated with the presence of MS at 313K and the absence of MS at 303K

## 2. Electronic energies, enthalpies and free energies of all structures

**Table S1.** Electronic energies, enthalpies and free energies (in hartrees) computed at the level of B3LYP-D3(BJ)-SMD (chloroform)/6-311+G(d,p)//B3LYP-D3(BJ)/ 6-31G(d,p)

Structure	ZPE	$\Delta H_{0 \rightarrow T}$	$\Delta G_{0 \rightarrow T}$	E	H	G
1	0.439513	0.466211	0.380929	-1249.391406	-1248.925195	-1249.010477
2	0.191621	0.203238	0.1544	-517.86539	-517.662152	-517.710990
TsOH	0.14221	0.154468	0.102797	-895.585512	-895.431044	-895.482715
H <sub>2</sub> O	0.021364	0.025207	0.003347	-76.466401	-76.441194	-76.463054
TS-1	0.580957	0.619690	0.506487	-2144.983359	-2144.363669	-2144.476872
INT-1	0.582606	0.622742	0.507609	-2145.005449	-2144.382707	-2144.497840
(S)-INT-2	0.556598	0.593863	0.48457	-2068.519499	-2067.925636	-2068.034929
(S)-TS-2	0.556173	0.592503	0.48596	-2068.481083	-2067.88858	-2067.995123
(S)-INT-3	0.559055	0.595279	0.488579	-2068.515322	-2067.920043	-2068.026743
(R)-INT-2	0.557357	0.594554	0.485883	-2068.52826	-2067.933706	-2068.042377
(R)-TS-2	0.556946	0.593096	0.487796	-2068.50208	-2067.908984	-2068.014284
(R)-INT-3	0.558722	0.595014	0.488047	-2068.519224	-2067.92421	-2068.031177
INT-4	0.753327	0.801133	0.67062	-2586.412305	-2585.611172	-2585.741685
TS-3	0.753615	0.800495	0.67162	-2586.404943	-2585.604448	-2585.733323
3	0.609607	0.645192	0.54041	-1690.814908	-1690.169716	-1690.274498
INT-5	0.753168	0.801236	0.669126	-2586.409888	-2585.608652	-2585.740762
TS-4	0.753341	0.800477	0.67073	-2586.398429	-2585.597952	-2585.727699
4	0.609331	0.645352	0.539787	-1690.823414	-1690.178062	-1690.283627
TS-1S	0.581188	0.619380	0.509197	-2144.983835	-2144.364455	-2144.474638
INT-1S	0.581904	0.621954	0.507527	-2145.006647	-2144.384693	-2144.499120
(S)-INT-2S	0.557271	0.593931	0.48732	-2068.529369	-2067.935438	-2068.042049
(S)-TS-2S	0.554701	0.590654	0.486189	-2068.484557	-2067.893903	-2067.998368
(S)-INT-3S	0.558018	0.594166	0.488332	-2068.523154	-2067.928988	-2068.034822
(R)-INT-2S	0.556748	0.593696	0.484836	-2068.529821	-2067.936125	-2068.044985
(R)-TS-2S	0.555185	0.591061	0.485969	-2068.499162	-2067.908101	-2068.013193
(R)-INT-3S	0.557991	0.594124	0.488808	-2068.527566	-2067.933442	-2068.038758
INT-4A	0.753283	0.801349	0.667953	-2586.404642	-2585.603293	-2585.736689
TS-3A	0.753535	0.800538	0.670858	-2586.40055	-2585.600012	-2585.729692
INT-4B	0.753195	0.801492	0.666999	-2586.405517	-2585.604025	-2585.738518
TS-3B	0.753665	0.800771	0.669119	-2586.395454	-2585.594683	-2585.726335
INT-4C	0.752463	0.800381	0.666745	-2586.423098	-2585.622717	-2585.756353
TS-3C	0.753218	0.800171	0.669347	-2586.389476	-2585.589305	-2585.720129
INT-4D	0.753218	0.800171	0.669347	-2586.389476	-2585.589305	-2585.720129
TS-3D	0.751657	0.800117	0.663084	-2586.423699	-2585.623582	-2585.760615
INT-5A	0.753413	0.801395	0.668955	-2586.403169	-2585.601774	-2585.734214
TS-4A	0.753395	0.800449	0.671139	-2586.399445	-2585.598996	-2585.728306
INT-5B	0.752798	0.801217	0.665338	-2586.404159	-2585.602942	-2585.738821
TS-4B	0.753131	0.800419	0.667596	-2586.394509	-2585.59409	-2585.726913
INT-5C	0.752707	0.801153	0.665581	-2586.413208	-2585.612055	-2585.747627
TS-4C	0.751966	0.79967	0.665098	-2586.388145	-2585.588475	-2585.723047
INT-5D	0.751348	0.799812	0.667277	-2586.407638	-2585.607826	-2585.740361
TS-4D	0.752709	0.799997	0.670815	-2586.379665	-2585.579668	-2585.708850
TS-3(R,R)	0.752488	0.799367	0.669725	-2586.391605	-2585.592238	-2585.721880
TS-4(R,R)	0.753409	0.800221	0.672132	-2586.38903	-2585.588809	-2585.716898

**Table S2.** Electronic energies, enthalpies and free energies (in hartrees) computed at the level of B3LYP-D3(BJ)-SMD(chloroform)/6-311+G(d,p)//B3LYP-D3(BJ)/ 6-31G(d,p) level

Structure	ZPE	$\Delta H_{0 \rightarrow T}$	$\Delta G_{0 \rightarrow T}$	E	H	G
<b>1(313.15K)</b>	0.439513	0.467907	0.378088	-1249.391406	-1248.923499	-1249.013318
<b>2(313.15K)</b>	0.191621	0.203937	0.152778	-517.86539	-517.661453	-517.712612
<b>TsOH(313.15K)</b>	0.14221	0.155148	0.10108	-895.585512	-895.430364	-895.484432
<b>H<sub>2</sub>O(313.15K)</b>	0.021364	0.025334	0.002624	-76.466401	-76.441067	-76.463777
<b>TS-1(313.15K)</b>	0.580957	0.62208	0.502714	-2144.983359	-2144.361279	-2144.480645
<b>INT-1(313.15K)</b>	0.582606	0.625189	0.503771	-2145.005449	-2144.38026	-2144.501678
<b>(S)-INT-6</b>	0.582698	0.62506	0.504589	-2145.000221	-2144.375161	-2144.495632
<b>(S)-TS-5</b>	0.58247	0.623612	0.507961	-2144.96564	-2144.342028	-2144.457679
<b>(S)-INT-7</b>	0.584373	0.625808	0.508273	-2145.000956	-2144.375148	-2144.492683
<b>(R)-INT-6</b>	0.582696	0.625175	0.505736	-2145.010578	-2144.385403	-2144.504842
<b>(R)-TS-5</b>	0.581943	0.623639	0.504905	-2144.981904	-2144.358265	-2144.476999
<b>(R)-INT-7</b>	0.583689	0.625693	0.505104	-2144.998362	-2144.372669	-2144.493258
<b>INT-8</b>	0.778893	0.832855	0.684783	-2662.890875	-2662.05802	-2662.206092
<b>TS-6</b>	0.779913	0.832314	0.68908	-2662.875596	-2662.043282	-2662.186516
<b>3(313.15K)</b>	0.609609	0.647468	0.536918	-1690.814911	-1690.167443	-1690.277993
<b>INT-9</b>	0.779592	0.832874	0.690414	-2662.891498	-2662.058624	-2662.201084
<b>TS-7</b>	0.779415	0.831868	0.69194	-2662.883318	-2662.05145	-2662.191378
<b>4(313.15K)</b>	0.609331	0.647642	0.536267	-1690.823414	-1690.175772	-1690.287147
<b>INT-8A</b>	0.778425	0.832546	0.685234	-2662.889892	-2662.057346	-2662.204658
<b>TS-6A</b>	0.779593	0.832242	0.688729	-2662.876403	-2662.044161	-2662.187674
<b>INT-8B</b>	0.778305	0.831957	0.686495	-2662.891142	-2662.059185	-2662.204647
<b>TS-6B</b>	0.779875	0.832228	0.689291	-2662.874882	-2662.042654	-2662.185591
<b>INT-9A</b>	0.77869	0.83285	0.68503	-2662.897642	-2662.064792	-2662.212612
<b>TS-7A</b>	0.778955	0.831918	0.688001	-2662.872425	-2662.040507	-2662.184424
<b>INT-9B</b>	0.778655	0.832584	0.685322	-2662.898308	-2662.065724	-2662.212986
<b>TS-7B</b>	0.778325	0.831496	0.684318	-2662.873236	-2662.04174	-2662.188918

**Table S3.** Electronic energies, enthalpies and free energies (in hartrees) computed at the B3LYP-D3(BJ)-SMD(chloroform)/6-311+G(d,p)//B3LYP-D3(BJ)/ 6-31G(d,p) level at 313.15K with 3Å MS

Structure	ZPE	$\Delta H_{0 \rightarrow T}$	$\Delta G_{0 \rightarrow T}$	E	H	G
<b>(S)-INT-2</b>	0.556599	0.596163	0.48093	-2068.519498	-2067.923335	-2068.038568
<b>(S)-TS-2</b>	0.556174	0.594769	0.482409	-2068.481085	-2067.886316	-2067.998676
<b>(S)-INT-3</b>	0.559054	0.597544	0.485023	-2068.515328	-2067.917784	-2068.030305
<b>(R)-INT-2</b>	0.557358	0.596851	0.482272	-2068.528256	-2067.931405	-2068.045984
<b>(R)-TS-2</b>	0.556946	0.595352	0.484286	-2068.50208	-2067.906728	-2068.017794
<b>(R)-INT-3</b>	0.558725	0.597282	0.484496	-2068.519221	-2067.921939	-2068.034725
<b>INT-4</b>	0.753328	0.804128	0.666269	-2586.412302	-2585.608174	-2585.746033
<b>TS-3</b>	0.753615	0.803444	0.667321	-2586.404943	-2585.601499	-2585.737622
<b>INT-5</b>	0.753167	0.804235	0.664715	-2586.409892	-2585.605657	-2585.745177
<b>TS-4</b>	0.753341	0.803439	0.666402	-2586.398429	-2585.59499	-2585.732027



**Table S4.** Electronic energies, enthalpies and free energies (in hartrees) computed at the B3LYP-D3(BJ)-SMD(chloroform)/6-311+G(d,p)//B3LYP-D3(BJ)/ 6-31G(d,p) level at 303.15K without 3Å MS

<b>Structure</b>	<b>ZPE</b>	<b><math>\Delta H_{0\rightarrow T}</math></b>	<b><math>\Delta G_{0\rightarrow T}</math></b>	<b>E</b>	<b>H</b>	<b>G</b>
<b>(S)-INT-6</b>	0.582697	0.622612	0.508392	-2145.000222	-2144.37761	-2144.491830
<b>(S)-TS-5</b>	0.58247	0.621204	0.511615	-2144.96564	-2144.344436	-2144.454025
<b>(S)-INT-7</b>	0.584374	0.623391	0.51199	-2145.000955	-2144.377564	-2144.488965
<b>(R)-INT-6</b>	0.582696	0.622727	0.509509	-2145.01058	-2144.387853	-2144.501071
<b>(R)-TS-5</b>	0.581943	0.621228	0.508657	-2144.981904	-2144.360676	-2144.473247
<b>(R)-INT-7</b>	0.58369	0.623272	0.508915	-2144.998362	-2144.37509	-2144.489447
<b>INT-8</b>	0.778892	0.829721	0.689458	-2662.890872	-2662.061151	-2662.201414
<b>TS-6</b>	0.779913	0.829233	0.693604	-2662.875596	-2662.046363	-2662.181992
<b>INT-9</b>	0.779592	0.829744	0.694913	-2662.8915	-2662.061756	-2662.196587
<b>TS-7</b>	0.779415	0.828772	0.696358	-2662.883318	-2662.054546	-2662.186960

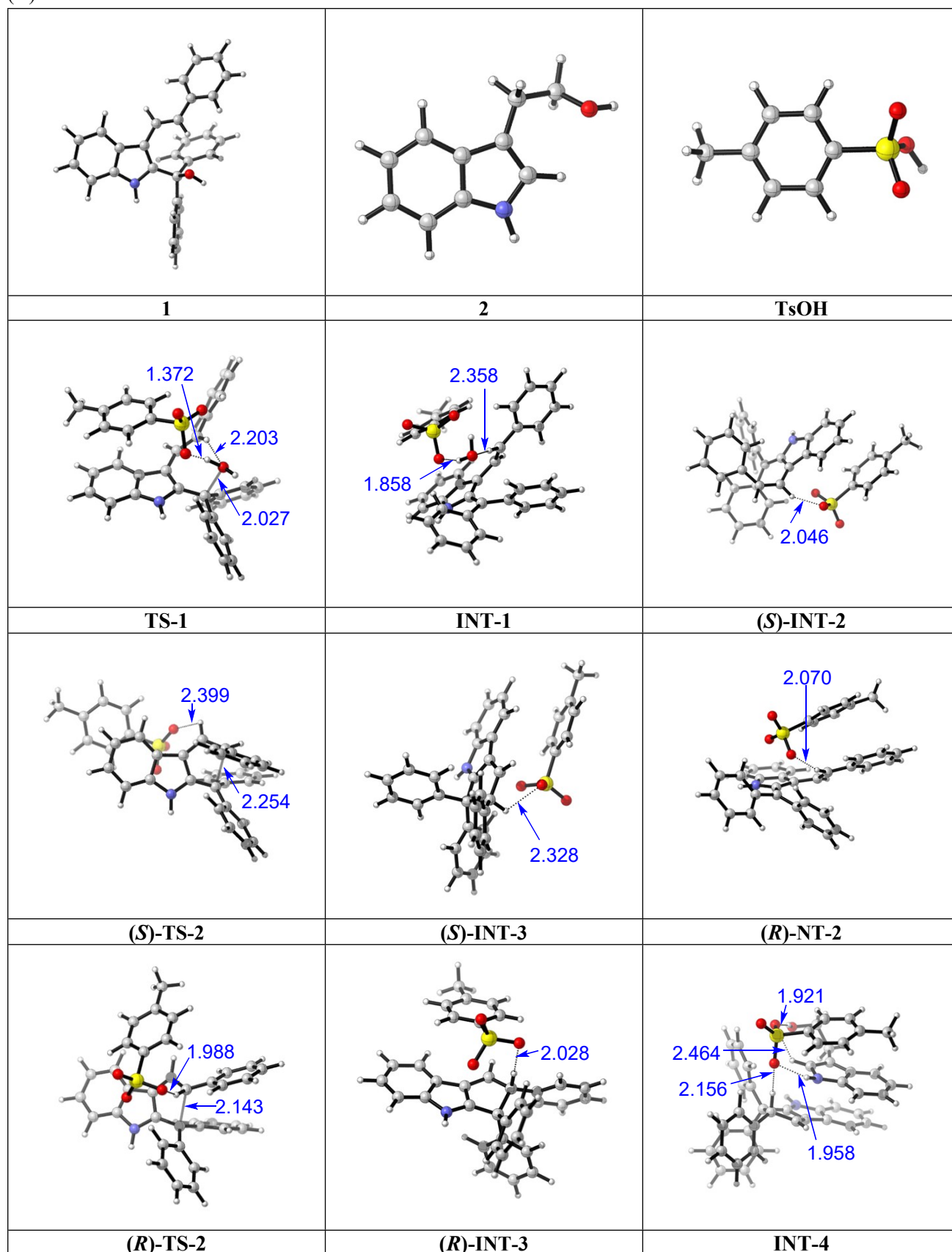
### 3. Imaginary frequencies of all TS structures

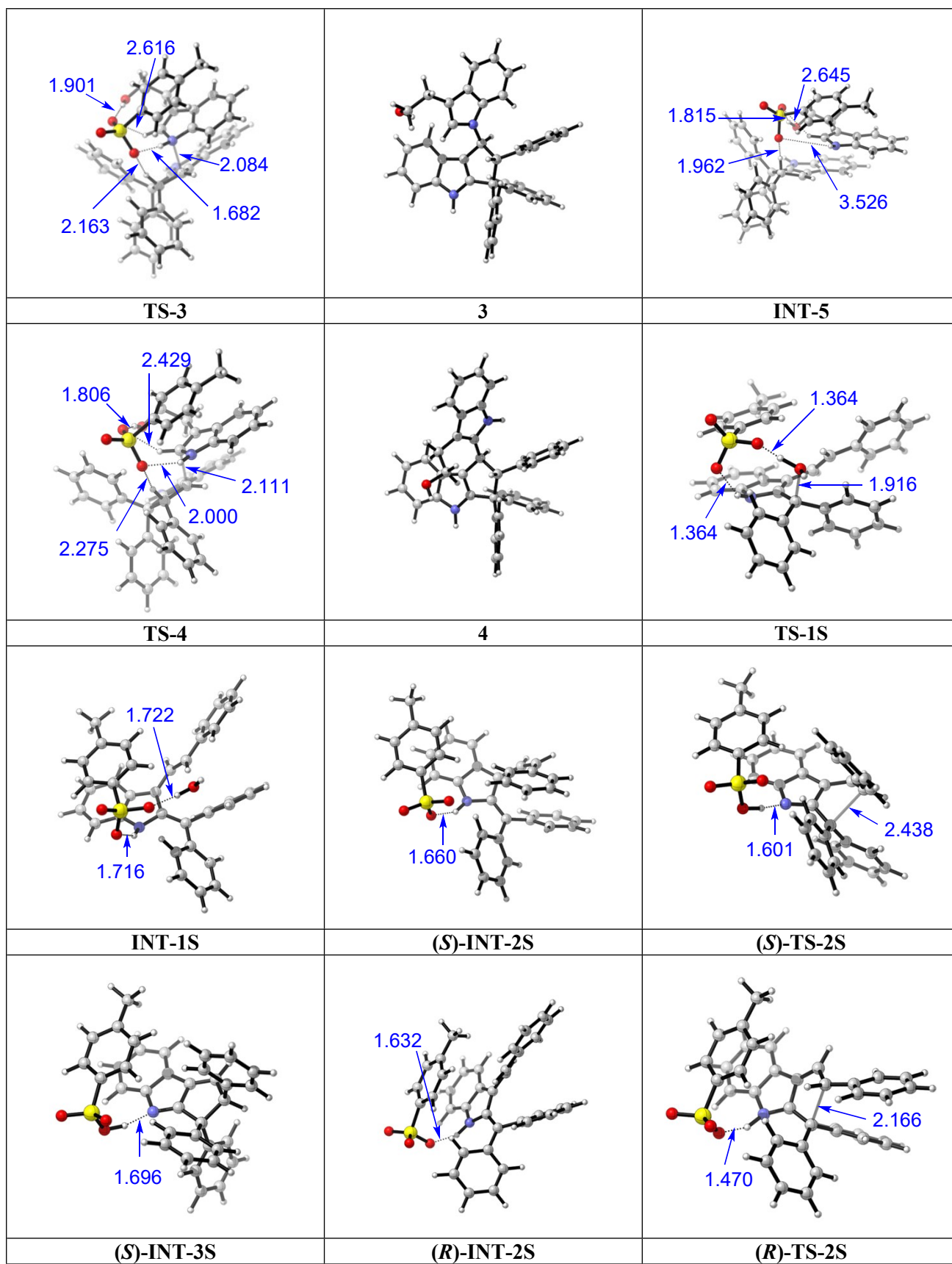
Table S5 Imaginary frequencies of all TS structures obtained for the cyclization reaction

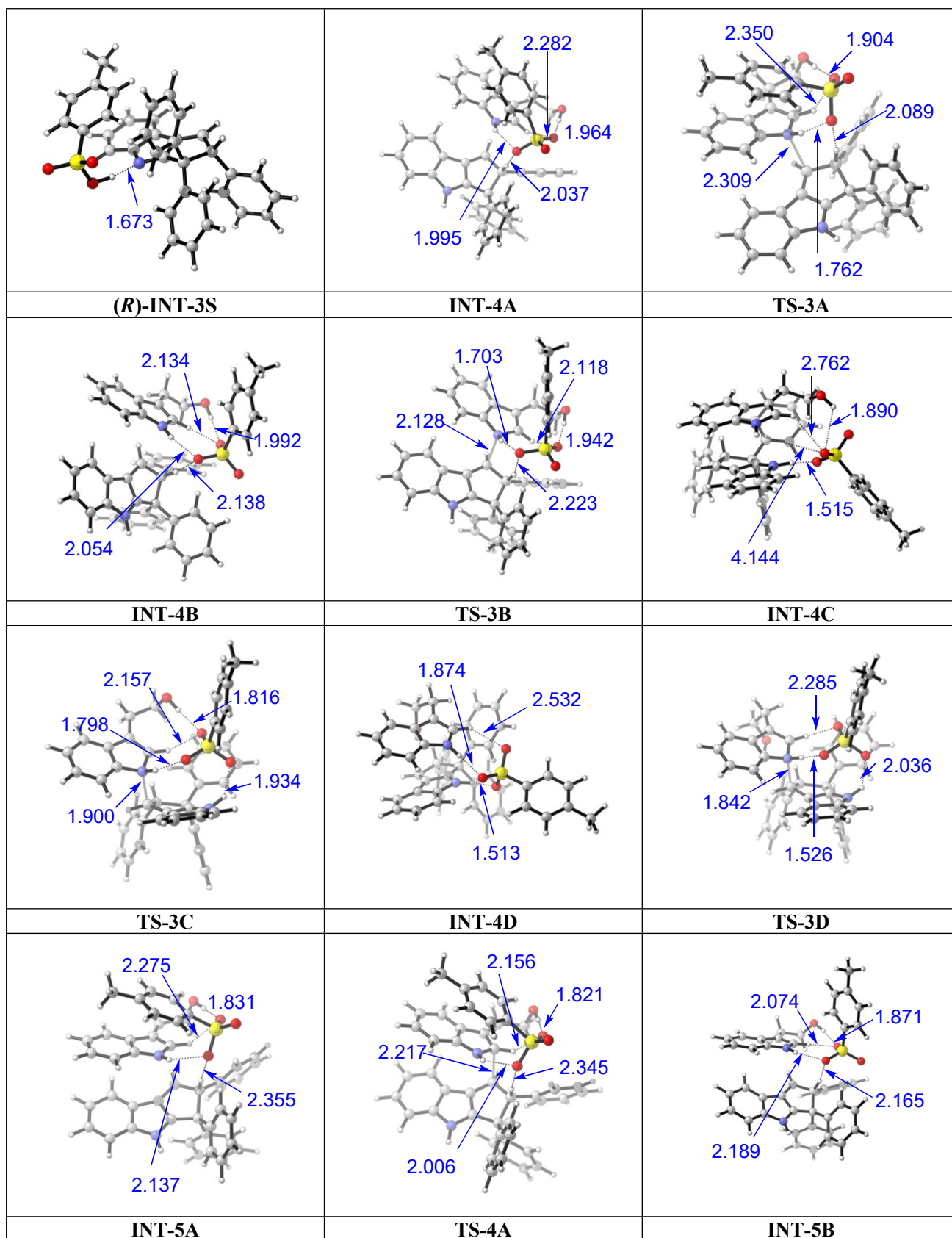
Structure	Freq	Infrared	Structure	Freq	Infrared
TS-1	-229.80	180.7787	<b>(S)</b> -TS-5	-199.91	91.8740
<b>(S)</b> -TS-2	-289.08	130.2505	<b>(R)</b> -TS-5	-196.85	119.7448
<b>(R)</b> -TS-2	-184.98	118.7559	TS-6	-196.76	432.3275
TS-3	-143.38	260.5229	TS-7	-229.96	576.5198
TS-4	-256.24	879.4298	TS-6A	-156.13	337.3217
TS-3A	-51.59	86.8241	TS-6B	-296.02	432.6581
TS-3B	-123.38	274.6119	TS-7A	-220.33	776.7593
TS-3C	-252.81	398.2547	TS-7B	-415.70	1326.1066
TS-3D	-225.72	334.6538	<b>(S)</b> -TS-2(313.15K)	-289.02	130.2540
TS-4A	-98.71	305.6275	<b>(R)</b> -TS-2(313.15K)	-184.98	118.7559
TS-4B	-292.04	652.0233	TS-3(313.15K)	-143.38	260.5229
TS-4C	-397.76	1249.7912	TS-4(313.15K)	-256.25	879.4398
TS-4D	-342.23	1111.2319	<b>(S)</b> -TS-5(303.15K)	-199.91	91.8729
TS-3( <b>R,R</b> )	-108.69	167.8863	<b>(R)</b> -TS-5(303.15K)	-196.86	119.7464
TS-4( <b>R,R</b> )	-181.26	497.7148	TS-6(303.15K)	-196.75	432.3121
TS-1(313.15K)	-229.80	180.7819	TS-7(303.15K)	-229.96	576.5166

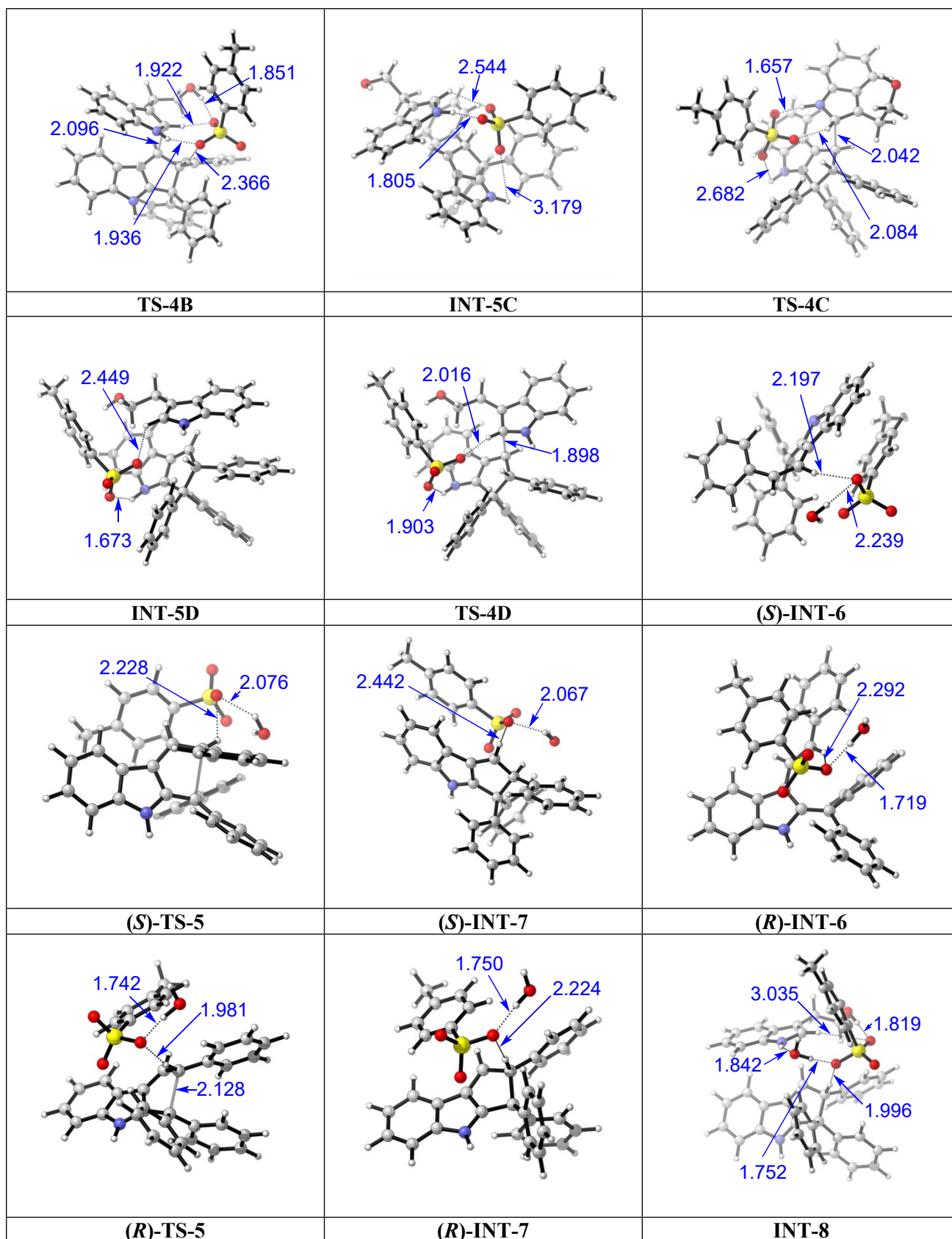
#### 4. Quantum chemistry method-optimized structures

Quantum chemistry method-optimized structures are illustrated using CYLView. Distances are shown in angstroms (Å).

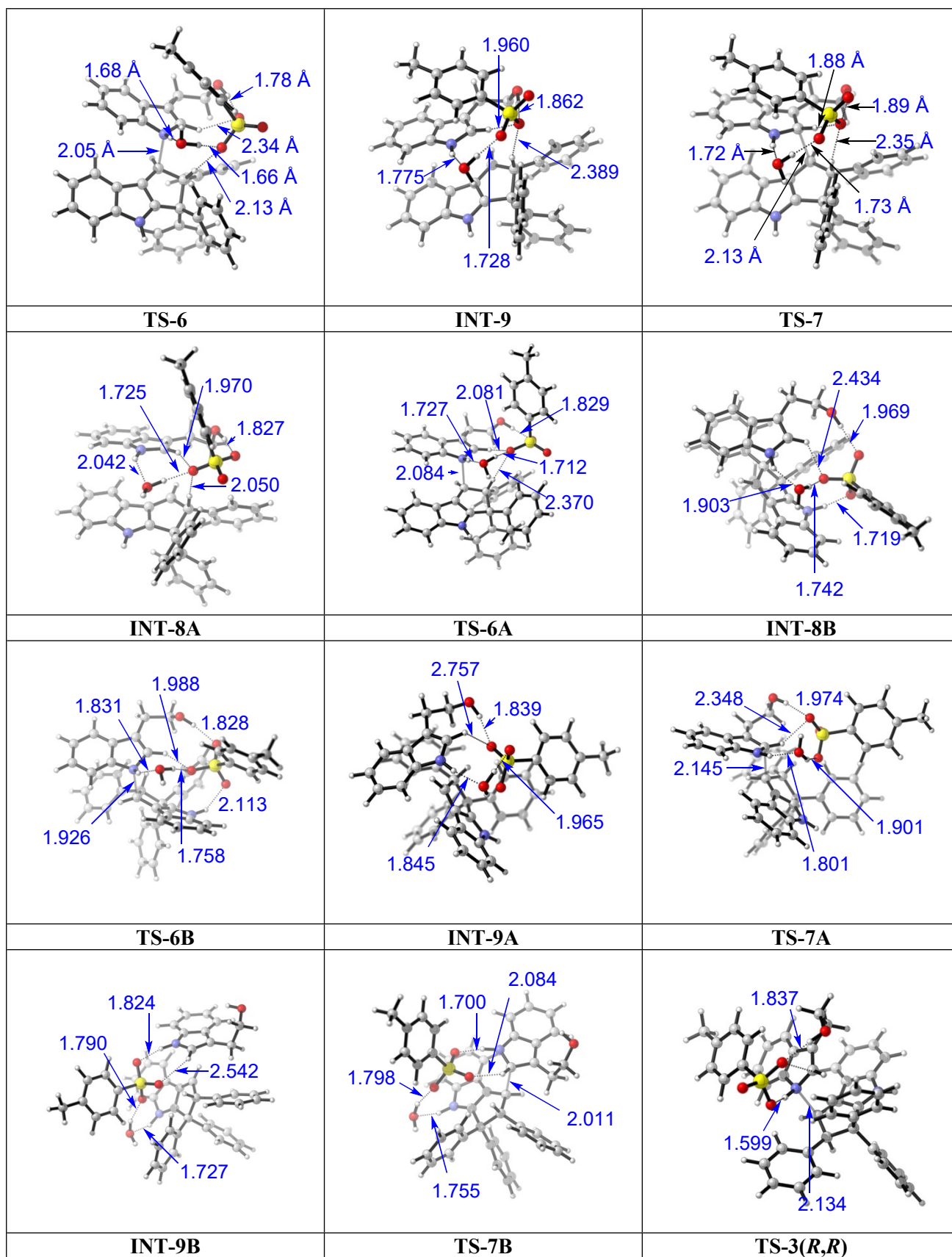














## 5. Cartesian coordinates of DFT-computed structures

### 1

C	0.98614300	2.75266900	0.07773500
C	2.36089500	2.40376200	0.03318800
C	3.37934900	3.34169900	0.22606000
C	2.99831600	4.65556500	0.46929500
C	1.63845100	5.02625500	0.51357100
C	0.63216900	4.09012000	0.31509100
C	0.22166100	1.54754100	-0.16149500
C	1.14900100	0.52231200	-0.32896400
H	4.42596900	3.05519200	0.18712300
H	3.76185900	5.41132800	0.62503500
H	1.37820000	6.06343100	0.70058300
H	-0.41173900	4.38773700	0.33636700
H	3.26510000	0.49932300	-0.27548700
N	2.42467600	1.05165100	-0.21859700
C	0.94723100	-0.96927600	-0.53312300
C	-0.08039200	-1.50708600	0.47460100
C	-1.05074300	-2.43121500	0.08620900
C	-0.05199500	-1.08005800	1.80675400
C	-1.98594900	-2.91033500	1.00321300
H	-1.11353700	-2.74665000	-0.94884500
C	-0.98036600	-1.56156500	2.72690700
H	0.68085500	-0.34166000	2.11456100
C	-1.95461300	-2.47728300	2.32717400
H	-2.74959200	-3.60854900	0.67516500
H	-0.95104000	-1.20952600	3.75360200
H	-2.68870600	-2.84105800	3.03917600
C	2.29149900	-1.71853600	-0.42233500
C	3.16846000	-1.66955000	-1.51860800
C	2.68653900	-2.41808100	0.72227200
C	4.41059600	-2.30039300	-1.46676100
H	2.86296800	-1.13244300	-2.40988100
C	3.92877100	-3.05232300	0.77117900
H	2.02051700	-2.47703600	1.57402500
C	4.79553800	-2.99520800	-0.31931300
H	5.07489200	-2.25094600	-2.32419900
H	4.21561500	-3.59579900	1.66620600
H	5.76080600	-3.49011700	-0.27766800
O	0.47090500	-1.12083100	-1.88682300
H	0.56081400	-2.05722000	-2.11533800
C	-1.22808100	1.48665900	-0.13758700
H	-1.70274600	2.22854800	0.50310700
C	-1.99918900	0.60821900	-0.80841600

H	-1.51627900	-0.06070800	-1.51297800
C	-3.44589200	0.44899400	-0.67718000
C	-4.19934400	1.04497300	0.35163400
C	-4.12559200	-0.36452700	-1.60148200
C	-5.57437800	0.85487100	0.43265700
H	-3.69782200	1.64410500	1.10457400
C	-5.50176400	-0.55923700	-1.51870500
H	-3.55685500	-0.84160000	-2.39506800
C	-6.23532100	0.05312500	-0.50217600
H	-6.13467400	1.32427900	1.23616100
H	-6.00245200	-1.18984300	-2.24770700
H	-7.30811500	-0.09825200	-0.43212800

### 2

C	-0.62148400	-0.34263800	-0.08218900
C	-1.28731700	0.91230800	0.01065200
C	-2.67755800	1.01445700	0.10871200
C	-3.41019500	-0.16696700	0.11151500
C	-2.77333700	-1.42079500	0.01964400
C	-1.39114900	-1.51736000	-0.07759900
C	0.79380400	-0.07406100	-0.16075500
C	0.93319500	1.29186300	-0.12075000
H	-3.16863200	1.98068700	0.17915300
H	-4.49239200	-0.12240800	0.18540600
H	-3.37655000	-2.32347100	0.02334000
H	-0.91207500	-2.48943600	-0.15244700
H	-0.47916000	2.87862400	0.03297100
N	-0.31285600	1.88766000	-0.01454800
H	1.83703500	1.87867500	-0.16166500
C	1.88060400	-1.10460400	-0.27410200
H	1.51079600	-2.05936800	0.11866700
H	2.14391000	-1.28682900	-1.32498200
C	3.16000000	-0.76087900	0.47853000
H	3.83675800	-1.62929400	0.46488100
H	2.91578700	-0.53694800	1.52781000
O	3.77392500	0.36186700	-0.15537400
H	4.54373700	0.61326700	0.36975300

### TsOH

C	-1.94433400	1.20939000	-0.03313400
C	-0.55347700	1.21219300	-0.08694400
C	0.12138700	-0.00751100	-0.07913400

C	-0.56556800	-1.22021900	-0.02507200
C	-1.95526700	-1.20073700	0.03161800
C	-2.66418500	0.00885900	0.02764400
H	-2.48071600	2.15362600	-0.04200800
H	0.00573200	2.13864300	-0.14778200
H	-0.01569500	-2.15406300	-0.03701900
H	-2.50057500	-2.13892000	0.07555500
C	-4.17115200	0.01436800	0.05380100
H	-4.56041400	0.94622000	0.47201900
H	-4.57715500	-0.08615000	-0.95987900
H	-4.56266900	-0.81790600	0.64519900
S	1.89739100	-0.01760200	-0.13145800
O	2.27409800	-0.08211900	1.47233100
H	2.78252500	0.72499600	1.65912600
O	2.34063600	-1.27059400	-0.72446300
O	2.37855300	1.27985600	-0.60968700

**H<sub>2</sub>O**

O	0.00000000	0.00000000	0.11920900
H	0.00000000	0.75932100	-0.47683700
H	0.00000000	-0.75932100	-0.47683700

**TS-1**

C	-4.18085200	-0.00766900	-0.03569600
C	-3.19799500	0.21960500	0.92811000
C	-2.53539000	-0.86403900	1.49489000
C	-2.84151000	-2.16854800	1.10185400
C	-3.82467600	-2.38110800	0.14373200
C	-4.51419300	-1.30544000	-0.43437800
H	-4.69826400	0.83824700	-0.48115200
H	-2.93780100	1.22274500	1.24315700
H	-2.31066900	-3.00263800	1.54720400
H	-4.05592500	-3.39406800	-0.17319500
C	-5.59993900	-1.55040900	-1.45118000
H	-6.56308400	-1.74336700	-0.96325500
H	-5.73559100	-0.68644400	-2.10856700
H	-5.37081800	-2.42068800	-2.07309600
S	-1.29809300	-0.59490000	2.76391600
O	-0.03467800	-1.22890300	2.15108900
H	0.93657500	-0.28080300	1.95361000
O	-1.12967100	0.87141400	2.88211800
O	-1.73834600	-1.32769500	3.95847100

C	-0.86257100	-1.30667100	-1.84734400
C	-0.23316500	-2.54609200	-1.53806000
C	-0.74746700	-3.77053500	-1.98870900
C	-1.89318100	-3.72707500	-2.76582500
C	-2.53007600	-2.50508900	-3.08935100
C	-2.03776500	-1.30120100	-2.62218600
C	-0.08665300	-0.26478100	-1.24614900
C	1.03781600	-0.89180600	-0.64982500
H	-0.26488100	-4.71046500	-1.74233900
H	-2.31616200	-4.65569400	-3.13637000
H	-3.42697700	-2.52171700	-3.69883700
H	-2.54688000	-0.36929700	-2.83981200
H	1.56577800	-2.95124900	-0.50367100
N	0.88122000	-2.27577900	-0.80143200
C	2.24096500	-0.32542300	-0.13014700
C	2.71382800	0.95844600	-0.74067200
C	3.32597000	1.97174400	0.00743800
C	2.64046300	1.09773900	-2.13542200
C	3.81460900	3.11389800	-0.62025800
H	3.37061100	1.88540300	1.08364100
C	3.14156400	2.23640600	-2.76189200
H	2.18726300	0.31035900	-2.72580000
C	3.72366400	3.25265600	-2.00592200
H	4.25957000	3.90248200	-0.02197100
H	3.07151900	2.32816600	-3.84117900
H	4.10371400	4.14604400	-2.49125100
C	3.29722100	-1.27752300	0.33590000
C	2.99698600	-2.28003900	1.28212500
C	4.59562300	-1.19896700	-0.18612200
C	3.97875700	-3.18399900	1.67644300
H	2.00437800	-2.32353900	1.72299200
C	5.57131900	-2.11292000	0.21111600
H	4.83386900	-0.42870100	-0.90983800
C	5.26725200	-3.10634300	1.14025800
H	3.73944800	-3.94303000	2.41436000
H	6.57095100	-2.04374100	-0.20585700
H	6.03007700	-3.81238600	1.45275300
O	1.75933800	0.36672400	1.71291000
H	2.46772000	0.10347200	2.31842700
C	-0.49575200	1.11796600	-1.19866000
H	-1.09522400	1.46444700	-2.03738400
C	-0.32416700	1.92218000	-0.12719300
H	0.14071800	1.52213100	0.76466000
C	-0.81785300	3.28873300	-0.01002900

C	-1.03748900	4.11772300	-1.12454500	H	1.04354700	-3.32189500	-0.86544800
C	-1.09452500	3.78826300	1.27666600	N	0.46520000	-2.53219100	-1.10165200
C	-1.53355500	5.40630500	-0.95844300	C	2.20580800	-0.86139900	-0.68398900
H	-0.78912100	3.75496500	-2.11739900	C	2.78854900	0.40783500	-1.14742500
C	-1.59880700	5.07632000	1.43618300	C	3.53853300	1.20810600	-0.26810100
H	-0.94132300	3.13592900	2.13120700	C	2.60864600	0.82009400	-2.47901700
C	-1.81908100	5.88876000	0.32223500	C	4.05544800	2.42125200	-0.71165500
H	-1.69063400	6.04120700	-1.82543800	H	3.61059300	0.90910400	0.77174300
H	-1.82138100	5.44693800	2.43211700	C	3.14537600	2.02488200	-2.91831200
H	-2.20590400	6.89540200	0.44931000	H	2.05111300	0.18586700	-3.15970200

### INT-1

C	-4.11811600	0.98995600	0.20060100	H	3.00845300	2.33352800	-3.94992600
C	-2.97991600	0.87003700	0.99924100	H	4.27060700	3.77963600	-2.37155700
C	-2.61515000	-0.37970100	1.49149500	C	3.06763200	-1.80705700	0.02521400
C	-3.38999100	-1.50404000	1.20085300	C	2.54723000	-2.65608900	1.02897600
C	-4.52561700	-1.37136600	0.40950800	C	4.44540500	-1.86075900	-0.27142800
C	-4.90465000	-0.12481700	-0.10801700	C	3.38944300	-3.53788100	1.69652500
H	-4.40642700	1.96834800	-0.17623000	H	1.50671600	-2.55538800	1.32596600
H	-2.38421600	1.73540000	1.26135100	C	5.27306800	-2.75874600	0.39035900
H	-3.10867300	-2.46584200	1.61520400	H	4.84860600	-1.20716900	-1.03619300
H	-5.12998300	-2.24674100	0.18653400	C	4.74756900	-3.59923300	1.37544100
C	-6.11263600	0.00103200	-1.00207500	H	2.98729900	-4.16296000	2.48701800
H	-6.90766200	-0.68794400	-0.70147800	H	6.32887900	-2.80240700	0.14328200
H	-6.51913100	1.01617500	-0.98725300	H	5.39897400	-4.29044200	1.90126200
H	-5.86107300	-0.23361000	-2.04506200	O	2.06016000	0.31205900	2.30314000
S	-1.14215400	-0.57585800	2.50555800	H	1.44429600	0.85338900	2.82213800
O	-0.15033000	-1.23332400	1.56990600	C	-0.36193300	1.03935700	-1.24212700
H	1.44298600	-0.39762900	2.03542500	H	-1.05253500	1.54218500	-1.91389700
O	-0.71281500	0.81086500	2.85800900	C	0.14888900	1.71157800	-0.18068600
O	-1.53162300	-1.43799200	3.63491300	H	0.68138200	1.16097300	0.58845800
C	-1.24068700	-1.25191100	-1.84894900	C	-0.03463500	3.13396600	0.05553300
C	-0.79461600	-2.58807300	-1.61296100	C	-0.19360800	4.05118500	-1.00046000
C	-1.60478800	-3.69422300	-1.90296200	C	-0.04923600	3.60789400	1.38155700
C	-2.86076100	-3.43570100	-2.42635900	C	-0.36798900	5.40471200	-0.73762500
C	-3.32465000	-2.11698000	-2.66012900	H	-0.14007400	3.69725500	-2.02533500
C	-2.53425500	-1.02684400	-2.36273200	C	-0.23660200	4.96284100	1.63836300
C	-0.20933600	-0.37267400	-1.42057200	H	0.03239800	2.88901400	2.18968800
C	0.89969200	-1.20503600	-1.01659800	C	-0.39331500	5.86392400	0.58311000
H	-1.26570600	-4.70736200	-1.71690500	H	-0.47625600	6.10656000	-1.55902700
H	-3.51625400	-4.26985800	-2.65658700	H	-0.26304000	5.31679100	2.66416900
H	-4.32333200	-1.97170200	-3.05639600	H	-0.53131000	6.92156800	0.78644500
H	-2.90214700	-0.01658800	-2.49669500				

**(S)-INT-2**

C	-1.15649700	-0.62817900	1.11926300
C	-1.05490900	-1.86480900	0.41477400
C	-2.04416000	-2.84604300	0.51438700
C	-3.12914200	-2.56349100	1.33384500
C	-3.24234600	-1.34875100	2.05032500
C	-2.26852800	-0.37633100	1.95263600
C	-0.02820200	0.15874500	0.78719600
C	0.75996400	-0.61319100	-0.14585500
H	-1.97615400	-3.77993500	-0.03289900
H	-3.92405700	-3.29710800	1.42214900
H	-4.12847900	-1.17017400	2.64711500
H	-2.36737500	0.58672900	2.43693800
H	0.34450800	-2.49954600	-1.03224900
N	0.12140700	-1.86085400	-0.28519600
C	1.94011400	-0.31447600	-0.80646400
C	2.42693600	1.05032700	-0.99484700
C	3.81080400	1.30998900	-0.91493800
C	1.53851400	2.10391700	-1.28852800
C	4.29113000	2.60262900	-1.08602800
H	4.49188300	0.50204200	-0.67449800
C	2.03307000	3.38888300	-1.47668800
H	0.47284000	1.90659100	-1.38163500
C	3.40281500	3.64454400	-1.36667200
H	5.35496500	2.79932800	-0.99837500
H	1.34218200	4.19205800	-1.71124100
H	3.77989500	4.65302100	-1.50840100
C	2.74079000	-1.40764000	-1.39022500
C	2.98705900	-2.59037900	-0.66653100
C	3.30634200	-1.26303700	-2.67061500
C	3.77242100	-3.59968600	-1.21463600
H	2.59367500	-2.68592000	0.33834900
C	4.07318400	-2.28457000	-3.22189600
H	3.12228800	-0.35181600	-3.22838300
C	4.30997500	-3.45354300	-2.49545400
H	3.97361900	-4.49757700	-0.63898000
H	4.48899700	-2.16833000	-4.21749700
H	4.91699900	-4.24525100	-2.92318200
C	0.29849800	1.42275900	1.43057900
H	-0.50898300	2.15538700	1.36128600
C	1.43034800	1.70871500	2.09870300
H	1.53769800	2.72486800	2.47219700
C	2.56218700	0.81023400	2.36417200
C	2.38900000	-0.55923400	2.63169100

C	3.86782900	1.32655500	2.35693200
C	3.48742600	-1.38933000	2.83483900
H	1.38522300	-0.96460100	2.69721300
C	4.96819900	0.49478600	2.55448800
H	4.01441200	2.38428000	2.16156800
C	4.78322800	-0.86856200	2.78487700
H	3.33320500	-2.44269900	3.05031400
H	5.97036400	0.91192800	2.52973000
H	5.63890100	-1.51750600	2.94330300
C	-4.85341800	-1.23531700	-1.24948100
C	-3.84213100	-0.28083700	-1.34299400
C	-3.91259700	0.87588000	-0.57157300
C	-4.99930700	1.08615900	0.27991000
C	-6.00392700	0.12810800	0.36472000
C	-5.94631600	-1.04913800	-0.39585800
H	-4.78888600	-2.14603500	-1.83986400
H	-2.98066200	-0.43074500	-1.98311100
H	-5.02745900	1.98245400	0.88959600
H	-6.84390800	0.28740200	1.03655200
C	-7.04770000	-2.07651400	-0.30964600
H	-6.69952100	-3.06403500	-0.62673900
H	-7.43643900	-2.16329000	0.70995400
H	-7.89314800	-1.80671100	-0.95440700
S	-2.60401200	2.10997300	-0.66006800
O	-2.42432600	2.54673700	0.75903500
O	-1.42129900	1.33641500	-1.17844900
O	-3.06389400	3.16892100	-1.57730900

**(S)-TS-2**

C	0.97942100	-1.36072300	0.00405700
C	0.68953600	-1.56825600	1.37319800
C	1.54457100	-2.26123000	2.21722000
C	2.72530800	-2.74990900	1.65418500
C	3.02794800	-2.55853900	0.29800400
C	2.15578200	-1.87222500	-0.54144300
C	-0.13148200	-0.60638500	-0.52542300
C	-1.00349400	-0.30634700	0.56933100
H	1.32055000	-2.40093000	3.26943300
H	3.43103400	-3.27902900	2.28608300
H	3.97670800	-2.90941900	-0.09149400
H	2.41170800	-1.67083200	-1.57354400
H	-0.86690400	-0.74412900	2.60594400
N	-0.53347900	-0.92728800	1.67040400





C	-3.33871900	3.28931800	1.43169400	C	1.89829200	1.74657400	1.32830300
H	-1.98704200	1.71095700	1.92453600	C	1.49914900	0.67867600	2.12791500
C	-4.12416800	3.33881000	-0.84054900	C	2.45311500	-0.15510000	2.71421100
H	-3.43511400	1.75685500	-2.11198900	C	3.80362000	0.06497000	2.46730100
C	-4.10479600	3.89542200	0.43733300	C	4.22599200	1.11154500	1.63461800
H	-3.29472800	3.71951700	2.42732500	H	3.56676800	2.78350400	0.45363200
H	-4.70181900	3.80656500	-1.63190600	H	1.13928100	2.39098200	0.90102900
H	-4.66963600	4.79697100	0.65242700	H	2.12901500	-0.96539900	3.35852500
C	-0.15314800	-0.16318400	1.35418600	H	4.54607200	-0.59036100	2.91517700
H	0.23033800	-0.49095900	2.30849000	C	5.68715500	1.29183500	1.31230000
C	-1.45089500	-0.67855200	0.77638400	H	5.99466800	0.59149200	0.52665900
H	-1.14386000	-1.61216400	0.29206600	H	5.89707600	2.30400200	0.95500600
C	-2.56123200	-1.02450700	1.73943800	H	6.31796100	1.10132900	2.18624000
C	-2.62890000	-0.50450900	3.03730700	S	-0.24651300	0.30404100	2.34376100
C	-3.54275600	-1.94195200	1.33955600	O	-0.46281400	0.09746300	3.78797800
C	-3.66439500	-0.86038600	3.90035000	O	-0.97293600	1.46289600	1.74300000
H	-1.86006000	0.17541700	3.39119300	O	-0.44749300	-0.95572000	1.53387100
C	-4.58702900	-2.28873600	2.19373000	C	-0.97098500	2.56840400	-1.62004300
H	-3.47881800	-2.39253400	0.35565700	C	-2.29061300	2.76979500	-1.12011000
C	-4.65504600	-1.74489900	3.47689100	C	-2.89927700	4.03405200	-1.12798600
H	-3.69406800	-0.44661300	4.90363200	C	-2.15730700	5.08981000	-1.62678100
H	-5.33853600	-2.99854100	1.86195300	C	-0.83682100	4.91577800	-2.11440000
H	-5.46429400	-2.02020900	4.14596300	C	-0.23908600	3.67163900	-2.10784400
C	5.45911600	-0.18231800	-0.49898800	C	-0.63932300	1.19126500	-1.44381400
C	4.24283900	-0.73629500	-0.88120800	C	-1.81134300	0.56324500	-0.87914300
C	3.44307100	-1.36864500	0.07120200	H	-3.90347600	4.17771300	-0.74437100
C	3.86210600	-1.45182800	1.39649800	H	-2.59409200	6.08348000	-1.63840900
C	5.08289600	-0.88861100	1.76967800	H	-0.29351500	5.77744700	-2.48683000
C	5.89888800	-0.24797100	0.83085800	H	0.77649500	3.54317000	-2.46699900
H	6.07362600	0.32457800	-1.23859000	H	-3.65319300	1.41301700	-0.24829000
H	3.88703300	-0.65407500	-1.90174700	N	-2.76303600	1.57343900	-0.69095500
H	3.22070100	-1.93915000	2.12216700	C	-2.10434400	-0.76479600	-0.56664000
H	5.40655800	-0.94630000	2.80589300	C	-1.41197200	-1.88473400	-1.22181300
C	7.22564000	0.34895400	1.23008700	C	-1.03750100	-3.01319800	-0.47182700
H	7.38414800	1.32374900	0.75681100	C	-1.15171300	-1.85543600	-2.60102000
H	7.29536300	0.48180500	2.31326100	C	-0.37295000	-4.06774800	-1.08932000
H	8.05841500	-0.29545000	0.92368900	H	-1.20819700	-3.00416000	0.59732600
S	1.87533900	-2.08735600	-0.43585200	C	-0.50207300	-2.92032200	-3.21499800
O	1.05824900	-2.13904300	0.83314300	H	-1.46155200	-0.99279600	-3.18044000
O	1.32973400	-1.09411900	-1.41250100	C	-0.10251400	-4.02465300	-2.45893100
O	2.15689100	-3.41604100	-1.00090600	H	-0.05858900	-4.92283300	-0.49936900
				H	-0.30740100	-2.89102100	-4.28235600
<b>(R)-INT-2</b>				H	0.41500800	-4.85054600	-2.93707000
C	3.25551600	1.95600000	1.08629600	C	-3.26720700	-1.08903600	0.27061800

C	-3.58133500	-0.32721800	1.41691100	O	-1.66455300	-1.41470300	1.53280700
C	-4.08113100	-2.18926500	-0.06334600	O	-0.57163200	0.36637900	2.86750800
C	-4.68725500	-0.66024600	2.19047200	C	-1.79636800	-1.58910700	-1.69031600
H	-2.91332400	0.47423400	1.71873200	C	-1.42002000	-2.89957100	-1.29915200
C	-5.19515200	-2.50268100	0.70797600	C	-2.24506800	-4.00000600	-1.49041100
H	-3.84265200	-2.78046700	-0.93995400	C	-3.48210900	-3.76869900	-2.09212100
C	-5.50026900	-1.74052700	1.83736600	C	-3.87422400	-2.48020600	-2.48692100
H	-4.90036400	-0.08734600	3.08704800	C	-3.04079900	-1.38195500	-2.28569000
H	-5.82270400	-3.34384600	0.43113000	C	-0.71735500	-0.72677400	-1.25354500
H	-6.36179700	-1.99494100	2.44713400	C	0.31065900	-1.57328300	-0.73471900
C	0.68477500	0.68886000	-1.66523400	H	-1.94914000	-4.99428800	-1.17359000
H	1.29472600	1.28416800	-2.33993100	H	-4.15676500	-4.60335300	-2.25124800
C	1.24104600	-0.33627700	-0.97537900	H	-4.84550800	-2.33848000	-2.94893600
H	0.63144300	-0.83325600	-0.22898600	H	-3.35092300	-0.38427800	-2.57367100
C	2.61162400	-0.80277000	-1.05213100	H	0.36992800	-3.62238300	-0.33777500
C	3.59241200	-0.24095100	-1.89216100	N	-0.13315200	-2.84165600	-0.73361200
C	2.97758500	-1.86933700	-0.21042800	C	1.57613800	-1.00185900	-0.31463000
C	4.88929100	-0.73695000	-1.89362500	C	2.44867400	-0.45871500	-1.39981300
H	3.33722700	0.58953400	-2.54222000	C	3.52664200	0.38759700	-1.08420000
C	4.27751500	-2.36440600	-0.21167200	C	2.21683100	-0.76896300	-2.74960700
H	2.22665500	-2.28396700	0.45375500	C	4.34320100	0.90312300	-2.08577400
C	5.23729400	-1.80121700	-1.05327900	H	3.70744300	0.65542500	-0.05042100
H	5.63645200	-0.29473800	-2.54556300	C	3.02769300	-0.23959200	-3.75144200
H	4.54490900	-3.18342400	0.44857000	H	1.40606900	-1.43752300	-3.01689400
H	6.25322800	-2.18428400	-1.05561100	C	4.09501000	0.59715500	-3.42433700

**(R)-TS-2**

C	-4.04368600	1.58280100	-0.49942400	H	5.16408900	1.56055700	-1.81810300
C	-3.54649100	0.63740700	0.39488400	H	2.83271300	-0.49543800	-4.78827200
C	-2.57867500	1.00983100	1.32945400	H	4.73047400	1.00289200	-4.20517700
C	-2.12579000	2.32808500	1.37511800	C	2.22471600	-1.63606100	0.86661300
C	-2.62224800	3.26470100	0.46987500	C	1.44238100	-1.94980200	1.99497500
C	-3.58794200	2.90916700	-0.48072700	C	3.58928800	-1.98292300	0.86881000
H	-4.79707300	1.28969900	-1.22699900	C	2.02211200	-2.56401000	3.10067700
H	-3.87427300	-0.39491600	0.35374400	H	0.38804600	-1.69585600	2.01439100
H	-1.36063000	2.59341200	2.09489900	C	4.15801700	-2.60499200	1.97639700
H	-2.25067600	4.28587300	0.49685800	H	4.19982300	-1.78349900	-0.00309400
C	-4.14753800	3.93303700	-1.43715200	C	3.37906300	-2.89056400	3.09914300
H	-3.41674600	4.71682300	-1.65720500	H	1.40582200	-2.77581700	3.96823500
H	-4.45232600	3.47510300	-2.38309400	H	5.21061600	-2.87031900	1.95970200
H	-5.03288900	4.42378500	-1.01474000	H	3.82768500	-3.36657200	3.96585400
S	-1.87724400	-0.23653900	2.43425300	C	-0.50541400	0.59392600	-0.92631800
O	-2.85123300	-0.45040500	3.51812000	H	-1.07496400	1.42338200	-1.33501100
				C	0.50071600	0.80907700	0.08205700
				H	0.24294200	0.37577000	1.05397700
				C	1.25964500	2.04467300	0.18404100

C	1.58666200	2.81117600	-0.94730400	N	-0.13424100	-2.63927000	-0.42369300
C	1.70248700	2.46065100	1.45399900	C	1.44371600	-0.60331200	-0.05595100
C	2.32960800	3.97935200	-0.81277100	C	2.48598600	-0.62062600	-1.19293200
H	1.27543100	2.46890900	-1.92995000	C	3.75521000	-0.09097400	-0.92442500
C	2.45111600	3.62586000	1.58229700	C	2.20797400	-1.07976200	-2.48348400
H	1.42117700	1.86938900	2.32034300	C	4.71716600	-0.01068400	-1.92530500
C	2.76488500	4.38571500	0.45105700	H	3.97843800	0.26998600	0.07266800
H	2.58157100	4.56650600	-1.69028800	C	3.17559000	-1.00130800	-3.48850100
H	2.78477600	3.94903700	2.56327300	H	1.23814000	-1.50006000	-2.72431700
H	3.34972500	5.29470300	0.55480600	C	4.43077900	-0.46427600	-3.21453300

**(R)-INT-3**

C	-4.58075100	0.92130700	-0.31337900
C	-3.77767300	0.30270900	0.63984800
C	-2.74448700	1.01971900	1.24626900
C	-2.52514900	2.35271600	0.89901600
C	-3.32890300	2.96048800	-0.06691900
C	-4.36918300	2.25724400	-0.68568800
H	-5.38284000	0.35830700	-0.78416000
H	-3.93573400	-0.73652400	0.90625800
H	-1.71801400	2.88942300	1.38433800
H	-3.15037400	3.99800200	-0.33829300
C	-5.26360600	2.92690600	-1.69945600
H	-4.74388400	3.73672200	-2.21964800
H	-5.62462800	2.21596000	-2.44911300
H	-6.14656100	3.36376700	-1.21722800
S	-1.68681100	0.20627500	2.46182100
O	-2.54776400	-0.14624700	3.60219100
O	-1.13500600	-0.97774700	1.72106300
O	-0.63162200	1.23588900	2.74552500
C	-1.80350700	-1.50617100	-1.53738900
C	-1.40617700	-2.77609000	-1.04674200
C	-2.18158100	-3.91376200	-1.19598400
C	-3.39839000	-3.76691600	-1.86926400
C	-3.80759600	-2.52460300	-2.36933700
C	-3.01800400	-1.38455400	-2.20616700
C	-0.75273000	-0.58429900	-1.13069900
C	0.23435600	-1.37234600	-0.45704800
H	-1.86729100	-4.87382400	-0.80132800
H	-4.03674100	-4.63389100	-2.00230100
H	-4.75856500	-2.44606700	-2.88552500
H	-3.34924900	-0.41963200	-2.57062800
H	0.34136800	-3.34996600	0.11799800

C	1.44371600	-0.60331200	-0.05595100
C	2.48598600	-0.62062600	-1.19293200
C	3.75521000	-0.09097400	-0.92442500
C	2.20797400	-1.07976200	-2.48348400
C	4.71716600	-0.01068400	-1.92530500
H	3.97843800	0.26998600	0.07266800
C	3.17559000	-1.00130800	-3.48850100
H	1.23814000	-1.50006000	-2.72431700
C	4.43077900	-0.46427600	-3.21453300
H	5.69047200	0.41271800	-1.69862200
H	2.94227700	-1.36649100	-4.48392600
H	5.18187500	-0.40295300	-3.99576800
C	2.05564400	-1.16401800	1.22904200
C	1.84875600	-0.60683000	2.49140600
C	2.80227300	-2.34956200	1.12206000
C	2.39609800	-1.21714700	3.62136200
H	1.21869600	0.26300300	2.62175900
C	3.33379600	-2.96359800	2.25408900
H	2.99499000	-2.77696300	0.14206100
C	3.13594800	-2.39254100	3.51176200
H	2.21859400	-0.77195500	4.59507500
H	3.90980200	-3.87827300	2.15043400
H	3.55195400	-2.86331500	4.39719000
C	-0.42540500	0.72398500	-0.94889000
H	-0.99057600	1.58330100	-1.28835600
C	0.75829500	0.86367100	-0.03447300
H	0.30156900	0.95807000	0.96638600
C	1.63378000	2.06333400	-0.25378500
C	2.00563000	2.47818400	-1.53871600
C	2.08418100	2.78909400	0.85505600
C	2.82494000	3.59060700	-1.71301400
H	1.67162700	1.90967800	-2.40181600
C	2.91057300	3.89879700	0.68163600
H	1.76651600	2.48857300	1.84830200
C	3.28406500	4.30003300	-0.60166400
H	3.11099600	3.89952600	-2.71374200
H	3.25463400	4.45483300	1.54820100
H	3.92661100	5.16488600	-0.73621500

**INT-4**

C	5.04724800	-1.23208000	0.30416700
C	3.92596200	-1.83357300	0.87217200
C	3.10435800	-2.63866000	0.08865400

C	3.42780100	-2.88111500	-1.24784200	C	-1.45917100	-1.94579300	3.29796700
C	4.55337400	-2.27876300	-1.80303900	H	-0.99941100	-1.98917900	1.21955100
C	5.36727200	-1.42718800	-1.04335300	C	-2.96771700	-0.22371800	4.04870300
H	5.67126800	-0.58187100	0.91134300	H	-3.74729300	1.07209200	2.52186700
H	3.66336500	-1.66714000	1.90915500	C	-2.14982600	-1.32042400	4.33072000
H	2.78763100	-3.51948200	-1.84787300	H	-0.79306800	-2.77897900	3.49003600
H	4.79849600	-2.45778500	-2.84676100	H	-3.52288600	0.26478500	4.84402200
C	6.52087600	-0.69225700	-1.67571000	H	-2.05053300	-1.67860400	5.35030200
H	6.19089300	0.28969900	-2.03589500	C	-0.94914200	0.62560000	-1.62211700
H	7.33139200	-0.52520300	-0.96025200	H	-0.48772500	0.46754200	-2.58853900
H	6.92718400	-1.24035800	-2.53079100	C	-1.69759100	-0.46996300	-0.90847100
S	1.53969400	-3.25309300	0.73655600	H	-0.91999900	-1.10078400	-0.46110000
O	1.57716900	-4.72279600	0.72198800	C	-2.52045800	-1.36895100	-1.79494400
O	1.40530600	-2.63135400	2.09125500	C	-3.36017200	-0.84512500	-2.78625400
O	0.53786900	-2.67474100	-0.24727100	C	-2.44063700	-2.75575500	-1.62335300
C	-0.26544900	3.06934000	-0.73329800	C	-4.12976900	-1.69241000	-3.57853100
C	-0.63906200	3.53511300	0.55524700	H	-3.43224600	0.23044200	-2.91655900
C	-0.16689500	4.72521000	1.08682300	C	-3.21630700	-3.60269900	-2.41523400
C	0.70252700	5.47278300	0.28799300	H	-1.74569300	-3.16335600	-0.89558200
C	1.08498000	5.02996300	-0.98540100	C	-4.06461300	-3.07426700	-3.38861400
C	0.61068800	3.82653100	-1.50660800	H	-4.78357200	-1.27556900	-4.33847300
C	-0.91877700	1.77692400	-0.88382400	H	-3.14768800	-4.67707100	-2.27634200
C	-1.65864400	1.54968100	0.30839800	H	-4.66761400	-3.73602700	-4.00304900
H	-0.44993900	5.05876000	2.07942400	C	2.72394800	1.70563800	-0.16917000
H	1.09564400	6.40942300	0.66875900	C	2.41160500	0.79307500	-1.21856400
H	1.78015900	5.62309300	-1.56906600	C	2.96934700	0.90271800	-2.49027400
H	0.95025500	3.46710100	-2.47108200	C	3.85285300	1.95808900	-2.71794100
H	-1.85514500	2.58953300	2.09180400	C	4.16642300	2.87664700	-1.69901700
N	-1.49759600	2.57040100	1.14484500	C	3.61067400	2.75726500	-0.42695200
C	-2.44876400	0.27971700	0.31379200	C	1.97170600	1.28499700	0.99322200
C	-3.91213900	0.54955000	-0.07267200	C	1.26314500	0.17203700	0.60972000
C	-4.83988000	-0.48672200	0.08913200	H	2.73889700	0.18148700	-3.26768600
C	-4.33444600	1.75492700	-0.63866400	H	4.30864400	2.06965200	-3.69692900
C	-6.15845000	-0.32454000	-0.32145900	H	4.85756300	3.68715200	-1.90935800
H	-4.51595800	-1.42565900	0.52306600	H	3.85610300	3.47425000	0.35060900
C	-5.66054500	1.91958400	-1.04616600	H	1.31055000	-1.06266700	-1.04710600
H	-3.63626400	2.57365600	-0.77729500	N	1.49041600	-0.11393200	-0.71822400
C	-6.57457900	0.88021300	-0.89255200	H	0.63450600	-0.46660400	1.20053800
H	-6.86143400	-1.14233000	-0.19947700	C	2.01593800	1.84243900	2.38121500
H	-5.97354300	2.86321300	-1.48234500	H	2.77970300	2.62684700	2.44596600
H	-7.60430300	1.00669200	-1.21166000	H	1.05951000	2.31532200	2.64416200
C	-2.36863400	-0.37406200	1.69705400	C	2.30947100	0.76305900	3.44451000
C	-1.57152400	-1.48109800	1.98512600	H	2.43957400	1.25874200	4.41575400
C	-3.07755100	0.24442900	2.74262000	H	3.26028800	0.27097700	3.19813900

O	1.25384200	-0.16611100	3.57766800	H	-4.04103400	2.15166200	-0.86979600
H	1.43761400	-0.97578300	3.06508200	C	-6.68993700	0.02847700	-0.83664200
				H	-6.66595400	-1.95695900	0.00668200
				H	-6.39883300	2.03066300	-1.57577300
				H	-7.72484000	-0.03020600	-1.15888900
<b>TS-3</b>				C	-2.36938100	-0.28760000	1.84026800
C	5.23225200	-1.00645400	0.30681400	C	-1.42964700	-1.22792700	2.26865900
C	4.13947400	-1.59380200	0.94161200	C	-3.16425400	0.35220700	2.80716600
C	3.25787000	-2.38121700	0.20683000	C	-1.25067600	-1.48579500	3.63041800
C	3.49068400	-2.61869000	-1.14922900	H	-0.79853900	-1.77253500	1.57893800
C	4.58983700	-2.03377400	-1.77005600	C	-2.99581000	0.08553700	4.16283500
C	5.46615400	-1.20315600	-1.05835200	H	-3.94393600	1.03964700	2.48839500
H	5.90821800	-0.37607800	0.87839800	C	-2.02663300	-0.82956900	4.58087200
H	3.95272800	-1.43842200	1.99668400	H	-0.48007400	-2.19131400	3.92000100
H	2.79907000	-3.23748300	-1.71092200	H	-3.62223300	0.59075200	4.89211000
H	4.76431700	-2.20849400	-2.82832200	H	-1.88172200	-1.02770800	5.63802000
C	6.60236700	-0.50240200	-1.75756100	C	-0.73822800	0.39025700	-1.36507800
H	6.26383000	0.45799500	-2.16410100	H	-0.34590900	0.20632800	-2.35742800
H	7.43005600	-0.29795100	-1.07250800	C	-1.64659500	-0.64139500	-0.70400200
H	6.98778100	-1.09605700	-2.59167500	H	-1.00984600	-1.33375400	-0.15832800
S	1.77258300	-3.04796500	0.97708000	C	-2.39562700	-1.48561800	-1.70923600
O	1.92018600	-4.50232400	1.11416700	C	-3.12297100	-0.91115800	-2.75894600
O	1.62529100	-2.29157100	2.25737200	C	-2.35392700	-2.87828200	-1.58705500
O	0.69682500	-2.65688200	-0.02922800	C	-3.82653500	-1.71477100	-3.65172400
C	-0.49728300	3.01909500	-0.80640600	H	-3.15972900	0.16892200	-2.85995000
C	-1.14037200	3.64300900	0.30013900	C	-3.05940300	-3.68334100	-2.48186700
C	-0.88098500	4.95979300	0.66731400	H	-1.74802600	-3.32430100	-0.80402100
C	0.04892200	5.66151500	-0.09830400	C	-3.80216900	-3.10392600	-3.51025400
C	0.69527900	5.06290200	-1.19322900	H	-4.39719400	-1.25818200	-4.45464000
C	0.43194000	3.74566700	-1.55655600	H	-3.02163100	-4.76321700	-2.37732900
C	-1.00733800	1.66395500	-0.83233900	H	-4.35401500	-3.73070600	-4.20418900
C	-1.90476400	1.53209400	0.22521800	C	2.69210200	1.59615400	-0.40443700
H	-1.37507600	5.42041700	1.51658400	C	2.11961500	0.64114600	-1.27469600
H	0.27917400	6.68982500	0.16042600	C	2.48540300	0.52962000	-2.60657400
H	1.42003300	5.63719400	-1.76081100	C	3.45702600	1.41751300	-3.08248400
H	0.95457600	3.28159300	-2.38556700	C	4.02977300	2.37833800	-2.23802500
H	-2.53596300	2.83785900	1.73859600	C	3.65759800	2.47380500	-0.89403600
N	-2.00111000	2.70004700	0.89371600	C	2.06213600	1.41750900	0.90111900
C	-2.52986200	0.17259800	0.37927000	C	1.16569900	0.40804400	0.76937300
C	-4.01162200	0.17364400	-0.01189000	H	2.05174500	-0.22774000	-3.25120500
C	-4.77104800	-0.97697000	0.23457300	H	3.77310300	1.35670000	-4.11871300
C	-4.61265300	1.25312700	-0.66229100	H	4.77789900	3.05702800	-2.63573900
C	-6.09582500	-1.05247400	-0.18040100	H	4.10820800	3.22035000	-0.24795100
H	-4.31090100	-1.81815400	0.74103100	H	1.05079200	-1.11867300	-0.61050800
C	-5.94664800	1.18223400	-1.07117200				



N	1.12672900	-0.07226600	-0.55888500	C	4.24223500	-2.29451900	2.52951700
H	0.53100800	-0.03438900	1.51482300	H	3.79190500	-2.29567500	0.43002000
C	2.39827900	2.10902400	2.18387400	C	3.98342100	-1.70691700	3.76975200
H	3.17036800	2.86906800	2.01768500	H	2.83309700	-0.21633800	4.81285100
H	1.51557400	2.62751900	2.57531600	H	4.99260500	-3.07431900	2.44049300
C	2.88773700	1.11468300	3.26221500	H	4.52566300	-2.02949100	4.65292600
H	3.16597900	1.68724100	4.15549100	C	-0.48473600	0.21587400	-0.61256100
H	3.79615400	0.61568200	2.89759900	H	-0.35642800	0.71436200	-1.57981000
O	1.89464000	0.19129900	3.64631200	C	0.68054400	0.61154000	0.37124600
H	1.93894100	-0.61709400	3.10115200	H	0.24606200	0.42910200	1.35644200
				C	1.06681000	2.06640600	0.29520100
<b>3</b>				C	1.52520000	2.65909000	-0.89214900
C	-0.99675200	-2.44531400	-1.14177300	C	0.88233200	2.88668300	1.41381600
C	-0.10039900	-3.53044900	-0.88275800	C	1.80323400	4.02268700	-0.94673400
C	-0.45772500	-4.85563900	-1.13384100	H	1.66400900	2.05526000	-1.78104500
C	-1.72713800	-5.09470000	-1.65209100	C	1.15816800	4.25271400	1.36319900
C	-2.62143100	-4.04022200	-1.91841800	H	0.49238500	2.45476200	2.33120400
C	-2.26794300	-2.71902300	-1.67115900	C	1.62322400	4.82528500	0.18102200
C	-0.30391100	-1.26425500	-0.71094400	H	2.15852100	4.45926300	-1.87520000
C	0.91744800	-1.64045700	-0.23604900	H	0.99916800	4.86800000	2.24335300
H	0.22746900	-5.67264900	-0.92890500	H	1.83629700	5.88880300	0.13491300
H	-2.03394100	-6.11601300	-1.85342000	C	-3.72684000	1.71793200	0.27012800
H	-3.60372200	-4.26574900	-2.32043600	C	-2.46339600	1.78630500	-0.38296800
H	-2.95652900	-1.90731600	-1.88590100	C	-2.07792800	2.90025700	-1.13647800
H	1.83069200	-3.53669500	0.04352300	C	-2.98563000	3.94733700	-1.24207700
N	1.07934800	-3.00158400	-0.36091000	C	-4.24525600	3.89580800	-0.61186300
C	1.81344400	-0.50589900	0.19708000	C	-4.62078100	2.79303600	0.14383900
C	2.81404200	-0.12535100	-0.90536100	C	-3.78644700	0.45477000	0.96295100
C	3.91929000	0.67601100	-0.59104900	C	-2.59134600	-0.17557600	0.71401700
C	2.60846100	-0.49083600	-2.23968900	H	-1.09945800	2.96264800	-1.59764000
C	4.78891900	1.11293100	-1.58655500	H	-2.71259300	4.82778400	-1.81567300
H	4.08732600	0.96998000	0.43894300	H	-4.92597300	4.73525200	-0.71524000
C	3.47924900	-0.05275400	-3.23931600	H	-5.58944200	2.76145600	0.63397400
H	1.75882600	-1.11137700	-2.50239200	N	-1.79172300	0.60709100	-0.11036400
C	4.57061600	0.75273500	-2.91732900	H	-2.23080200	-1.13970000	1.03830500
H	5.63425000	1.74116500	-1.32303100	C	-4.93994900	-0.06545900	1.77352000
H	3.30262500	-0.34590000	-4.26980900	H	-4.96769100	0.42004700	2.76017700
H	5.24751200	1.09353300	-3.69468100	H	-5.87966100	0.19955100	1.27324500
C	2.56902500	-0.86630400	1.48040900	C	-4.91071600	-1.58397000	1.97376000
C	2.33019500	-0.27838700	2.72387700	H	-5.76598200	-1.88866300	2.58443800
C	3.54863900	-1.87057600	1.40014600	H	-4.00173100	-1.86464700	2.53206500
C	3.03309600	-0.69344400	3.85829300	O	-5.01744000	-2.31214700	0.76152100
H	1.60622800	0.51927200	2.82290500	H	-4.28016100	-2.04119700	0.19650300

**INT-5**

C	4.89300600	-1.93540700	0.77948400
C	3.65895400	-2.17186900	1.38118300
C	2.67735500	-2.87616200	0.68905500
C	2.94275700	-3.38178700	-0.58507500
C	4.18444600	-3.14577500	-1.17475100
C	5.17037600	-2.40097700	-0.51100200
H	5.64464500	-1.35676900	1.30925800
H	3.43064800	-1.78288900	2.36607700
H	2.16975600	-3.92767500	-1.11517400
H	4.38934700	-3.53396500	-2.16939000
C	6.47532800	-2.06139300	-1.18507000
H	6.44895800	-1.03636600	-1.57456400
H	7.31465400	-2.12217900	-0.48566000
H	6.68107800	-2.73298800	-2.02332500
S	1.01836200	-3.05023900	1.36959200
O	0.84013300	-4.44642400	1.79925300
O	0.93663700	-2.03814700	2.47386300
O	0.15424200	-2.64942300	0.20069500
C	-0.20543300	3.05249100	-0.32662400
C	-0.86983300	3.54973200	0.82319100
C	-0.51518800	4.74108100	1.43512700
C	0.55340000	5.44594900	0.87029500
C	1.23088400	4.96528700	-0.25788000
C	0.86024700	3.76521100	-0.86731300
C	-0.83333100	1.77338100	-0.61225000
C	-1.85965200	1.59068400	0.36088100
H	-1.02658800	5.10441200	2.31986500
H	0.86862200	6.37893000	1.32532700
H	2.07101600	5.52388100	-0.65544100
H	1.41262600	3.38051000	-1.71615100
H	-2.42276100	2.64131000	2.04733000
N	-1.88131700	2.61881300	1.19230700
C	-2.64300500	0.33045200	0.19724000
C	-3.96542700	0.61262800	-0.53679300
C	-4.92292400	-0.40797300	-0.58768700
C	-4.21462400	1.80936500	-1.21295100
C	-6.09594400	-0.23991600	-1.31494900
H	-4.73317700	-1.34037800	-0.06906000
C	-5.39626300	1.98031900	-1.93828600
H	-3.49035400	2.61681100	-1.19170100
C	-6.33734400	0.95571500	-1.99539300
H	-6.82110000	-1.04640400	-1.35437800

H	-5.57527700	2.91716200	-2.45683900
H	-7.25372200	1.08648100	-2.56221100
C	-2.90957300	-0.29982600	1.56694400
C	-2.20793200	-1.40378400	2.04610600
C	-3.85168400	0.32475300	2.40204400
C	-2.42196500	-1.86579800	3.34645600
H	-1.46767900	-1.90312500	1.43763100
C	-4.06643000	-0.13848200	3.69745800
H	-4.44384500	1.15327500	2.02143700
C	-3.34639100	-1.23640900	4.17562300
H	-1.83839700	-2.70970800	3.69829200
H	-4.80060300	0.35192700	4.32976100
H	-3.50919200	-1.59583400	5.18689900
C	-0.70750900	0.60871200	-1.30834600
H	0.02743600	0.39958000	-2.07697400
C	-1.63750800	-0.44910300	-0.80360400
H	-0.98470200	-1.10255500	-0.19902300
C	-2.26065800	-1.31656300	-1.86752700
C	-2.75693900	-0.75873900	-3.05260400
C	-2.36926200	-2.69615600	-1.65959400
C	-3.37534200	-1.56136500	-4.00727100
H	-2.68721700	0.31338600	-3.21153100
C	-2.99410400	-3.49790600	-2.61460400
H	-1.93266200	-3.13380800	-0.76842000
C	-3.50215000	-2.93382100	-3.78538800
H	-3.76395100	-1.11651800	-4.91821200
H	-3.07445700	-4.56733400	-2.44606500
H	-3.98905700	-3.56129900	-4.52586900
C	3.59863400	1.80788800	-0.36630000
C	3.65798100	0.87689000	-1.44376400
C	4.57182400	1.01066100	-2.49138100
C	5.43069600	2.10652400	-2.46386200
C	5.37249100	3.05174000	-1.42081000
C	4.46486700	2.91248900	-0.37620100
C	2.57877400	1.34469200	0.54592300
C	2.06321900	0.19879800	-0.00586700
H	4.60906900	0.28618100	-3.29950800
H	6.15428600	2.23669300	-3.26268300
H	6.05224700	3.89842700	-1.43414000
H	4.42950300	3.64357800	0.42650800
H	2.69929500	-1.00730800	-1.60396600
N	2.67668500	-0.07167800	-1.22199600
H	1.31492900	-0.46955900	0.37749700
C	2.20601800	1.98467100	1.85020900

H 3.12162300 2.32618600 2.35353900  
H 1.61126700 2.88939700 1.68135600  
C 1.45848400 1.06960200 2.82010200  
H 1.27553000 1.62260500 3.75420400  
H 2.08604300 0.20611600 3.06481500  
O 0.21757400 0.61678700 2.28628700  
H 0.25214500 -0.36164800 2.34900600

**TS-4**

C 5.37535900 -0.10321500 0.92819800  
C 4.24032400 -0.66422600 1.51129900  
C 3.67985500 -1.81516200 0.96447700  
C 4.27336300 -2.42685500 -0.14141100  
C 5.40927600 -1.86047600 -0.71256800  
C 5.96934000 -0.68230500 -0.19770100  
H 5.80079700 0.80443000 1.34798000  
H 3.77537600 -0.21983100 2.38239500  
H 3.83744400 -3.33093500 -0.55386000  
H 5.86856000 -2.33406400 -1.57645700  
C 7.15080500 -0.03108800 -0.86823300  
H 6.81176600 0.70489100 -1.60766000  
H 7.78115100 0.49644700 -0.14659700  
H 7.77079900 -0.76439600 -1.39186900  
S 2.13269900 -2.47523400 1.61134800  
O 2.40056300 -3.81741400 2.14626100  
O 1.69265300 -1.46750700 2.63286200  
O 1.23026200 -2.46814100 0.39955700  
C -1.62096800 3.18811300 -0.24554200  
C -2.75356900 3.39490700 0.59373800  
C -3.19760900 4.66623200 0.94244200  
C -2.49163300 5.75284100 0.42746100  
C -1.37773700 5.57071600 -0.40972900  
C -0.93415300 4.29641300 -0.75207300  
C -1.47713000 1.75259000 -0.35619100  
C -2.51605200 1.17413400 0.36530100  
H -4.05869600 4.80912800 1.58718300  
H -2.81176300 6.75880500 0.67798600  
H -0.85548500 6.44077900 -0.79409600  
H -0.06547700 4.15809800 -1.38774100  
H -4.05972600 1.96630200 1.54812000  
N -3.27131900 2.13531000 0.94160200  
C -2.61967900 -0.31956900 0.26758500  
C -3.88602800 -0.76530800 -0.47105700

C -4.20273700 -2.12973500 -0.48815200  
C -4.69155400 0.12196200 -1.18798800  
C -5.28917500 -2.59578600 -1.21977800  
H -3.58234300 -2.82456700 0.06698500  
C -5.78956500 -0.34372100 -1.91550900  
H -4.45953300 1.18146200 -1.20179900  
C -6.08893700 -1.70307000 -1.93778700  
H -5.51176900 -3.65812200 -1.23177300  
H -6.40455600 0.36053700 -2.46767300  
H -6.93812400 -2.06714300 -2.50761800  
C -2.60163400 -0.89732000 1.69475500  
C -1.46086900 -1.42531800 2.29802200  
C -3.77639100 -0.79055600 2.45865500  
C -1.48215100 -1.82658600 3.63510200  
H -0.53553300 -1.55867900 1.75959300  
C -3.79973600 -1.18993800 3.79192400  
H -4.68748700 -0.42316200 1.99360500  
C -2.64687700 -1.70719800 4.38792400  
H -0.56849000 -2.22202900 4.06555900  
H -4.71975200 -1.10434600 4.36277300  
H -2.66265900 -2.01848700 5.42784400  
C -0.65650700 0.74634200 -0.91748100  
H -0.12624600 0.88529300 -1.85242700  
C -1.30153900 -0.62337200 -0.62799400  
H -0.62545800 -1.22360100 -0.02669900  
C -1.51605900 -1.41964500 -1.89585700  
C -2.12876600 -0.86448900 -3.02611500  
C -1.08085900 -2.74898200 -1.93840700  
C -2.33310000 -1.63340700 -4.16833900  
H -2.46777600 0.16636200 -3.00230100  
C -1.28504300 -3.51877000 -3.08423500  
H -0.56803500 -3.16680200 -1.07684900  
C -1.91648500 -2.96611600 -4.19800400  
H -2.82055900 -1.19517600 -5.03397500  
H -0.94619100 -4.55011200 -3.10514100  
H -2.07870200 -3.56683600 -5.08789200  
C 2.69263600 1.96566800 -0.85839800  
C 2.78252300 0.69576600 -1.53022700  
C 3.67632200 0.49049000 -2.59442700  
C 4.47739500 1.55419100 -2.96643000  
C 4.41036700 2.81372800 -2.31188400  
C 3.53092000 3.02722200 -1.27108100  
C 1.73613100 1.82383000 0.17805100  
C 1.20207700 0.51636800 0.05580900

H	3.74210200	-0.47207500	-3.08770800	C	-2.36350600	0.00687700	1.60137900
H	5.18120000	1.42566800	-3.78302800	C	-1.70897000	-0.35171800	2.78297100
H	5.06296300	3.61438700	-2.64389900	C	-3.66058100	0.53804800	1.70352800
H	3.48046800	3.98969900	-0.77156700	C	-2.32628400	-0.18484400	4.02511900
H	1.84982700	-1.17108000	-0.99123100	H	-0.71003600	-0.76644800	2.75499400
N	1.90180400	-0.15541900	-0.94460100	C	-4.27476100	0.71568900	2.94016800
H	0.79938900	-0.04325900	0.87993400	H	-4.20062700	0.78946500	0.79537900
C	1.40707100	2.74277900	1.30152100	C	-3.60775500	0.35303700	4.11168100
H	2.01323200	3.65330300	1.24008400	H	-1.79754600	-0.48047300	4.92633800
H	0.35723000	3.04643700	1.25538700	H	-5.27775500	1.12900200	2.98836600
C	1.60133100	2.06965700	2.68397700	H	-4.08490400	0.48301300	5.07789100
H	1.50071000	2.85156500	3.44905800	C	0.55723000	0.01444300	-0.91943100
H	2.61877900	1.66621900	2.75623200	H	0.39026600	-0.41147300	-1.91909700
O	0.62329000	1.08008600	2.90924600	C	-0.30907600	-0.78668900	0.13370300
H	1.03652400	0.19277100	2.90329000	H	0.18355200	-0.57939500	1.08286800
				C	-0.29049200	-2.28084200	-0.06877500
				C	-0.57531800	-2.86985200	-1.31112400
<b>4</b>				C	0.06746300	-3.12041900	0.99228000
C	0.10871300	2.71607600	-1.32909800	C	-0.50784600	-4.25132100	-1.47934200
C	-1.06206600	3.43384600	-0.92373700	H	-0.87259300	-2.24759200	-2.14776400
C	-1.22483500	4.79294200	-1.19431000	C	0.13185100	-4.50430700	0.82987400
C	-0.20939500	5.43697800	-1.89440800	H	0.31285700	-2.68394400	1.95564600
C	0.94463800	4.74629900	-2.31180800	C	-0.15549000	-5.07522200	-0.40884500
C	1.11365000	3.39540600	-2.03493900	H	-0.73763300	-4.68472000	-2.44801300
C	-0.06769500	1.37504500	-0.84467100	H	0.41553300	-5.13272800	1.66852600
C	-1.27852300	1.31875800	-0.21915200	H	-0.10263600	-6.15146000	-0.54121400
H	-2.11332500	5.32870300	-0.87395200	C	4.12926300	-0.11592500	0.20405100
H	-0.30956700	6.49351800	-2.12212300	C	3.96125200	-1.28557200	-0.58718500
H	1.71593200	5.28283600	-2.85528400	C	4.98275000	-2.22131100	-0.76650400
H	2.01046500	2.86857300	-2.34518800	C	6.19710900	-1.97365300	-0.13585800
H	-2.74275900	2.78965600	0.23773000	C	6.38913000	-0.81899800	0.64873900
N	-1.90841800	2.54276900	-0.26951900	C	5.36988700	0.10921400	0.82184300
C	-1.72689700	-0.05521600	0.20650500	C	2.88117300	0.61171500	0.18162200
C	-2.70106000	-0.67163000	-0.80697300	C	2.01577700	-0.12184400	-0.60774800
C	-3.43095900	-1.81627900	-0.46020900	H	4.83309800	-3.10973100	-1.37288900
C	-2.80966600	-0.17656900	-2.11033500	H	7.01172100	-2.68203500	-0.25132000
C	-4.24295800	-2.45410700	-1.39362400	H	7.35080300	-0.65584800	1.12557800
H	-3.34696900	-2.21561300	0.54459900	H	5.52827700	0.99369400	1.43182800
C	-3.62318400	-0.81569500	-3.04834800	H	2.21060300	-2.00899900	-1.55600700
H	-2.24961200	0.70649800	-2.39753800	N	2.67589500	-1.25141900	-1.08095000
C	-4.34106300	-1.95693900	-2.69450400	C	2.62418000	1.87892800	0.94830600
H	-4.79388500	-3.34463400	-1.10685500	H	3.58170300	2.31530200	1.25173800
H	-3.69525400	-0.41622200	-4.05551800	H	2.11888000	2.63019700	0.33834400
H	-4.97348600	-2.45380200	-3.42381900	C	1.79825000	1.65664600	2.21444900

H	2.25084100	0.84708500	2.81035200
H	0.78306500	1.34127700	1.93567900
O	1.76785600	2.88305500	2.93742000
H	1.15218000	2.77645400	3.67288000

**TS-1S**

C	-2.46862200	-3.63438700	-0.03985500
C	-3.06799100	-2.48387400	-0.53407500
C	-2.33873900	-1.63224000	-1.36754900
C	-1.02501300	-1.93846500	-1.71003100
C	-0.43045300	-3.09095900	-1.19601100
C	-1.13850600	-3.95108200	-0.35398000
H	-3.02863700	-4.28518500	0.62482400
H	-4.08626100	-2.22993300	-0.26310400
H	-0.47471800	-1.27707100	-2.36751400
H	0.60362000	-3.31290600	-1.44246500
C	-0.49345700	-5.18297900	0.22687700
H	0.55671600	-5.26033300	-0.06632400
H	-0.54074500	-5.16507900	1.32125400
H	-1.00323100	-6.09481000	-0.10389400
S	-3.13026100	-0.14928800	-1.99307200
O	-1.97637100	0.64648700	-2.60516300
H	-0.81770500	1.02663500	-1.99394400
O	-4.11859400	-0.53637000	-3.00258700
O	-3.68748400	0.54998500	-0.79474600
C	-0.71452000	-1.23703800	1.98251600
C	-1.94894700	-0.53900000	1.89419900
C	-3.12399000	-1.03525100	2.47798400
C	-3.02761900	-2.22291800	3.18175400
C	-1.80038500	-2.92181500	3.30098800
C	-0.64971900	-2.44768600	2.69910600
C	0.24262500	-0.50127400	1.21391700
C	-0.41896500	0.66669100	0.75881700
H	-4.06431800	-0.50676100	2.36960900
H	-3.91517700	-2.63468500	3.65207200
H	-1.77326100	-3.84907900	3.86424400
H	0.28234500	-2.99941700	2.76694700
H	-2.52242300	1.00194400	0.63349700
N	-1.75288200	0.61077600	1.18156500
C	0.14369700	1.85844700	0.16541500
C	1.61744400	2.07941200	0.41509200
C	2.53694400	2.39903300	-0.58627400
C	2.05832200	2.02926600	1.74609400

C	3.87866000	2.61069000	-0.27203700
H	2.22617900	2.42500100	-1.62123400
C	3.39534600	2.25688900	2.05960800
H	1.35008200	1.79310000	2.53191300
C	4.31497700	2.53745500	1.04897900
H	4.58492100	2.82022700	-1.06880900
H	3.71827800	2.20408200	3.09458200
H	5.36136900	2.69571100	1.28899700
C	-0.67312500	3.12344700	0.15571300
C	-1.93513600	3.19035600	-0.46142000
C	-0.17400600	4.27180200	0.79343100
C	-2.67885600	4.36532300	-0.41799300
H	-2.34368200	2.34190600	-0.99394300
C	-0.92849800	5.44224600	0.83921000
H	0.79954000	4.24792100	1.26524900
C	-2.18350500	5.49459200	0.23528900
H	-3.64899600	4.39030100	-0.90321500
H	-0.52768000	6.31493900	1.34503200
H	-2.76808700	6.40870600	0.26733900
O	0.13360600	1.46209500	-1.70877600
H	0.11034200	2.32857400	-2.14515700
C	1.58660300	-0.96663700	0.94575700
H	2.06690100	-1.52882600	1.74368900
C	2.21581200	-0.81164700	-0.23674900
H	1.66832500	-0.33860200	-1.04636500
C	3.58039100	-1.21658000	-0.55450900
C	4.52436000	-1.56273800	0.43006700
C	3.98513100	-1.23706600	-1.90089000
C	5.81497700	-1.93768500	0.07547700
H	4.24882300	-1.51162500	1.47822500
C	5.27790900	-1.61212900	-2.25597100
H	3.26886300	-0.95862500	-2.66895700
C	6.19787200	-1.96717900	-1.26881900
H	6.53129500	-2.19840100	0.84879700
H	5.56838400	-1.62583000	-3.30199500
H	7.20792000	-2.25640800	-1.54173400

**INT-1S**

C	-3.15613300	-3.16192000	-0.26448500
C	-3.54022500	-1.89890200	-0.69530600
C	-2.61768200	-1.08231600	-1.35520100
C	-1.32667800	-1.54164100	-1.59805300
C	-0.95302900	-2.81327200	-1.15943900

C	-1.85348700	-3.63669800	-0.48155100	H	-1.57601900	2.54299000	-0.89049600
H	-3.87001400	-3.78813500	0.26386200	C	0.29244800	5.59093700	0.60717100
H	-4.54578900	-1.53463700	-0.51660500	H	1.62510300	4.17063100	1.50609800
H	-0.61610200	-0.90811700	-2.11268700	C	-0.83928800	5.77219400	-0.19394500
H	0.06118100	-3.15995800	-1.33635800	H	-2.37346600	4.79043600	-1.35594900
C	-1.44203000	-4.99426100	0.02847000	H	0.81774500	6.44957300	1.01303700
H	-0.40501500	-5.22124800	-0.23303700	H	-1.19054000	6.77503500	-0.41741800
H	-1.53439800	-5.04488300	1.11975500	O	0.79921600	1.06727400	-2.35319400
H	-2.07452000	-5.78760400	-0.38486800	H	0.97864800	1.16928200	-3.29572200
S	-3.12744800	0.56796600	-1.86358100	C	1.34114900	-1.28976800	1.06595000
O	-1.89744600	1.17635700	-2.47331000	H	1.65307000	-2.09591500	1.72482100
H	-0.18455700	1.12935300	-2.30611600	C	1.96380300	-1.07882900	-0.11928100
O	-4.25750400	0.40545500	-2.78694300	H	1.53458700	-0.34626500	-0.79794600
O	-3.50201800	1.27077300	-0.58047300	C	3.14404100	-1.75458500	-0.62400300
C	-0.97569700	-1.15525400	2.06842000	C	3.94627000	-2.61249800	0.15294500
C	-2.06566800	-0.24568800	1.89934900	C	3.50992700	-1.51627000	-1.96292400
C	-3.36351200	-0.56649600	2.33357300	C	5.06895100	-3.21716800	-0.39738800
C	-3.53178300	-1.77825700	2.97223300	H	3.69606500	-2.78942100	1.19396000
C	-2.45596700	-2.69014800	3.16640400	C	4.63400300	-2.12448000	-2.51200400
C	-1.19213200	-2.40040700	2.70417600	H	2.89174800	-0.84800000	-2.55462200
C	0.14338000	-0.58311500	1.41744300	C	5.41615800	-2.97748700	-1.73148900
C	-0.25792900	0.75983400	1.01429800	H	5.68205900	-3.87398600	0.21195200
H	-4.18678200	0.11350700	2.15157400	H	4.90231100	-1.93426100	-3.54648000
H	-4.51945700	-2.05571200	3.32737100	H	6.29518700	-3.45185300	-2.15657900
H	-2.64784800	-3.63111500	3.67089400				
H	-0.37730800	-3.10662000	2.82408400				
H	-2.30571600	1.37102400	0.64543500				
N	-1.63557200	0.88194400	1.27473400	<b>(S)-INT-2S</b>			
C	0.56417200	1.84770000	0.73180300	C	5.52495000	-0.16002200	-0.00656200
C	2.03059800	1.75118600	0.92777400	C	4.74778800	0.97522600	-0.23193500
C	2.89377000	2.08600700	-0.12527700	C	3.48791000	1.07356300	0.35492400
C	2.56371800	1.36387300	2.16482900	C	3.02329200	0.05526600	1.18876900
C	4.27041700	1.96805500	0.04298500	C	3.80579800	-1.07314000	1.40757000
H	2.46174800	2.35927400	-1.08098400	C	5.06283700	-1.20534800	0.80295200
C	3.94225000	1.27465700	2.33555800	H	6.50748700	-0.23740800	-0.46511200
H	1.89114800	1.13147100	2.98364500	H	5.10912700	1.78966100	-0.85048200
C	4.79784400	1.56294600	1.27078800	H	2.06013100	0.17062700	1.66938000
H	4.93406000	2.18795200	-0.78724100	H	3.43511700	-1.86804700	2.04955000
H	4.34887300	0.97855200	3.29749400	C	5.88896000	-2.44733400	1.02475000
H	5.87230800	1.47702400	1.39898400	H	6.12943300	-2.58416800	2.08491500
C	0.06251600	3.17766600	0.38690100	H	5.34536300	-3.34253500	0.70097300
C	-1.07035500	3.37621300	-0.42540700	H	6.83075500	-2.40632000	0.47120400
C	0.74997600	4.31002500	0.88275300	S	2.42692800	2.47697300	-0.03326000
C	-1.50848400	4.66345000	-0.71379400	O	1.42855900	2.50620300	1.07544500
				O	3.31075100	3.64765300	-0.14244500





C	2.20898300	0.38411100	-0.35649800	C	2.23322700	-1.54159300	0.11833700
C	3.26283800	1.40591400	-0.59486400	C	2.67231900	-1.54349500	-1.20213100
C	4.58323000	1.24555800	-0.13430600	C	3.91843000	-1.00668000	-1.55140600
C	2.94665900	2.56458500	-1.32269900	H	5.71991600	-0.11107300	-0.78634500
C	5.54671200	2.21462900	-0.38381300	H	4.93911700	-0.08505100	1.57890200
H	4.83745100	0.36610500	0.44760400	H	1.27396900	-1.96516200	0.39022500
C	3.91534300	3.53726100	-1.57076600	H	2.03836400	-1.96335700	-1.97784100
H	1.94228600	2.68888200	-1.71144900	C	4.34596400	-0.92938300	-2.99295700
C	5.21624300	3.36831900	-1.10279600	H	5.43049800	-1.02292200	-3.09716100
H	6.55601400	2.07842400	-0.00764000	H	3.87300200	-1.70900400	-3.59621600
H	3.64977200	4.42449800	-2.13706200	H	4.05585200	0.04029000	-3.41492900
H	5.96999000	4.12541700	-1.29463100	S	2.43375700	-0.81003600	2.76781500
C	2.44721200	-1.00391700	-0.70733600	O	1.38007800	-1.81109500	2.95263000
C	1.45250700	-1.96480600	-0.43290400	O	3.56136300	-0.73984900	3.68842600
C	3.64910500	-1.44485000	-1.31239200	O	1.78793500	0.66565500	2.75723500
C	1.64819400	-3.30754200	-0.72768800	C	1.17046000	1.78399600	-1.72254600
H	0.51689900	-1.66696200	0.01159700	C	1.53760100	1.79193400	-0.34861600
C	3.84463400	-2.78817200	-1.59660600	C	2.76479200	2.28455500	0.06608800
H	4.40880100	-0.72570700	-1.58928700	C	3.64010300	2.76115800	-0.91740200
C	2.84846600	-3.72619200	-1.29976100	C	3.29601800	2.74234500	-2.27273900
H	0.84662800	-4.00592100	-0.52039300	C	2.05263500	2.25283300	-2.68953600
H	4.76790100	-3.10711600	-2.07027200	C	-0.17405300	1.23037400	-1.73007600
H	3.00523900	-4.77498700	-1.53335800	C	-0.48591900	0.97211900	-0.31669900
C	1.45959600	1.97644100	1.80024400	H	3.03185800	2.28742700	1.11592300
H	1.60805800	2.88104500	2.38897700	H	4.60837200	3.15044600	-0.61915900
C	2.26612000	0.82879700	2.03948400	H	3.99775700	3.12020600	-3.00941900
H	3.27958100	1.00852000	2.39862200	H	1.78302900	2.24918900	-3.74118500
C	1.75221000	-0.49815100	2.37122700	H	1.13502900	0.81631500	1.99245700
C	0.37741200	-0.76928100	2.52554000	N	0.49602000	1.26287800	0.48617500
C	2.66096500	-1.55615700	2.56379200	C	-1.94474400	0.57859200	-0.17319900
C	-0.06356900	-2.05104500	2.83377700	C	-2.64888600	1.90259000	0.22518500
H	-0.33767100	0.03703600	2.41016000	C	-3.08486100	2.83884300	-0.71709800
C	2.21546200	-2.83675800	2.87686200	C	-2.77866800	2.21081300	1.58584700
H	3.72446900	-1.36604200	2.45052800	C	-3.67190700	4.03832200	-0.31174800
C	0.85102400	-3.09321200	3.00777000	H	-2.95865800	2.65337100	-1.77764500
H	-1.12681100	-2.24120500	2.93907400	C	-3.35764600	3.41057300	1.99114100
H	2.93580900	-3.63817800	3.00729500	H	-2.42963400	1.50213000	2.32780200
H	0.50033500	-4.09247100	3.24314500	C	-3.81328400	4.32820900	1.04367400
				H	-4.01195500	4.74707800	-1.06066200
				H	-3.45263800	3.62678800	3.05070400
				H	-4.26777600	5.26208800	1.35929000
				C	-2.30960800	-0.52264100	0.80681500
				C	-1.36193400	-1.18682400	1.57935000
				C	-3.65687100	-0.89140300	0.92305400
<b>(S)-INT-3S</b>							
C	4.74091300	-0.50743500	-0.53382000				
C	4.31318500	-0.48599200	0.78983200				
C	3.04938700	-0.98285100	1.10145000				



C	6.00505500	-1.91787900	-0.48283000
H	4.52916500	-1.86907600	1.07090700
C	5.35717900	-0.96651700	-2.60743700
H	3.35276600	-0.19124200	-2.71095800
C	6.31486900	-1.58977600	-1.80661000
H	6.75113000	-2.39338400	0.14627700
H	5.59159400	-0.70507600	-3.63448100
H	7.29838100	-1.81442100	-2.20689000

**(R)-TS-2S**

C	3.95478600	-1.60178000	1.36824000
C	4.14496300	-0.38610200	0.71877100
C	3.26840900	0.67291900	0.95549200
C	2.24563500	0.52751700	1.89221300
C	2.05215500	-0.69959700	2.52664200
C	2.88915200	-1.78783600	2.25852000
H	4.63239400	-2.42684700	1.16897100
H	4.96941100	-0.24149500	0.03058600
H	1.63699600	1.38744100	2.14524400
H	1.24879100	-0.81003300	3.25089400
C	2.64585000	-3.13273400	2.89366100
H	1.96440000	-3.05831900	3.74554600
H	2.20218100	-3.82840100	2.17017500
H	3.57817600	-3.58709000	3.24313700
S	3.44081000	2.20559900	0.01268400
O	2.75888800	3.22978900	0.83485000
O	4.88186700	2.37242900	-0.22701200
O	2.69312000	1.93144900	-1.29339500
C	1.23152200	-2.21584700	-0.87660200
C	1.88530900	-1.14022000	-1.52841500
C	3.13600100	-1.27352900	-2.11893600
C	3.73135700	-2.53242500	-2.05849000
C	3.10436400	-3.61051800	-1.41158800
C	1.85769000	-3.46198500	-0.80669100
C	0.00765800	-1.64248400	-0.35311500
C	-0.06562000	-0.28951900	-0.87635400
H	3.62229700	-0.41941000	-2.57518500
H	4.70824200	-2.67828200	-2.50783300
H	3.60161100	-4.57445300	-1.38093300
H	1.38039700	-4.29850500	-0.30649000
H	1.59539200	0.98257400	-1.52875600
N	1.07908600	0.01772000	-1.48866100
C	-1.33316400	0.42321200	-0.73118100

C	-2.46779600	-0.20731100	-1.47691100
C	-3.80539300	0.05874300	-1.13110700
C	-2.21807200	-1.07306100	-2.55538900
C	-4.85189400	-0.52857400	-1.83537000
H	-4.02366500	0.71430400	-0.29830200
C	-3.26823800	-1.66420900	-3.25432200
H	-1.19753300	-1.26554700	-2.86615700
C	-4.58908800	-1.39639300	-2.89623300
H	-5.87531300	-0.31490800	-1.54413600
H	-3.05100500	-2.32469300	-4.08776700
H	-5.40726300	-1.85372500	-3.44361700
C	-1.32089700	1.89061200	-0.56280000
C	-0.25599500	2.49233800	0.12951200
C	-2.30787500	2.72855200	-1.12105300
C	-0.17194500	3.87108000	0.27632100
H	0.53522500	1.88147100	0.53745700
C	-2.23539900	4.10776900	-0.95848600
H	-3.10897400	2.30674200	-1.71280500
C	-1.17319800	4.68324100	-0.25769700
H	0.69978900	4.28086600	0.77139200
H	-3.00092400	4.73720900	-1.40156800
H	-1.11478200	5.76172100	-0.14816500
C	-0.90051000	-1.85602200	0.65024400
H	-1.11558900	-2.83202100	1.07795400
C	-1.55835600	-0.65854000	1.13176800
H	-0.88545900	0.08408400	1.54808500
C	-2.89226900	-0.66446900	1.70883300
C	-3.81298700	-1.68666500	1.41609100
C	-3.30752900	0.41521000	2.51059400
C	-5.10226800	-1.64572800	1.93675400
H	-3.51888700	-2.49718500	0.75681800
C	-4.60214400	0.46289900	3.01506900
H	-2.60633500	1.21757000	2.72116600
C	-5.50092500	-0.57060400	2.73371600
H	-5.80339300	-2.44150300	1.70634500
H	-4.91269400	1.30149600	3.62994600
H	-6.51078200	-0.53366700	3.12992600

**(R)-INT-3S**

C	-4.98702500	0.81291200	0.00709700
C	-4.57126400	-0.31361300	-0.69654000
C	-3.44799900	-1.01054500	-0.25358900
C	-2.76716300	-0.62276200	0.89883700



C	-2.06261600	3.85583100	0.48095900	H	-2.26304400	-0.68257500	-2.90437500
C	-2.17367100	5.19382300	0.83137600	C	-1.18996200	-4.05678200	-1.33162200
C	-1.26092200	6.07575600	0.24802900	H	-0.73551500	-2.91806200	0.43358900
C	-0.27520500	5.62454900	-0.64162300	C	-1.63032500	-4.01320400	-2.65456900
C	-0.16930900	4.27663700	-0.98527800	H	-2.34637800	-2.75378400	-4.25349200
C	-1.28008800	1.94100700	-0.49345300	H	-0.86241600	-4.99241100	-0.89082300
C	-2.37508700	1.63446500	0.35287900	H	-1.66551900	-4.92226000	-3.24703500
H	-2.92766400	5.54139200	1.52953400	C	2.99113800	0.86717700	-2.00971400
H	-1.31321200	7.13034000	0.49695600	C	2.53750500	1.41079700	-0.77015800
H	0.42411500	6.33723300	-1.06546100	C	2.86948200	2.70102900	-0.35550600
H	0.61452700	3.92856600	-1.64805900	C	3.66328900	3.46752000	-1.20639000
H	-3.58749800	2.77454200	1.59771200	C	4.10935800	2.95678400	-2.44126300
N	-2.83107400	2.74563000	0.92597400	C	3.78113400	1.66643400	-2.84828800
C	-2.76433400	0.19245200	0.36575500	C	2.50377500	-0.49701500	-2.07980500
C	-3.93986000	-0.07027300	-0.58853200	C	1.80359300	-0.70804000	-0.92651700
C	-4.55035600	-1.33025400	-0.55367200	H	2.52899400	3.08624900	0.60028200
C	-4.36931500	0.86536800	-1.53293400	H	3.94673100	4.47294500	-0.91001600
C	-5.56266700	-1.64920300	-1.45224000	H	4.72712100	3.58011500	-3.08057000
H	-4.21440100	-2.06392900	0.16992500	H	4.14143500	1.27924900	-3.79678000
C	-5.38779800	0.54509400	-2.43403900	H	1.53088700	0.36278600	0.83216400
H	-3.91220000	1.84795000	-1.58452400	N	1.76468600	0.44466300	-0.15513400
C	-5.98496000	-0.71251600	-2.39809500	H	1.32899400	-1.59738900	-0.55537300
H	-6.01699800	-2.63415700	-1.41858300	C	2.77190600	-1.53498900	-3.12794700
H	-5.71132400	1.28370000	-3.16085500	H	2.36905200	-1.21599900	-4.10089700
H	-6.77469200	-0.96231200	-3.09946700	H	3.85593200	-1.64370800	-3.26727900
C	-3.11134000	-0.22982200	1.79825600	C	2.18958600	-2.91729600	-2.78933300
C	-2.21098800	-0.87881800	2.64602400	H	2.32754100	-3.56843400	-3.66186100
C	-4.37090000	0.14575900	2.29901200	H	1.10799500	-2.83035800	-2.62348000
C	-2.57216300	-1.15762800	3.96721000	O	2.83723500	-3.53869400	-1.69136200
H	-1.21673100	-1.16483300	2.32041700	H	2.31434400	-3.44704500	-0.87515900
C	-4.72017000	-0.12289600	3.61993800				
H	-5.09394000	0.61618000	1.63818800				
C	-3.81886300	-0.78093000	4.46024400	<b>TS-3A</b>			
H	-1.85644400	-1.67016100	4.60218000	C	4.48936700	1.07142300	2.28564600
H	-5.69961400	0.16819000	3.98751100	C	3.44591500	0.19476900	2.56310100
H	-4.09184700	-1.00035600	5.48777400	C	3.32923300	-0.99406600	1.83760200
C	-0.77605800	0.76076900	-0.98261100	C	4.26786500	-1.31740500	0.86116300
H	-0.03634100	0.64083000	-1.76188400	C	5.30644600	-0.42586600	0.59285000
C	-1.41696600	-0.41562600	-0.30340300	C	5.42761700	0.78245300	1.28502900
H	-0.72965700	-0.64498300	0.52703300	H	4.57312400	2.00062200	2.84324600
C	-1.52322000	-1.66631800	-1.13341200	H	2.70996000	0.43299300	3.32356000
C	-1.95371700	-1.62690500	-2.46571800	H	4.17064900	-2.22848800	0.28510300
C	-1.13719500	-2.88834800	-0.57215100	H	6.02517700	-0.66928500	-0.18490600
C	-2.00947200	-2.79432500	-3.22226000	C	6.50719100	1.77209000	0.92903200

H	6.16002800	2.44406500	0.13538700	C	-0.80612600	0.61434500	-1.03148300
H	6.78592300	2.38943600	1.78816500	H	-0.29024600	0.45283500	-1.96688800
H	7.40701700	1.26868500	0.56365300	C	-1.46984900	-0.51568200	-0.26222600
S	1.88402600	-2.02863500	2.13142900	H	-0.80998500	-0.71233300	0.58723200
O	1.94488200	-2.54261200	3.50693600	C	-1.59761600	-1.81426600	-1.01363500
O	0.75030500	-1.02587900	1.93967500	C	-2.08024600	-1.86590400	-2.32745200
O	1.87262500	-3.06323800	1.05427200	C	-1.14948200	-2.99118200	-0.40226600
C	-1.13631700	3.27738200	-0.65106600	C	-2.11980800	-3.07517200	-3.01646300
C	-2.13444900	3.81578600	0.20847500	H	-2.43745500	-0.95969000	-2.80734600
C	-2.28951400	5.18186200	0.41282000	C	-1.18425900	-4.20152800	-1.09471400
C	-1.41800900	6.02811100	-0.27230100	H	-0.71321900	-2.94996700	0.58975900
C	-0.42574600	5.51852000	-1.12502100	C	-1.67165900	-4.24645800	-2.40106200
C	-0.27125700	4.14778500	-1.31905400	H	-2.49716500	-3.10379600	-4.03406900
C	-1.29136900	1.83600600	-0.56881000	H	-0.81038100	-5.10045200	-0.61573900
C	-2.37151500	1.58674600	0.29353500	H	-1.69426300	-5.18746000	-2.94214600
H	-3.05352300	5.57463500	1.07550000	C	3.01172600	0.68743700	-1.87992600
H	-1.50836400	7.10103000	-0.13921500	C	2.27190900	1.23485900	-0.80015000
H	0.23716300	6.20666700	-1.63879000	C	2.48675800	2.52235900	-0.32401900
H	0.51404200	3.76034500	-1.95720900	C	3.45736100	3.29218900	-0.96782000
H	-3.65154000	2.81602000	1.39332100	C	4.18647100	2.77724700	-2.05215400
N	-2.86956900	2.74112000	0.75743300	C	3.97521300	1.47694200	-2.51346900
C	-2.79843800	0.15468600	0.37377400	C	2.58622100	-0.69953700	-2.02958000
C	-3.98663700	-0.11906200	-0.56012500	C	1.64205400	-0.91497700	-1.07806000
C	-4.63529700	-1.35721400	-0.46649400	H	1.92682600	2.90943200	0.52000800
C	-4.39107800	0.78197700	-1.54877700	H	3.65489100	4.30107900	-0.61970500
C	-5.66027600	-1.68818000	-1.34648500	H	4.93492500	3.40021400	-2.53235700
H	-4.31991500	-2.06578400	0.29075900	H	4.55905400	1.08194700	-3.33905600
C	-5.42135800	0.44997600	-2.43207800	H	1.15979600	0.10204400	0.64954500
H	-3.90321400	1.74559100	-1.64838200	N	1.37231600	0.25896200	-0.35246200
C	-6.05723500	-0.78545900	-2.33515800	H	1.13390800	-1.81896600	-0.79718100
H	-6.14389700	-2.65635900	-1.26510700	C	3.14741200	-1.73827400	-2.95065400
H	-5.72413600	1.16245000	-3.19323100	H	2.85988300	-1.52625500	-3.99126800
H	-6.85666400	-1.04404000	-3.02232000	H	4.24372300	-1.69032500	-2.91904400
C	-3.14119900	-0.20082600	1.82607100	C	2.71891800	-3.17338300	-2.59683800
C	-2.23002000	-0.78577800	2.70963400	H	3.08166100	-3.84020900	-3.38790500
C	-4.40417900	0.18327500	2.31066300	H	1.62083600	-3.24381000	-2.60028200
C	-2.58434100	-0.99465500	4.04515800	O	3.26867100	-3.64058000	-1.38096400
H	-1.23124100	-1.07243700	2.40092500	H	2.68566300	-3.43614200	-0.62597900
C	-4.74807200	-0.01607700	3.64529600				
H	-5.13359200	0.61051500	1.62851800				
C	-3.83658500	-0.61179200	4.51939200	<b>INT-4B</b>			
H	-1.86040400	-1.45687900	4.70871200	C	-6.06704800	-0.42626200	-0.29128100
H	-5.73085300	0.28232300	3.99788300	C	-4.77024500	-0.87650400	-0.05441900
H	-4.10412400	-0.77709100	5.55843600	C	-4.07018900	-1.50321800	-1.08658200

C	-4.66041800	-1.68931200	-2.33574600	C	1.02659400	-3.29198600	-3.06580600
C	-5.95833400	-1.23479700	-2.55489500	H	0.18562700	-1.98702000	-1.61331200
C	-6.68029400	-0.59594300	-1.53887400	C	3.42334200	-3.22865700	-3.32238000
H	-6.61406200	0.06203200	0.51078800	H	4.48313800	-1.94653200	-1.96197400
H	-4.31867200	-0.75136200	0.92319400	C	2.17964600	-3.73636600	-3.70822700
H	-4.10320300	-2.19728600	-3.11491500	H	0.04363200	-3.66752400	-3.32986300
H	-6.42077500	-1.38044300	-3.52773400	H	4.33001500	-3.57186300	-3.81177800
C	-8.09766500	-0.13410900	-1.77024900	H	2.11648300	-4.47604400	-4.50047100
H	-8.81751000	-0.90665100	-1.47280600	C	1.12731000	1.04979100	0.41903800
H	-8.32536600	0.76284700	-1.18675500	H	0.49980700	1.56704400	1.13430700
H	-8.27803000	0.09030800	-2.82553700	C	1.20725500	-0.44699900	0.38259000
S	-2.36786700	-2.01321100	-0.84713500	H	0.29623500	-0.73877600	-0.17069900
O	-1.54019700	-0.81645100	-1.26182300	C	1.18903800	-1.13049900	1.72294900
O	-2.22748700	-2.28255000	0.62006100	C	1.81161800	-0.54829200	2.83367000
O	-2.12642100	-3.18387500	-1.71580100	C	0.58284200	-2.38394200	1.85449000
C	2.20894800	2.84784600	-1.27468500	C	1.83414600	-1.20891500	4.05888400
C	3.05949400	2.46134000	-2.34348900	H	2.30124400	0.41611900	2.73236800
C	3.56076800	3.36279800	-3.27002500	C	0.61007800	-3.04712700	3.08085200
C	3.19401900	4.70153000	-3.10740600	H	0.05171800	-2.81963500	1.01727600
C	2.35909100	5.10572900	-2.05705400	C	1.23637000	-2.46451400	4.18295300
C	1.85632200	4.18867000	-1.13230900	H	2.32015900	-0.74767600	4.91292000
C	1.89802500	1.61590700	-0.56073600	H	0.12345400	-4.01238900	3.17552800
C	2.61448200	0.57255700	-1.21231500	H	1.25070700	-2.98123400	5.13761700
H	4.20582400	3.04802400	-4.08332600	C	-1.67700700	2.99658900	1.82096600
H	3.56431900	5.43955700	-3.81100000	C	-1.61222300	2.94766900	0.39088300
H	2.09403100	6.15334200	-1.96204200	C	-1.45212700	4.09860800	-0.38482700
H	1.19349900	4.50492900	-0.33569300	C	-1.33840900	5.31700600	0.27983500
H	3.81964500	0.49399300	-2.89736000	C	-1.38154300	5.38649500	1.68736100
N	3.27157500	1.05606300	-2.25783600	C	-1.55246400	4.24214700	2.45838100
C	2.49018300	-0.76260600	-0.56480500	C	-1.86566400	1.64017500	2.28512800
C	3.70075400	-1.03140300	0.34710200	C	-1.89729700	0.85601600	1.16091800
C	3.86626300	-2.32169200	0.86661600	H	-1.41796200	4.04295500	-1.46867000
C	4.58141900	-0.02296100	0.74577300	H	-1.22160600	6.22984900	-0.29696400
C	4.88065300	-2.59018200	1.77887300	H	-1.29082800	6.35322500	2.17340300
H	3.18358400	-3.10781900	0.56777900	H	-1.59701800	4.30917900	3.54154500
C	5.60461500	-0.29513200	1.65707600	H	-1.76060900	1.19125900	-0.88789400
H	4.47638500	0.98700400	0.36366000	N	-1.72347200	1.62347500	0.02820600
C	5.75410500	-1.57683600	2.17973600	H	-2.00054900	-0.20784400	1.06506900
H	4.98457600	-3.59214400	2.18251700	C	-2.04426300	1.14131500	3.68961400
H	6.28084200	0.49995400	1.95544600	H	-1.27850300	1.57703000	4.34770200
H	6.54524900	-1.78754000	2.89227600	H	-3.01285400	1.47572900	4.08653500
C	2.34692400	-1.84735400	-1.63754900	C	-1.96581800	-0.38709800	3.81719900
C	1.10864200	-2.34032500	-2.04767700	H	-1.99925500	-0.64714700	4.88436500
C	3.50855400	-2.29614100	-2.29086600	H	-1.00250200	-0.73136500	3.42977600



O	-3.04553200	-1.04254000	3.16232500	H	4.38520100	1.33933900	0.37237300
H	-2.70757400	-1.56624400	2.41605200	C	6.02575900	-1.16296600	1.97234800
				H	5.48533700	-3.24924000	1.87830400
				H	6.30328000	0.97049200	1.86190800
<b>TS-3B</b>				H	6.86835400	-1.32324100	2.63770300
C	-5.91319800	-0.18865500	-0.52503800	C	2.49951000	-1.59498000	-1.72588900
C	-4.63577000	-0.69386100	-0.29741000	C	1.29355400	-2.13153500	-2.18063200
C	-3.97356000	-1.35440600	-1.33336900	C	3.68330900	-1.93376400	-2.40397500
C	-4.57851400	-1.51541300	-2.57832000	C	1.26684000	-3.01362900	-3.26146200
C	-5.85699500	-1.00369300	-2.78832800	H	0.34930300	-1.85770200	-1.73606600
C	-6.54254100	-0.33283200	-1.76833800	C	3.65517300	-2.80064700	-3.49470400
H	-6.43398800	0.32112200	0.28119000	H	4.63478100	-1.54308000	-2.05624400
H	-4.17871300	-0.59779300	0.68093200	C	2.44532800	-3.35168600	-3.92288700
H	-4.04657600	-2.04495700	-3.36050100	H	0.30694300	-3.41845300	-3.56476700
H	-6.33191300	-1.12922600	-3.75783400	H	4.58177200	-3.05502700	-4.00093100
C	-7.94029300	0.18963500	-1.98940600	H	2.42616600	-4.03791700	-4.76409600
H	-8.69018800	-0.54662700	-1.67488000	C	1.07985800	1.03111500	0.61718900
H	-8.12113700	1.10229100	-1.41377500	H	0.90066500	1.43428800	1.60583700
H	-8.12251400	0.41018300	-3.04508600	C	1.29771800	-0.46880400	0.39969000
S	-2.29336100	-1.93282500	-1.10579100	H	0.44490600	-0.80883000	-0.19100100
O	-1.43120700	-0.71485200	-1.38039500	C	1.35468800	-1.30042000	1.65456600
O	-2.18829100	-2.36114400	0.32714700	C	2.01572200	-0.85194400	2.80446200
O	-2.04734400	-3.00412100	-2.08881100	C	0.72990000	-2.55253300	1.67329300
C	2.04366600	3.05514300	-0.93368000	C	2.05207000	-1.63767700	3.95308400
C	2.94050700	2.84232000	-2.02119000	H	2.52653600	0.10608900	2.79507500
C	3.44401400	3.88290300	-2.79482100	C	0.76639900	-3.34041800	2.82406300
C	3.05323500	5.17644900	-2.45506600	H	0.17395800	-2.89212600	0.80650900
C	2.18892700	5.41351500	-1.37386800	C	1.42683000	-2.88615400	3.96581800
C	1.67786700	4.36671200	-0.61123400	H	2.57119300	-1.27795100	4.83615700
C	1.75100400	1.73307100	-0.40752800	H	0.26511100	-4.30304100	2.82774700
C	2.51020300	0.82461200	-1.15006000	H	1.45117900	-3.49827200	4.86223900
H	4.11957000	3.69624200	-3.62319400	C	-2.03953900	2.42162300	2.08041600
H	3.42859800	6.01381100	-3.03390700	C	-1.48977000	2.45502700	0.77563000
H	1.91409800	6.43402000	-1.12800200	C	-1.44897600	3.61165300	0.01128600
H	1.00472100	4.56140000	0.21470400	C	-1.94569000	4.78298700	0.59159200
H	3.83327000	1.01447100	-2.75884100	C	-2.46406600	4.77876800	1.89441100
N	3.20132800	1.46278200	-2.11098600	C	-2.52062400	3.60381500	2.64706400
C	2.57211600	-0.56215300	-0.59415000	C	-2.01358200	1.02750200	2.52260300
C	3.84094900	-0.74795000	0.25464500	C	-1.45636800	0.31403800	1.51703400
C	4.17303000	-2.03789800	0.69066800	H	-1.05102800	3.60579100	-0.99713500
C	4.62101700	0.32842000	0.68595000	H	-1.93540400	5.70574500	0.02044800
C	5.25270100	-2.24359100	1.54274500	H	-2.84136500	5.70396400	2.31877700
H	3.56769900	-2.87824600	0.37200700	H	-2.94622800	3.60622000	3.64556700
C	5.70783600	0.12181000	1.53933700	H	-1.20706600	0.70766200	-0.47055100

N	-1.03822100	1.15352700	0.45566800
H	-1.33185100	-0.74675100	1.39746100
C	-2.57742700	0.44556500	3.78129700
H	-1.99130600	0.77588000	4.65126300
H	-3.59515400	0.82871400	3.93137000
C	-2.63088800	-1.09139400	3.76473000
H	-2.98060300	-1.43199800	4.74748200
H	-1.61879300	-1.49577400	3.62656900
O	-3.52975600	-1.58331800	2.78643000
H	-3.04557500	-1.92903800	2.01470000

**INT-4C**

C	5.76662000	3.03154400	0.08407700
C	4.76700600	2.15308500	0.49201000
C	4.87805000	0.79842200	0.17992700
C	5.97387900	0.32252100	-0.53685300
C	6.96707000	1.21341100	-0.93837500
C	6.88289500	2.57669300	-0.63098200
H	5.67913000	4.08896500	0.31949500
H	3.89597600	2.50758000	1.03106400
H	6.02933000	-0.73146700	-0.78428200
H	7.81986800	0.84572500	-1.50276600
C	7.97733700	3.53106700	-1.03917200
H	7.57883600	4.52529900	-1.26189000
H	8.71513800	3.64905500	-0.23609000
H	8.51218900	3.17205300	-1.92296000
S	3.63012600	-0.35669100	0.74178000
O	3.64566300	-1.49247000	-0.21582200
O	3.97725900	-0.71796800	2.13731000
O	2.33892500	0.44065800	0.66074000
C	-0.65798200	-1.13982500	-2.74516500
C	0.58005000	-0.97972300	-2.07717800
C	1.77857100	-1.44393800	-2.59846300
C	1.71019100	-2.09783700	-3.83395000
C	0.49433000	-2.27298600	-4.51085900
C	-0.70280600	-1.79417100	-3.97335100
C	-1.64647900	-0.55359300	-1.85727800
C	-0.91948600	-0.04575500	-0.71472600
H	2.70271600	-1.34476400	-2.03821700
H	2.62431700	-2.48224000	-4.27487000
H	0.48383200	-2.78718000	-5.46642500
H	-1.64415800	-1.93534300	-4.49360600
H	1.17204200	-0.05669400	-0.16845100

N	0.36060900	-0.31307800	-0.83248300
C	-1.80234200	0.76502300	0.20299200
C	-1.61890400	2.26391600	-0.12498900
C	-2.16434500	3.21266500	0.74933100
C	-0.99789800	2.70728300	-1.29601500
C	-2.10771100	4.56928800	0.44923600
H	-2.64548400	2.88183100	1.66184400
C	-0.93405900	4.07032200	-1.59326100
H	-0.55437600	2.00277600	-1.99001000
C	-1.49304400	5.00517200	-0.72609500
H	-2.54458200	5.28745400	1.13590900
H	-0.44069200	4.39493400	-2.50408400
H	-1.44443200	6.06443000	-0.95808100
C	-1.54939200	0.54279100	1.69698800
C	-2.50972200	0.03658000	2.57717400
C	-0.31410800	0.94895400	2.21924300
C	-2.24458300	-0.06070400	3.94499600
H	-3.47529700	-0.28883800	2.21688000
C	-0.04239000	0.83715600	3.57934100
H	0.45365200	1.34733100	1.56791100
C	-1.00984300	0.33754600	4.45163600
H	-3.00833600	-0.45308900	4.60933900
H	0.93445300	1.13045400	3.94848500
H	-0.80017500	0.25401800	5.51314300
C	-2.97052800	-0.36449700	-1.66315800
H	-3.77096100	-0.65521500	-2.33216200
C	-3.24976300	0.28114500	-0.33037900
H	-3.56952100	-0.54131400	0.31684700
C	-4.33979200	1.32586900	-0.37463700
C	-4.42701500	2.21607300	-1.45287300
C	-5.26644800	1.43867800	0.66591600
C	-5.40438300	3.20657700	-1.48094700
H	-3.70297000	2.15081100	-2.25872500
C	-6.24605600	2.43119200	0.64252900
H	-5.22044800	0.75272200	1.50531200
C	-6.31549800	3.31994600	-0.42965600
H	-5.45033900	3.89439100	-2.31941400
H	-6.95509300	2.50735500	1.46102600
H	-7.07547700	4.09483600	-0.44739000
C	-1.46903400	-3.26719300	0.61507100
C	-1.21865000	-3.64205300	-0.74198400
C	-2.24747400	-3.81639700	-1.66871900
C	-3.55066200	-3.57957200	-1.24144400
C	-3.82536500	-3.21738800	0.09568100

C	-2.80097400	-3.06977700	1.02320500	C	0.23251400	-0.04331200	4.09012900
C	-0.19681100	-3.17746500	1.28164200	C	-1.06399500	-0.26227100	1.81001600
C	0.75827800	-3.46721400	0.33239700	C	-1.02422800	-1.28147000	0.86752400
H	-2.03442000	-4.10646500	-2.69238900	H	1.72311400	-3.50129700	2.95433300
H	-4.37291500	-3.70457300	-1.93966800	H	2.46979300	-2.42078700	5.07558000
H	-4.85640000	-3.06553300	0.40206800	H	1.53198400	-0.25086200	5.78683800
H	-3.01991600	-2.80987000	2.05358400	H	-0.17359400	0.91141900	4.41125000
H	0.63326600	-3.89159300	-1.74612100	H	0.37395500	-2.80738300	0.63320500
N	0.14451900	-3.77114700	-0.87363500	N	-0.21628300	-2.28832800	1.29013400
H	1.83192100	-3.46990000	0.43855300	C	-1.92156100	-1.05784600	-0.32984900
C	0.01822400	-2.88808400	2.73945500	C	-3.18761800	-1.93215700	-0.21918200
H	-0.81251200	-2.28100000	3.11364400	C	-4.07038900	-1.99507300	-1.30452300
H	-0.00020100	-3.82750000	3.30962500	C	-3.51727600	-2.61727000	0.95312200
C	1.31782200	-2.15657000	3.05692800	C	-5.26523200	-2.70097500	-1.20981800
H	1.31515800	-1.88198000	4.12547100	H	-3.82060000	-1.48097400	-2.22552500
H	1.35474500	-1.22389900	2.48694600	C	-4.71005900	-3.33720800	1.04486100
O	2.42741700	-2.98006800	2.74451400	H	-2.84958000	-2.58950700	1.80606500
H	3.16945100	-2.36720700	2.58528200	C	-5.59205900	-3.37573700	-0.03193200

**TS-3C**

C	6.35794700	-0.50817500	-1.26856500	H	-5.94140500	-2.72669600	-2.05885200
C	4.96914900	-0.56716500	-1.39132600	H	-4.94599600	-3.86551700	1.96370200
C	4.20701600	-0.95560800	-0.29439000	H	-6.52232700	-3.93058700	0.04090500
C	4.81510300	-1.27948600	0.92076600	C	-1.24878400	-1.35518900	-1.67716700
C	6.19931200	-1.21809100	1.02624400	C	-1.25970200	-0.47558700	-2.76369500
C	6.99259200	-0.83554700	-0.06672700	C	-0.66085900	-2.61351900	-1.85736500
H	6.95603600	-0.19803100	-2.12096300	C	-0.64957700	-0.82064700	-3.97103300
H	4.47556500	-0.30220300	-2.31899500	H	-1.74453000	0.49021500	-2.69262300
H	4.20266600	-1.56011400	1.77117100	C	-0.03412600	-2.95309500	-3.05041400
H	6.67704000	-1.46454700	1.97102400	H	-0.70735100	-3.34765700	-1.06161200
C	8.49550400	-0.79518800	0.05591100	C	-0.01682500	-2.05159600	-4.11302700
H	8.92024000	-1.80623300	0.03805300	H	-0.66957000	-0.11783400	-4.79830500
H	8.94799100	-0.23301200	-0.76523200	H	0.44544800	-3.92149500	-3.14451700
H	8.80692300	-0.33155000	0.99747300	H	0.47666000	-2.31001000	-5.04425000
S	2.42511100	-1.04367500	-0.41272500	C	-1.53497000	0.92285400	1.17284400
O	1.92571700	-0.18848900	0.71282400	H	-1.92585200	1.77957300	1.71198000
O	2.06870800	-0.50095700	-1.76109000	C	-2.27745300	0.50583000	-0.09807900
O	2.06810500	-2.48195000	-0.24169200	H	-1.86133300	1.07902100	-0.92405000
C	-0.19311600	-0.63906600	2.89907700	C	-3.74943200	0.84291400	-0.02470500
C	0.34271000	-1.89992500	2.51991700	C	-4.51094300	0.54741300	1.11252800
C	1.30339500	-2.55595100	3.27985300	C	-4.37861800	1.44006100	-1.12036300
C	1.72002100	-1.93719600	4.45755300	C	-5.87442900	0.82705800	1.14366000
C	1.18795900	-0.70096000	4.86108200	H	-4.03648900	0.07253400	1.96495400
				C	-5.74433700	1.72090400	-1.09324400
				H	-3.79604600	1.67953000	-2.00574700
				C	-6.49663300	1.41133900	0.03900300

H	-6.45364100	0.58259200	2.02865200	O	-3.57920100	0.95063300	-0.33052000
H	-6.21842700	2.18067800	-1.95497100	O	-3.03815700	-0.24371700	1.80474200
H	-7.56079000	1.62457200	0.06215900	O	-2.24396300	-1.13626400	-0.38604700
C	0.24613500	3.99047500	-0.06515900	C	1.06440000	1.72116300	-2.30339500
C	0.08647700	3.16887300	1.06577200	C	-0.23292600	1.26631700	-1.96560800
C	-0.06247500	3.66901700	2.34675900	C	-1.38688800	1.78752300	-2.52662900
C	-0.04833100	5.06233200	2.49303800	C	-1.21387800	2.81520900	-3.45904200
C	0.10285900	5.89901900	1.38223700	C	0.05749100	3.29355200	-3.79960200
C	0.25372900	5.37455200	0.09426500	C	1.21051200	2.75488500	-3.22522700
C	0.42148900	3.10847100	-1.22643000	C	1.96984300	0.89403200	-1.51731700
C	0.31135800	1.83856600	-0.78276200	C	1.13632000	0.00593400	-0.73392700
H	-0.16264400	3.01177900	3.20409100	H	-2.36459700	1.43513200	-2.21659400
H	-0.15137000	5.49540100	3.48239300	H	-2.08947600	3.26292100	-3.91738400
H	0.10848200	6.97496000	1.52437700	H	0.14759700	4.10440700	-4.51448300
H	0.38235000	6.03149500	-0.75976000	H	2.19226800	3.13321900	-3.48939600
H	0.77096900	1.15153200	1.03737200	H	-0.99286300	-0.33567200	-0.67234400
N	0.06286200	1.79859400	0.63397200	N	-0.12779900	0.21990600	-1.00244000
H	0.50252600	0.90209500	-1.28245100	C	1.92555900	-0.97210000	0.09926200
C	0.78715500	3.53590800	-2.61398200	C	1.78192100	-2.39714600	-0.46039600
H	-0.09726400	3.93365000	-3.13348700	C	2.21334600	-3.47664900	0.31891300
H	1.50194100	4.36501700	-2.54305900	C	1.31444500	-2.64268700	-1.75400800
C	1.42335100	2.41611800	-3.45858900	C	2.19583700	-4.77001700	-0.19253200
H	1.61368900	2.81998800	-4.46186900	H	2.57024900	-3.29732500	1.32622100
H	0.70874800	1.59044300	-3.57626400	C	1.28755000	-3.94166600	-2.26398100
O	2.64403700	1.96957500	-2.91581900	H	0.96566000	-1.82790300	-2.37870100
H	2.48583600	1.13293500	-2.43499800	C	1.73372300	-5.00839500	-1.48817800

#### INT-4D

C	-6.30815900	-2.99724700	1.01332700	H	1.71455300	-6.01865900	-1.88466300
C	-5.16964200	-2.21169300	1.17893500	C	1.49040000	-0.94086800	1.57510100
C	-4.79982300	-1.32740600	0.16846500	C	2.36691000	-0.67911200	2.63210700
C	-5.55819600	-1.21616600	-0.99615800	C	0.15433500	-1.23722800	1.87353800
C	-6.69318900	-2.00708900	-1.14709900	C	1.91506900	-0.69787000	3.95306200
C	-7.08216200	-2.91243400	-0.15028100	H	3.40718500	-0.44837300	2.44944300
H	-6.60491200	-3.68268400	1.80249600	C	-0.30502300	-1.22794000	3.18788600
H	-4.57708800	-2.26086300	2.08506800	H	-0.55109800	-1.47758400	1.08696900
H	-5.26782600	-0.50175600	-1.75787300	C	0.57610000	-0.96017300	4.23617400
H	-7.29256700	-1.91739500	-2.04908800	H	2.61530900	-0.49328800	4.75732700
C	-8.29607700	-3.78790600	-0.33686100	H	-1.35835600	-1.40809200	3.36894700
H	-8.03579300	-4.71197200	-0.86759700	H	0.22254300	-0.95507600	5.26252600
H	-8.73302700	-4.07523200	0.62351400	C	3.26682900	0.62021700	-1.25012700
H	-9.06724200	-3.28190900	-0.92493200	H	4.13237400	1.09583700	-1.69810000
S	-3.31437900	-0.35288900	0.35601900	C	3.41746200	-0.41158000	-0.16648800
				H	3.70125100	0.17972400	0.70864700



C	0.06546400	-1.89700800	-4.30412000
H	-0.81889800	-0.01014400	-4.84823300
H	0.77357400	-3.75071600	-3.45974400
H	0.51316400	-2.06715600	-5.27811200
C	-1.20069400	0.73357700	1.13165100
H	-1.59695800	1.54842400	1.72918200
C	-2.09068600	0.26652700	-0.02900500
H	-1.87929900	0.88239900	-0.89760200
C	-3.55667700	0.46350300	0.29620700
C	-4.07658500	0.15395800	1.55901000
C	-4.42442400	0.94608300	-0.68972400
C	-5.43205500	0.32482100	1.82862200
H	-3.41876300	-0.24146300	2.32607100
C	-5.78240500	1.11901000	-0.42071200
H	-4.04408900	1.17602400	-1.68038800
C	-6.29022600	0.80828700	0.83950300
H	-5.82025200	0.07418400	2.81107000
H	-6.44026500	1.49392500	-1.19865600
H	-7.34705500	0.93894200	1.05048100
C	0.02685800	3.95148600	0.17199200
C	0.28968400	2.94414900	1.12001700
C	0.49777000	3.21106200	2.46109300
C	0.43266600	4.55134300	2.86320600
C	0.15755900	5.56739000	1.94140900
C	-0.04484900	5.28036700	0.58787200
C	-0.06082800	3.29587500	-1.13695100
C	0.11847400	1.97172400	-0.93724200
H	0.73123100	2.41769000	3.16137900
H	0.60513600	4.80330700	3.90429000
H	0.11033500	6.59678500	2.28195000
H	-0.23854300	6.07741600	-0.12304400
H	1.06715300	0.97710100	0.61061100
N	0.23953100	1.66584300	0.46235900
H	0.25931700	1.16738100	-1.64378800
C	-0.35476800	3.94528900	-2.44973600
H	0.21457900	4.87631600	-2.56226900
H	-0.05538100	3.27266200	-3.25882000
C	-1.85638600	4.25991400	-2.59769000
H	-2.05158500	4.63691600	-3.60557600
H	-2.14733900	5.04540500	-1.88568200
O	-2.67260500	3.10687100	-2.43618600
H	-2.70737200	2.90197300	-1.49279500

**INT-5A**

C	4.82811100	-0.85415700	2.25484700
C	3.73049000	-1.70995400	2.27727900
C	3.27492100	-2.28221500	1.08725800
C	3.94508500	-2.03959000	-0.10972000
C	5.04181000	-1.17869600	-0.11697200
C	5.48534000	-0.55479400	1.05324000
H	5.17317600	-0.39832900	3.17947900
H	3.21135600	-1.92092700	3.20641500
H	3.58477500	-2.46756500	-1.03626700
H	5.54241600	-0.96605000	-1.05762600
C	6.60019000	0.45868600	1.01032800
H	6.20334100	1.44836000	0.75165200
H	7.10421000	0.54507900	1.97733700
H	7.34924400	0.19996000	0.25613300
S	1.68659500	-3.13314600	1.11480900
O	1.40577300	-3.54539700	-0.29800600
O	1.76921600	-4.23038300	2.08996800
O	0.74912700	-2.01970400	1.53752700
C	-0.41340300	3.16877700	-0.53933600
C	-0.95923100	3.76336200	0.63148100
C	-0.63362100	5.04883600	1.04410200
C	0.26953700	5.75782500	0.25149000
C	0.82257000	5.19045200	-0.90624100
C	0.48741600	3.90084000	-1.31226400
C	-0.95507400	1.81846600	-0.58032200
C	-1.81531600	1.69163300	0.53407800
H	-1.05664300	5.48179500	1.94451600
H	0.55373500	6.76344500	0.54286400
H	1.53454000	5.76086100	-1.49233700
H	0.94587600	3.46077100	-2.18795700
H	-2.35418200	2.96297800	2.09163600
N	-1.82143400	2.82215800	1.24358000
C	-2.57963400	0.40747100	0.59132700
C	-3.96676500	0.55756900	-0.05074000
C	-4.88001900	-0.49415100	0.09584400
C	-4.32582600	1.66267600	-0.82730300
C	-6.12182300	-0.44503600	-0.52904600
H	-4.60415700	-1.35770800	0.69017600
C	-5.57334900	1.71200800	-1.45402300
H	-3.63724200	2.49015000	-0.95971600
C	-6.47326200	0.65850400	-1.30906200
H	-6.81259100	-1.27402800	-0.41308800
H	-5.83778700	2.57835200	-2.05245400



C	-4.28788900	1.56910100	-0.90754900	H	4.45147000	3.87015400	0.89545300
C	-6.08930800	-0.52228300	-0.53896100	H	4.81905400	3.91458100	-1.54603200
H	-4.59763500	-1.36886200	0.75662200	H	3.68308400	2.28182700	-3.03198700
C	-5.52201500	1.58466800	-1.56199400	H	1.44331700	-0.19993200	1.22311300
H	-3.59373000	2.38657000	-1.06897400	N	1.60498200	0.27126500	0.33511800
C	-6.42498300	0.53923800	-1.38182200	H	0.82339500	-1.35165600	-0.79444000
H	-6.78189000	-1.34559300	-0.39559300	C	1.72446900	-0.19606800	-3.34132700
H	-5.77353300	2.41813100	-2.21080100	H	1.03786100	0.47415700	-3.88556400
H	-7.38320700	0.55051700	-1.89172100	H	2.69457200	-0.10332200	-3.84326600
C	-2.70704800	-0.01096300	2.07421800	C	1.22565100	-1.64722800	-3.49249400
C	-1.88158000	-0.94590400	2.70423800	H	1.09791200	-1.84547900	-4.56466600
C	-3.66749300	0.66839400	2.84467100	H	0.23248500	-1.75608200	-3.03417700
C	-2.01813000	-1.19350000	4.07313100	O	2.14225800	-2.58156600	-2.96872400
H	-1.11459400	-1.49311500	2.17003500	H	1.81950100	-2.93003500	-2.11349800
C	-3.79295400	0.42719100	4.21009100				
H	-4.34420700	1.36687600	2.35999100				
C	-2.96529000	-0.51031800	4.83146600	<b>INT-5B</b>			
H	-1.36756700	-1.92867000	4.53603200	C	-6.06258200	-0.94896900	-0.06746500
H	-4.54425200	0.96096200	4.78450300	C	-4.70463700	-1.11126700	0.19266800
H	-3.06471800	-0.70810000	5.89427100	C	-3.93925100	-1.90664600	-0.66234000
C	-0.82303100	0.48980500	-1.17909500	C	-4.52254600	-2.54138000	-1.75658900
H	-0.72986600	0.32933000	-2.24452300	C	-5.88341700	-2.36998500	-2.00150100
C	-1.59024200	-0.51189000	-0.30681000	C	-6.67151100	-1.56798900	-1.16744400
H	-0.87099900	-0.92206300	0.40084300	H	-6.66272000	-0.33771600	0.60126000
C	-2.16238200	-1.67646600	-1.07011700	H	-4.25223100	-0.64523800	1.06114500
C	-2.93639100	-1.49755900	-2.22612500	H	-3.91189800	-3.17552400	-2.38940400
C	-1.85285900	-2.97498400	-0.65070300	H	-6.34301000	-2.87146000	-2.84914500
C	-3.40634100	-2.59837100	-2.93674700	C	-8.13840900	-1.36013100	-1.45155600
H	-3.18702700	-0.49514600	-2.55917000	H	-8.72210600	-1.31940600	-0.52692000
C	-2.32193700	-4.07747900	-1.36503800	H	-8.30717700	-0.41523700	-1.98275500
H	-1.20600900	-3.11756900	0.20700000	H	-8.54275900	-2.16287300	-2.07440000
C	-3.10241800	-3.89189900	-2.50504800	S	-2.17473900	-2.06422600	-0.39339900
H	-4.00981700	-2.44768800	-3.82671000	O	-1.54780700	-0.90000900	-1.11562000
H	-2.05824900	-5.07734700	-1.03639600	O	-1.98119500	-1.94954800	1.08866000
H	-3.46458500	-4.74985900	-3.06338000	O	-1.74849300	-3.36810900	-0.95334300
C	2.65570100	1.30685300	-1.38570000	C	1.80709000	2.95159500	-0.61737800
C	2.47059400	1.28429400	0.03793000	C	2.54388200	2.85061600	-1.82764400
C	3.11500600	2.20469300	0.87459600	C	2.85919800	3.94927500	-2.61182600
C	3.94118500	3.14029800	0.27461400	C	2.42033000	5.19518600	-2.15402500
C	4.15033100	3.16916600	-1.12840200	C	1.69015200	5.31749400	-0.96517800
C	3.52121900	2.26233500	-1.95864700	C	1.37031300	4.20267400	-0.18896100
C	1.86646700	0.25414600	-1.92375500	C	1.67896600	1.58533700	-0.12574500
C	1.20279300	-0.34288400	-0.83468400	C	2.37912600	0.75166100	-1.04302100
H	2.97301200	2.17759200	1.94893600	H	3.41884800	3.85074300	-3.53591100



H	2.64529400	6.08139000	-2.73801100	C	-1.82931800	3.17178800	-0.10664600
H	1.34465500	6.29388500	-0.64557600	C	-1.81632200	4.21409000	-1.03539600
H	0.77257700	4.30807200	0.70825200	C	-1.74000300	5.51489800	-0.54848400
H	3.37333900	1.10301500	-2.82896900	C	-1.67950100	5.77681100	0.83628300
N	2.86481300	1.48063000	-2.03944000	C	-1.70190800	4.74050700	1.76334700
C	2.45583200	-0.68090300	-0.63690700	C	-1.80959300	2.12829600	1.95684500
C	3.79011200	-0.96328200	0.07983800	C	-1.86667300	1.19283200	0.94690300
C	4.13737100	-2.29721700	0.32756300	H	-1.85465800	4.01495500	-2.10186100
C	4.61958700	0.05329800	0.55982200	H	-1.72760200	6.34465900	-1.24853500
C	5.28158800	-2.60498800	1.05530400	H	-1.62675200	6.80538700	1.18034100
H	3.49443900	-3.09058600	-0.03432600	H	-1.66738000	4.95175300	2.82830400
C	5.77279700	-0.25715800	1.28457300	H	-1.89582300	1.26099200	-1.13132400
H	4.37527600	1.09584400	0.38626600	N	-1.87534700	1.80864600	-0.28127700
C	6.10468000	-1.58541000	1.53818300	H	-1.90938200	0.12197000	1.00969400
H	5.52707100	-3.64384400	1.25088700	C	-1.81993200	1.81504900	3.42523700
H	6.40765200	0.54464700	1.64875900	H	-1.00354200	2.34856200	3.93554100
H	6.99790900	-1.82666500	2.10565600	H	-2.74959700	2.18409300	3.87984000
C	2.29741800	-1.58997800	-1.85764500	C	-1.69712300	0.31693800	3.74762700
C	1.13125700	-2.29833400	-2.14119600	H	-1.60285100	0.20778900	4.83761200
C	3.37612900	-1.66701900	-2.75705000	H	-0.77422600	-0.08859300	3.30862500
C	1.04244100	-3.07366300	-3.29948200	O	-2.82902000	-0.41378600	3.30818400
H	0.26848600	-2.26101700	-1.49673100	H	-2.55030700	-1.05555600	2.63018000
C	3.27912600	-2.42620700	-3.92001200				
H	4.31205900	-1.16744300	-2.51890000				
C	2.10686400	-3.13603800	-4.19460000	<b>TS-4B</b>			
H	0.12301100	-3.62062000	-3.47942000	C	6.11285400	-0.25397100	-0.05460200
H	4.12310700	-2.47821600	-4.60132000	C	4.76561500	-0.57068600	-0.19697000
H	2.03304500	-3.73779200	-5.09518600	C	4.22210900	-1.59930300	0.57549700
C	1.11710300	0.77859400	0.82777800	C	5.01344600	-2.30870000	1.47443400
H	0.55842000	1.10707700	1.69300300	C	6.36186400	-1.97954000	1.60495300
C	1.27583800	-0.67237400	0.47778900	C	6.92980500	-0.94718700	0.85000400
H	0.33549200	-0.90948900	-0.04796100	H	6.54209000	0.53774200	-0.66301200
C	1.44344900	-1.60920700	1.64256500	H	4.15021300	-0.04594200	-0.92012300
C	2.16427400	-1.21161100	2.77550700	H	4.57102700	-3.11730200	2.04523000
C	0.91021900	-2.90161300	1.58845400	H	6.98465800	-2.53732400	2.29920000
C	2.35883700	-2.09071500	3.83748400	C	8.38294800	-0.57575500	1.01162300
H	2.60036800	-0.21707000	2.81241200	H	8.84255300	-0.33394700	0.04833400
C	1.11221200	-3.78331800	2.64887400	H	8.49585700	0.30593300	1.65447300
H	0.31477600	-3.21192200	0.73823300	H	8.95494000	-1.38887300	1.46672200
C	1.83588400	-3.38292600	3.77251300	S	2.47331200	-1.96660700	0.45359300
H	2.92224800	-1.77080200	4.70855400	O	1.78725200	-0.92981500	1.30254900
H	0.68699400	-4.78058300	2.60036400	O	2.13711200	-1.78047600	-1.00209300
H	1.98630800	-4.07239200	4.59772100	O	2.25649300	-3.34043100	0.94553900
C	-1.77862900	3.41297700	1.30633100	C	-1.98096000	2.92657400	0.28924600

C	-2.77279100	2.89952700	1.47702600	H	-2.62222900	-0.66166500	-2.75874100
C	-3.22242100	4.05763600	2.10609000	C	-0.84656600	-4.06314100	-2.28725200
C	-2.88532400	5.27572800	1.52174000	H	-0.05030900	-3.24253400	-0.47239000
C	-2.12289700	5.32768700	0.34216900	C	-1.62901400	-3.83814000	-3.41939800
C	-1.67080600	4.16827500	-0.27775000	H	-2.86941400	-2.41811300	-4.46796700
C	-1.69601400	1.53842200	-0.02126600	H	-0.34400100	-5.01523300	-2.14986200
C	-2.34057100	0.76827500	0.93968700	H	-1.74814500	-4.61842500	-4.16511700
H	-3.81687500	4.01215600	3.01305000	C	1.40150900	3.20572100	-1.17618700
H	-3.22027100	6.19829600	1.98453200	C	1.45854300	2.91361700	0.23288000
H	-1.87742400	6.29125000	-0.09215600	C	1.64354900	3.93283100	1.18026900
H	-1.07018500	4.22634400	-1.17581300	C	1.76423200	5.22642300	0.70707400
H	-3.51583000	1.22569700	2.61815300	C	1.72855700	5.53300900	-0.68017200
N	-2.97870900	1.55972800	1.83190600	C	1.55597200	4.53928500	-1.62021600
C	-2.37667100	-0.70327200	0.66392800	C	1.17785200	1.97934800	-1.84267000
C	-3.69920700	-1.09660800	-0.01621000	C	1.03358100	0.98804600	-0.83717300
C	-4.01382400	-2.45641100	-0.14198100	H	1.67183500	3.71185700	2.24140500
C	-4.55472400	-0.15316700	-0.59154600	H	1.89626300	6.03715600	1.41676900
C	-5.14742700	-2.86181900	-0.83808600	H	1.84176400	6.56534400	-0.99385600
H	-3.35137600	-3.19680800	0.29091300	H	1.52708800	4.76976100	-2.68056200
C	-5.69713100	-0.55954000	-1.28545400	H	1.46611500	0.97604800	1.19541800
H	-4.33214600	0.90536200	-0.51521400	N	1.28185200	1.57679100	0.39467700
C	-5.99545800	-1.91377300	-1.41439600	H	1.28220100	-0.05941800	-0.96019700
H	-5.36481300	-3.92068400	-0.93686400	C	1.10768300	1.68673900	-3.30434700
H	-6.35121000	0.18826100	-1.72379900	H	0.10684600	1.92804600	-3.69928500
H	-6.88079900	-2.22986700	-1.95736800	H	1.80581900	2.34917600	-3.82882800
C	-2.18042500	-1.50331700	1.95721900	C	1.44348200	0.22053500	-3.64160300
C	-0.97014100	-2.08543400	2.33830500	H	1.39908600	0.10446200	-4.73320100
C	-3.27363300	-1.59121600	2.83776500	H	0.67877000	-0.44581600	-3.22215900
C	-0.85807700	-2.74709100	3.56356400	O	2.73364700	-0.12276000	-3.17784900
H	-0.08650400	-2.02398500	1.72089200	H	2.64445100	-0.82068700	-2.50088100
C	-3.15636700	-2.23707200	4.06548800				
H	-4.23492300	-1.18208100	2.53874600				
C	-1.94310200	-2.82354000	4.43262600				
H	0.09447400	-3.19774700	3.82263800	<b>INT-5C</b>			
H	-4.01540700	-2.29498200	4.72746300	C	-5.42592700	-3.06504500	-1.90959300
H	-1.85050100	-3.33822600	5.38411100	C	-4.09469900	-2.95393300	-1.52131500
C	-1.03596700	0.67416600	-0.94907500	C	-3.68756400	-1.84385300	-0.78041100
H	-1.08477100	0.83857100	-2.01784800	C	-4.60215800	-0.85678300	-0.42257900
C	-1.17826400	-0.76879400	-0.42228800	C	-5.93264100	-0.97923400	-0.82132100
H	-0.28033000	-0.98604400	0.15341800	C	-6.36478900	-2.08047300	-1.56834900
C	-1.31651600	-1.82228600	-1.49169800	H	-5.74563300	-3.92928800	-2.48601500
C	-2.09853900	-1.60437900	-2.63413300	H	-3.37165800	-3.72082200	-1.77572400
C	-0.68686800	-3.06171400	-1.33022800	H	-4.26469300	-0.00917700	0.16042700
C	-2.25383300	-2.60229300	-3.59271400	H	-6.64706600	-0.20789000	-0.54540100
				C	-7.81019200	-2.22564200	-1.97506100

H	-7.90100800	-2.59356700	-3.00191400	C	1.33796800	0.14416600	0.63294800
H	-8.33252800	-2.94128700	-1.32857200	H	2.17274700	-0.50078100	0.38702400
H	-8.34205500	-1.27266600	-1.90730800	C	0.65911900	0.98711000	-0.40548900
S	-1.95714700	-1.65032000	-0.35849300	H	-0.04105800	0.27369900	-0.87633100
O	-1.46993200	-3.00986500	0.01991900	C	1.54951600	1.56145700	-1.47102400
O	-1.28829200	-1.14407300	-1.60376700	C	2.81042100	2.08419200	-1.15995500
O	-1.92875800	-0.65522200	0.75328800	C	1.12095400	1.57153800	-2.80257800
C	0.50476800	-0.41377100	3.12369700	C	3.62347900	2.61658000	-2.15687300
C	-0.64434000	0.19832800	3.68457000	H	3.14682300	2.08827200	-0.12761200
C	-1.16225700	-0.16428900	4.91643400	C	1.93125000	2.10926800	-3.80250500
C	-0.49364000	-1.17999600	5.60725200	H	0.15661500	1.14258400	-3.05434100
C	0.64529400	-1.79507200	5.07333300	C	3.18351400	2.63463700	-3.48139200
C	1.15651600	-1.42231700	3.82794000	H	4.59857100	3.01869700	-1.90039500
C	0.68657400	0.21821000	1.82471400	H	1.58771600	2.10967800	-4.83236100
C	-0.34968900	1.19672000	1.69944100	H	3.81600900	3.05023700	-4.25970800
H	-2.04866200	0.30840500	5.32563700	C	3.47298400	-2.45980300	-0.34150300
H	-0.86989500	-1.49716100	6.57414800	C	2.30146600	-3.06094000	0.21620900
H	1.13693100	-2.58205100	5.63547800	C	2.32103200	-3.73319700	1.44340200
H	2.02614400	-1.91459300	3.40782900	C	3.53235100	-3.79632200	2.12385200
H	-1.97017500	1.71746000	2.86823200	C	4.70010900	-3.20247800	1.59704800
N	-1.10630000	1.19818300	2.78108300	C	4.68307600	-2.53940200	0.37682200
C	-0.25484100	2.01021000	0.45201600	C	3.07210500	-1.83704100	-1.58314700
C	0.57333800	3.28558300	0.71237600	C	1.72120500	-2.08582400	-1.71451100
C	0.59914600	4.26808100	-0.28602200	H	1.41684200	-4.18046300	1.84380500
C	1.34943800	3.47077900	1.86007900	H	3.58303800	-4.31842200	3.07503300
C	1.39251700	5.40156600	-0.14552500	H	5.62903600	-3.27411900	2.15465300
H	0.00482800	4.13026000	-1.18167100	H	5.58855500	-2.10426700	-0.03389800
C	2.14345400	4.61141600	2.00240000	H	0.26989400	-3.02602700	-0.45995700
H	1.35195000	2.73050600	2.65200700	N	1.25940500	-2.81783600	-0.64403300
C	2.17069400	5.57792700	1.00029300	H	1.02359900	-1.75732300	-2.46983800
H	1.40725900	6.14538900	-0.93579000	C	3.94507600	-1.08076900	-2.54015000
H	2.73790400	4.73904100	2.90175600	H	3.32319100	-0.45999200	-3.19452200
H	2.78963900	6.46273200	1.11058900	H	4.60160500	-0.39619900	-1.98995700
C	-1.63753800	2.38704800	-0.08052700	C	4.81982600	-1.99518700	-3.40919600
C	-2.22379900	1.80076400	-1.20192600	H	5.44150200	-1.39069500	-4.07843700
C	-2.36479100	3.34978400	0.63829300	H	4.17091900	-2.62733100	-4.03581200
C	-3.51161800	2.17010400	-1.59528000	O	5.72232900	-2.78623400	-2.64775500
H	-1.72252300	1.00727900	-1.73787600	H	5.18668400	-3.33962100	-2.06203700
C	-3.65555500	3.70611600	0.25366000				
H	-1.90137300	3.84943400	1.48504200				
C	-4.23370300	3.11677700	-0.87177700	<b>TS-4C</b>			
H	-3.95594200	1.68859600	-2.46012000	C	6.23396200	0.99200000	-1.33345800
H	-4.20137000	4.45167600	0.82394300	C	4.96839900	1.08934500	-0.75695700
H	-5.23721900	3.39366800	-1.17958400	C	4.22933300	-0.06843700	-0.53096200

C	4.74533000	-1.31909100	-0.87334300	C	1.72021700	-3.89512400	-1.46107800
C	6.00867900	-1.40130000	-1.45085700	H	0.72099900	-2.03982600	-1.78608400
C	6.77253800	-0.25000300	-1.68893100	C	1.11124600	-5.11478500	0.52085300
H	6.81462100	1.89411900	-1.50801600	H	-0.46974100	-4.25975700	1.69375500
H	4.55159500	2.04758600	-0.46885600	C	1.89703000	-4.99562600	-0.62590600
H	4.15818500	-2.20905000	-0.67400100	H	2.33127200	-3.78156200	-2.35139900
H	6.41420800	-2.37385200	-1.71838200	H	1.23432800	-5.96634400	1.18329700
C	8.15558600	-0.35358100	-2.28271800	H	2.63885100	-5.75206200	-0.86312700
H	8.45197400	0.57923900	-2.77062000	C	-1.52229200	0.48673100	0.25029600
H	8.90261200	-0.57022000	-1.50908900	H	-2.47503500	1.00046900	0.24792600
H	8.21372000	-1.15792300	-3.02239400	C	-1.35944300	-0.78688900	-0.60870100
S	2.56961300	0.02414500	0.13706600	H	-0.42054500	-0.65842000	-1.14343000
O	2.50112400	1.33578000	0.87019000	C	-2.46137800	-1.03658400	-1.60222300
O	1.66489400	0.02106700	-1.06110500	C	-3.81417000	-0.90619800	-1.25697900
O	2.42216700	-1.16476400	1.00475900	C	-2.13838400	-1.38319000	-2.91921400
C	-0.40301500	0.84118400	2.71567000	C	-4.81363500	-1.10772300	-2.20481500
C	0.26432300	-0.19185900	3.43789700	H	-4.08610400	-0.66350300	-0.23508300
C	0.87595800	0.03557800	4.66552300	C	-3.13749400	-1.58943700	-3.87128300
C	0.79873700	1.32292900	5.19330700	H	-1.09495600	-1.48762700	-3.20003100
C	0.12004500	2.34805400	4.51365800	C	-4.47868100	-1.44844800	-3.51692000
C	-0.47884600	2.11979800	3.27851300	H	-5.85554700	-1.00418300	-1.91788300
C	-0.83715000	0.22826100	1.48156300	H	-2.86641200	-1.85473400	-4.88857400
C	-0.46062200	-1.10678100	1.53686100	H	-5.25824800	-1.60428400	-4.25627700
H	1.39568800	-0.75897400	5.19068400	C	-1.43367800	4.00891600	-0.48655300
H	1.26935800	1.53458800	6.14800800	C	-0.25168100	3.86176000	0.32699500
H	0.06656600	3.33689800	4.95823500	C	0.17105800	4.88884300	1.19584300
H	-0.98988600	2.92194600	2.75943800	C	-0.58600800	6.04195200	1.22881600
H	0.74925000	-2.18811400	2.83502300	C	-1.75485600	6.20871700	0.42987300
N	0.14929800	-1.38505000	2.71122900	C	-2.18685700	5.21181100	-0.41472200
C	-1.02565000	-1.96345000	0.44176500	C	-1.57435000	2.81767900	-1.22519400
C	-2.34222700	-2.62468500	0.88755300	C	-0.53023000	1.93582700	-0.79205400
C	-2.89565200	-3.63434300	0.08845400	H	1.05258400	4.76147700	1.81382700
C	-3.05477200	-2.19479200	2.01121400	H	-0.28564100	6.85237800	1.88600000
C	-4.13266700	-4.19150400	0.39735300	H	-2.30861000	7.13905600	0.49854500
H	-2.35398200	-3.97275100	-0.78744700	H	-3.06592800	5.33803200	-1.03696600
C	-4.29549700	-2.75525400	2.32370300	H	1.15656800	2.22684300	0.49257800
H	-2.64930300	-1.41755400	2.64839000	N	0.27906300	2.64471800	0.10296500
C	-4.84072600	-3.75223000	1.51741300	H	-0.00056100	1.22309900	-1.41309000
H	-4.54649800	-4.96566100	-0.24146100	C	-2.60776200	2.50487500	-2.25496500
H	-4.83099000	-2.41079300	3.20333800	H	-2.65816900	1.42669800	-2.42617400
H	-5.80548000	-4.18674800	1.76062400	H	-3.59684400	2.83356000	-1.91519200
C	-0.02231000	-3.02688700	-0.01640900	C	-2.31429100	3.19627200	-3.60398800
C	0.77381900	-2.91564200	-1.15713800	H	-3.09135100	2.91097700	-4.31887400
C	0.15755300	-4.14399900	0.81482800	H	-1.35102200	2.83689000	-3.99401600

O -2.34877700 4.61099300 -3.52594300  
H -1.58604800 4.89534900 -3.00433400

**INT-5D**

C 5.41346900 0.86549400 -1.77537700  
C 4.30370100 0.09720700 -2.11957100  
C 3.79867400 -0.83264800 -1.21096600  
C 4.43536400 -1.03132900 0.01104800  
C 5.54598400 -0.25838100 0.34734900  
C 6.03460200 0.72267400 -0.52750700  
H 5.79659300 1.60021500 -2.47829400  
H 3.81765600 0.21401900 -3.08216800  
H 4.05501100 -1.78234500 0.68849300  
H 6.03830600 -0.41606800 1.30423200  
C 7.16171900 1.63324000 -0.11287200  
H 7.87335300 1.12241100 0.54238500  
H 7.70745300 2.01861400 -0.97831000  
H 6.76354200 2.49411000 0.43815800  
S 2.20706500 -1.59719400 -1.54901300  
O 1.23804100 -0.56230200 -1.05237100  
O 2.15542100 -1.83453600 -3.00063900  
O 2.16600700 -2.84644700 -0.70074800  
C 1.06964100 -0.18490500 2.50429100  
C 1.55156400 -1.49117300 2.23536500  
C 2.69975000 -1.99644200 2.82113300  
C 3.39843600 -1.15025600 3.68983200  
C 2.95102800 0.14918300 3.95190300  
C 1.78348300 0.64385500 3.36481500  
C -0.12520900 -0.04707800 1.67837900  
C -0.28281200 -1.30410500 0.99520800  
H 3.04567500 -3.00034500 2.60149100  
H 4.30673800 -1.50932200 4.16278900  
H 3.52275600 0.78888400 4.61525100  
H 1.45567900 1.65727200 3.56305800  
H 1.09557200 -2.78682200 0.58414700  
N 0.68302100 -2.14519600 1.31240900  
C -1.53642300 -1.36709400 0.17935800  
C -2.68455100 -1.93012400 1.04897400  
C -3.88130300 -2.29111000 0.41557800  
C -2.61274700 -2.01522700 2.44256500  
C -4.98218900 -2.70567100 1.15755000  
H -3.94861100 -2.23604200 -0.66372200  
C -3.71562200 -2.44002400 3.18700800

H -1.70080900 -1.75567300 2.96697100  
C -4.90541600 -2.78063100 2.54940800  
H -5.90251700 -2.96934200 0.64593500  
H -3.63611200 -2.50498800 4.26782700  
H -5.76337100 -3.10724500 3.12870800  
C -1.37250500 -2.19155900 -1.09540500  
C -1.21056700 -1.63222400 -2.36358200  
C -1.31805800 -3.58611100 -0.96598000  
C -1.00757700 -2.44456500 -3.47715800  
H -1.18354800 -0.55846700 -2.48903800  
C -1.10437300 -4.39836600 -2.07578500  
H -1.44816800 -4.03676800 0.01274100  
C -0.95322500 -3.82866800 -3.33909900  
H -0.85565200 -1.98806100 -4.44915000  
H -1.05130100 -5.47522400 -1.95074400  
H -0.77653500 -4.45721800 -4.20576400  
C -1.00870800 0.83513200 1.14721200  
H -1.11865500 1.88310800 1.39346000  
C -1.78540400 0.21370200 0.01379600  
H -1.22260700 0.51624400 -0.87614800  
C -3.21458600 0.66182300 -0.13693100  
C -3.94206300 1.13551100 0.95758000  
C -3.84526100 0.58627400 -1.38391800  
C -5.26725000 1.53991500 0.81013400  
H -3.47296500 1.17582900 1.93580300  
C -5.17383400 0.97616800 -1.53261300  
H -3.29491500 0.20802900 -2.23870100  
C -5.88810500 1.46039300 -0.43573300  
H -5.81614100 1.91015700 1.67035100  
H -5.65031300 0.90742900 -2.50596500  
H -6.92214400 1.77019400 -0.55122200  
C -0.75679700 3.73661300 -0.34045700  
C -1.50279100 3.35004200 -1.48841500  
C -2.82564200 3.74926200 -1.68634100  
C -3.41529000 4.53236000 -0.70092700  
C -2.69992300 4.92021200 0.44869700  
C -1.37689300 4.53564400 0.63438800  
C 0.54066400 3.10730900 -0.43303000  
C 0.53941400 2.38250400 -1.60013100  
H -3.38656600 3.43149200 -2.55850800  
H -4.44978000 4.83875800 -0.81538400  
H -3.19234100 5.53154200 1.19861900  
H -0.82898000 4.84552000 1.51978100  
H -0.90895700 2.13923000 -3.13985000

N	-0.68801400	2.51762300	-2.23368300
H	1.27751800	1.70013800	-1.99032700
C	1.63715800	3.20001200	0.58698200
H	2.06683100	4.21068200	0.60597200
H	1.22232200	3.03883500	1.59135100
C	2.74926200	2.18659600	0.35963300
H	3.22384900	2.36990400	-0.61458600
H	2.32394600	1.17819900	0.32351900
O	3.70162100	2.31510100	1.41336100
H	4.25863800	1.52609900	1.36481700

**TS-4D**

C	5.55115600	0.14627200	-1.89305900
C	4.33015000	-0.46349100	-2.16615500
C	3.69130200	-1.21028100	-1.17503500
C	4.28736200	-1.36822500	0.07279400
C	5.51441300	-0.75621200	0.33798000
C	6.15815700	0.02172600	-0.63488000
H	6.04402400	0.73229400	-2.66422600
H	3.86554200	-0.37707200	-3.14229000
H	3.79103400	-1.97009800	0.82228300
H	5.97683100	-0.88352600	1.31353800
C	7.44327500	0.74637700	-0.32380400
H	7.99195100	0.26072200	0.48791800
H	8.09794700	0.79450300	-1.19881100
H	7.23507300	1.77749700	-0.01290600
S	2.04375300	-1.86793800	-1.48916200
O	1.14316300	-0.69571900	-1.19777200
O	2.03228900	-2.27381600	-2.90710900
O	1.87493500	-2.97660700	-0.49947900
C	0.86640800	0.24476300	2.31413100
C	1.35226400	-1.09606100	2.39463300
C	2.46425100	-1.43807900	3.15542800
C	3.09829500	-0.42158400	3.86983700
C	2.60680500	0.89286100	3.84704500
C	1.48895200	1.22923300	3.08879800
C	-0.23855000	0.19578600	1.37848400
C	-0.40246000	-1.14415700	1.04234300
H	2.81724600	-2.46334100	3.19517200
H	3.97269600	-0.65594700	4.46832300
H	3.10382200	1.65857400	4.43332200
H	1.10593700	2.24365700	3.10115300
H	0.88577400	-2.73609200	1.10890700

N	0.51569100	-1.93440200	1.63742300
C	-1.65169700	-1.44435200	0.27361400
C	-2.82289400	-1.73296300	1.23677200
C	-4.01577600	-2.24384900	0.70611400
C	-2.77697100	-1.42516900	2.59952500
C	-5.13607300	-2.42486500	1.51058100
H	-4.06248100	-2.49152500	-0.34801000
C	-3.89938900	-1.61334000	3.41001700
H	-1.86752000	-1.03416200	3.03950500
C	-5.08387400	-2.10789300	2.86934500
H	-6.05175700	-2.81262600	1.07475100
H	-3.83979200	-1.37447800	4.46766700
H	-5.95610200	-2.25195400	3.49962700
C	-1.46951600	-2.61006300	-0.70206200
C	-1.21583900	-2.46423600	-2.06598800
C	-1.46459500	-3.90425000	-0.15909300
C	-0.95635700	-3.57635800	-2.86650600
H	-1.14506600	-1.48519500	-2.51927200
C	-1.20555500	-5.01476000	-0.95533900
H	-1.66352000	-4.03791600	0.89924100
C	-0.95188300	-4.85430400	-2.31728800
H	-0.71972600	-3.42968400	-3.91421200
H	-1.19474700	-6.00452100	-0.50909900
H	-0.73513700	-5.71633800	-2.94008000
C	-1.07332700	1.00550700	0.53449100
H	-1.62398800	1.85566800	0.93266400
C	-1.85856700	0.00220600	-0.36992600
H	-1.29877900	-0.06437800	-1.30089800
C	-3.27437600	0.40559400	-0.69205900
C	-4.12066100	0.97128300	0.27168500
C	-3.76931600	0.21740000	-1.98978400
C	-5.42050200	1.34533200	-0.05545200
H	-3.76779900	1.09044100	1.29038200
C	-5.07347500	0.59128100	-2.32038100
H	-3.13359600	-0.24444900	-2.73967100
C	-5.90117500	1.16033600	-1.35402400
H	-6.06332800	1.77559800	0.70616900
H	-5.43918600	0.43428200	-3.33039100
H	-6.91556500	1.45243000	-1.60713000
C	-0.27116800	4.25740800	-0.35364200
C	-1.40766600	3.86264100	-1.13213200
C	-2.45401200	4.75907400	-1.41724200
C	-2.31749900	6.05289400	-0.95293500
C	-1.17833500	6.47757400	-0.21262400

C -0.16141400 5.59963100 0.08845500  
 C 0.55648600 3.12763400 -0.20594300  
 C -0.14035400 2.00498400 -0.78154900  
 H -3.32516500 4.44288200 -1.98068300  
 H -3.10268400 6.77349400 -1.15949400  
 H -1.12353500 7.50845200 0.12016900  
 H 0.70387700 5.91708000 0.66081600  
 H -2.00348300 2.01006900 -1.86216900  
 N -1.24472200 2.56936800 -1.49583900  
 H 0.40366400 1.17974000 -1.24127300  
 C 1.93283500 3.14285000 0.37088600  
 H 2.43005400 4.06589500 0.04622000  
 H 1.89187300 3.20873700 1.46180300  
 C 2.81095300 1.95272700 -0.00097400  
 H 2.96039900 1.92393100 -1.09061800  
 H 2.32269000 1.01325400 0.27214700  
 O 4.03646300 2.13112700 0.69012400  
 H 4.50215800 1.28318200 0.65836400

**TS-3(R,R)**

C -5.28050300 0.02536000 0.33130000  
 C -4.28307600 -0.68615200 0.99500100  
 C -3.66869700 -1.76232800 0.36312100  
 C -4.06706600 -2.14717400 -0.91828000  
 C -5.06820600 -1.43392200 -1.56875000  
 C -5.68186000 -0.32981200 -0.96039500  
 H -5.74803900 0.87582000 0.82015100  
 H -3.96448600 -0.41489300 1.99346000  
 H -3.58383000 -2.99162400 -1.39796800  
 H -5.37686300 -1.72965200 -2.56818300  
 C -6.71877600 0.48052800 -1.69453100  
 H -6.25190500 1.33769700 -2.19470900  
 H -7.47698700 0.87493600 -1.01157300  
 H -7.22558100 -0.11380000 -2.46012200  
 S -2.32021000 -2.64544500 1.15865000  
 O -2.75587700 -4.02801200 1.39624900  
 O -1.99479100 -1.85712800 2.38273600  
 O -1.22217600 -2.55234900 0.11258500  
 C 0.95086500 3.07328200 -0.77413100  
 C 1.85672900 3.55707700 0.21153800  
 C 1.83154700 4.87228900 0.66664600  
 C 0.87709600 5.71978400 0.10767700  
 C -0.01640600 5.26486700 -0.87777200

C 0.01213700 3.94901700 -1.32835300  
 C 1.29498100 1.68016900 -0.95919300  
 C 2.35592800 1.38969100 -0.10535700  
 H 2.52384300 5.22423600 1.42459500  
 H 0.82591600 6.75160300 0.43937700  
 H -0.74571800 5.95378300 -1.29118100  
 H -0.69305800 3.60052000 -2.07390700  
 H 3.43050000 2.55030000 1.28094100  
 N 2.70325500 2.49731600 0.58464700  
 C 2.86045500 -0.03463700 -0.16155500  
 C 4.36629700 -0.06060600 -0.48704400  
 C 5.23286000 -1.00019500 0.08080100  
 C 4.88563100 0.85660400 -1.41068400  
 C 6.58251700 -1.02604400 -0.27193300  
 H 4.85117700 -1.71138400 0.80364000  
 C 6.23403600 0.83465500 -1.76132400  
 H 4.22936500 1.59693500 -1.86046400  
 C 7.08925000 -0.10926000 -1.19192800  
 H 7.23732700 -1.76586900 0.17783300  
 H 6.61528700 1.55600300 -2.47747600  
 H 8.14020100 -0.12863700 -1.46232800  
 C 2.54087900 -0.69885300 1.18906300  
 C 1.55849400 -1.67399900 1.37095100  
 C 3.21643700 -0.21232900 2.32229300  
 C 1.23606100 -2.12808700 2.65327600  
 H 0.98816700 -2.07414900 0.54656900  
 C 2.90419900 -0.67121000 3.59726500  
 H 4.01308300 0.51745900 2.20395400  
 C 1.90013800 -1.62691800 3.76791200  
 H 0.42591200 -2.83831200 2.76407900  
 H 3.43580100 -0.27469100 4.45691700  
 H 1.63266800 -1.96753500 4.76263100  
 C 0.87628900 0.49444600 -1.59215600  
 H 0.25558500 0.47296200 -2.47794100  
 C 2.00712100 -0.51708500 -1.43962600  
 H 2.65414400 -0.21728600 -2.27989900  
 C 1.73520900 -1.98632800 -1.68754700  
 C 0.52067900 -2.42520400 -2.21862500  
 C 2.75255000 -2.92896400 -1.48016700  
 C 0.30523000 -3.77454300 -2.49422000  
 H -0.28737000 -1.72701400 -2.39373400  
 C 2.53987600 -4.27562400 -1.75676800  
 H 3.71277500 -2.61045300 -1.09638800  
 C 1.31117100 -4.70641000 -2.26025700

H	-0.66146300	-4.09329300	-2.86882900	O	-3.39747000	-2.95785300	2.86052000
H	3.33580100	-4.99111900	-1.57431500	O	-2.74204700	-0.58013000	3.31465600
H	1.13978100	-5.75901800	-2.46093900	O	-1.44186800	-1.93442300	1.69267800
C	-2.19934400	1.85174900	-0.18176800	C	2.25531400	3.06608700	-0.03138100
C	-1.84388100	0.79784000	-1.05279500	C	3.44322100	3.01012200	0.75066200
C	-2.38290300	0.67425200	-2.32292900	C	4.02937400	4.14815300	1.29748900
C	-3.29782000	1.65119000	-2.73551500	C	3.41350900	5.37054600	1.03728800
C	-3.65181200	2.70909400	-1.88982500	C	2.25131300	5.45032400	0.24987400
C	-3.11251500	2.81512900	-0.60428200	C	1.66606500	4.30919200	-0.28866800
C	-1.44555600	1.65606200	1.05216700	C	1.96177400	1.69660000	-0.39296500
C	-0.68376300	0.54703000	0.87653000	C	2.98414100	0.90175600	0.11490500
H	-2.12799900	-0.15893300	-2.96963900	H	4.93109300	4.08880500	1.89836700
H	-3.74462900	1.57859100	-3.72159700	H	3.84356700	6.27838600	1.44708800
H	-4.36178300	3.45345100	-2.23672000	H	1.80475900	6.42116300	0.06141300
H	-3.39513000	3.63491900	0.04832300	H	0.76267800	4.37271400	-0.88654200
H	-0.96404800	-1.05464900	-0.38596900	H	4.62317600	1.32333100	1.37161800
N	-0.84016500	0.00547500	-0.42167200	N	3.85494000	1.66921900	0.81761000
H	-0.03319500	0.06083600	1.57832500	C	2.88891900	-0.56316800	-0.22051800
C	-1.56117200	2.42819000	2.32665200	C	4.11116900	-1.10696000	-0.97703700
H	-2.21780000	3.29569500	2.19354900	C	3.97941000	-2.30001900	-1.70751300
H	-0.57770100	2.81139900	2.62130800	C	5.35263800	-0.46464300	-0.98823200
C	-2.09820900	1.54853500	3.48115500	C	5.05721400	-2.83653900	-2.40661600
H	-2.17615800	2.17352800	4.37985900	H	3.02570500	-2.81392900	-1.72468300
H	-3.11388300	1.21212500	3.22995100	C	6.43457500	-1.00069800	-1.68999600
O	-1.24522700	0.46886300	3.77691600	H	5.48986900	0.47674700	-0.47225900
H	-1.53200000	-0.32082700	3.27747900	C	6.29416500	-2.19043000	-2.39897900

**TS-4(R,R)**

C	-5.21282100	0.53873800	-0.01356200	H	7.13497900	-2.60737800	-2.94413100
C	-4.42043600	0.10458500	1.04834600	C	2.59412600	-1.35578800	1.06983300
C	-3.82636900	-1.15420800	1.00134500	C	1.75989700	-0.78896100	2.04301000
C	-4.02674800	-1.97773200	-0.10893300	C	3.10194700	-2.64088900	1.29292000
C	-4.81633100	-1.53410000	-1.16642300	C	1.39064300	-1.50518600	3.17779500
C	-5.42850400	-0.27259000	-1.13239100	H	1.34577100	0.20391200	1.92474300
H	-5.66579200	1.52607300	0.02291900	C	2.74320000	-3.35295900	2.43800300
H	-4.25938300	0.72305600	1.92327600	H	3.77119200	-3.09873300	0.57682900
H	-3.56499000	-2.95821100	-0.13828600	C	1.87847600	-2.79510400	3.37815300
H	-4.97146600	-2.17845400	-2.02864000	H	0.70711200	-1.04609100	3.88131600
C	-6.31834700	0.18911300	-2.25856900	H	3.13903500	-4.35318500	2.58651100
H	-6.23892800	1.26959500	-2.40816000	H	1.58230500	-3.36149400	4.25506600
H	-7.37060500	-0.03775600	-2.04856400	C	0.99422400	0.89507800	-1.06205100
H	-6.06196600	-0.30449900	-3.20101800	H	0.39629100	1.28107000	-1.88220400
S	-2.77058700	-1.73022100	2.34508100	C	1.67933200	-0.46934500	-1.28499800
				H	2.20754200	-0.27669700	-2.22919400



C	0.78507800	-1.65270100	-1.57409600	C	-0.40997100	0.78200100	0.52113000
C	0.44248800	-1.87855300	-2.91861100	H	2.06421900	3.81827900	2.00240500
C	0.20205900	-2.45974000	-0.59200100	H	3.97817000	2.93369200	3.30698000
C	-0.47900900	-2.86087700	-3.27161100	H	4.31710700	0.50917900	3.62113300
H	0.89302200	-1.26234100	-3.69272100	H	2.72429600	-1.13260400	2.63425100
C	-0.72364900	-3.44442100	-0.94421900	H	-0.04226900	2.86859000	0.38007500
H	0.39976100	-2.30590200	0.45543000	N	0.15211400	2.02346400	0.89445700
C	-1.07080400	-3.64746900	-2.27884400	C	-1.48854500	0.73895000	-0.35174200
H	-0.73493300	-3.01164400	-4.31602400	C	-1.92220600	-0.44391000	-1.08303900
H	-1.18629200	-4.01847700	-0.14963000	C	-3.29078000	-0.60490800	-1.39484300
H	-1.79743600	-4.40866400	-2.54622500	C	-1.00429700	-1.41352400	-1.52790100
C	-1.98901600	2.32495400	-0.82663200	C	-3.72182300	-1.70908900	-2.11959000
C	-2.26373000	1.16636500	-1.62726600	H	-4.01011400	0.11625600	-1.02572800
C	-3.06927700	1.23764600	-2.77566800	C	-1.43948600	-2.50955400	-2.25773000
C	-3.61609300	2.46699100	-3.09010100	H	0.05300700	-1.33484300	-1.31807300
C	-3.37994900	3.62258500	-2.29718700	C	-2.79790700	-2.66193600	-2.55555300
C	-2.57467900	3.56380600	-1.17943600	H	-4.77817900	-1.83226900	-2.33473000
C	-1.13884800	1.91697900	0.23087600	H	-0.70247100	-3.23079600	-2.59331000
C	-0.82242100	0.54223600	-0.00337400	H	-3.13518100	-3.52097600	-3.12766700
H	-3.26499600	0.35542800	-3.37348500	C	-2.22421100	1.99371100	-0.61810600
H	-4.24948900	2.55462000	-3.96724800	C	-2.66626300	2.81066600	0.43910300
H	-3.83905900	4.56190300	-2.58661500	C	-2.51544100	2.37243000	-1.94093900
H	-2.39127900	4.44733400	-0.57631200	C	-3.37993700	3.97608300	0.17599900
H	-1.70873300	-0.85676300	-1.33747300	H	-2.47134300	2.50453300	1.46053900
N	-1.60829500	0.11304900	-1.07720000	C	-3.20861100	3.55124200	-2.19920000
H	-0.55004500	-0.17911800	0.75845800	H	-2.17954300	1.74180300	-2.75645200
C	-0.70919500	2.71726800	1.40631300	C	-3.64524100	4.35297100	-1.14259200
H	-1.00130200	3.76443400	1.27551200	H	-3.73480900	4.58782900	0.99917500
H	0.37880500	2.69543600	1.50624200	H	-3.41217900	3.84254900	-3.22446300
C	-1.26662700	2.17425400	2.74423400	H	-4.19550000	5.26623100	-1.34548300
H	-1.06196500	2.93904000	3.50991500	C	0.18782600	-1.66858900	1.29572200
H	-2.35479400	2.05309600	2.67875500	H	1.11828100	-2.22788300	1.22128400
O	-0.63951000	0.96515700	3.06636600	C	-0.93699300	-2.39369400	1.47787600
H	-1.35502700	0.28675300	3.20185400	H	-0.78521300	-3.46983100	1.41866400
				C	-2.29892000	-1.91783700	1.70700300
				C	-2.58536600	-0.72458200	2.39503200
				C	-3.37349200	-2.68044300	1.21963100
				C	-3.89538200	-0.28249200	2.53573800
				H	-1.77148300	-0.15663500	2.83205200
				C	-4.68708600	-2.23737500	1.36009100
				H	-3.16328000	-3.60818200	0.69723800
				C	-4.95282200	-1.03277300	2.00932600
				H	-4.09998100	0.63763000	3.07522500
				H	-5.50214600	-2.83366600	0.96199400
<b>(S)-INT-6</b>							
C	1.45890600	0.42106400	1.80825700				
C	1.29337300	1.82368100	1.61510500				
C	2.19397500	2.75213800	2.15141800				
C	3.25842900	2.24361800	2.87730300				
C	3.45012300	0.85080600	3.06680500				
C	2.56284800	-0.06638200	2.54510300				
C	0.37274000	-0.24418100	1.18117500				

H	-5.97566900	-0.68799200	2.12536200	H	0.94666900	-2.46653200	1.18901000
C	2.07712700	1.73258700	-1.99767200	C	-1.12463000	-0.45793100	3.77838300
C	2.11735000	0.33810900	-1.92927000	H	-0.26916800	1.30029900	2.88742800
C	3.06588700	-0.29133500	-1.12835900	C	-1.17784600	-1.85162300	3.76650000
C	4.00668900	0.47326700	-0.43438200	H	-0.49889800	-3.64564500	2.78153300
C	3.97089700	1.85942400	-0.52269700	H	-1.71830500	0.10672300	4.49058700
C	2.99817500	2.51343800	-1.29520400	H	-1.82382300	-2.37861000	4.46105200
H	1.32158800	2.21815400	-2.61148700	C	2.84056900	0.06872800	1.15898200
H	1.41674000	-0.26729200	-2.49019100	C	3.71769500	0.84563900	0.37006100
H	4.73847200	-0.02427200	0.19130600	C	3.39811600	-0.94499000	1.96664400
H	4.69373500	2.45047000	0.03284700	C	5.08555600	0.60752400	0.37382600
C	2.96135400	4.01983100	-1.36379700	H	3.31824400	1.61211600	-0.28047000
H	2.04381900	4.37730400	-1.84077100	C	4.76731700	-1.18000100	1.96590400
H	3.02360800	4.46604500	-0.36469600	H	2.75092600	-1.54347500	2.59424600
H	3.80565000	4.41493200	-1.94062800	C	5.61673200	-0.41000600	1.16768200
S	3.10487600	-2.09013700	-0.97251000	H	5.73492200	1.20380300	-0.25847400
O	4.27571400	-2.55188600	-1.73522800	H	5.17464700	-1.96762400	2.59141100
O	3.19429300	-2.32020300	0.50821300	H	6.68485600	-0.60300800	1.16482400
O	1.77739900	-2.53054400	-1.52460100	C	-0.49727800	0.38468900	-0.94156900
H	1.19169200	-3.99928200	-0.36518600	H	-1.46583100	0.14432800	-1.36935700
O	1.19048400	-4.50745300	0.46765100	C	0.52815900	-0.60877100	-0.94718200
H	2.03752900	-4.20881200	0.83381200	H	0.19871600	-1.63630700	-0.81229300

**(S)-TS-5**

C	-0.63342700	2.97233700	-0.40658400	C	2.67565800	-1.57513100	-1.65653400
C	0.32838400	3.71184900	0.32975800	C	3.32430700	0.70344000	-3.13816000
C	0.27952700	5.09847700	0.43107900	H	1.42419300	1.48228000	-2.51088400
C	-0.76472100	5.74652600	-0.22838200	C	3.88240600	-1.51025000	-2.34635000
C	-1.72101500	5.03248400	-0.96949000	H	2.39341100	-2.46712200	-1.10536200
C	-1.66018900	3.64536400	-1.07286300	C	4.21384100	-0.37368500	-3.08509800
C	-0.21882900	1.58684100	-0.31911700	H	3.56398400	1.57810500	-3.73519800
C	0.88959300	1.53191300	0.57768100	H	4.56249400	-2.35531300	-2.31299600
H	1.01903000	5.65448900	0.99782200	H	5.15045400	-0.33197800	-3.63240300
H	-0.83669300	6.82746400	-0.16803300	C	-3.40937100	0.42618800	1.04140800
H	-2.51897300	5.57253700	-1.46761300	C	-2.96944700	-0.85821400	0.72481400
H	-2.40086100	3.08790900	-1.63514500	C	-3.20039700	-1.37579200	-0.54929400
H	1.95291700	3.04666700	1.57215200	C	-3.88615200	-0.61475900	-1.49864700
N	1.25175200	2.80788800	0.88622300	C	-4.31715900	0.67076700	-1.17244500
C	1.39681200	0.26996700	1.05867300	C	-4.08519000	1.21270300	0.10101500
C	0.47028000	-0.49631900	1.94416800	H	-3.21835700	0.82321700	2.03455700
C	0.40471500	-1.89877500	1.93677400	H	-2.44243200	-1.46683200	1.44646600
C	-0.31233300	0.21599000	2.86891700	H	-4.07108300	-1.03124000	-2.48302100
C	-0.41801400	-2.56656200	2.83803700	H	-4.85374000	1.26082400	-1.91160700
				C	-4.57505100	2.59295000	0.46422200

H	-5.40136200	2.54123200	1.18262600
H	-3.78136500	3.19180700	0.92246900
H	-4.93725600	3.13346000	-0.41479300
S	-2.49967000	-2.96732500	-1.03632600
O	-3.60751700	-3.73687800	-1.62629500
O	-1.42880400	-2.56881900	-2.01527400
O	-1.91733200	-3.52633400	0.22625500
H	-0.12162800	-3.98532100	-0.12794800
O	0.69493600	-3.89921700	-0.66258500
H	0.27864000	-3.63097500	-1.50111900

**(S)-INT-7**

C	-1.58467300	1.69687100	-0.73307900
C	-1.60644400	2.23208800	0.58043500
C	-2.68187100	2.95061500	1.07906400
C	-3.77577900	3.12458700	0.22789300
C	-3.78316200	2.59006300	-1.06663500
C	-2.69307000	1.87175100	-1.55770500
C	-0.32107300	0.98424000	-0.84202000
C	0.33709200	1.13214900	0.40798000
H	-2.68357500	3.34692600	2.08892300
H	-4.64183100	3.67201400	0.58461000
H	-4.65944600	2.72148800	-1.69162900
H	-2.71599200	1.43741900	-2.55036200
H	-0.18559600	2.00807800	2.20704300
N	-0.39042100	1.88146300	1.22465300
C	1.66686800	0.45657800	0.48857600
C	1.86200500	-0.17959900	1.86852000
C	1.70771300	-1.54394400	2.12188700
C	2.14707400	0.68228500	2.94038000
C	1.84518700	-2.03110500	3.42311500
H	1.46400900	-2.24350200	1.33182400
C	2.26743100	0.19445800	4.23947400
H	2.31108500	1.73934600	2.74809900
C	2.11832500	-1.17116900	4.48445000
H	1.72291700	-3.09475100	3.60122500
H	2.49026300	0.87744700	5.05375700
H	2.21702500	-1.55968500	5.49335500
C	2.80100600	1.45135100	0.18831700
C	4.12128100	1.04230300	0.41637000
C	2.57284200	2.71234000	-0.36864300
C	5.18742900	1.86959600	0.08124900
H	4.30689900	0.06314500	0.84219300

C	3.64371200	3.54585600	-0.70087100
H	1.56149000	3.05498600	-0.55828000
C	4.95318900	3.12645700	-0.48078400
H	6.20360800	1.52962700	0.25404300
H	3.44749100	4.52324000	-1.13097700
H	5.78548800	3.77263400	-0.74164500
C	0.34244500	0.02521200	-1.55422400
H	0.09638600	-0.33745500	-2.54153200
C	1.48954500	-0.54467800	-0.76344700
H	1.07063000	-1.46746200	-0.35388000
C	2.72076500	-0.89539600	-1.55444200
C	3.37129600	-2.11125900	-1.31603100
C	3.23634500	-0.02066500	-2.51914100
C	4.53499700	-2.43193300	-2.01565700
H	2.94551200	-2.81219300	-0.60487700
C	4.39489800	-0.34346400	-3.22011100
H	2.74227400	0.92949200	-2.69923400
C	5.05150400	-1.54873600	-2.96392500
H	5.03208200	-3.37817100	-1.82524400
H	4.78863300	0.34640200	-3.96027200
H	5.95758600	-1.80048600	-3.50683600
C	-5.31321600	-0.81483000	-1.59006300
C	-4.05259200	-1.37035500	-1.37564100
C	-3.44075900	-1.22116400	-0.13352000
C	-4.08178700	-0.52729300	0.89222900
C	-5.33994000	0.02016400	0.66610100
C	-5.97311100	-0.10992100	-0.57742500
H	-5.79060800	-0.92643000	-2.56010800
H	-3.52961500	-1.90187300	-2.16235800
H	-3.57802900	-0.40402100	1.84390400
H	-5.83618900	0.56979300	1.46178800
C	-7.31653700	0.53048800	-0.82208200
H	-8.00135200	0.35623600	0.01389200
H	-7.22034200	1.61767900	-0.93700000
H	-7.78561400	0.14364000	-1.73056100
S	-1.81451800	-1.92055700	0.16043400
O	-1.15092900	-0.96948900	1.09792100
O	-1.99464000	-3.28404300	0.71392200
O	-1.16941300	-1.94223000	-1.20606500
O	0.75426400	-3.81503100	-0.15340700
H	0.01171800	-3.99338200	0.44976900
H	0.27044100	-3.38879600	-0.88169400

**(R)-INT-6**

C	2.57875900	2.74153200	0.91442100
C	1.28797600	2.41228200	1.33078700
C	1.06196000	1.19001200	1.95445800
C	2.12206800	0.31462300	2.20169900
C	3.40394600	0.65949900	1.79139200
C	3.65082300	1.86871600	1.12649200
H	2.75118900	3.68808600	0.40835100
H	0.44997900	3.07406500	1.15020400
H	1.93099000	-0.65257000	2.65364200
H	4.22038700	-0.04010000	1.94695300
C	5.03866300	2.19229500	0.63309200
H	5.06662800	3.15651200	0.11794300
H	5.75814400	2.23256700	1.45857700
H	5.39079100	1.42265000	-0.06335700
S	-0.60994300	0.68855400	2.37904300
O	-0.65381800	0.49660100	3.84018100
O	-1.48843000	1.75545100	1.82193200
O	-0.80032900	-0.61649400	1.62577900
C	-0.36970400	2.44503000	-1.66852600
C	-1.71668300	2.82403400	-1.39621300
C	-2.13946600	4.16017200	-1.47494300
C	-1.18788800	5.10411800	-1.81504100
C	0.16204700	4.75136100	-2.07767600
C	0.57702100	3.43830700	-2.00120400
C	-0.25013600	1.04172700	-1.44601800
C	-1.57458900	0.58013000	-1.08468700
H	-3.16459400	4.43966300	-1.25850500
H	-1.47738900	6.14865000	-1.87312500
H	0.87193700	5.53195600	-2.32880100
H	1.61418500	3.17261300	-2.17104600
H	-3.35844400	1.67957200	-0.73539400
N	-2.40964200	1.70588200	-1.07200100
C	-2.08048600	-0.68639500	-0.80044200
C	-1.38204900	-1.91011200	-1.21545600
C	-1.21850000	-2.95668800	-0.29298700
C	-0.86735600	-2.04258900	-2.51469200
C	-0.48498800	-4.08459700	-0.64616100
H	-1.58533100	-2.83488000	0.71767900
C	-0.17010600	-3.18960900	-2.87374900
H	-1.00976700	-1.23728400	-3.22707100
C	0.03726400	-4.20461400	-1.93485900
H	-0.30478500	-4.85286900	0.09739700
H	0.22314300	-3.29006800	-3.88029500

H	0.60913900	-5.08559200	-2.20908000
C	-3.40646500	-0.85788700	-0.19446500
C	-3.85806600	-0.02745400	0.85372400
C	-4.24114300	-1.89551900	-0.65711100
C	-5.12085700	-0.22970200	1.40058900
H	-3.18286600	0.71323400	1.27589400
C	-5.50912000	-2.07404800	-0.11611800
H	-3.89243500	-2.54209500	-1.45421000
C	-5.95211400	-1.24189300	0.91451100
H	-5.44765200	0.39427800	2.22619200
H	-6.14952300	-2.86517400	-0.49273300
H	-6.93690500	-1.39135100	1.34655800
C	1.02391900	0.38326300	-1.48508500
H	1.76927600	0.89515900	-2.08695700
C	1.39800400	-0.68882800	-0.74532400
H	0.67794200	-1.10789100	-0.05511700
C	2.71431300	-1.30188300	-0.72467400
C	3.77861900	-0.88000600	-1.54495100
C	2.93745500	-2.35244700	0.18760700
C	5.02770200	-1.48018000	-1.44851200
H	3.62993600	-0.07473400	-2.25674400
C	4.19064600	-2.95082300	0.27859500
H	2.13282500	-2.66751500	0.84786400
C	5.23999300	-2.51755000	-0.53386800
H	5.83998000	-1.14264900	-2.08520700
H	4.35066200	-3.75284600	0.99264000
H	6.21840300	-2.98222600	-0.45790400
H	0.55004700	-2.78799500	3.40917500
O	0.54838300	-2.80989800	2.44427400
H	0.02546500	-2.01014100	2.20084400

**(R)-TS-5**

C	-3.92179100	1.49216100	-1.06315100
C	-3.53224400	0.64613700	-0.02671500
C	-2.63460800	1.10318900	0.93912400
C	-2.14443800	2.40987300	0.88236800
C	-2.53472700	3.24115200	-0.16619400
C	-3.42489000	2.79982900	-1.15450600
H	-4.62031200	1.13372600	-1.81570400
H	-3.88763500	-0.37642600	0.02317100
H	-1.44563600	2.76379600	1.63414300
H	-2.13388400	4.24989700	-0.22140700
C	-3.86208300	3.71956800	-2.26749000

H	-4.15809700	3.15903100	-3.15916200	C	-0.45101800	0.36508300	-1.10132700
H	-4.72479100	4.32399600	-1.96187100	H	-1.00541300	1.12317500	-1.64649100
H	-3.06458000	4.41362200	-2.54895000	C	0.54616400	0.74151600	-0.12331100
S	-2.09375300	-0.03308700	2.23262700	H	0.24884500	0.51300400	0.90698300
O	-3.08564100	0.03375200	3.31855300	C	1.31617000	1.96772200	-0.27986500
O	-1.96432000	-1.34714500	1.54198000	C	1.66920100	2.44143000	-1.55673600
O	-0.73113900	0.49544600	2.62806400	C	1.72477400	2.68610600	0.85842400
C	-1.72295300	-1.90642600	-1.59239500	C	2.40361800	3.61331800	-1.69571200
C	-1.37208000	-3.14446900	-0.99729600	H	1.38538600	1.86678500	-2.43382000
C	-2.18952600	-4.26422000	-1.06810700	C	2.45935200	3.85893500	0.71387000
C	-3.39285200	-4.12777500	-1.76073800	H	1.42767300	2.35311300	1.84587700
C	-3.75848500	-2.91256600	-2.35949500	C	2.80159400	4.32241300	-0.55910000
C	-2.93250500	-1.79313300	-2.27709200	H	2.67621100	3.96916500	-2.68434600
C	-0.66196900	-0.98680200	-1.23213700	H	2.75167500	4.41733800	1.59699700
C	0.33680100	-1.74590700	-0.54872100	H	3.37673700	5.23728000	-0.66655300
H	-1.91372600	-5.20073700	-0.59551600	H	-0.75110800	3.27790500	4.14967300
H	-4.06124100	-4.97940500	-1.83185600	O	-0.09431900	2.97128200	3.51288800
H	-4.70311000	-2.84375900	-2.88849800	H	-0.35283200	2.03831300	3.34262100
H	-3.22206400	-0.85006000	-2.72581700				
H	0.36911200	-3.71498800	0.14240100				
N	-0.11382700	-2.99995100	-0.38218900	<b>(R)-INT-7</b>			
C	1.58646800	-1.11501600	-0.16104600	C	-4.25102000	0.77566200	-1.00633700
C	2.52549600	-0.78343100	-1.27711600	C	-3.63836900	0.30230400	0.14954100
C	3.60608300	0.08914000	-1.05768300	C	-2.71420700	1.10418300	0.82515800
C	2.35089800	-1.31882800	-2.56313100	C	-2.42067900	2.38386800	0.35031800
C	4.48392000	0.40796500	-2.08883500	C	-3.03629500	2.84218500	-0.81613900
H	3.73970800	0.53509600	-0.07972300	C	-3.95688400	2.05097000	-1.51276700
C	3.22211800	-0.98466500	-3.59824200	H	-4.97189200	0.14946800	-1.52644700
H	1.53737700	-2.01017800	-2.75366500	H	-3.85474900	-0.69276400	0.52178300
C	4.29367800	-0.12250500	-3.36524300	H	-1.70737000	3.01186700	0.87380400
H	5.30603200	1.08974000	-1.89674700	H	-2.79373100	3.83365400	-1.18942000
H	3.07017500	-1.41253200	-4.58431900	C	-4.64398100	2.56679000	-2.75254400
H	4.97602900	0.13110100	-4.17035500	H	-4.85514100	1.75964100	-3.46076100
C	2.15846800	-1.57539500	1.13713000	H	-5.60286800	3.03696800	-2.50274200
C	1.29763000	-1.75598700	2.23705100	H	-4.03593300	3.31888800	-3.26299400
C	3.52002900	-1.89985500	1.28402700	S	-1.89868600	0.43676900	2.29154200
C	1.79540000	-2.21539300	3.45205200	O	-2.93547500	0.29611600	3.32479200
H	0.24622400	-1.50986000	2.15344900	O	-1.29229000	-0.84721900	1.82493400
C	4.00850800	-2.36521700	2.50173000	O	-0.83542200	1.45721100	2.60293000
H	4.19308100	-1.80764300	0.44100900	C	-1.67736900	-2.18691800	-1.20092100
C	3.15072300	-2.51774500	3.59208100	C	-1.19257100	-3.27169000	-0.42665500
H	1.11711500	-2.32396700	4.29192900	C	-1.87228500	-4.47214800	-0.30769500
H	5.06114200	-2.61357500	2.59590600	C	-3.08240000	-4.58556100	-0.99909700
H	3.53653900	-2.87180900	4.54321500	C	-3.57692400	-3.53136500	-1.77671400

C -2.88254300 -2.32430100 -1.88363800  
 C -0.71033800 -1.11404800 -1.01706100  
 C 0.32611000 -1.64444800 -0.18744600  
 H -1.49179600 -5.28517400 0.30096200  
 H -3.64770300 -5.50859800 -0.92741600  
 H -4.51919300 -3.65341100 -2.30027200  
 H -3.27528600 -1.50355500 -2.47153400  
 H 0.57738100 -3.41860200 0.83483200  
 N 0.05098800 -2.88990100 0.15028200  
 C 1.45684400 -0.70500400 0.04267800  
 C 2.53266200 -0.88660500 -1.04516900  
 C 3.74155800 -0.19586900 -0.88991000  
 C 2.33872400 -1.65700800 -2.19478200  
 C 4.72719200 -0.26392300 -1.86829000  
 H 3.89726900 0.40705400 -0.00290400  
 C 3.33022700 -1.72698300 -3.17687200  
 H 1.41582400 -2.20653800 -2.34317600  
 C 4.52481200 -1.02910000 -3.01882100  
 H 5.65234800 0.28751900 -1.73464000  
 H 3.16346600 -2.33254500 -4.06236600  
 H 5.29436800 -1.08267900 -3.78243500  
 C 2.06705400 -0.92149300 1.42883200  
 C 1.78092800 -0.11935300 2.53284100  
 C 2.89699500 -2.04343500 1.59839500  
 C 2.32733800 -0.42742900 3.78034500  
 H 1.09529600 0.71301500 2.45891100  
 C 3.42930100 -2.35474700 2.84734900  
 H 3.15357900 -2.65702200 0.73933500  
 C 3.14810000 -1.54047600 3.94563500  
 H 2.08669200 0.20632400 4.62772500  
 H 4.07100300 -3.22372300 2.95797400  
 H 3.56421900 -1.77532600 4.92046200  
 C -0.50959300 0.22871000 -1.11337100  
 H -1.13890200 0.94303800 -1.63016800  
 C 0.65168800 0.66950400 -0.26188500  
 H 0.18964700 0.94578600 0.69626600  
 C 1.41070400 1.85946900 -0.77776000  
 C 1.78513300 1.95282700 -2.12534800  
 C 1.71766800 2.91134900 0.09163200  
 C 2.47241700 3.06965300 -2.59190200  
 H 1.55539100 1.13625800 -2.80360200  
 C 2.40492600 4.03082100 -0.37673800  
 H 1.38681100 2.88289500 1.12306300  
 C 2.78884300 4.10991200 -1.71521800

H 2.76314000 3.12766300 -3.63640900  
 H 2.62223500 4.84498500 0.30687200  
 H 3.32403100 4.98226900 -2.07832700  
 H -0.87674200 4.63789400 2.87818300  
 O -0.26974100 4.09881700 2.35688100  
 H -0.51848800 3.17854500 2.58464100

**INT-8**

C -5.95036400 0.32697200 0.01474200  
 C -4.85680900 -0.42151600 0.44596800  
 C -4.33059900 -1.40384400 -0.39482300  
 C -4.90295200 -1.64894800 -1.64385600  
 C -5.99466600 -0.88923600 -2.06132800  
 C -6.53313900 0.11171800 -1.24092700  
 H -6.35560500 1.09678300 0.66585600  
 H -4.41388100 -0.22900800 1.41691500  
 H -4.48492400 -2.42731300 -2.27264700  
 H -6.43858300 -1.07783700 -3.03533800  
 C -7.73184300 0.91310100 -1.68329200  
 H -7.79435600 0.97145200 -2.77369900  
 H -8.66268600 0.45553800 -1.32663600  
 H -7.69901500 1.93224400 -1.28719100  
 S -2.80175200 -2.25477400 0.02181900  
 O -2.74152400 -2.33608700 1.51204500  
 O -2.81889500 -3.54726400 -0.68116900  
 O -1.74613600 -1.29793800 -0.50411200  
 C 3.05931700 2.45647400 -0.34855700  
 C 4.08538800 2.07702100 -1.24943800  
 C 4.99064000 2.98271300 -1.77957600  
 C 4.84454900 4.31746100 -1.38694700  
 C 3.83486400 4.71170300 -0.49926300  
 C 2.93198300 3.78888000 0.03240500  
 C 2.33762900 1.23215200 -0.04030400  
 C 2.97331200 0.17723300 -0.76153200  
 H 5.77109600 2.67856900 -2.46888300  
 H 5.52859000 5.06057300 -1.78306800  
 H 3.74561700 5.75670200 -0.22261800  
 H 2.14619000 4.10091400 0.70986500  
 H 4.55062100 0.13866900 -2.11577500  
 N 3.98618300 0.67061200 -1.46666100  
 C 2.24787400 -1.13041200 -0.68023600  
 C 3.07414900 -2.34198200 -0.28603600  
 C 2.41823200 -3.57741000 -0.20322900

C	4.42881800	-2.26707100	0.03665000	H	0.43565600	6.38719600	-0.81823200
C	3.11004200	-4.71366800	0.20032900	H	0.58577600	6.57546800	1.64610900
H	1.36321700	-3.63948000	-0.45040100	H	-0.23384000	4.75301200	3.11299900
C	5.12595100	-3.41039600	0.43603300	H	-1.81983500	1.85184200	-1.19067400
H	4.94976800	-1.31528400	0.00322100	N	-1.51656100	2.21041200	-0.27863100
C	4.46843300	-4.63440200	0.52010400	H	-2.31939500	0.59643500	0.85327600
H	2.58742700	-5.66218500	0.26903800	C	-1.62092900	1.92423200	3.43108900
H	6.17933200	-3.33674600	0.68796700	H	-0.77404200	2.31909100	4.00887700
H	5.00666000	-5.52239800	0.83588600	H	-2.52155200	2.38946200	3.85528800
C	1.64257000	-1.28724300	-2.10095900	C	-1.70540600	0.41486900	3.67366600
C	0.52180300	-0.54730800	-2.48511600	H	-1.65290700	0.22657400	4.75804200
C	2.28974100	-2.08803400	-3.05136800	H	-0.83516900	-0.07519500	3.21981500
C	0.01835000	-0.64381600	-3.78104000	O	-2.91550600	-0.10207200	3.14741000
H	0.01927600	0.09914700	-1.77857600	H	-2.75155000	-0.95225400	2.69194300
C	1.79457200	-2.17303600	-4.35194300	O	-2.51007700	0.57732400	-2.32815500
H	3.15953000	-2.66974800	-2.76800700	H	-2.25587300	-0.19560400	-1.76658200
C	0.65492100	-1.45642600	-4.71823600	H	-3.47642700	0.55722100	-2.31740800
H	-0.88340800	-0.09382300	-4.02529900				
H	2.29456900	-2.81210400	-5.07343500				
H	0.26271000	-1.53563700	-5.72738100				
C	1.24862900	0.72049900	0.60620200	<b>TS-6</b>			
H	0.53365500	1.26769500	1.21249000	C	5.09097700	0.40963900	0.50347600
C	1.14940700	-0.76163200	0.43005100	C	4.26626900	-0.68918400	0.26391300
H	0.14459400	-1.03669200	0.08019200	C	3.75451000	-1.40684500	1.34385800
C	1.34585000	-1.40340300	1.80011900	C	4.10862400	-1.06306800	2.65110000
C	2.47000400	-1.10761500	2.58197500	C	4.93473400	0.03689500	2.87514400
C	0.37709200	-2.28254600	2.29286600	C	5.42792200	0.79907600	1.80489200
C	2.63936900	-1.70827500	3.82729600	H	5.47520400	0.97659300	-0.34023200
H	3.22164400	-0.41606700	2.21463300	H	4.02946700	-0.97960700	-0.75190600
C	0.54617300	-2.87695800	3.54297900	H	3.72536200	-1.65183000	3.47790100
H	-0.52196500	-2.48322700	1.72246100	H	5.20532300	0.30707800	3.89265600
C	1.67677300	-2.59621000	4.31044200	C	6.33238200	1.98104200	2.04854200
H	3.51812000	-1.47831500	4.42200400	H	6.14686000	2.43299600	3.02720000
H	-0.21648300	-3.55453900	3.91316900	H	7.38676500	1.68027300	2.02267400
H	1.80516500	-3.05993100	5.28372400	H	6.19535000	2.75116900	1.28386900
C	-0.86530200	3.50793800	1.45483000	S	2.46965100	-2.65119000	1.12141100
C	-0.93106000	3.41771200	0.02799200	O	2.48407300	-3.05082000	-0.31612900
C	-0.46363400	4.44129300	-0.80265900	O	2.73485500	-3.72099300	2.09260700
C	0.07314200	5.57289900	-0.19830200	O	1.20708700	-1.86098600	1.42626300
C	0.16129600	5.67787700	1.20599900	C	-1.92151700	3.23462500	0.21816300
C	-0.29522500	4.65596000	2.03275400	C	-2.95329600	3.29872000	1.20051100
C	-1.46209800	2.30362800	1.98524400	C	-3.48555000	4.50145400	1.65549100
C	-1.85883000	1.56562400	0.89273400	C	-2.98600600	5.67353800	1.09308400
H	-0.52802200	4.35686400	-1.88312900	C	-1.98954800	5.63566400	0.10371500
				C	-1.45141100	4.43038500	-0.33763100

C	-1.64774600	1.82006900	0.03450800	H	-0.21684800	-4.74858000	-1.90360800
C	-2.54391300	1.12593100	0.84250000	H	-1.21006700	-4.27936200	-4.13980700
H	-4.26498500	4.52459500	2.41020800	C	2.13576800	1.88607200	-2.26907300
H	-3.37990000	6.63007700	1.42041300	C	1.60387100	2.15882700	-0.99088600
H	-1.63326200	6.56595500	-0.32665100	C	1.61939700	3.42220900	-0.42137100
H	-0.68081900	4.41613800	-1.09784100	C	2.15966100	4.46009700	-1.18800500
H	-4.04968700	1.71776200	2.17746200	C	2.65717800	4.22060000	-2.47694900
N	-3.30474700	1.98542900	1.55155600	C	2.65382300	2.93731300	-3.02876300
C	-2.62669300	-0.35080500	0.61634300	C	2.07056100	0.43750400	-2.46391000
C	-3.83604700	-0.70804900	-0.25440300	C	1.54405800	-0.08942900	-1.33126300
C	-4.10033300	-2.05631300	-0.54174700	H	1.22679400	3.59437400	0.57440000
C	-4.63187300	0.26802400	-0.86199400	H	2.19508400	5.46352600	-0.77624300
C	-5.13492400	-2.41468600	-1.39931300	H	3.06726700	5.04675600	-3.04937200
H	-3.47387100	-2.82675700	-0.10934600	H	3.06659600	2.75792700	-4.01627700
C	-5.66882300	-0.09046100	-1.72689500	H	1.23005100	0.81262600	0.58876300
H	-4.44472000	1.32035400	-0.68130000	N	1.11299500	0.94454500	-0.44642900
C	-5.92571900	-1.43180300	-1.99718800	H	1.39667900	-1.11728300	-1.04675300
H	-5.31300700	-3.46405100	-1.61143400	C	2.52850700	-0.30458100	-3.68151200
H	-6.27201400	0.68560700	-2.18808000	H	1.85926300	-0.06184700	-4.52013400
H	-6.73014600	-1.71077000	-2.67054200	H	3.52528300	0.05241700	-3.97132400
C	-2.60018200	-1.06749400	1.97511200	C	2.59402500	-1.82605600	-3.51087700
C	-1.49029900	-0.87265100	2.80844100	H	2.77155400	-2.27310100	-4.49921400
C	-3.68262500	-1.80444600	2.47043400	H	1.62646200	-2.20519100	-3.15740600
C	-1.43294200	-1.45049300	4.07210700	O	3.64770900	-2.18905400	-2.64013600
H	-0.66603300	-0.25173400	2.48497700	H	3.27545200	-2.61969700	-1.84543300
C	-3.62889900	-2.37838400	3.74220800	O	1.41716300	0.61932200	2.24864200
H	-4.57176300	-1.93950800	1.86808800	H	1.39723500	-0.37014200	2.12285500
C	-2.50047000	-2.21563000	4.54276000	H	2.33258900	0.80179800	2.50423100
H	-0.54863900	-1.30155800	4.68277000				
H	-4.47506900	-2.95616900	4.10157600				
H	-2.45493700	-2.67442400	5.52550300				
C	-0.91051300	0.88647800	-0.74260600	<b>INT-9</b>			
H	-0.67598300	1.06046900	-1.78667500	C	4.77633900	-1.95890700	-0.88582700
C	-1.26609300	-0.52756500	-0.26372600	C	3.71589500	-2.76338900	-0.48048400
H	-0.50348400	-0.84230700	0.45115300	C	3.15992700	-2.57580900	0.78625600
C	-1.28051000	-1.56446400	-1.35814000	C	3.71916500	-1.65290600	1.66856700
C	-1.82880800	-1.30202900	-2.61978500	C	4.78187400	-0.85605100	1.24899100
C	-0.71096100	-2.81750800	-1.10827300	C	5.30054200	-0.96813400	-0.04524500
C	-1.80692400	-2.27474500	-3.61532900	H	5.18701700	-2.08493900	-1.88404900
H	-2.29754900	-0.34244800	-2.81787900	H	3.29252200	-3.48687400	-1.16452700
C	-0.68616300	-3.79154200	-2.10631500	H	3.30432800	-1.53915000	2.66187200
H	-0.24645400	-3.00634900	-0.14758300	H	5.19294400	-0.11342200	1.92736500
C	-1.23450300	-3.52355300	-3.36064400	C	6.35494000	-0.01071700	-0.53855600
H	-2.23851700	-2.06057600	-4.58832700	H	7.02089900	0.30614400	0.26946600
				H	6.96429000	-0.45556200	-1.33056300



H	5.88540500	0.89236500	-0.94868400	C	-1.54022800	-0.35219900	-0.68541700
S	1.61887600	-3.40829400	1.19990500	H	-0.79561700	-0.97773900	-0.19241700
O	0.63160200	-2.85732900	0.17602300	C	-2.21960200	-1.22044100	-1.71283800
O	1.81697300	-4.85728700	1.08374800	C	-2.96158500	-0.66287600	-2.76225100
O	1.26469000	-2.91258800	2.57188100	C	-2.09131200	-2.61162700	-1.62500300
C	-0.44136800	3.28335200	-0.13931900	C	-3.58215200	-1.48283100	-3.69999100
C	-1.01449900	3.64551400	1.11031100	H	-3.07241600	0.41514400	-2.82969800
C	-0.78652400	4.87448100	1.71449600	C	-2.71589000	-3.43144200	-2.56514500
C	0.03385400	5.77230800	1.02956800	H	-1.47851400	-3.04687200	-0.84134800
C	0.60598100	5.43758700	-0.20639700	C	-3.46406500	-2.87081600	-3.59986300
C	0.37941800	4.19692600	-0.79874300	H	-4.15967100	-1.04052700	-4.50588600
C	-0.89932800	1.92618700	-0.39911700	H	-2.60348600	-4.50844500	-2.49333700
C	-1.74687200	1.56751400	0.67435300	H	-3.94704800	-3.51118600	-4.33161100
H	-1.22623800	5.12870500	2.67321100	C	2.72639400	1.70010900	-1.30745600
H	0.23662800	6.74380200	1.46770100	C	2.57792100	1.90754200	0.09909000
H	1.25365400	6.14994700	-0.70497300	C	3.08155600	3.04099000	0.73451800
H	0.86457500	3.93278700	-1.73029000	C	3.73888900	3.98251200	-0.05282300
H	-2.34312000	2.53605100	2.41934100	C	3.90032300	3.79806200	-1.44135900
N	-1.80547100	2.56103700	1.56336900	C	3.40250500	2.66422900	-2.07415400
C	-2.45663100	0.26188800	0.49906900	C	2.11216100	0.43402400	-1.61615400
C	-3.88356100	0.48755900	-0.02721700	C	1.63254800	-0.05421100	-0.40567600
C	-4.76463300	-0.60105400	-0.04495900	H	2.95609100	3.18743600	1.80225900
C	-4.30640200	1.70962900	-0.55624700	H	4.14199200	4.87577200	0.41417600
C	-6.03664400	-0.47191400	-0.59184200	H	4.42897400	4.54973800	-2.01922400
H	-4.43982200	-1.55473400	0.35492600	H	3.54034500	2.52098500	-3.14193700
C	-5.58610100	1.84030400	-1.10111700	H	1.65293000	0.60698000	1.58444000
H	-3.64272200	2.56764200	-0.56150400	N	1.88856800	0.82658500	0.60559300
C	-6.45295300	0.75055600	-1.12349400	H	1.20143900	-1.01717900	-0.18511500
H	-6.70170700	-1.32935500	-0.60837500	C	2.12502000	-0.25031100	-2.95088000
H	-5.89991400	2.79708100	-1.50692600	H	1.94094900	0.49956100	-3.73500400
H	-7.44606100	0.85110200	-1.54976600	H	3.13741200	-0.63477300	-3.13696100
C	-2.48799500	-0.50295700	1.82621300	C	1.14707400	-1.42051500	-3.17748700
C	-1.64852600	-1.57857000	2.12231700	H	1.16609400	-1.64681200	-4.25065800
C	-3.36477000	-0.03367500	2.82158600	H	0.11766000	-1.11590000	-2.94790800
C	-1.67818700	-2.16814000	3.39198500	O	1.48915200	-2.61218800	-2.51131600
H	-0.94897300	-1.98367800	1.40084700	H	1.10542800	-2.65509300	-1.61341100
C	-3.38846900	-0.61683300	4.08518800	O	1.04305200	-0.24172300	3.01860200
H	-4.06054500	0.76797100	2.58753900	H	1.16330600	-1.21469500	2.87550100
C	-2.53991000	-1.68876900	4.37510400	H	0.10208600	-0.16959500	3.21990300
H	-0.99036700	-2.98303800	3.58893400				
H	-4.07433300	-0.24145000	4.83866500				
H	-2.55518900	-2.14636600	5.35919300	<b>TS-7</b>			
C	-0.80233300	0.84744100	-1.25188900	C	4.71187200	-1.54781700	-0.60883400
H	-0.38937800	0.85473000	-2.24786000	C	3.57288200	-2.32984000	-0.44652600

C	3.00548500	-2.45990700	0.82386300	C	-3.38673600	0.16795600	2.91605300
C	3.60737600	-1.85269500	1.92472200	C	-1.91401900	-2.11485300	3.49651500
C	4.74984900	-1.07389800	1.74539400	H	-1.18020900	-2.01754300	1.50853200
C	5.30954700	-0.89384200	0.47646900	C	-3.46595400	-0.40497600	4.18184500
H	5.13526300	-1.42725300	-1.60256000	H	-3.99994000	1.03390100	2.68046300
H	3.10904000	-2.78701100	-1.31156300	C	-2.72320600	-1.55096100	4.47860000
H	3.16472300	-1.96853700	2.90625200	H	-1.30867900	-2.99194100	3.69669000
H	5.20476700	-0.58824500	2.60449000	H	-4.11094100	0.03918700	4.93409700
C	6.49578600	0.01197300	0.26656400	H	-2.77928100	-1.99797900	5.46609600
H	7.02486900	0.20257900	1.20433000	C	-0.63970300	0.73112500	-1.11703400
H	7.20715600	-0.41888500	-0.44488500	H	-0.53728600	0.81619000	-2.19039600
H	6.17425500	0.97957200	-0.13632800	C	-1.56989800	-0.35901700	-0.54964500
S	1.47009500	-3.37881100	1.04887600	H	-0.94752000	-1.07413600	-0.02036100
O	0.55438300	-2.87825400	-0.05994300	C	-2.31486300	-1.14133300	-1.60215600
O	1.75879400	-4.81387500	0.95018400	C	-2.98416200	-0.50491800	-2.65656900
O	0.96367400	-2.91899600	2.38580500	C	-2.31924000	-2.53972000	-1.53864600
C	-0.19277900	3.19627700	-0.04901200	C	-3.65827200	-1.25044200	-3.61915900
C	-0.82103200	3.67178700	1.13996900	H	-2.99725800	0.57896300	-2.71034800
C	-0.53703200	4.92039200	1.68745600	C	-2.99526100	-3.28644100	-2.50443900
C	0.39026600	5.71489000	1.01777000	H	-1.75899200	-3.03991000	-0.75531500
C	1.01476900	5.27035400	-0.16093000	C	-3.66844800	-2.64501900	-3.54322400
C	0.73447200	4.01956900	-0.69907900	H	-4.17862000	-0.74405600	-4.42638500
C	-0.73261500	1.87069500	-0.26875400	H	-2.98262600	-4.37032300	-2.44857000
C	-1.64677300	1.62213700	0.74656900	H	-4.19237500	-3.22700300	-4.29529400
H	-1.01984700	5.26234700	2.59730400	C	2.82379600	1.34788800	-1.60291100
H	0.63441300	6.69460400	1.41524400	C	2.75302900	1.47360500	-0.17165400
H	1.73669600	5.91169900	-0.65549200	C	3.51884900	2.42653100	0.51791100
H	1.24311400	3.67741900	-1.59287600	C	4.33530500	3.24995500	-0.23498400
H	-2.30622000	2.74770600	2.39905800	C	4.42262400	3.14135500	-1.65023900
N	-1.70721100	2.68124500	1.59029500	C	3.68286000	2.19897600	-2.33538000
C	-2.45847300	0.36835300	0.58636900	C	1.93520700	0.30854200	-1.96881700
C	-3.86101000	0.68622600	0.04699300	C	1.29167100	-0.11049200	-0.77251600
C	-4.83075800	-0.32471700	0.04940000	H	3.45526400	2.51571500	1.59620000
C	-4.17928100	1.92385800	-0.51861300	H	4.93438500	4.00285900	0.26792300
C	-6.08401000	-0.10689900	-0.51310900	H	5.08687500	3.80833100	-2.18956200
H	-4.59012200	-1.29078900	0.47857100	H	3.75313200	2.11070100	-3.41506400
C	-5.43977100	2.14528900	-1.07831600	H	1.58194400	0.38450100	1.27670000
H	-3.44245800	2.71935900	-0.54130300	N	1.85565000	0.57194100	0.29435300
C	-6.39423800	1.13082500	-1.08061400	H	0.90985900	-1.10715000	-0.58728600
H	-6.81787500	-0.90664400	-0.51325200	C	1.69230900	-0.25934600	-3.33029800
H	-5.67042900	3.11341700	-1.51246700	H	1.23946600	0.51128500	-3.97522700
H	-7.37264600	1.30144100	-1.51875700	H	2.66671300	-0.48429400	-3.78283500
C	-2.56137300	-0.38424100	1.91980400	C	0.81920900	-1.52715500	-3.39954900
C	-1.83705500	-1.54012600	2.22332600	H	0.68555900	-1.76801500	-4.46185500

H -0.18065700 -1.32602100 -3.00104500  
O 1.40880900 -2.64324300 -2.76886500  
H 0.99526200 -2.81077500 -1.89874900  
O 0.93706400 -0.22666700 2.74690300  
H 0.97690800 -1.21412700 2.67290800  
H 0.00473400 -0.05360000 2.92820800

**INT-8A**

C -5.99985800 0.25551200 -0.13280700  
C -4.78775000 -0.31047200 0.24628000  
C -4.35764900 -1.47778300 -0.39232400  
C -5.12559400 -2.07308500 -1.38795200  
C -6.33988800 -1.49133200 -1.75356700  
C -6.79430100 -0.32294600 -1.13455100  
H -6.33895100 1.16366600 0.35867700  
H -4.19021200 0.14190000 1.03165300  
H -4.76444100 -2.97851800 -1.86176600  
H -6.94267600 -1.95301600 -2.53111100  
C -8.11710100 0.29521400 -1.51344300  
H -8.87130300 0.11887300 -0.73715200  
H -8.02988200 1.37968100 -1.63616400  
H -8.50095300 -0.12279200 -2.44793600  
S -2.78318800 -2.20383700 0.05619100  
O -1.77305400 -1.11831800 -0.26976300  
O -2.80800900 -2.44507000 1.52796100  
O -2.59666700 -3.41033000 -0.77601000  
C 2.30523800 2.64285400 -0.71095400  
C 2.78494300 2.37866300 -2.02153400  
C 3.22320900 3.37564400 -2.87864400  
C 3.19186600 4.68523800 -2.38956200  
C 2.73189900 4.96758200 -1.09753100  
C 2.27776700 3.95642500 -0.24922100  
C 1.95222300 1.34235500 -0.15753000  
C 2.28951000 0.37169600 -1.14283700  
H 3.58118900 3.15361800 -3.87843600  
H 3.52909300 5.49567500 -3.02717100  
H 2.70449700 5.99425800 -0.75086100  
H 1.88977700 4.19354900 0.73426300  
H 3.03005700 0.49363500 -3.07627000  
N 2.75377500 0.97298300 -2.22992800  
C 2.19034300 -1.03960300 -0.66429200  
C 3.56967100 -1.51622700 -0.16348600  
C 3.72818000 -2.87708900 0.12730500

C 4.63698500 -0.64543500 0.07323200  
C 4.92258700 -3.35279100 0.65725200  
H 2.90302500 -3.55752300 -0.04791900  
C 5.83837100 -1.12504900 0.60082900  
H 4.54563700 0.41420800 -0.13830800  
C 5.98386600 -2.47773300 0.89775300  
H 5.02202700 -4.40855100 0.88813500  
H 6.65775100 -0.43500800 0.77715200  
H 6.91632300 -2.84947600 1.31062000  
C 1.69855000 -1.97736200 -1.76716100  
C 0.47261700 -2.63721100 -1.72640000  
C 2.53329500 -2.17220600 -2.88077100  
C 0.06480200 -3.44808900 -2.78785800  
H -0.20266000 -2.51549400 -0.89644800  
C 2.12568200 -2.97293400 -3.94506900  
H 3.52993700 -1.73630700 -2.89074100  
C 0.88272300 -3.61061400 -3.90386200  
H -0.90392900 -3.93066600 -2.71279300  
H 2.78414800 -3.11180600 -4.79738400  
H 0.56532700 -4.23825500 -4.73089300  
C 1.38800200 0.68699800 0.90231100  
H 1.07261600 1.12943800 1.83578200  
C 1.22913300 -0.78330500 0.61651000  
H 0.19503300 -0.90162100 0.26173900  
C 1.40855400 -1.66839800 1.82414100  
C 2.45010700 -1.44108700 2.73438900  
C 0.50878800 -2.71183100 2.06624600  
C 2.60198200 -2.25286500 3.85457700  
H 3.15792700 -0.63826900 2.55075600  
C 0.66086600 -3.52504000 3.18908700  
H -0.33591800 -2.87107300 1.40843100  
C 1.70844100 -3.30173800 4.08191400  
H 3.41709100 -2.06903400 4.54781100  
H -0.05440200 -4.32123400 3.36767000  
H 1.82429400 -3.93490200 4.95637700  
C -0.88109900 3.72858800 1.47344100  
C -0.95535000 3.76736100 0.04557300  
C -0.69906700 4.93251800 -0.67683500  
C -0.34427400 6.07325400 0.03791600  
C -0.24834600 6.05521700 1.44407300  
C -0.51895300 4.89669700 2.16554600  
C -1.21350000 2.38601200 1.87818900  
C -1.45689500 1.68390400 0.71445400  
H -0.75847400 4.94479900 -1.76055500

H	-0.13845200	6.99455900	-0.49854600	C	2.54495000	1.09499200	-0.62933800
H	0.02739500	6.96436900	1.96970200	C	2.77739100	-0.16581500	-1.18050400
H	-0.45806600	4.89573100	3.25009600	H	5.55074300	1.19278500	-3.90848600
H	-1.23564400	2.12775400	-1.31939100	H	6.06404900	3.61756100	-3.67852200
N	-1.31183100	2.50666200	-0.38001000	H	4.95166600	4.98428400	-1.94658700
H	-1.75486000	0.65573800	0.58667600	H	3.25885700	3.99538100	-0.43493400
C	-1.31298600	1.85227100	3.27850000	H	4.02683900	-0.85896100	-2.71620700
H	-0.40331400	2.11034300	3.84172000	N	3.68242100	-0.07920000	-2.17650100
H	-2.13974000	2.34523300	3.80826100	C	2.18085700	-1.31323300	-0.42096800
C	-1.52571800	0.33928300	3.37235800	C	3.24627400	-1.97662300	0.46973600
H	-1.43037200	0.03850400	4.42845600	C	2.94872900	-3.21013000	1.06265100
H	-0.73195800	-0.18540400	2.82325500	C	4.46123400	-1.35658500	0.77406800
O	-2.80127800	0.00425600	2.86433000	C	3.84021900	-3.80176800	1.95138900
H	-2.78434300	-0.91830100	2.53417900	H	2.00515900	-3.69438600	0.83897500
O	-0.56611700	0.38507900	-2.14601600	C	5.35980800	-1.95470400	1.66049400
H	-0.57064100	-0.04880700	-3.00752600	H	4.71355600	-0.39642800	0.33741000
H	-1.10479200	-0.21688800	-1.57966900	C	5.05116600	-3.17605000	2.25445100
<b>TS-6A</b>				H	3.58592300	-4.75114100	2.41183500
C	-6.20583400	0.99677300	-0.79825400	H	6.29996500	-1.45991700	1.88449900
C	-5.05888300	0.38740700	-0.30228100	H	5.74740600	-3.63878100	2.94685100
C	-4.72976000	-0.89686000	-0.74597200	C	1.57411800	-2.35469700	-1.36857300
C	-5.53128900	-1.56265800	-1.66760900	C	0.20720300	-2.62156400	-1.45973100
C	-6.67807900	-0.93465500	-2.15464100	C	2.45419000	-3.08109000	-2.19033600
C	-7.03230600	0.34904000	-1.72922800	C	-0.27781700	-3.57061000	-2.36569300
H	-6.46849400	1.99458300	-0.45627500	H	-0.51787200	-2.11684100	-0.83827900
H	-4.43694800	0.89335000	0.42882000	C	1.97326000	-4.01514300	-3.10269600
H	-5.24736400	-2.55691600	-1.99229200	H	3.52783400	-2.95297600	-2.07387800
H	-7.30605200	-1.45061900	-2.87603200	C	0.59996400	-4.26003500	-3.19702300
C	-8.28242400	1.02173600	-2.23945200	H	-1.34763100	-3.75143900	-2.38230500
H	-9.05214100	1.06789200	-1.45980300	H	2.67076600	-4.56495600	-3.72761400
H	-8.08121600	2.05127600	-2.55362500	H	0.22539300	-4.99597800	-3.90165000
H	-8.70626400	0.48402500	-3.09174800	C	1.59100300	0.97683200	0.40994400
S	-3.24675800	-1.69137300	-0.13220800	H	1.58781900	1.59776500	1.29774100
O	-2.12773400	-0.74355500	-0.51857700	C	1.13908700	-0.48595300	0.49469900
O	-3.36178000	-1.75081200	1.35683400	H	0.18117500	-0.55197200	-0.01926200
O	-3.13754500	-3.00191600	-0.80502000	C	0.93356000	-0.97929900	1.90684200
C	3.42900700	2.02643000	-1.30841400	C	1.84835800	-0.68275100	2.92558000
C	4.11100200	1.25386900	-2.29227400	C	-0.19771500	-1.74034900	2.21259200
C	5.05070800	1.80033700	-3.16123700	C	1.64013700	-1.14864600	4.22075200
C	5.33340200	3.15684800	-3.02202200	H	2.74000000	-0.10520900	2.70169500
C	4.69667300	3.93373200	-2.03980900	C	-0.41041800	-2.20458000	3.51056200
C	3.74738700	3.38397500	-1.18334400	H	-0.94363300	-1.94215800	1.45624900
				C	0.50929000	-1.91356300	4.51718200
				H	2.36099300	-0.91612300	4.99867500



C	-2.04296400	0.12911700	-0.29120300	C	-4.65691200	-0.01060600	0.59117300
H	-1.45757700	-0.60582100	0.28606800	C	-4.96502700	1.20645900	-0.01951100
C	-3.48706300	-0.20370200	-0.07851500	C	-6.25178700	1.41817000	-0.50362900
C	-4.43669200	-0.06334800	-1.09229100	C	-7.24287700	0.43337500	-0.38408100
C	-3.89343800	-0.66047400	1.18133300	H	-7.65988800	-1.55734400	0.31939300
C	-5.77356300	-0.37924100	-0.85613600	H	-5.35024800	-1.94838300	1.18016900
H	-4.13191700	0.30473800	-2.06715800	H	-4.20102100	1.96748400	-0.13423100
C	-5.23110500	-0.95763700	1.42516700	H	-6.49208200	2.36141600	-0.98685900
H	-3.15273900	-0.78068200	1.96578600	C	-8.64232900	0.68764600	-0.88609100
C	-6.17458300	-0.82063300	0.40413300	H	-9.22373300	1.26190700	-0.15453000
H	-6.50188900	-0.27315000	-1.65394900	H	-8.63492800	1.26370500	-1.81645100
H	-5.53645500	-1.30838200	2.40611400	H	-9.17817100	-0.24793100	-1.06839200
H	-7.21664300	-1.06145700	0.59036300	S	-3.00306700	-0.28681400	1.21971300
C	-2.14266800	-3.38780300	-0.22497800	O	-2.10559300	0.29259400	0.15828900
C	-1.54332400	-3.09554200	-1.48754900	O	-2.87663800	0.46788400	2.50154300
C	-2.27039700	-3.14060000	-2.68216700	O	-2.85344700	-1.75895900	1.36094400
C	-3.62331700	-3.45828600	-2.60512700	C	-0.81756300	-1.03332100	-2.37449200
C	-4.23623200	-3.73783000	-1.36783800	C	-1.54291500	-1.98889700	-1.60788700
C	-3.50757900	-3.71477700	-0.18566500	C	-2.81300200	-2.42402600	-1.97288200
C	-1.11747400	-3.23249700	0.77951400	C	-3.34456800	-1.92836900	-3.16028100
C	0.02485300	-2.85449700	0.10367800	C	-2.61992500	-1.03140200	-3.96641300
H	-1.79255500	-2.94176000	-3.63796000	C	-1.35954400	-0.57681900	-3.58235000
H	-4.21453900	-3.49686900	-3.51498900	C	0.35875800	-0.73991600	-1.59094500
H	-5.29540500	-3.97272800	-1.34107200	C	0.33449300	-1.57440100	-0.48365500
H	-3.99229500	-3.93062000	0.76117800	H	-3.37191100	-3.10037400	-1.33685500
H	0.51372700	-2.51848200	-1.90536300	H	-4.33527500	-2.24266200	-3.47140800
N	-0.22934300	-2.75218600	-1.24595800	H	-3.05220500	-0.68761200	-4.90096200
H	1.00424300	-2.64774900	0.49655200	H	-0.81126400	0.12385600	-4.20550300
C	-1.23414700	-3.53433800	2.24683200	H	-1.23125200	-2.67761300	0.36681300
H	-2.27147500	-3.38197600	2.57424700	N	-0.78303500	-2.34019100	-0.48318900
H	-1.01301800	-4.59590100	2.42530200	C	1.59850200	-1.55819400	0.33531500
C	-0.32513800	-2.69499000	3.14887100	C	2.56713900	-2.64297200	-0.15787900
H	-0.53530200	-2.95659400	4.19889600	C	3.86432000	-2.72063500	0.37501900
H	-0.58639300	-1.63981400	3.02484300	C	2.21492100	-3.54932000	-1.16435100
O	1.03923400	-2.93592200	2.84793700	C	4.77284100	-3.67222400	-0.08029300
H	1.54332800	-2.10258900	2.84462100	H	4.17188300	-2.02321900	1.14366600
O	2.30758600	-1.90256400	-2.06333500	C	3.12584800	-4.50196500	-1.62445100
H	2.61511100	-1.30106400	-2.75292900	H	1.22273600	-3.52303900	-1.59762500
H	2.25929700	-1.33616800	-1.26129700	C	4.40850600	-4.56808500	-1.08563500
				H	5.77008900	-3.70449100	0.34739900
				H	2.82468900	-5.19352000	-2.40539800
				H	5.11693600	-5.30884300	-1.44347900
<b>TS-6B</b>				C	1.28639900	-1.64431200	1.83537800
C	-6.90667500	-0.77934100	0.22779400	C	0.25985400	-0.82892200	2.33236100
C	-5.62109600	-1.00666900	0.71689500				

C 1.89090200 -2.55200000 2.71225800  
 C -0.15004700 -0.90531600 3.66023600  
 H -0.26265200 -0.15980500 1.66115000  
 C 1.50192700 -2.61160100 4.05205400  
 H 2.65122000 -3.23447900 2.35778100  
 C 0.48365200 -1.79078700 4.53199300  
 H -0.99064300 -0.30067300 3.98094700  
 H 1.98847800 -3.32174200 4.71415600  
 H 0.16932200 -1.85696800 5.56905100  
 C 1.41205000 0.21072300 -1.44725500  
 H 2.00501000 0.55632200 -2.28653000  
 C 2.12403700 -0.08431800 -0.12385300  
 H 1.67889900 0.57867500 0.62055700  
 C 3.59952200 0.20133600 -0.13388500  
 C 4.41863300 -0.16618000 -1.20828500  
 C 4.17410600 0.86384900 0.95577100  
 C 5.78030000 0.12396100 -1.19423000  
 H 3.99217300 -0.70600600 -2.04835800  
 C 5.53873900 1.14842500 0.97762300  
 H 3.54228700 1.15800500 1.78881700  
 C 6.34516300 0.78059600 -0.09951200  
 H 6.40278300 -0.17039100 -2.03355400  
 H 5.96935600 1.66385900 1.83056600  
 H 7.40711100 1.00584300 -0.08768400  
 C 1.97286000 3.55441000 -0.13929300  
 C 1.74679400 2.89664100 -1.36310000  
 C 2.54428700 3.09305100 -2.47706700  
 C 3.61549200 3.98571800 -2.34932000  
 C 3.86443300 4.64068300 -1.13877800  
 C 3.04565400 4.43591900 -0.02464800  
 C 0.93499300 3.10970200 0.79628300  
 C 0.17334900 2.20077600 0.14743200  
 H 2.34972400 2.58624700 -3.41683400  
 H 4.26079600 4.16806800 -3.20204800  
 H 4.70644000 5.32143100 -1.06597000  
 H 3.24085400 4.95321000 0.90905500  
 H -0.14756000 1.97931200 -1.83735500  
 N 0.66543200 1.96597100 -1.18209900  
 H -0.71876800 1.68403800 0.46161000  
 C 0.73222500 3.61657600 2.19105000  
 H 1.69280200 3.61088100 2.72481700  
 H 0.41837200 4.66815000 2.13962600  
 C -0.29955400 2.82809500 3.00283500  
 H -0.31089600 3.23119000 4.02901000

H 0.02865900 1.78347900 3.07326000  
 O -1.56712900 2.94174100 2.39382800  
 H -2.06233800 2.10456000 2.50944200  
 O -1.97003300 1.94278400 -2.00525400  
 H -2.29434000 1.39133600 -2.73021200  
 H -2.16770600 1.38926000 -1.21471800

**INT-9A**

C -5.50306900 -0.85902600 -2.12228400  
 C -4.17498500 -1.26137900 -2.01621800  
 C -3.59952400 -1.39364400 -0.75167800  
 C -4.34087700 -1.13004700 0.39590400  
 C -5.66902400 -0.72548100 0.27564600  
 C -6.27031200 -0.58487300 -0.98007900  
 H -5.95231600 -0.74913100 -3.10568500  
 H -3.57716300 -1.44810800 -2.90152300  
 H -3.86131300 -1.21617700 1.36375900  
 H -6.24591300 -0.50579700 1.16998700  
 C -7.71460800 -0.16907600 -1.10614700  
 H -7.87407700 0.46206900 -1.98554200  
 H -8.36729100 -1.04391500 -1.21314000  
 H -8.05034400 0.38295100 -0.22382000  
 S -1.87597100 -1.86704700 -0.61821200  
 O -1.78996300 -3.32766600 -0.87915900  
 O -1.19194300 -1.05176800 -1.68148400  
 O -1.46048500 -1.47152800 0.76236700  
 C 0.88794700 -1.09054100 2.86593200  
 C -0.18621800 -0.58163900 3.63978100  
 C -0.62190700 -1.18169000 4.80930600  
 C 0.05160200 -2.33906100 5.21219100  
 C 1.11695600 -2.85735900 4.46647500  
 C 1.54665900 -2.24041600 3.29011500  
 C 0.98222600 -0.21450600 1.70603100  
 C -0.00579100 0.79879900 1.88243700  
 H -1.45162000 -0.78220300 5.38259800  
 H -0.26339200 -2.84548900 6.11825100  
 H 1.61146800 -3.76189700 4.80284000  
 H 2.36782900 -2.64171000 2.71147300  
 H -1.50045700 1.11622100 3.27490600  
 N -0.68489800 0.58582500 2.99530800  
 C -0.03696200 1.81657000 0.79305100  
 C 0.83181900 3.03433700 1.16405100  
 C 0.69757600 4.20596500 0.40904000

C	1.81194200	2.98149600	2.15926600	H	6.10963100	-2.31877300	1.56592900
C	1.53416400	5.29428000	0.63589000	H	6.66092900	-0.87921700	-0.37053800
H	-0.05685700	4.25690000	-0.36648300	H	5.09962100	-0.67216000	-2.28462900
C	2.64645300	4.07662700	2.39101500	H	1.42992100	-3.73130800	0.25195600
H	1.94463100	2.08687600	2.75704400	N	2.04099300	-3.29686100	-0.45140100
C	2.51371000	5.23431600	1.62848800	H	0.57303900	-3.14714500	-1.99193900
H	1.42256300	6.18922600	0.03203100	C	2.38714000	-1.41109500	-3.65259900
H	3.40044700	4.01788700	3.16972400	H	3.11652300	-0.59283700	-3.71922800
H	3.16574600	6.08372800	1.80556800	H	2.66528400	-2.13585400	-4.42999900
C	-1.48441900	2.22395300	0.50978000	C	1.00948400	-0.83764900	-4.00753200
C	-2.23056000	1.73097200	-0.56174400	H	1.08246700	-0.34917500	-4.99016300
C	-2.11504100	3.06463500	1.44381600	H	0.74755400	-0.06207900	-3.28091600
C	-3.57992000	2.06708800	-0.69367900	O	-0.00261300	-1.82692300	-4.07156300
H	-1.79496800	1.04424400	-1.27530800	H	-0.54229400	-1.71658000	-3.26830600
C	-3.46258900	3.39209700	1.31386400	O	-0.09065400	-4.04916600	1.24822700
H	-1.53475000	3.48963600	2.25829700	H	-0.37884200	-3.15654800	1.50416900
C	-4.20160800	2.88994700	0.24089500	H	-0.69844100	-4.20346800	0.49969900
H	-4.14790700	1.64881000	-1.51710600				
H	-3.93094100	4.04409100	2.04506600				
H	-5.25366400	3.13604300	0.13782200				
C	1.46984000	-0.10081000	0.43862500	<b>TS-7A</b>			
H	2.20488500	-0.73916800	-0.03394500	C	-6.33020400	-2.23466300	-0.60517100
C	0.75603500	0.96856000	-0.32783700	C	-4.96221100	-2.27692800	-0.86036900
H	0.00369100	0.37954800	-0.88131800	C	-4.13503200	-1.30579500	-0.29852900
C	1.58891000	1.74704400	-1.30832200	C	-4.66002500	-0.30037200	0.51223200
C	2.97514300	1.84956600	-1.15960200	C	-6.03100200	-0.27063900	0.75530000
C	0.97149000	2.38685600	-2.38964800	C	-6.88520600	-1.23396600	0.20368300
C	3.73381500	2.56970700	-2.08058600	H	-6.97906300	-2.99067700	-1.03900100
H	3.46894900	1.35796600	-0.32744000	H	-4.52924700	-3.05598900	-1.47756300
C	1.72637900	3.11722700	-3.30426900	H	-3.99629900	0.43912300	0.94386200
H	-0.10365400	2.30593500	-2.51508900	H	-6.44527800	0.51132900	1.38616300
C	3.11115900	3.20812500	-3.15310100	C	-8.36403600	-1.21579600	0.49973900
H	4.81042800	2.63242200	-1.95727300	H	-8.94538900	-1.59280900	-0.34667700
H	1.23578400	3.60443200	-4.14108900	H	-8.59983500	-1.84865900	1.36409100
H	3.70144000	3.77055700	-3.86982800	H	-8.71295600	-0.20530400	0.73040600
C	3.61680700	-1.98333900	-1.40405400	S	-2.39117900	-1.29484200	-0.68883300
C	3.30258300	-2.78412100	-0.25925000	O	-1.98677900	-2.72957000	-0.86444800
C	4.19740900	-2.92441200	0.80937500	O	-2.21796500	-0.49197900	-1.93058100
C	5.39830900	-2.22586600	0.75086400	O	-1.71606000	-0.66872800	0.49912800
C	5.71377600	-1.41027900	-0.35594900	C	1.71157000	-0.33838300	2.80323800
C	4.84207100	-1.29319600	-1.43167900	C	0.95816500	0.47436000	3.70307500
C	2.48551300	-2.04960200	-2.29561400	C	0.95757600	0.26791100	5.07866100
C	1.55676900	-2.85258900	-1.66784500	C	1.75141000	-0.76590800	5.57094200
H	3.97387500	-3.58321200	1.64343000	C	2.52385000	-1.56145000	4.70876000
				C	2.50907600	-1.36128300	3.33172600



C	1.42191300	0.17294700	1.48084500	H	0.24877700	2.03141500	-5.17727100
C	0.57871300	1.26725400	1.64494900	H	2.62852800	2.69632500	-5.46053800
H	0.36812700	0.89149000	5.74311900	C	3.06138200	-3.06455500	-1.01648000
H	1.77622600	-0.95420800	6.63921200	C	2.70787300	-3.37631900	0.34214900
H	3.14328700	-2.34875300	5.12619100	C	3.50440200	-4.22555600	1.13038700
H	3.11376300	-1.97749000	2.67834800	C	4.64455100	-4.74941900	0.54746500
H	-0.31187200	2.17665600	3.31280800	C	5.01339100	-4.45114300	-0.79150900
N	0.29548000	1.45652600	2.95175300	C	4.23730400	-3.62060400	-1.57234500
C	0.41065000	2.11207500	0.42003500	C	2.03875500	-2.23921500	-1.54084700
C	1.46795200	3.23234700	0.38407700	C	1.15526500	-1.96459800	-0.45901700
C	1.31960600	4.26264500	-0.55418100	H	3.22386700	-4.46716900	2.14994000
C	2.60916300	3.22033600	1.19183300	H	5.27738200	-5.41344600	1.12838700
C	2.29216400	5.24825900	-0.68969000	H	5.91843400	-4.88990500	-1.19808100
H	0.44196700	4.27792900	-1.19014100	H	4.51517500	-3.39718100	-2.59726900
C	3.58396900	4.21210400	1.05911900	H	0.87803600	-2.88621500	1.40258100
H	2.75263200	2.43511500	1.92518300	N	1.55574200	-2.72505700	0.64012700
C	3.43133800	5.22693300	0.11698200	H	0.10985600	-1.72684400	-0.53079000
H	2.16244800	6.03034500	-1.43125200	C	1.85810500	-1.81501100	-2.96143600
H	4.46130200	4.18774000	1.69845200	H	2.23090300	-0.79629600	-3.12588500
H	4.19025500	5.99623100	0.01322500	H	2.46079400	-2.47794200	-3.59126800
C	-0.99147200	2.71931700	0.35262800	C	0.38280700	-1.89341700	-3.40318700
C	-1.99615300	2.27964100	-0.50741400	H	0.34188000	-1.69646100	-4.48341900
C	-1.28952700	3.75012800	1.26115700	H	-0.19873500	-1.10645400	-2.91758200
C	-3.27240100	2.84571200	-0.45308400	O	-0.16540500	-3.16831600	-3.13108800
H	-1.82732000	1.47164700	-1.20276800	H	-0.83928800	-3.06557900	-2.43505600
C	-2.56463500	4.30620800	1.32437300	O	-0.84985500	-2.91168800	1.90997400
H	-0.50311500	4.14280300	1.90055100	H	-1.14100700	-1.99411600	1.73453800
C	-3.56610100	3.85248300	0.46347200	H	-1.24308500	-3.35640000	1.13941100
H	-4.03761800	2.47499500	-1.12757100				
H	-2.77156600	5.10020700	2.03575300				
H	-4.56087200	4.28551200	0.50470600				
C	1.73412500	0.02515500	0.09636600	<b>INT-9B</b>			
H	2.74536700	-0.15938600	-0.24032200	C	-5.58611000	-3.19069200	-1.50894000
C	0.81103600	0.98598700	-0.67415600	C	-4.28933300	-2.98863900	-1.04118400
H	-0.11893800	0.44417500	-0.84613900	C	-3.83710900	-1.68970200	-0.82054000
C	1.33346600	1.48333300	-1.99477000	C	-4.67139400	-0.59801200	-1.06136800
C	2.67101500	1.86486900	-2.16342200	C	-5.96440000	-0.81454200	-1.52829500
C	0.46777600	1.55486000	-3.09274800	C	-6.44247600	-2.11150600	-1.75880900
C	3.13577900	2.29789200	-3.40291100	H	-5.94089900	-4.20339700	-1.68024500
H	3.34917600	1.84086800	-1.31648300	H	-3.62767100	-3.82186700	-0.83473400
C	0.93090500	1.99168400	-4.33372700	H	-4.31156200	0.40755700	-0.87899600
H	-0.56297800	1.23635300	-2.98098900	H	-6.61626600	0.03513200	-1.71373000
C	2.26625100	2.36166600	-4.49328700	C	-7.85642200	-2.33985800	-2.23136300
H	4.17531500	2.58994900	-3.51605700	H	-8.54558900	-2.42606600	-1.38235600
				H	-8.20874100	-1.51190200	-2.85333600

H	-7.93894400	-3.26244300	-2.81273500	C	0.93594400	0.90818100	-0.46517200
S	-2.14799300	-1.41935100	-0.29067800	H	0.17465600	0.27041500	-0.93958200
O	-1.71348800	-2.67953600	0.37288000	C	1.95981600	1.29017600	-1.49612800
O	-1.35655600	-1.11147100	-1.52140800	C	3.27311500	1.60439400	-1.12853400
O	-2.20929600	-0.24208100	0.63782100	C	1.60306500	1.34246900	-2.84761900
C	0.37959400	-0.22735100	3.11494200	C	4.21126000	1.96907500	-2.09049400
C	-0.75373600	0.52213700	3.51745500	H	3.55417000	1.57973400	-0.07995000
C	-1.44434000	0.26194800	4.68937500	C	2.53869300	1.71435500	-3.81284200
C	-0.96367800	-0.78146700	5.48705200	H	0.59069700	1.08512500	-3.14205300
C	0.16287100	-1.52472600	5.11310700	C	3.84496800	2.02880400	-3.43599100
C	0.84537300	-1.26066700	3.92283400	H	5.22620800	2.20985900	-1.79031300
C	0.74554100	0.31108500	1.81195600	H	2.24936900	1.75055700	-4.85860100
C	-0.16338400	1.39405000	1.55428700	H	4.57494200	2.31425600	-4.18705800
H	-2.32277900	0.83384700	4.96670500	C	3.24454800	-2.85381200	-0.11951600
H	-1.47796300	-1.01982900	6.41225600	C	2.00989700	-3.24248400	0.48688800
H	0.50711700	-2.32792100	5.75629400	C	1.95224800	-3.80204600	1.76830700
H	1.70166000	-1.85390100	3.62302500	C	3.15136800	-3.96839700	2.45244300
H	-1.97679600	1.94256000	2.41532700	C	4.38254300	-3.58739000	1.87567100
N	-1.02620000	1.52440600	2.54047300	C	4.44127900	-3.03593600	0.60254000
C	0.12734300	2.10353700	0.26791200	C	2.91742400	-2.28826700	-1.40924000
C	1.11665800	3.26030000	0.52191600	C	1.54445000	-2.36204400	-1.51995800
C	1.38874600	4.14136900	-0.53369300	H	1.00077200	-4.08674300	2.20592400
C	1.79800100	3.42944000	1.73046200	H	3.14193800	-4.40659900	3.44622400
C	2.32840000	5.15601800	-0.38830400	H	5.29948500	-3.73565500	2.43789300
H	0.87035000	4.01754200	-1.47713500	H	5.39225100	-2.76424100	0.15566900
C	2.74006700	4.45065400	1.87727000	H	-0.00192000	-2.97852400	-0.18176700
H	1.60623300	2.77167000	2.57018800	N	1.00033200	-2.93491600	-0.39184500
C	3.01135300	5.31413300	0.81922900	H	0.88944900	-2.00985100	-2.30233200
H	2.53180900	5.82000400	-1.22244000	C	3.87491400	-1.74110200	-2.42574400
H	3.25668700	4.56724300	2.82484600	H	3.33701100	-1.09572100	-3.12906000
H	3.74484200	6.10602700	0.93357700	H	4.62470300	-1.11060700	-1.93367100
C	-1.13497200	2.63354500	-0.41376200	C	4.60588500	-2.83540400	-3.21611200
C	-1.77211600	1.98242600	-1.47202500	H	5.29563700	-2.37889000	-3.93413900
C	-1.70889400	3.80891800	0.09617800	H	3.86942500	-3.42273900	-3.78712200
C	-2.95442600	2.49736300	-2.00885700	O	5.40197800	-3.67639900	-2.39217200
H	-1.39981500	1.04068400	-1.85095500	H	4.80395800	-4.10143500	-1.76137700
C	-2.89712200	4.31512200	-0.42903700	O	-3.58226700	1.79304200	1.79623100
H	-1.21851100	4.33386200	0.90937000	H	-3.33930200	0.94996900	1.34926200
C	-3.52624700	3.65799900	-1.48993300	H	-3.66153000	2.43162700	1.07296000
H	-3.43412000	1.97032400	-2.82746100				
H	-3.32423900	5.22341500	-0.01541100				
H	-4.44801100	4.05098100	-1.90740500				
C	1.43232600	0.05416800	0.66929500				
H	2.16808500	-0.72505900	0.51411700				
				<b>TS-7B</b>			
				C	6.31748300	0.26777000	-1.20034000
				C	5.05060100	0.36750300	-0.62809300

C	4.18408100	-0.72045900	-0.69220400	C	-1.23546300	-4.16344600	0.17670100
C	4.57515100	-1.90368600	-1.31936000	C	0.61673800	-4.02696300	-1.88282900
C	5.84226500	-1.98923100	-1.88779900	H	0.31862200	-1.91748400	-1.83785100
C	6.73253700	-0.90752200	-1.83731100	C	-0.61346100	-5.32702000	-0.27578500
H	6.99694600	1.11438800	-1.14874300	H	-1.95801600	-4.22737200	0.98245500
H	4.73108700	1.27094900	-0.12165200	C	0.31707200	-5.26306900	-1.31562800
H	3.89115300	-2.74492200	-1.34314900	H	1.35075800	-3.95544900	-2.67958300
H	6.15042700	-2.91044000	-2.37541400	H	-0.86164200	-6.28049700	0.18097700
C	8.11671400	-1.02244800	-2.42572600	H	0.80232000	-6.16594600	-1.67331100
H	8.80942000	-1.48973500	-1.71506400	C	-1.40695200	0.83646300	0.29448100
H	8.11643800	-1.63830800	-3.33006800	H	-2.20083300	1.56770700	0.38100600
H	8.52468000	-0.04080900	-2.68222100	C	-1.58564200	-0.33764700	-0.69656000
S	2.52458200	-0.59179300	-0.03214400	H	-0.64847700	-0.40565000	-1.24422300
O	2.58039000	0.48790600	1.00415000	C	-2.70547100	-0.18594100	-1.68842200
O	1.65488700	-0.22051400	-1.19286400	C	-3.96873800	0.29466600	-1.31620800
O	2.21646200	-1.93895400	0.51227000	C	-2.48329100	-0.51636800	-3.03035800
C	-0.23439400	0.61253100	2.74623400	C	-4.97675600	0.45328900	-2.26330400
C	0.15973000	-0.63329600	3.32077900	H	-4.16931700	0.52767400	-0.27563400
C	0.82268500	-0.71174800	4.54148700	C	-3.49296100	-0.36405800	-3.98128900
C	1.07250400	0.48214900	5.21467300	H	-1.50976800	-0.89384900	-3.32859700
C	0.66480900	1.71744700	4.68224300	C	-4.74169900	0.12627800	-3.60031900
C	0.01829500	1.79444000	3.45233100	H	-5.94913400	0.82605500	-1.95652800
C	-0.81120300	0.27357100	1.46822600	H	-3.30123500	-0.62306300	-5.01806300
C	-0.78112900	-1.11618500	1.36859600	H	-5.52768300	0.25111200	-4.33875600
H	1.13249900	-1.66905400	4.94679400	C	-0.44349700	4.27940800	-0.12341100
H	1.58842800	0.45636500	6.16922300	C	0.63327600	3.76326200	0.68542600
H	0.86177200	2.62805500	5.23966400	C	1.27580100	4.56782300	1.64860900
H	-0.28146300	2.75484600	3.04931700	C	0.84163100	5.87150600	1.77608700
H	0.15440600	-2.63126600	2.50606200	C	-0.21559700	6.40313500	0.98159900
N	-0.23906400	-1.67211700	2.47095100	C	-0.86172100	5.62680400	0.04688200
C	-1.58693700	-1.66426800	0.22301200	C	-0.86365200	3.23266400	-0.96654800
C	-3.03325600	-1.95323000	0.66404800	C	-0.10023400	2.07311500	-0.60430400
C	-3.89224000	-2.62214500	-0.22013600	H	2.07167300	4.16425700	2.26421000
C	-3.55174300	-1.49779400	1.88008600	H	1.31772400	6.51737700	2.50753800
C	-5.23149400	-2.82369200	0.09835300	H	-0.51222400	7.43643800	1.12689500
H	-3.50637300	-2.97557100	-1.16944200	H	-1.65687700	6.02871100	-0.57114200
C	-4.89640300	-1.69926400	2.20094300	H	1.54933400	1.80975800	0.72414300
H	-2.91203100	-0.98176200	2.58591900	N	0.84101300	2.47513700	0.35428100
C	-5.74172000	-2.35966800	1.31207800	H	0.25910100	1.32385600	-1.30021000
H	-5.87853600	-3.33681200	-0.60641200	C	-1.90493200	3.29111100	-2.03311800
H	-5.27703200	-1.34129300	3.15278200	H	-2.22891700	2.28305200	-2.30247500
H	-6.78644700	-2.51591900	1.56280700	H	-2.78553100	3.83831900	-1.67714400
C	-0.94442400	-2.91319700	-0.39355700	C	-1.39261600	3.99259200	-3.30991600
C	-0.00186200	-2.86319000	-1.42434400	H	-2.19096100	3.98245400	-4.05743500

H	-0.54274100	3.42707600	-3.71865000
O	-1.06044700	5.35501200	-3.10462700
H	-0.26813100	5.38460800	-2.55147700
O	1.32042000	-3.90309400	2.18351900
H	1.86042700	-3.25794200	1.68040900
H	0.91420900	-4.43718000	1.48511300