

## Electronic Supplementary Information (ESI) for Chemical Communications

### Insights into the Reaction between a Primary Amine and a Cavitand with an Introverted Aldehyde Group: An Enzyme-like Mechanism

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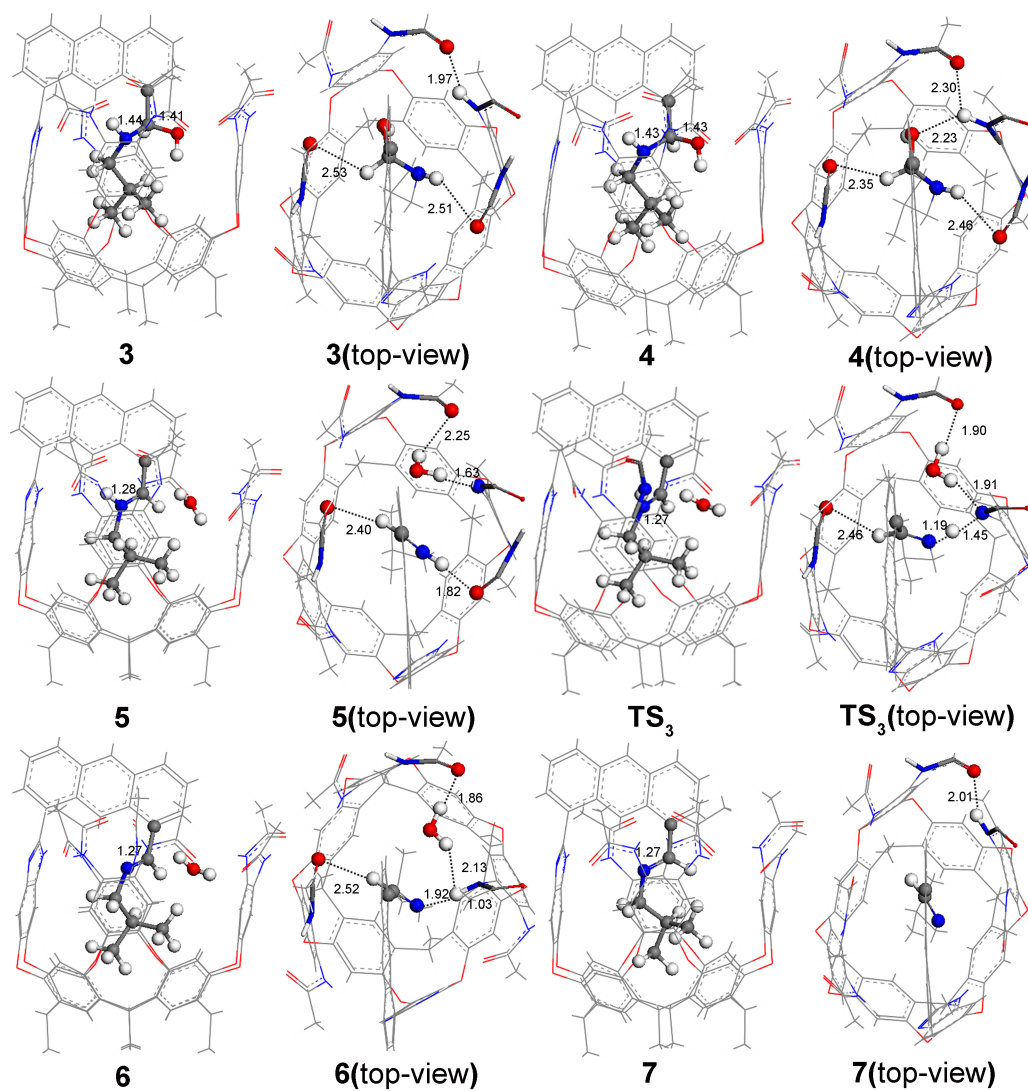
### Computational details:

Geometries of stationary points for the studied reaction and the model reaction were fully optimized using the M06-2X functional<sup>S1</sup> with the 6-31G (d,p) basis set implemented in the Gaussian09 program<sup>S2</sup>. Vibrational frequency calculation was carried out for each stationary point to verify whether it is a minimum or a transition state and obtain the thermodynamic data (enthalpy, entropy and Gibbs free energy) at 298.15K and 1atm. All the transition states were verified by intrinsic reaction coordinate (IRC)<sup>S3</sup> calculations. The polarizable-continuum model (PCM)<sup>S4</sup> was employed to compute the solvation Gibbs free energy for each species in the solvent (mesitylene) at its gas-phase optimized structure. To gain more accurate electronic energies, we carried out single point M06-2X calculations for stationary points of the encapsulated reaction and the model reaction. The large cc-pVTZ<sup>S5</sup> basis set was employed for all the atoms.

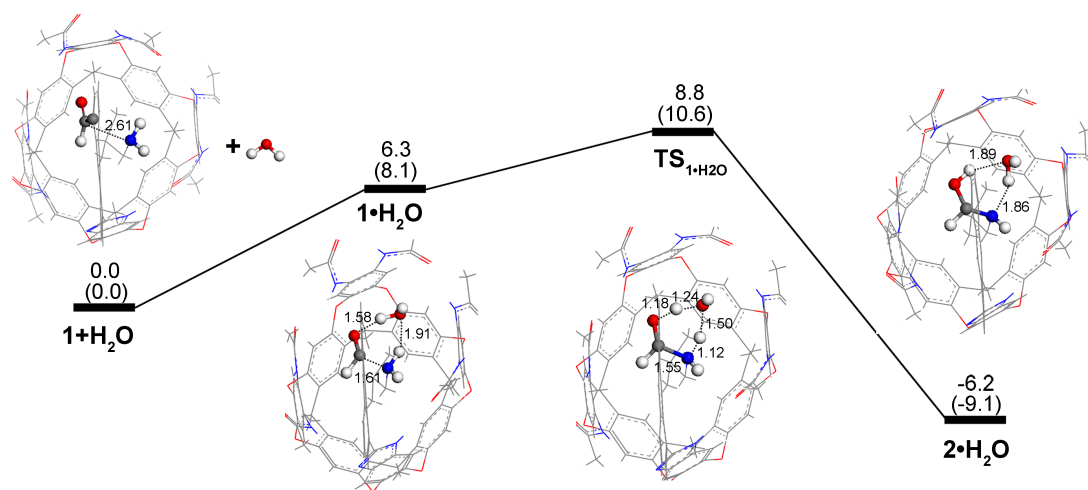
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**Figure S1.** The optimized geometries of some stationary points in the imine formation.



**Figure S2.** Gibbs free energy profile of the hemiaminal formation (the nucleophilic addition) from isobutylamine and the cavitand with a water molecule as the catalyst in the gas phase (298.15K and 1atm). The corresponding free energies in the solvent are also presented in parentheses. Energies are in kcal/mol.

### Cartesian coordinates of optimized geometries of all the species

<b>1</b>			
C	-3.072442	-2.777292	2.330690
C	-3.282227	-2.850837	3.830447
H	-3.139216	-1.852760	4.255093
H	-4.308723	-3.165229	4.026579
H	-2.589237	-3.539771	4.316924
C	0.656156	-4.836028	2.757052
C	1.913935	-5.094191	3.550603
H	1.897200	-6.143433	3.851903
H	2.825519	-4.872671	2.994556
H	1.885780	-4.487836	4.461008
N	0.829658	-4.202101	1.562102
H	1.799802	-3.999846	1.316718
N	-1.896113	-3.326374	1.930607
H	-1.432063	-3.920332	2.627854
O	-3.895025	-2.246021	1.586787
O	-0.442636	-5.181033	3.188692
C	3.924921	2.706971	2.017665
C	4.547238	2.720522	3.394792
H	5.616570	2.521881	3.297064
H	4.398395	3.663934	3.921643
H	4.108482	1.906055	3.977470
C	1.180312	5.797511	2.658668
C	0.154765	6.255196	3.670864
H	-0.843416	6.328559	3.237065
H	0.129096	5.547460	4.504701
H	0.470685	7.223182	4.058800
N	0.677272	5.061939	1.634277
H	-0.341162	4.948594	1.590565
N	3.284934	3.835697	1.661639
H	3.238770	4.630988	2.306860
O	3.993047	1.704452	1.297914
O	2.371371	6.070759	2.797635
C	-2.940159	4.095085	2.007998
C	-2.999732	4.516096	3.461254
H	-2.067370	4.210485	3.943409
H	-3.074512	5.604169	3.522689
H	-3.841195	4.067376	3.992310
C	-5.506380	0.880004	2.684049
C	-5.684501	-0.231291	3.692729
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H	-4.938241	-0.108941	4.484940

H	-6.672357	-0.130729	4.142548
N	-4.810001	0.526824	1.577509
H	-4.472545	-0.437475	1.530211
N	-3.927387	3.256183	1.643340
H	-4.670891	3.029024	2.314088
O	-2.048232	4.487296	1.251052
O	-5.939591	2.013767	2.899387
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H	0.884277	4.274514	-7.278359
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**TS<sub>1</sub>**

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C	3.562505	-5.926521	3.235491
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H	3.569426	-5.442924	4.215265
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H	3.208893	-4.761671	1.054358
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H	0.226748	-4.588247	2.739398
O	-2.093942	-2.610377	1.937960
O	1.177312	-6.001708	3.126149
C	3.877503	2.415324	1.827807
C	4.624006	2.464772	3.138744
H	5.682296	2.273813	2.946106
H	4.516650	3.419797	3.654356
H	4.250085	1.658044	3.774598
C	1.126924	5.412066	2.553933
C	0.161642	5.864457	3.625137
H	-0.864539	5.901962	3.256631
H	0.209196	5.172604	4.471443
H	0.477011	6.847838	3.972115

N	0.586798	4.593256	1.611254
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O	2.306254	5.759363	2.575792
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H	-3.056453	5.081904	3.715873
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C	3.285847	-1.966740	5.305920
C	3.319389	-1.941643	3.870164
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H	2.224492	-1.337286	7.062166

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H	-3.810782	1.235450	-6.961720
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C	-2.846369	-0.958068	-4.427408
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C	-2.894786	-2.464856	-2.520024
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C	-1.985956	-3.299871	-3.155090
C	-1.524414	-3.027278	-4.447801
C	-1.952635	-1.837040	-5.042863
H	-1.600683	-1.602525	-6.043524
C	-0.653946	-4.048246	-5.169655
H	-0.912930	-5.018702	-4.739618
C	-0.940087	-4.111305	-6.673714
H	-2.005689	-4.279003	-6.849500
H	-0.655269	-3.194884	-7.197779
C	0.826601	-3.841735	-4.888826
C	1.489930	-4.617100	-3.936297
C	2.845598	-4.460741	-3.703271
H	3.344156	-5.106897	-2.994435
C	3.551351	-3.446281	-4.334208
C	2.928202	-2.617145	-5.270232
C	1.577059	-2.858823	-5.535842
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C	3.677496	-1.472285	-5.937846
H	4.741287	-1.667689	-5.782198
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H	4.669931	1.793797	-2.758673
C	2.959997	2.300681	-3.950456
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C	2.373601	0.728075	-5.647210

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H	1.869953	3.159611	-7.498249
H	0.539585	2.002253	-7.420155
C	-0.248200	2.689974	-4.778991
C	-0.599096	3.426555	-3.644682
C	-1.818049	3.237524	-3.010733
H	-2.088547	3.841886	-2.152883
C	-2.695916	2.267887	-3.479067
C	-2.375437	1.475000	-4.585766
C	-1.149098	1.715342	-5.206576
H	-0.876205	1.101983	-6.061293
C	-3.916756	1.571380	-1.600855
C	-3.815421	2.361617	-0.463953
H	-3.730468	3.437404	-0.553439
C	-3.823918	1.771453	0.799099
C	-3.953477	0.384596	0.921954
C	-4.108186	-0.391473	-0.221486
H	-4.256346	-1.459429	-0.114615
C	-4.085062	0.189871	-1.477589
C	-0.693571	-4.543867	-1.576694
C	-0.972295	-4.145640	-0.273236
H	-1.934363	-3.717453	-0.028690
C	-0.020328	-4.305492	0.742088
C	1.224460	-4.885716	0.430019
C	1.477699	-5.296351	-0.878447
H	2.418420	-5.787033	-1.102828
C	0.538945	-5.124386	-1.885893
C	4.989766	-2.721635	-2.699936
C	4.988806	-3.544883	-1.588069
H	5.023830	-4.622524	-1.698074
C	4.897167	-2.939689	-0.328574
C	4.824933	-1.539863	-0.235021
C	4.928253	-0.696121	-1.339241
H	4.912363	0.379746	-1.224179
C	5.018311	-1.310601	-2.575234
C	2.281706	3.665650	-2.129070
C	0.963419	4.132333	-2.026056
C	0.432466	4.416331	-0.778125
H	-0.570085	4.821795	-0.695246
C	1.191214	4.237270	0.382997
C	2.489095	3.722502	0.281614

C	3.030037	3.459302	-0.978874
H	4.060053	3.130575	-1.051722
O	-3.931243	2.133764	-2.863400
O	-4.335265	-0.546354	-2.613483
O	-1.655375	-4.508416	-2.561896
O	0.792451	-5.550932	-3.177064
O	4.885438	-3.252965	-3.976925
O	5.187363	-0.591892	-3.738546
O	2.842483	3.557626	-3.379891
O	0.260614	4.414832	-3.175016
H	-4.112444	-0.511429	-6.862433
H	0.197101	3.726653	-7.310809
H	3.741423	-2.354276	-7.910138
H	-0.376924	-4.932591	-7.123358
H	4.467673	-0.341983	1.478773
H	2.220245	0.611170	-0.796387
C	1.571549	-0.111795	-0.285537
H	2.220562	-0.905867	0.104695
N	0.937112	0.587725	0.849857
C	0.565020	-0.700440	-1.268618
H	-0.147065	-1.340740	-0.728988
C	1.337374	-1.561422	-2.261955
H	0.648717	-2.023437	-2.973885
H	2.044583	-0.947470	-2.835094
H	1.902607	-2.358956	-1.761107
C	-0.223832	0.388785	-1.985579
H	-0.826279	-0.050717	-2.786681
H	-0.902536	0.911456	-1.304203
H	0.461008	1.114248	-2.445442
H	1.640300	1.092021	1.392249
H	-0.127028	1.078792	0.634422
<b>2</b>			
C	-2.381814	-2.492298	2.227062
C	-2.546725	-2.385908	3.728724
H	-2.589037	-1.328327	3.999869
H	-3.491556	-2.855751	4.016906
H	-1.731802	-2.866368	4.273552
C	0.783938	-5.324982	2.637823
C	2.002184	-5.709529	3.443214
H	1.960588	-6.789117	3.606248
H	2.938582	-5.439891	2.953352
H	1.942874	-5.222445	4.419407
N	1.039747	-4.746967	1.434321

H	2.021545	-4.552713	1.228290
N	-1.442895	-3.389659	1.843310
H	-1.103398	-4.034239	2.562583
O	-3.050273	-1.812556	1.447595
O	-0.350772	-5.533746	3.063908
C	3.670101	2.481225	2.086194
C	4.262748	2.457060	3.475203
H	5.315749	2.174514	3.405987
H	4.177116	3.414867	3.990262
H	3.746336	1.683901	4.049904
C	1.029199	5.356185	2.753970
C	0.011858	5.549624	3.856839
H	-0.923977	5.941599	3.453153
H	-0.199250	4.587825	4.335205
H	0.421356	6.240249	4.591528
N	0.562860	4.647162	1.692210
H	-0.439287	4.440189	1.677941
N	3.246663	3.679396	1.650198
H	3.227857	4.479055	2.287287
O	3.581881	1.449769	1.410884
O	2.172755	5.794389	2.853779
C	-3.222055	3.997069	1.941815
C	-3.408924	4.631797	3.301033
H	-2.627559	4.257755	3.966833
H	-3.288673	5.714285	3.213153
H	-4.387544	4.413241	3.731226
C	-5.457123	0.856425	2.680524
C	-5.370276	-0.108700	3.842102
H	-5.198010	-1.132129	3.503600
H	-4.535967	0.183911	4.488806
H	-6.294421	-0.048214	4.415281
N	-4.689037	0.517174	1.618908
H	-4.117335	-0.332140	1.679222
N	-4.296264	3.337804	1.479560
H	-5.099208	3.170766	2.092229
O	-2.158522	4.075889	1.316769
O	-6.154341	1.869958	2.739197
C	3.604609	-2.414687	2.106707
N	3.709372	-3.462426	1.309854
N	3.879384	-1.240144	1.476317
C	-1.684512	1.250776	3.646106
C	-0.687169	0.540261	3.038270
C	0.259176	-0.191622	3.848582
C	0.105127	-0.171595	5.277646

C	-0.946386	0.604544	5.860350
C	-1.807127	1.302167	5.067224
C	1.301789	-0.947487	3.294960
C	0.967193	-0.932703	6.069062
C	1.994912	-1.698169	5.515021
C	2.188367	-1.682358	4.092265
C	3.279387	-2.456375	3.547282
C	4.061708	-3.220529	4.370080
C	3.838728	-3.258306	5.775402
C	2.845711	-2.508079	6.331097
H	1.421389	-0.977533	2.218858
H	-2.427779	1.732256	3.017458
H	-1.044665	0.616725	6.942122
H	-2.609794	1.884967	5.511403
H	0.828434	-0.937777	7.147898
H	4.872013	-3.796589	3.933654
H	4.477950	-3.874374	6.398736
H	2.678569	-2.513190	7.404514
C	-0.658469	0.413687	1.520512
H	-0.725123	-0.663754	1.295433
O	-1.809040	0.979243	0.938044
C	-3.182958	1.138352	-5.481303
H	-4.182763	1.455562	-5.177505
C	-3.149340	1.090814	-7.010397
H	-3.384607	2.076804	-7.418348
H	-2.175125	0.795004	-7.408863
C	-2.938283	-0.218677	-4.829821
C	-3.588707	-0.530674	-3.633301
C	-3.367118	-1.731439	-2.975109
H	-3.921857	-1.981360	-2.080613
C	-2.492101	-2.656747	-3.525211
C	-1.860248	-2.423192	-4.750934
C	-2.084208	-1.186752	-5.362632
H	-1.597768	-0.983260	-6.312389
C	-1.016842	-3.520867	-5.385003
H	-1.417157	-4.465782	-5.009650
C	-1.123717	-3.542156	-6.913316
H	-2.171493	-3.604990	-7.218261
H	-0.692587	-2.652301	-7.380191
C	0.430534	-3.457871	-4.922421
C	0.899884	-4.298805	-3.911800
C	2.229063	-4.279210	-3.524272
H	2.579242	-4.979579	-2.779366
C	3.098735	-3.339418	-4.057314



C	2.671759	-2.450348	-5.046917
C	1.342904	-2.552109	-5.465128
H	0.987795	-1.858253	-6.223483
C	3.607162	-1.395426	-5.617722
H	4.619637	-1.703195	-5.345989
C	3.533004	-1.320092	-7.145592
H	2.539029	-1.046710	-7.509810
H	4.240634	-0.576822	-7.521741
C	3.380603	-0.044882	-4.948892
C	4.091866	0.268364	-3.786128
C	4.001845	1.521314	-3.198171
H	4.643511	1.781288	-2.366779
C	3.136969	2.464881	-3.734255
C	2.369087	2.190972	-4.867249
C	2.517654	0.930035	-5.452916
H	1.952008	0.707085	-6.353427
C	1.443439	3.264069	-5.421225
H	1.836325	4.218935	-5.065861
C	1.432129	3.303671	-6.952434
H	2.447015	3.450862	-7.330267
H	1.042678	2.385364	-7.399953
C	0.044848	3.133537	-4.834218
C	-0.338900	3.874674	-3.711743
C	-1.635382	3.813220	-3.220054
H	-1.928992	4.431391	-2.379720
C	-2.557527	2.956645	-3.808644
C	-2.207033	2.151988	-4.896602
C	-0.904521	2.272847	-5.382683
H	-0.611824	1.655862	-6.227837
C	-4.068599	2.383449	-2.095578
C	-4.058334	3.155723	-0.943959
H	-3.866343	4.220687	-1.005297
C	-4.307854	2.566824	0.294366
C	-4.575945	1.199564	0.386632
C	-4.638296	0.440438	-0.780013
H	-4.899093	-0.608935	-0.713612
C	-4.388597	1.023319	-2.011476
C	-1.526061	-4.019077	-1.830824
C	-1.906463	-3.570123	-0.571452
H	-2.842861	-3.047345	-0.437562
C	-1.089162	-3.792398	0.542336
C	0.116149	-4.501082	0.380045
C	0.470770	-4.961303	-0.888076
H	1.382853	-5.536677	-1.003353

C	-0.327409	-4.716288	-1.996244
C	4.419166	-2.750051	-2.273336
C	4.190741	-3.555893	-1.172469
H	4.097820	-4.629830	-1.284094
C	4.043958	-2.933822	0.073242
C	4.157159	-1.536933	0.166475
C	4.482624	-0.722357	-0.916933
H	4.591126	0.348166	-0.796803
C	4.611737	-1.351987	-2.141276
C	2.476993	3.891022	-1.975985
C	1.168695	4.392554	-1.943695
C	0.562164	4.641666	-0.720324
H	-0.439071	5.057550	-0.685720
C	1.240792	4.396993	0.477726
C	2.543696	3.891944	0.437766
C	3.156464	3.655231	-0.789994
H	4.185246	3.315760	-0.812112
O	-3.864685	2.947802	-3.336369
O	-4.570930	0.331679	-3.182806
O	-2.358731	-3.896010	-2.921361
O	0.034556	-5.167188	-3.252944
O	4.397122	-3.281460	-3.554951
O	4.977960	-0.663707	-3.279020
O	3.107215	3.740720	-3.190296
O	0.563982	4.755552	-3.128607
H	-3.887611	0.374324	-7.379397
H	0.806016	4.129390	-7.299174
H	3.783485	-2.292299	-7.576838
H	-0.590183	-4.409515	-7.309330
H	3.817548	-0.283732	1.834638
H	1.998974	0.652707	-0.515763
C	1.119149	0.127455	-0.121472
H	1.479833	-0.836816	0.288328
N	0.528109	0.973281	0.914359
C	0.163394	-0.198201	-1.267683
H	-0.749841	-0.656820	-0.858416
C	0.837180	-1.206782	-2.192539
H	0.168409	-1.493080	-3.010673
H	1.739365	-0.768142	-2.639761
H	1.135745	-2.116473	-1.654249
C	-0.231415	1.057680	-2.026377
H	-0.927189	0.821043	-2.839260
H	-0.702960	1.791262	-1.366374
H	0.661954	1.519079	-2.469041

H	1.234683	1.254351	1.585462
H	-1.598243	1.910556	0.755849
<b>3</b>			
C	-2.337483	-2.352761	2.244255
C	-2.497412	-2.253966	3.747119
H	-2.521645	-1.198237	4.027116
H	-3.449352	-2.710692	4.033557
H	-1.690099	-2.753455	4.286261
C	0.756616	-5.271105	2.617562
C	1.973587	-5.680501	3.412351
H	1.911199	-6.758968	3.576108
H	2.911059	-5.430653	2.914142
H	1.933215	-5.192180	4.388912
N	1.014244	-4.695530	1.413244
H	1.998041	-4.519001	1.198098
N	-1.438656	-3.288700	1.852823
H	-1.116838	-3.947013	2.568087
O	-2.976052	-1.636222	1.472470
O	-0.378390	-5.459736	3.051942
C	3.528085	2.361295	2.045564
C	3.940053	2.260356	3.495965
H	5.014391	2.073017	3.547227
H	3.692557	3.153283	4.071399
H	3.426783	1.397968	3.934506
C	0.465225	4.997751	2.766452
C	-0.704306	5.184645	3.701014
H	-1.400348	5.901999	3.260323
H	-1.232503	4.236876	3.842220
H	-0.332295	5.552488	4.655205
N	0.149340	4.396844	1.587356
H	-0.845911	4.272719	1.405368
N	2.850272	3.473752	1.714321
H	2.647760	4.182490	2.429657
O	3.770890	1.449282	1.247613
O	1.597448	5.369142	3.071736
C	-3.622628	4.712065	1.767933
C	-4.074080	5.458910	3.007874
H	-3.609284	5.015354	3.893557
H	-3.751102	6.496849	2.929557
H	-5.157203	5.416389	3.134964
C	-5.382346	1.071011	2.729940
C	-5.271135	0.112898	3.895448
H	-5.099302	-0.909855	3.553708

H	-4.425879	0.407900	4.526623
H	-6.186480	0.169071	4.482533
N	-4.557714	0.782522	1.696204
H	-3.959950	-0.046847	1.761014
N	-4.387812	3.639272	1.468257
H	-5.161326	3.377122	2.086033
O	-2.632932	5.055500	1.121741
O	-6.143675	2.037442	2.758600
C	3.632598	-2.416254	2.040710
N	3.693473	-3.458429	1.232130
N	3.938011	-1.245689	1.418028
C	-1.548563	1.381392	3.639393
C	-0.596231	0.619800	3.018484
C	0.340934	-0.139969	3.813389
C	0.210069	-0.109894	5.244895
C	-0.805743	0.701030	5.842375
C	-1.646713	1.435417	5.062309
C	1.360954	-0.918770	3.248451
C	1.063915	-0.889631	6.027025
C	2.068198	-1.677640	5.462614
C	2.244772	-1.667076	4.037653
C	3.319127	-2.457686	3.483543
C	4.097596	-3.233927	4.298387
C	3.888095	-3.268490	5.705838
C	2.913559	-2.501281	6.270720
H	1.468685	-0.951278	2.171297
H	-2.263036	1.920640	3.023670
H	-0.886389	0.717324	6.925503
H	-2.412575	2.057485	5.517507
H	0.940133	-0.886637	7.107640
H	4.895217	-3.821584	3.854120
H	4.523828	-3.894066	6.323175
H	2.757828	-2.501796	7.345843
C	-0.596691	0.485491	1.508100
H	-0.681847	-0.592283	1.282406
O	-1.758263	1.138339	1.035775
C	-3.235274	1.250810	-5.456948
H	-4.231438	1.568356	-5.141026
C	-3.221752	1.194555	-6.986015
H	-3.472714	2.175953	-7.395441
H	-2.249302	0.907677	-7.395403
C	-2.979601	-0.100617	-4.799544
C	-3.590616	-0.389196	-3.575974
C	-3.375876	-1.592237	-2.920075

H	-3.914212	-1.827850	-2.011666
C	-2.542333	-2.540168	-3.496267
C	-1.940401	-2.323435	-4.739816
C	-2.161889	-1.087260	-5.353318
H	-1.706141	-0.900524	-6.321430
C	-1.124207	-3.434158	-5.386147
H	-1.529420	-4.373393	-5.001954
C	-1.254147	-3.457601	-6.912447
H	-2.307104	-3.504634	-7.202096
H	-0.815170	-2.576307	-7.388191
C	0.330929	-3.385237	-4.945118
C	0.806606	-4.230498	-3.941015
C	2.142444	-4.225718	-3.576495
H	2.497046	-4.933433	-2.840803
C	3.011767	-3.290839	-4.118867
C	2.577310	-2.390504	-5.095369
C	1.242543	-2.483288	-5.497297
H	0.880879	-1.783627	-6.247308
C	3.514768	-1.335677	-5.666076
H	4.527886	-1.657233	-5.413808
C	3.418465	-1.239880	-7.191525
H	2.421279	-0.954892	-7.537496
H	4.125880	-0.496982	-7.568707
C	3.312945	0.009415	-4.976457
C	4.042885	0.305539	-3.820417
C	3.955722	1.548159	-3.207256
H	4.603893	1.796517	-2.376962
C	3.087419	2.504984	-3.716743
C	2.320424	2.253973	-4.857829
C	2.455286	0.998953	-5.459462
H	1.884345	0.794629	-6.360926
C	1.414689	3.340256	-5.418768
H	1.818574	4.288322	-5.057490
C	1.417694	3.382375	-6.950232
H	2.439531	3.494103	-7.321376
H	0.997113	2.479731	-7.401540
C	0.006534	3.233614	-4.851367
C	-0.377069	4.009494	-3.754391
C	-1.673854	3.973481	-3.263577
H	-1.969528	4.619917	-2.445984
C	-2.599402	3.104492	-3.826272
C	-2.253676	2.270734	-4.893872
C	-0.949041	2.369130	-5.382792
H	-0.658887	1.726101	-6.209756

C	-4.062535	2.576635	-2.071028
C	-4.067278	3.383535	-0.942870
H	-3.922144	4.452644	-1.042985
C	-4.281665	2.827044	0.321580
C	-4.478179	1.447481	0.449782
C	-4.519750	0.651378	-0.695333
H	-4.732887	-0.405544	-0.587705
C	-4.328257	1.207719	-1.949726
C	-1.577308	-3.918742	-1.818163
C	-1.933369	-3.463792	-0.553985
H	-2.861618	-2.930220	-0.406188
C	-1.104741	-3.698186	0.548664
C	0.085228	-4.428711	0.369782
C	0.416439	-4.893152	-0.903990
H	1.317601	-5.483292	-1.031625
C	-0.391752	-4.633597	-2.001808
C	4.371352	-2.728331	-2.354006
C	4.141867	-3.540223	-1.257369
H	4.022957	-4.610508	-1.377275
C	4.029581	-2.928010	-0.003554
C	4.189072	-1.536988	0.102399
C	4.517897	-0.719604	-0.976930
H	4.662810	0.344660	-0.846240
C	4.597687	-1.336581	-2.211097
C	2.367521	3.902293	-1.951890
C	1.083720	4.458195	-1.974595
C	0.395852	4.646253	-0.784519
H	-0.595746	5.086958	-0.789346
C	0.963520	4.280785	0.435321
C	2.264558	3.762121	0.460907
C	2.958997	3.584440	-0.735190
H	3.972274	3.203381	-0.708385
O	-3.898740	3.110743	-3.332518
O	-4.539506	0.494333	-3.102862
O	-2.422232	-3.782094	-2.896807
O	-0.056408	-5.088545	-3.264828
O	4.318513	-3.246365	-3.639947
O	4.940341	-0.634680	-3.347799
O	3.062885	3.766654	-3.136158
O	0.544787	4.870988	-3.175133
H	-3.957417	0.468751	-7.341984
H	0.823536	4.230550	-7.298921
H	3.655210	-2.208191	-7.638915
H	-0.740488	-4.334464	-7.313555

H	3.924041	-0.289976	1.778899
H	2.055458	0.627320	-0.553502
C	1.159557	0.129272	-0.160776
H	1.487182	-0.850285	0.241112
N	0.583478	0.994409	0.857919
C	0.187930	-0.150517	-1.309036
H	-0.734308	-0.593638	-0.894641
C	0.807262	-1.176129	-2.249955
H	0.117091	-1.426259	-3.061530
H	1.720989	-0.769949	-2.703016
H	1.074123	-2.100882	-1.722325
C	-0.166924	1.127913	-2.059631
H	-0.927753	0.941163	-2.825929
H	-0.522052	1.921011	-1.390409
H	0.727571	1.518819	-2.562030
H	1.271876	1.387673	1.485665
H	-1.669877	1.218430	0.077645

#### 4

C	-2.200296	-2.435917	2.243473
C	-2.377138	-2.328332	3.742925
H	-2.389496	-1.271337	4.019187
H	-3.338523	-2.770941	4.020202
H	-1.583136	-2.837903	4.292292
C	0.848465	-5.381479	2.625340
C	2.062000	-5.775115	3.432791
H	2.017445	-6.855728	3.587924
H	3.000441	-5.505114	2.947077
H	2.001494	-5.294452	4.411949
N	1.111210	-4.800435	1.425640
H	2.092094	-4.586085	1.227183
N	-1.344991	-3.408990	1.860283
H	-1.038748	-4.074378	2.576655
O	-2.797562	-1.690144	1.461084
O	-0.289183	-5.588672	3.045218
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C	4.125172	2.334460	3.517437
H	5.202069	2.155450	3.535283
H	3.893149	3.241723	4.076655
H	3.635202	1.480873	3.995993
C	0.484418	4.692404	2.816695
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H	-0.763254	5.570890	4.290367
H	-1.533755	4.184792	3.459413

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N	0.232597	4.060627	1.644518
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N	3.014959	3.515551	1.722155
H	2.794723	4.228870	2.424725
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C	-3.398484	4.651594	1.610189
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H	-4.669086	6.104038	2.529227
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H	-6.017451	0.138765	4.562596
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O	-2.480692	4.947677	0.854199
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C	0.341878	-0.125464	3.850496
C	0.177126	-0.166891	5.281550
C	-0.857531	0.597907	5.905015
C	-1.699863	1.351897	5.148705
C	1.369885	-0.895687	3.284639
C	1.014055	-0.974620	6.052089
C	2.031524	-1.740359	5.484363
C	2.231217	-1.682041	4.064565
C	3.309187	-2.466244	3.506941
C	4.075517	-3.263334	4.313863
C	3.848605	-3.334052	5.716811
C	2.862524	-2.585075	6.285113
H	1.502555	-0.895217	2.212201
H	-2.282844	1.937633	3.138287
H	-0.953182	0.556728	6.986297
H	-2.486960	1.937416	5.615911



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H	4.877003	-3.841853	3.864648
H	4.476835	-3.974270	6.326794
H	2.687014	-2.614665	7.356777
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H	-4.208044	1.419792	-5.114673
C	-3.199487	1.047545	-6.960630
H	-3.465881	2.023683	-7.372883
H	-2.223889	0.773855	-7.371602
C	-2.939766	-0.235101	-4.768387
C	-3.550204	-0.538416	-3.547453
C	-3.320424	-1.743332	-2.898984
H	-3.860872	-1.989451	-1.994240
C	-2.471775	-2.676417	-3.477232
C	-1.868413	-2.443548	-4.716855
C	-2.105634	-1.207580	-5.323212
H	-1.648871	-1.008894	-6.288343
C	-1.031785	-3.536454	-5.366474
H	-1.421776	-4.484850	-4.989261
C	-1.155556	-3.553557	-6.893368
H	-2.206466	-3.617316	-7.187223
H	-0.730300	-2.662109	-7.362605
C	0.420134	-3.462731	-4.919121
C	0.907986	-4.307834	-3.920951
C	2.241893	-4.279568	-3.549382
H	2.607403	-4.987398	-2.819196
C	3.094505	-3.323489	-4.081147
C	2.647494	-2.425865	-5.054323
C	1.316039	-2.538848	-5.461098
H	0.944475	-1.841219	-6.208209
C	3.573567	-1.358696	-5.619315
H	4.589504	-1.669413	-5.364955
C	3.480688	-1.263114	-7.145274
H	2.481719	-0.987816	-7.493936
H	4.181787	-0.513053	-7.519985
C	3.357925	-0.015124	-4.931651
C	4.093177	0.299309	-3.783580
C	4.001190	1.548637	-3.184462
H	4.648111	1.807646	-2.356287
C	3.125169	2.495695	-3.700722
C	2.346393	2.221390	-4.827964

C	2.485516	0.960241	-5.415132
H	1.904116	0.739545	-6.305980
C	1.412335	3.281853	-5.389195
H	1.788570	4.241253	-5.028284
C	1.414731	3.323252	-6.920665
H	2.432498	3.470487	-7.290566
H	1.027146	2.406011	-7.372247
C	0.008650	3.133457	-4.820142
C	-0.383116	3.884638	-3.708166
C	-1.682384	3.836959	-3.225407
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C	-2.596163	2.967711	-3.807507
C	-2.236633	2.142431	-4.875696
C	-0.933516	2.261984	-5.364147
H	-0.635713	1.634342	-6.200192
C	-4.049280	2.425172	-2.064101
C	-4.025165	3.244527	-0.947905
H	-3.883180	4.310731	-1.070340
C	-4.180848	2.707920	0.332753
C	-4.375451	1.328009	0.482243
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H	-4.656586	-0.539454	-0.528870
C	-4.294077	1.055924	-1.921928
C	-1.484932	-4.049166	-1.807840
C	-1.843381	-3.596487	-0.543865
H	-2.775473	-3.069222	-0.397050
C	-1.009318	-3.819808	0.555950
C	0.184184	-4.542708	0.379170
C	0.519288	-5.004968	-0.894275
H	1.425754	-5.586530	-1.022394
C	-0.290322	-4.749714	-1.991946
C	4.437121	-2.728412	-2.314222
C	4.200152	-3.538618	-1.218251
H	4.085777	-4.609431	-1.336545
C	4.071169	-2.924577	0.032292
C	4.227518	-1.533433	0.139866
C	4.565001	-0.717319	-0.938017
H	4.704619	0.348215	-0.809186
C	4.656203	-1.335251	-2.171489
C	2.420809	3.877996	-1.932334
C	1.096918	4.333628	-1.927937
C	0.405383	4.432088	-0.727768
H	-0.626599	4.766815	-0.698713
C	1.028438	4.098177	0.473942

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C	3.066949	3.620208	-0.729296
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O	-2.332091	-3.920119	-2.884991
O	0.057557	-5.188989	-3.256787
O	4.398319	-3.253097	-3.597874
O	5.001208	-0.628900	-3.305010
O	3.093841	3.764227	-3.132239
O	0.531706	4.743114	-3.117425
H	-3.925395	0.309850	-7.312163
H	0.791719	4.149920	-7.270713
H	3.728452	-2.228870	-7.592317
H	-0.625233	-4.419148	-7.297307
H	3.948796	-0.287677	1.817514
H	2.104621	0.449774	-0.483678
C	1.181230	0.014530	-0.079588
H	1.456710	-0.972930	0.342985
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C	0.210997	-0.250781	-1.234181
H	-0.727486	-0.666639	-0.829507
C	0.825825	-1.303582	-2.149753
H	0.139871	-1.562307	-2.962198
H	1.748628	-0.917334	-2.602853
H	1.078727	-2.219599	-1.601208
C	-0.107705	1.018763	-2.013832
H	-0.852446	0.828005	-2.795585
H	-0.473030	1.823919	-1.367238
H	0.802459	1.396296	-2.499300
H	1.388945	1.389993	1.477742
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## TS<sub>2</sub>

C	-2.435360	-2.061910	2.170768
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H	-3.831125	-2.171599	3.776524
H	-2.223057	-2.799946	4.209176
C	0.608916	-4.983990	2.584571
C	1.812674	-5.372230	3.408008
H	1.747385	-6.445853	3.597998
H	2.757875	-5.133381	2.919082
H	1.758275	-4.859767	4.371802

N	0.882934	-4.370838	1.401656
H	1.869466	-4.195696	1.198128
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H	-1.387767	-3.790175	2.509469
O	-2.875340	-1.214583	1.385122
O	-0.532028	-5.221781	2.978358
C	3.417765	2.767143	2.164512
C	3.951893	2.797125	3.574921
H	5.043754	2.746531	3.550080
H	3.646288	3.706104	4.096422
H	3.582523	1.916875	4.105152
C	0.602711	4.865529	2.871521
C	-0.367672	4.644939	4.018081
H	-1.324388	4.248816	3.673125
H	0.071979	3.940115	4.731752
H	-0.517954	5.591898	4.541538
N	0.219164	4.334430	1.710624
H	-0.930169	3.467209	1.465382
N	3.065238	3.946978	1.652905
H	2.818503	4.715803	2.326094
O	3.317265	1.693121	1.533936
O	1.655126	5.504972	3.114272
C	-3.506496	4.994906	1.271905
C	-3.547197	5.828767	2.531892
H	-4.239195	6.662721	2.384308
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H	-2.549027	6.234062	2.697960
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C	-5.386520	0.486359	3.864809
H	-4.353876	0.266126	4.146322
H	-5.911738	0.946627	4.699953
H	-5.877826	-0.456161	3.605470
N	-4.647273	1.067016	1.636580
H	-4.109055	0.200130	1.708992
N	-4.379009	3.942949	1.248181
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O	-2.758100	5.270127	0.344232
O	-6.139731	2.435806	2.691169
C	3.521074	-2.127526	2.007015
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C	-1.808462	1.513379	3.566014
C	-0.751700	0.897564	2.944400
C	0.172515	0.087699	3.723459

C	-0.030165	0.031333	5.150049
C	-1.113325	0.745393	5.748249
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C	1.219872	-0.674849	3.181989
C	0.813626	-0.748877	5.942306
C	1.866839	-1.482560	5.400335
C	2.084908	-1.430261	3.983969
C	3.187463	-2.189264	3.443252
C	3.966012	-2.959044	4.263852
C	3.723364	-3.024382	5.665086
C	2.710603	-2.298892	6.217300
H	1.363802	-0.706058	2.109847
H	-2.499914	2.088451	2.960912
H	-1.229318	0.698242	6.827324
H	-2.811342	1.991143	5.428007
H	0.633615	-0.792729	7.013846
H	4.787479	-3.520108	3.828846
H	4.360976	-3.643180	6.287184
H	2.523850	-2.325980	7.287003
C	-0.609901	0.968997	1.455963
H	-1.376207	0.478637	0.862304
O	-1.652927	2.727202	1.171345
C	-3.460772	1.377475	-5.512438
H	-4.459290	1.706872	-5.219450
C	-3.415791	1.313291	-7.040835
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H	-2.434026	1.030301	-7.430009
C	-3.230349	0.029524	-4.842258
C	-3.898693	-0.300363	-3.657725
C	-3.674639	-1.514918	-3.020493
H	-4.244968	-1.783393	-2.139787
C	-2.748667	-2.405676	-3.548261
C	-2.086223	-2.142247	-4.751639
C	-2.337261	-0.910839	-5.357933
H	-1.832752	-0.683453	-6.292378
C	-1.204309	-3.205646	-5.393252
H	-1.571672	-4.164530	-5.019875
C	-1.327281	-3.224357	-6.921142
H	-2.375845	-3.317589	-7.214953
H	-0.928139	-2.320377	-7.389251
C	0.248428	-3.108716	-4.951818
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C	2.074916	-3.932537	-3.587334
H	2.439710	-4.641654	-2.858075

C	2.933189	-2.990560	-4.135993
C	2.485922	-2.097984	-5.113409
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H	0.781940	-1.508830	-6.265673
C	3.417900	-1.042763	-5.690620
H	4.432891	-1.356220	-5.436329
C	3.321169	-0.955062	-7.216522
H	2.322605	-0.677005	-7.563997
H	4.024293	-0.209604	-7.596283
C	3.200222	0.300516	-5.005970
C	3.925818	0.617547	-3.853265
C	3.817345	1.861425	-3.247112
H	4.462411	2.128334	-2.420064
C	2.922456	2.795734	-3.754449
C	2.135880	2.508466	-4.872599
C	2.305727	1.260928	-5.479353
H	1.723416	1.035090	-6.368452
C	1.161885	3.549808	-5.395438
H	1.515285	4.513032	-5.022094
C	1.137400	3.622419	-6.925752
H	2.142412	3.822008	-7.306096
H	0.784330	2.698456	-7.391935
C	-0.228321	3.352290	-4.806271
C	-0.630764	4.075780	-3.675725
C	-1.945097	4.033713	-3.223164
H	-2.248578	4.649906	-2.382413
C	-2.857210	3.203647	-3.868724
C	-2.475663	2.381715	-4.929585
C	-1.159925	2.488176	-5.380955
H	-0.849695	1.877363	-6.224803
C	-4.403831	2.693182	-2.223032
C	-4.391300	3.547143	-1.137296
H	-4.272954	4.608324	-1.305208
C	-4.485812	3.055450	0.165206
C	-4.637401	1.672378	0.355104
C	-4.751613	0.828608	-0.756952
H	-4.935824	-0.227871	-0.595080
C	-4.635179	1.326062	-2.048227
C	-1.711094	-3.710609	-1.862251
C	-2.088996	-3.266887	-0.601348
H	-3.043180	-2.775646	-0.462382
C	-1.254752	-3.459950	0.503401
C	-0.031558	-4.130165	0.340368
C	0.334837	-4.569223	-0.931727

H	1.264289	-5.113766	-1.055437
C	-0.483509	-4.359640	-2.032113
C	4.296381	-2.410292	-2.381125
C	4.083204	-3.228614	-1.286180
H	3.988949	-4.301053	-1.409170
C	3.948431	-2.622618	-0.032126
C	4.066363	-1.226594	0.077737
C	4.386017	-0.400606	-1.000138
H	4.501473	0.668556	-0.871296
C	4.493939	-1.013186	-2.236445
C	2.254355	4.166489	-1.968910
C	0.902681	4.538898	-1.903041
C	0.269481	4.627352	-0.672063
H	-0.766812	4.947784	-0.606187
C	0.965467	4.383643	0.528628
C	2.337829	4.087578	0.440645
C	2.970101	3.979105	-0.795303
H	4.033043	3.766896	-0.836511
O	-4.193381	3.199403	-3.484730
O	-4.869384	0.554576	-3.167887
O	-2.571134	-3.636260	-2.934843
O	-0.118342	-4.817878	-3.282790
O	4.243442	-2.930631	-3.665801
O	4.835902	-0.307236	-3.368371
O	2.877657	4.063989	-3.198494
O	0.273121	4.931377	-3.070631
H	-4.141630	0.584324	-7.410137
H	0.473986	4.427905	-7.249760
H	3.564117	-1.923809	-7.659753
H	-0.772291	-4.074119	-7.325713
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C	0.968884	0.911447	-0.461445
H	1.961163	0.452162	-0.408932
N	0.571215	1.125607	0.933365
C	0.008353	0.042115	-1.265772
H	-0.380166	-0.758781	-0.617675
C	0.775584	-0.609120	-2.414323
H	0.090882	-1.179898	-3.049013
H	1.248337	0.158628	-3.040394
H	1.555247	-1.290020	-2.050953
C	-1.151031	0.860927	-1.828238
H	-1.827235	0.212971	-2.387994
H	-1.739627	1.372425	-1.058377

H	-0.760924	1.619970	-2.516562
H	1.325486	1.504536	1.506340
H	-1.923652	2.976233	0.274950
<b>5</b>			
C	-2.355696	-2.053008	2.285937
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H	-3.482992	-2.831986	3.919594
H	-1.843245	-2.333672	4.374648
C	0.853569	-4.859275	2.804676
C	2.048166	-5.325541	3.599046
H	1.869336	-6.369146	3.866549
H	2.989326	-5.230913	3.056420
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N	1.127972	-4.292716	1.594236
H	2.115752	-4.249938	1.340925
N	-1.385358	-2.937525	1.955658
H	-1.079969	-3.586146	2.692647
O	-2.919216	-1.308206	1.479993
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H	5.153302	2.292214	3.755128
H	3.737442	3.224833	4.306321
H	3.693894	1.434413	4.268247
C	0.654601	4.442161	3.050120
C	-0.373374	4.289393	4.155637
H	-1.310331	3.871549	3.780728
H	0.032799	3.638541	4.936338
H	-0.554245	5.267087	4.610428
N	0.275184	3.980446	1.869182
H	-1.041822	3.081262	1.513402
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C	-0.280051	0.335615	3.032843
C	0.693386	-0.368281	3.842295
C	0.516547	-0.344595	5.269335
C	-0.581345	0.380619	5.830505
C	-1.486538	1.010353	5.030008
C	1.751683	-1.112945	3.312628
C	1.398963	-1.056423	6.083710
C	2.465223	-1.785317	5.553328
C	2.660329	-1.791913	4.133109
C	3.777971	-2.528603	3.598774
C	4.593302	-3.245942	4.429851
C	4.370134	-3.266137	5.836080
C	3.347647	-2.547046	6.381921
H	1.864174	-1.205042	2.239000
H	-2.072817	1.467260	2.969146
H	-0.678746	0.411316	6.912091
H	-2.310838	1.566119	5.465940
H	1.240972	-1.054738	7.159534
H	5.424326	-3.799021	4.003232
H	5.032230	-3.845984	6.469974
H	3.182880	-2.541288	7.455502
C	-0.176009	0.363080	1.563375
H	-1.054059	0.120201	0.970695
O	-1.752355	2.451316	1.159894
C	-3.212200	1.182149	-5.477942
H	-4.217703	1.521704	-5.223222
C	-3.112629	1.104230	-7.002712
H	-3.338402	2.081245	-7.436437
H	-2.118804	0.813945	-7.353740
C	-3.010660	-0.158653	-4.784638
C	-3.702718	-0.455794	-3.604508

C	-3.484299	-1.648406	-2.925641
H	-4.063364	-1.892513	-2.043282
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C	-1.877688	-2.331546	-4.619497
C	-2.118626	-1.117920	-5.265694
H	-1.601827	-0.919116	-6.200056
C	-0.994803	-3.417907	-5.220378
H	-1.366830	-4.361726	-4.814190
C	-1.117657	-3.489470	-6.747065
H	-2.166498	-3.588737	-7.037797
H	-0.714898	-2.603465	-7.245299
C	0.461374	-3.319609	-4.787438
C	0.946995	-4.135165	-3.764587
C	2.288499	-4.143123	-3.424614
H	2.647105	-4.839214	-2.679555
C	3.160692	-3.238956	-4.013109
C	2.716127	-2.352193	-4.998219
C	1.372951	-2.442302	-5.378594
H	1.008353	-1.761030	-6.144155
C	3.646835	-1.300510	-5.587837
H	4.663920	-1.618327	-5.347435
C	3.530437	-1.204783	-7.111271
H	2.528633	-0.921195	-7.444523
H	4.231200	-0.459839	-7.496353
C	3.437821	0.039002	-4.889264
C	4.150078	0.326369	-3.720432
C	4.029274	1.550056	-3.076652
H	4.664682	1.798131	-2.236703
C	3.139052	2.498146	-3.566464
C	2.379915	2.247998	-4.712572
C	2.559318	1.018517	-5.354235
H	1.991651	0.820593	-6.259395
C	1.421382	3.310078	-5.219277
H	1.778224	4.259189	-4.814300
C	1.419429	3.425090	-6.747399
H	2.432469	3.618749	-7.109350
H	1.057142	2.520015	-7.242619
C	0.017369	3.116060	-4.661366
C	-0.413340	3.843476	-3.543868
C	-1.746508	3.831169	-3.145959
H	-2.069892	4.450464	-2.314277
C	-2.649070	3.019218	-3.827430
C	-2.239357	2.181446	-4.865786
C	-0.905426	2.262670	-5.265567

H	-0.572975	1.641126	-6.093215
C	-4.281480	2.566484	-2.244160
C	-4.337424	3.440226	-1.175741
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C	-4.650340	1.590723	0.335448
C	-4.704069	0.727194	-0.765289
H	-4.892634	-0.327057	-0.594312
C	-4.516126	1.201468	-2.055702
C	-1.495318	-3.772414	-1.675772
C	-1.858932	-3.257904	-0.437454
H	-2.808657	-2.753286	-0.322023
C	-1.015230	-3.386817	0.672071
C	0.204062	-4.075109	0.531975
C	0.557215	-4.578286	-0.720326
H	1.485798	-5.129239	-0.823876
C	-0.269991	-4.428995	-1.823890
C	4.576815	-2.714970	-2.278897
C	4.418427	-3.548707	-1.185743
H	4.325664	-4.620376	-1.319126
C	4.349627	-2.958265	0.082536
C	4.474596	-1.563035	0.200334
C	4.729611	-0.720882	-0.881465
H	4.856544	0.345226	-0.742863
C	4.773741	-1.318126	-2.128156
C	2.419545	3.816996	-1.754092
C	1.074614	4.220988	-1.717224
C	0.406111	4.287615	-0.504227
H	-0.624692	4.628975	-0.463766
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C	3.092570	3.575544	-0.564250
H	4.150460	3.335853	-0.579698
O	-4.000756	3.047920	-3.502315
O	-4.689712	0.409554	-3.172162
O	-2.365789	-3.753646	-2.742308
O	0.081167	-4.957615	-3.050389
O	4.480726	-3.212656	-3.569305
O	5.067696	-0.605956	-3.266906
O	3.081300	3.745523	-2.967742
O	0.487155	4.666462	-2.890010
H	-3.828233	0.375377	-7.391792
H	0.773153	4.249723	-7.057322
H	3.764061	-2.171881	-7.562910

H	-0.565523	-4.354736	-7.121569
H	4.191361	-0.346044	1.917745
H	1.360344	1.571689	-0.826503
C	1.222043	0.544249	-0.468491
H	2.198679	0.048752	-0.526746
N	0.930443	0.619279	0.968678
C	0.175778	-0.180605	-1.299203
H	-0.173547	-1.062616	-0.741257
C	0.840256	-0.658052	-2.585484
H	0.092336	-1.096034	-3.250504
H	1.292979	0.190819	-3.112609
H	1.620212	-1.406582	-2.395563
C	-1.000767	0.732376	-1.636994
H	-1.774710	0.164561	-2.155142
H	-1.444612	1.213279	-0.760694
H	-0.652255	1.522929	-2.310751
H	1.766141	0.899207	1.507820
H	-2.107880	2.930129	0.399469

**TS<sub>3</sub>**

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H	-3.704440	-2.802446	3.948109
H	-1.979925	-2.861260	4.370220
C	0.785875	-5.109888	2.758748
C	1.995799	-5.524263	3.559181
H	1.906820	-6.595749	3.752234
H	2.937542	-5.309750	3.052799
H	1.970066	-5.009635	4.523242
N	1.047690	-4.506891	1.566479
H	2.035442	-4.374370	1.339265
N	-1.494079	-3.242679	1.949685
H	-1.183785	-3.912312	2.664370
O	-2.980995	-1.568313	1.513497
O	-0.351323	-5.319170	3.178516
C	3.930919	2.456397	2.040719
C	4.410771	2.493780	3.471887
H	5.499814	2.588908	3.494896
H	3.976188	3.350218	3.994860
H	4.123505	1.567058	3.969224
C	1.361779	4.057373	2.830310
C	0.697433	3.460654	4.058666
H	-0.390554	3.523060	3.969004

H	0.953590	2.400258	4.163936
H	1.025136	4.009548	4.940936
N	1.036405	3.441420	1.665262
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H	3.760154	4.450853	2.052838
O	3.646862	1.402090	1.464605
O	2.116998	5.029408	2.952467
C	-4.026903	4.753142	1.605611
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H	-5.012425	6.400832	2.523446
H	-5.112203	4.911566	3.492493
H	-3.582002	5.831701	3.380924
C	-5.612470	0.959088	2.705480
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H	-4.696140	0.249047	4.507768
H	-6.459045	0.047699	4.431581
H	-5.381054	-1.041306	3.507051
N	-4.765708	0.680294	1.682867
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N	-4.639102	3.554480	1.415339
H	-5.360625	3.249208	2.071169
O	-3.171517	5.208938	0.852019
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C	3.728852	-2.392885	2.112846
N	3.841833	-3.440862	1.316242
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C	-1.702836	1.094756	3.426391
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C	0.021382	-0.342209	5.163018
C	-1.075796	0.419639	5.678095
C	-1.899526	1.116081	4.841226
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C	0.881034	-1.071373	5.989436
C	1.975009	-1.774607	5.476984
C	2.232033	-1.742538	4.064007
C	3.388736	-2.440445	3.553366
C	4.192910	-3.144870	4.406496
C	3.917526	-3.197340	5.803583
C	2.849332	-2.527516	6.323078
H	1.529620	-1.059991	2.164842
H	-2.346668	1.664494	2.760171
H	-1.232627	0.438878	6.752903

H	-2.713435	1.708074	5.249229
H	0.698927	-1.086198	7.061505
H	5.055521	-3.667821	4.004881
H	4.575533	-3.766601	6.451388
H	2.644002	-2.551076	7.389510
C	-0.353892	0.293052	1.455164
H	-0.849767	-0.502634	0.893976
O	-1.641761	2.835798	0.907631
C	-3.223926	1.116494	-5.407417
H	-4.211187	1.468950	-5.103802
C	-3.193625	1.061229	-6.936412
H	-3.394637	2.053467	-7.347473
H	-2.231637	0.729466	-7.336133
C	-3.017726	-0.241044	-4.750268
C	-3.711122	-0.561201	-3.580245
C	-3.513778	-1.775361	-2.934836
H	-4.094246	-2.034295	-2.058009
C	-2.576890	-2.669830	-3.435466
C	-1.891635	-2.418995	-4.629375
C	-2.123836	-1.189465	-5.248730
H	-1.596941	-0.968484	-6.172666
C	-1.008829	-3.493447	-5.252138
H	-1.378626	-4.444808	-4.862143
C	-1.137099	-3.537790	-6.779278
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H	-0.744705	-2.639549	-7.263750
C	0.446054	-3.397697	-4.816602
C	0.926013	-4.213968	-3.790842
C	2.262521	-4.211851	-3.431469
H	2.616055	-4.904471	-2.681107
C	3.137466	-3.307378	-4.015526
C	2.701939	-2.437005	-5.017109
C	1.362483	-2.527426	-5.409283
H	1.007645	-1.856732	-6.188373
C	3.648292	-1.411475	-5.619940
H	4.658583	-1.731958	-5.355151
C	3.555416	-1.361717	-7.147960
H	2.561106	-1.078738	-7.503743
H	4.268869	-0.635576	-7.545362
C	3.452444	-0.044888	-4.975146
C	4.187858	0.298585	-3.834717
C	4.144304	1.581262	-3.307022
H	4.804603	1.856539	-2.494086
C	3.282557	2.522114	-3.861906

C	2.441795	2.191789	-4.925455
C	2.572013	0.913472	-5.476976
H	1.959809	0.656865	-6.337361
C	1.425302	3.204337	-5.424934
H	1.778016	4.183536	-5.094773
C	1.325948	3.237387	-6.953426
H	2.304950	3.464506	-7.382840
H	0.990540	2.288816	-7.381490
C	0.066459	2.999871	-4.759691
C	-0.283816	3.714797	-3.605494
C	-1.585727	3.697683	-3.111846
H	-1.857751	4.323055	-2.267562
C	-2.541538	2.897971	-3.733255
C	-2.208573	2.084817	-4.819083
C	-0.904163	2.163699	-5.307806
H	-0.640159	1.563323	-6.173902
C	-4.154717	2.418374	-2.086812
C	-4.233797	3.247875	-0.980260
H	-4.076576	4.311307	-1.105032
C	-4.505914	2.723976	0.287028
C	-4.669292	1.338164	0.427878
C	-4.687925	0.527120	-0.709605
H	-4.909868	-0.528103	-0.595640
C	-4.457154	1.056864	-1.969420
C	-1.547708	-3.929079	-1.713604
C	-1.934666	-3.461161	-0.463042
H	-2.896089	-2.981262	-0.338437
C	-1.104537	-3.625899	0.651768
C	0.129661	-4.284097	0.502788
C	0.505741	-4.739394	-0.760013
H	1.443050	-5.273529	-0.869735
C	-0.312224	-4.565107	-1.866657
C	4.507084	-2.719313	-2.274968
C	4.305284	-3.526238	-1.169895
H	4.228858	-4.601556	-1.281354
C	4.158198	-2.906407	0.076428
C	4.243922	-1.505986	0.163770
C	4.551080	-0.686159	-0.927278
H	4.640320	0.388809	-0.814273
C	4.685813	-1.316295	-2.153052
C	2.758230	3.948764	-2.112898
C	1.388925	4.185569	-1.942833
C	0.834140	4.112128	-0.670202
H	-0.238634	4.201478	-0.547773

C	1.634680	3.847297	0.451116
C	3.026893	3.794810	0.269174
C	3.580276	3.825081	-1.001559
H	4.653618	3.734120	-1.128656
O	-3.869161	2.952564	-3.324452
O	-4.667006	0.321019	-3.116737
O	-2.404016	-3.886675	-2.792013
O	0.057045	-5.054540	-3.103217
O	4.451007	-3.258628	-3.552165
O	5.055952	-0.636547	-3.294872
O	3.285359	3.826493	-3.382917
O	0.651521	4.568027	-3.045090
H	-3.957915	0.370463	-7.301404
H	0.618147	4.008569	-7.267041
H	3.785673	-2.344758	-7.565789
H	-0.579973	-4.391624	-7.172335
H	3.894363	-0.253716	1.838379
H	1.293267	1.645065	-0.915019
C	1.126826	0.692438	-0.404149
H	2.118263	0.265699	-0.207024
N	0.567536	0.991417	0.924486
C	0.271209	-0.214348	-1.275351
H	0.068601	-1.158885	-0.747454
C	1.045751	-0.565512	-2.541278
H	0.397446	-1.105150	-3.238536
H	1.384069	0.348870	-3.044751
H	1.919123	-1.192283	-2.328215
C	-1.038900	0.482859	-1.640119
H	-1.742614	-0.243748	-2.046902
H	-1.513109	1.007311	-0.802084
H	-0.834495	1.229652	-2.415670
H	0.868006	2.017219	1.441256
H	-2.134568	3.631806	0.652629
<b>6</b>			
C	-2.602838	-2.214017	2.358756
C	-2.932402	-2.235588	3.833909
H	-3.340737	-1.269631	4.124786
H	-3.685858	-3.009232	4.013491
H	-2.054374	-2.456611	4.445635
C	0.794523	-4.786071	2.902284
C	2.008383	-5.161407	3.716266
H	1.900232	-6.211942	3.994157
H	2.947547	-5.004462	3.184564



H	2.008192	-4.571618	4.637623
N	1.047152	-4.201059	1.697142
H	2.033562	-4.082265	1.460438
N	-1.558490	-3.009895	2.031119
H	-1.199552	-3.623543	2.772152
O	-3.250982	-1.546299	1.548281
O	-0.339627	-5.005137	3.323729
C	4.262185	2.740010	2.080706
C	4.835841	2.879101	3.472170
H	5.891420	3.157081	3.408972
H	4.309404	3.658527	4.030454
H	4.750093	1.925166	3.991477
C	1.532735	3.983993	2.940477
C	1.132617	3.147285	4.137811
H	0.062258	2.921343	4.120650
H	1.662466	2.187623	4.116971
H	1.382834	3.691996	5.046621
N	1.245242	3.390183	1.735831
H	-0.863450	3.180124	1.538452
N	4.016292	3.912576	1.438382
H	3.922768	4.728737	2.036505
O	4.050973	1.654619	1.549324
O	2.064688	5.078771	3.045208
C	-4.004515	4.862853	1.681089
C	-4.495635	5.653395	2.871896
H	-5.041300	6.527034	2.506605
H	-5.150239	5.073352	3.524552
H	-3.629683	6.012439	3.429243
C	-5.771588	1.115452	2.685796
C	-5.811142	0.120037	3.825232
H	-5.057512	0.393989	4.570951
H	-6.793128	0.172357	4.293412
H	-5.606833	-0.897576	3.485662
N	-4.875359	0.816954	1.711419
H	-4.371254	-0.071139	1.785448
N	-4.657054	3.693895	1.460790
H	-5.417669	3.413117	2.083485
O	-3.082282	5.271458	0.978252
O	-6.483112	2.117105	2.688549
C	3.860070	-2.215348	2.224687
N	3.938527	-3.261468	1.423063
N	4.090912	-1.036691	1.584172
C	-1.756898	0.903489	3.473434
C	-0.667687	0.260489	2.948159

C	0.289357	-0.383410	3.819914
C	0.077115	-0.334897	5.239049
C	-1.062901	0.370281	5.740774
C	-1.941948	0.972975	4.887550
C	1.417062	-1.051028	3.328962
C	0.986672	-0.975055	6.088529
C	2.120266	-1.625779	5.595076
C	2.356667	-1.632610	4.179663
C	3.553739	-2.259196	3.674175
C	4.411440	-2.888664	4.532543
C	4.150968	-2.918103	5.934272
C	3.051274	-2.296819	6.450131
H	1.575209	-1.109674	2.261564
H	-2.448465	1.406672	2.801125
H	-1.208400	0.421896	6.816304
H	-2.791762	1.522200	5.282977
H	0.807852	-0.963112	7.161297
H	5.302389	-3.366054	4.136625
H	4.848637	-3.427566	6.590526
H	2.862745	-2.301592	7.520060
C	-0.420408	0.198612	1.481608
H	-1.196098	-0.262485	0.856588
O	-1.632933	2.875671	1.038498
C	-3.193148	1.248190	-5.374520
H	-4.183190	1.595647	-5.073503
C	-3.157772	1.191839	-6.903001
H	-3.356672	2.183370	-7.316855
H	-2.195036	0.857842	-7.298981
C	-2.979286	-0.107969	-4.713732
C	-3.648127	-0.405974	-3.523302
C	-3.429287	-1.598908	-2.849769
H	-3.993403	-1.839685	-1.957873
C	-2.517692	-2.512993	-3.360784
C	-1.852782	-2.285671	-4.570484
C	-2.095794	-1.067604	-5.211043
H	-1.583278	-0.863999	-6.147154
C	-0.964080	-3.368542	-5.170344
H	-1.333592	-4.314159	-4.766005
C	-1.080321	-3.439602	-6.697120
H	-2.126937	-3.553065	-6.990822
H	-0.689748	-2.547127	-7.193640
C	0.488837	-3.261881	-4.725273
C	0.967338	-4.054788	-3.680005
C	2.304802	-4.049523	-3.323468

H	2.656018	-4.728958	-2.560015
C	3.178659	-3.152264	-3.919205
C	2.742501	-2.296299	-4.932870
C	1.405781	-2.400443	-5.330155
H	1.050779	-1.743532	-6.120925
C	3.685218	-1.267030	-5.535147
H	4.696316	-1.582175	-5.266743
C	3.596629	-1.219950	-7.063551
H	2.602609	-0.939762	-7.422442
H	4.309593	-0.493184	-7.460789
C	3.485413	0.102513	-4.895659
C	4.224646	0.457417	-3.760306
C	4.186015	1.747616	-3.249731
H	4.846169	2.028881	-2.438190
C	3.326398	2.683727	-3.815287
C	2.476132	2.341414	-4.865749
C	2.602078	1.055482	-5.401431
H	1.981812	0.788758	-6.252867
C	1.454709	3.344052	-5.374191
H	1.798756	4.327302	-5.046097
C	1.365559	3.370440	-6.903461
H	2.345202	3.606276	-7.326570
H	1.044286	2.416143	-7.329460
C	0.092935	3.133879	-4.717251
C	-0.256251	3.831558	-3.554432
C	-1.559456	3.831018	-3.070209
H	-1.825123	4.444272	-2.214722
C	-2.516735	3.036131	-3.694154
C	-2.184627	2.224178	-4.782601
C	-0.880819	2.307410	-5.273316
H	-0.618883	1.714108	-6.144785
C	-4.123382	2.563866	-2.034805
C	-4.202839	3.387515	-0.924311
H	-4.034114	4.450678	-1.038842
C	-4.505017	2.859742	0.335696
C	-4.700971	1.477954	0.466884
C	-4.695648	0.669928	-0.673184
H	-4.937813	-0.381694	-0.569550
C	-4.431682	1.203501	-1.923322
C	-1.530882	-3.765285	-1.616235
C	-1.955415	-3.305303	-0.376404
H	-2.934064	-2.859088	-0.271764
C	-1.134879	-3.415566	0.751484
C	0.127638	-4.026881	0.624089

C	0.531763	-4.493840	-0.627496
H	1.488906	-4.996291	-0.715928
C	-0.278384	-4.368527	-1.747049
C	4.545140	-2.547380	-2.179560
C	4.353651	-3.350064	-1.070176
H	4.274741	-4.425765	-1.175863
C	4.231348	-2.726774	0.177116
C	4.333662	-1.327507	0.263181
C	4.616255	-0.511068	-0.837076
H	4.710458	0.563363	-0.728200
C	4.725306	-1.144334	-2.063251
C	2.826568	4.096481	-2.068402
C	1.444605	4.221559	-1.879770
C	0.914431	4.025805	-0.606211
H	-0.159469	3.981664	-0.458372
C	1.768209	3.831310	0.482452
C	3.153458	3.940137	0.304342
C	3.678844	4.042189	-0.974906
H	4.752835	4.052976	-1.124675
O	-3.840437	3.094738	-3.275134
O	-4.612772	0.475863	-3.077458
O	-2.360801	-3.730090	-2.714870
O	0.103063	-4.880567	-2.971836
O	4.490198	-3.092042	-3.454522
O	5.092877	-0.469169	-3.210969
O	3.336024	3.997363	-3.343849
O	0.696868	4.640631	-2.956684
H	-3.921294	0.500848	-7.269123
H	0.651507	4.132324	-7.225657
H	3.829901	-2.203439	-7.478670
H	-0.515290	-4.296451	-7.071887
H	4.060947	-0.086715	1.959695
H	1.594281	1.302961	-0.688598
C	1.138051	0.374703	-0.313692
H	1.973715	-0.334212	-0.217233
N	0.698010	0.617561	1.051314
C	0.132894	-0.144998	-1.331188
H	-0.336791	-1.063815	-0.948356
C	0.889566	-0.488340	-2.609357
H	0.194020	-0.760500	-3.408649
H	1.456657	0.386949	-2.952714
H	1.592578	-1.317952	-2.461166
C	-0.925164	0.907772	-1.633315
H	-1.643382	0.522741	-2.360492

H	-1.463895	1.274284	-0.753005
H	-0.425708	1.767288	-2.090060
H	1.086378	2.368247	1.746704
H	-2.103711	3.695230	0.807736
<b>7</b>			
C	-2.098273	-2.272071	2.294184
C	-2.294848	-2.207028	3.793448
H	-2.270154	-1.163872	4.112097
H	-3.276965	-2.623278	4.037864
H	-1.531324	-2.769147	4.334605
C	0.893217	-5.268390	2.676426
C	2.101625	-5.716055	3.461738
H	1.989423	-6.786707	3.648828
H	3.043324	-5.520270	2.947752
H	2.097237	-5.207266	4.429032
N	1.153106	-4.714635	1.460522
H	2.140191	-4.607990	1.220729
N	-1.275452	-3.268118	1.904793
H	-0.980304	-3.940337	2.621877
O	-2.664132	-1.490713	1.521672
O	-0.242801	-5.413636	3.125840
C	3.254141	1.890027	2.074348
C	3.483807	1.700987	3.561178
H	4.448217	2.146117	3.820982
H	2.701445	2.159909	4.169334
H	3.529944	0.634117	3.791409
C	-0.088764	4.400828	2.842209
C	-1.357576	4.683757	3.614281
H	-1.642658	5.727044	3.449983
H	-2.186523	4.043394	3.301091
H	-1.146373	4.534637	4.672237
N	-0.274981	4.101310	1.526365
H	-1.217959	4.276932	1.182810
N	2.323900	2.828004	1.790279
H	1.942433	3.355169	2.583550
O	3.903339	1.256219	1.241386
O	1.003162	4.466186	3.400519
C	-3.656861	5.109596	1.444910
C	-4.293379	5.998243	2.489443
H	-4.505656	5.448310	3.410079
H	-3.634927	6.841203	2.693323
H	-5.241663	6.379780	2.099824
C	-4.970899	1.252458	2.786179

C	-4.870125	0.293509	3.950609
H	-4.814952	-0.740055	3.601306
H	-3.960947	0.503492	4.523548
H	-5.739231	0.431398	4.591325
N	-4.113729	0.978041	1.764702
H	-3.600190	0.091160	1.815011
N	-4.175954	3.854873	1.383892
H	-4.907928	3.574845	2.043863
O	-2.744151	5.498963	0.720289
O	-5.750219	2.201578	2.796652
C	3.953721	-2.684988	2.122804
N	3.979859	-3.708986	1.288882
N	4.209879	-1.496366	1.506365
C	-1.104110	1.173471	3.453499
C	-0.156198	0.354007	2.897711
C	0.704681	-0.428211	3.759161
C	0.554299	-0.309704	5.183942
C	-0.438260	0.579378	5.705751
C	-1.236949	1.301875	4.866473
C	1.680898	-1.297076	3.261196
C	1.376726	-1.067344	6.026910
C	2.383385	-1.895314	5.522690
C	2.562413	-1.974143	4.102654
C	3.663643	-2.741689	3.573850
C	4.461967	-3.460426	4.419009
C	4.231077	-3.444538	5.826649
C	3.240820	-2.673997	6.363422
H	1.785025	-1.401313	2.192401
H	-1.760818	1.739029	2.794511
H	-0.536443	0.673250	6.783700
H	-1.978731	1.984459	5.271846
H	1.234405	-1.001138	7.103190
H	5.289202	-4.033291	4.011183
H	4.875711	-4.031275	6.472554
H	3.091285	-2.634017	7.438731
C	-0.057887	0.265831	1.419421
H	-1.007316	0.364776	0.875121
C	-3.153657	1.161785	-5.435954
H	-4.157539	1.470949	-5.135266
C	-3.114550	1.106254	-6.964712
H	-3.383671	2.081534	-7.376842
H	-2.126297	0.847766	-7.355078
C	-2.899334	-0.187391	-4.773747
C	-3.457372	-0.436148	-3.515174

C	-3.254996	-1.636547	-2.852641
H	-3.769630	-1.846210	-1.924284
C	-2.463551	-2.612469	-3.442901
C	-1.906015	-2.431976	-4.712133
C	-2.142096	-1.209326	-5.349137
H	-1.726337	-1.052827	-6.340237
C	-1.081297	-3.546804	-5.339159
H	-1.479846	-4.483611	-4.941827
C	-1.199967	-3.594242	-6.865500
H	-2.250535	-3.645334	-7.163395
H	-0.755391	-2.720560	-7.350033
C	0.374864	-3.481577	-4.892553
C	0.854993	-4.322747	-3.887195
C	2.190666	-4.317306	-3.523388
H	2.546872	-5.022211	-2.785673
C	3.062562	-3.391281	-4.073379
C	2.626508	-2.490439	-5.049862
C	1.288117	-2.579719	-5.445816
H	0.924780	-1.877649	-6.193358
C	3.570998	-1.443129	-5.628013
H	4.582473	-1.773443	-5.380115
C	3.466301	-1.346856	-7.152200
H	2.467401	-1.060839	-7.492490
H	4.172740	-0.605167	-7.533670
C	3.375447	-0.102789	-4.929026
C	4.065061	0.159965	-3.740363
C	3.939313	1.376824	-3.082440
H	4.557553	1.605433	-2.224357
C	3.073824	2.339914	-3.584944
C	2.366266	2.129323	-4.771825
C	2.539174	0.902086	-5.417771
H	2.013041	0.730849	-6.352517
C	1.491583	3.241389	-5.326294
H	1.911608	4.176420	-4.949103
C	1.505912	3.305273	-6.857399
H	2.533375	3.378451	-7.223041
H	1.046319	2.428405	-7.321574
C	0.072312	3.162522	-4.783827
C	-0.350628	4.001551	-3.748935
C	-1.670788	4.002156	-3.324976
H	-1.992533	4.684822	-2.547331
C	-2.576148	3.104018	-3.876318
C	-2.191120	2.201481	-4.870535
C	-0.863272	2.266108	-5.300381

H	-0.534895	1.566653	-6.066042
C	-3.980236	2.622691	-2.105475
C	-3.974975	3.477616	-1.019714
H	-3.923189	4.546567	-1.184578
C	-4.048970	2.975045	0.284766
C	-4.104572	1.589141	0.484212
C	-4.154446	0.734235	-0.623657
H	-4.262539	-0.330465	-0.451638
C	-4.120277	1.243004	-1.911154
C	-1.482541	-3.960931	-1.747338
C	-1.809380	-3.479311	-0.485791
H	-2.728986	-2.932612	-0.329206
C	-0.959204	-3.697830	0.603306
C	0.216631	-4.448144	0.422642
C	0.520186	-4.938748	-0.847918
H	1.411009	-5.542828	-0.980859
C	-0.307944	-4.693374	-1.933855
C	4.461901	-2.889767	-2.313198
C	4.294115	-3.730718	-1.227230
H	4.185474	-4.800024	-1.368280
C	4.243118	-3.148512	0.046987
C	4.389244	-1.757526	0.174084
C	4.651705	-0.909176	-0.900709
H	4.790087	0.152302	-0.746536
C	4.675609	-1.497638	-2.149622
C	2.234827	3.692854	-1.831392
C	1.013268	4.367453	-1.907300
C	0.259046	4.529130	-0.755401
H	-0.685793	5.062406	-0.800087
C	0.669707	3.993795	0.466652
C	1.900777	3.314292	0.545828
C	2.680397	3.200994	-0.610368
H	3.637705	2.703618	-0.540998
O	-3.883158	3.111216	-3.392352
O	-4.362895	0.482727	-3.024812
O	-2.339090	-3.841675	-2.818482
O	-0.002760	-5.172986	-3.194463
O	4.374233	-3.372473	-3.611231
O	4.970529	-0.780143	-3.288767
O	3.008408	3.581471	-2.968595
O	0.558154	4.849145	-3.123350
H	-3.824825	0.362356	-7.335155
H	0.949968	4.182830	-7.196062
H	3.699019	-2.315391	-7.601139



H	-0.683391	-4.477160	-7.248949
H	4.171549	-0.544183	1.870603
H	1.967049	0.528237	-0.914185
C	1.214977	-0.185562	-0.543432
H	1.706624	-1.169782	-0.616060
N	1.065198	0.056906	0.872263
C	-0.006067	-0.168681	-1.454385
H	-0.792437	-0.806288	-1.018358
C	0.430619	-0.759930	-2.789902
H	-0.354462	-0.664687	-3.544145
H	1.313421	-0.224246	-3.161991
H	0.698205	-1.818698	-2.691468
C	-0.544905	1.238761	-1.680345
H	-1.395783	1.209044	-2.366406
H	-0.860750	1.754775	-0.766256
H	0.234017	1.845659	-2.154766

**1·H<sub>2</sub>O**

C	-2.824247	-2.643659	2.334345
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H	-4.053590	-2.959683	4.049509
H	-2.351068	-3.409239	4.326694
C	0.784896	-4.977059	2.702016
C	2.038022	-5.324033	3.469840
H	1.957367	-6.371989	3.764565
H	2.951898	-5.160076	2.897109
H	2.069728	-4.723767	4.384238
N	0.977786	-4.317177	1.520673
H	1.952260	-4.182039	1.256281
N	-1.692885	-3.288436	1.926276
H	-1.258434	-3.893904	2.625629
O	-3.619669	-2.067986	1.601470
O	-0.324645	-5.270304	3.137103
C	3.293153	2.419425	2.175582
C	3.771659	2.377654	3.607555
H	4.847020	2.185066	3.612663
H	3.564842	3.298889	4.153632
H	3.280713	1.536603	4.106646
C	0.705869	5.701559	2.649707
C	-0.371143	6.285475	3.533594
H	-1.279978	6.498360	2.968309
H	-0.600384	5.577908	4.336802
H	0.020340	7.194580	3.989326

N	0.244192	5.042489	1.558616
H	-0.765864	5.059547	1.389767
N	2.723579	3.569021	1.787255
H	2.648923	4.356010	2.448296
O	3.407776	1.421279	1.443917
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C	-3.471839	4.907484	1.773859
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H	-3.112301	5.199919	3.865556
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H	-4.836348	5.170111	3.458639
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H	-4.877174	3.454762	2.115088
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N	4.039245	-3.496506	1.253482
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C	-0.496316	-0.050641	3.154891
C	0.568211	-0.625724	3.936442
C	0.510127	-0.530471	5.371345
C	-0.572043	0.179569	5.980524
C	-1.545312	0.742067	5.211341
C	1.653647	-1.287914	3.353326
C	1.492506	-1.154450	6.141685
C	2.558852	-1.841447	5.556991
C	2.665399	-1.866658	4.127655
C	3.794397	-2.534164	3.537893
C	4.690816	-3.206456	4.321638
C	4.549361	-3.223694	5.738610
C	3.530456	-2.542557	6.337494
H	1.703927	-1.397848	2.274128
H	-2.324303	0.997592	3.183397
H	-0.599020	0.254779	7.063850
H	-2.364648	1.282290	5.676961
H	1.417797	-1.116911	7.226156

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H	5.273582	-3.765522	6.337224
H	3.431206	-2.529302	7.419157
C	-0.584911	-0.229874	1.629453
H	-0.276141	-1.264404	1.377553
O	-1.700801	0.175990	1.083061
C	-3.114474	1.383042	-5.462345
H	-4.113134	1.706787	-5.161295
C	-3.077509	1.327812	-6.991287
H	-3.314585	2.311161	-7.404386
H	-2.100612	1.033892	-7.385027
C	-2.879741	0.028795	-4.803683
C	-3.506729	-0.241001	-3.583553
C	-3.330221	-1.449040	-2.925922
H	-3.878057	-1.672240	-2.020367
C	-2.507070	-2.414924	-3.488385
C	-1.875609	-2.208381	-4.718836
C	-2.073873	-0.973055	-5.344647
H	-1.600052	-0.797119	-6.306313
C	-1.039181	-3.317174	-5.339281
H	-1.435778	-4.254859	-4.942618
C	-1.156950	-3.368180	-6.866149
H	-2.207108	-3.437024	-7.161163
H	-0.730305	-2.487208	-7.353561
C	0.414580	-3.248607	-4.891235
C	0.878848	-4.067687	-3.859673
C	2.218508	-4.094491	-3.512719
H	2.563628	-4.795046	-2.765168
C	3.107283	-3.203195	-4.096268
C	2.682595	-2.310148	-5.082828
C	1.341013	-2.382190	-5.472294
H	0.990765	-1.697543	-6.241502
C	3.630765	-1.275785	-5.675540
H	4.642176	-1.604030	-5.424992
C	3.526109	-1.191715	-7.200379
H	2.528874	-0.903266	-7.543100
H	4.236219	-0.456674	-7.587859
C	3.432832	0.070695	-4.988420
C	4.128610	0.344784	-3.807802
C	4.013432	1.567498	-3.161541
H	4.646301	1.808410	-2.317662
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C	2.421569	2.302790	-4.840749
C	2.589277	1.069665	-5.477033

H	2.054293	0.889726	-6.405064
C	1.545192	3.411930	-5.399114
H	1.972783	4.349293	-5.036501
C	1.545743	3.460167	-6.930387
H	2.569491	3.535664	-7.305980
H	1.087432	2.577022	-7.383344
C	0.135750	3.337190	-4.833145
C	-0.259525	4.156804	-3.774563
C	-1.562153	4.143860	-3.300007
H	-1.861045	4.804669	-2.495055
C	-2.490251	3.269770	-3.851898
C	-2.135385	2.399498	-4.888194
C	-0.818825	2.461844	-5.347921
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C	-3.937298	2.763125	-2.094831
C	-3.901911	3.566671	-0.964981
H	-3.760402	4.636246	-1.060928
C	-4.068122	3.001059	0.303087
C	-4.245011	1.617738	0.423406
C	-4.316848	0.826249	-0.720557
H	-4.506561	-0.233575	-0.601300
C	-4.186766	1.391953	-1.974284
C	-1.611718	-3.770695	-1.766584
C	-2.054865	-3.388515	-0.505429
H	-3.035512	-2.951791	-0.376667
C	-1.252585	-3.579767	0.626080
C	0.031088	-4.144337	0.464179
C	0.441443	-4.554312	-0.805134
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C	-0.368554	-4.388653	-1.918981
C	4.507362	-2.699752	-2.352199
C	4.346350	-3.530669	-1.258722
H	4.267106	-4.604108	-1.386752
C	4.262596	-2.933925	0.005341
C	4.353188	-1.536126	0.118744
C	4.609039	-0.695977	-0.962474
H	4.729586	0.370542	-0.827484
C	4.691521	-1.302307	-2.201775
C	2.368742	3.937581	-1.904955
C	1.150064	4.627181	-1.976758
C	0.481631	4.957242	-0.811435
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C	0.995169	4.611670	0.439600
C	2.186059	3.876589	0.512207

C	2.872190	3.561484	-0.666278
H	3.825361	3.050775	-0.599008
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O	-4.424141	0.679006	-3.124755
O	-2.421375	-3.656420	-2.875584
O	0.000100	-4.880296	-3.158388
O	4.425437	-3.198473	-3.642101
O	5.019483	-0.600340	-3.338216
O	3.096949	3.770335	-3.061311
O	0.661196	5.028832	-3.200307
H	-3.812800	0.607491	-7.359059
H	0.982178	4.331659	-7.271862
H	3.754140	-2.165004	-7.641221
H	-0.626317	-4.242815	-7.249942
H	4.075779	-0.330750	1.839826
H	1.973313	0.686345	-0.606068
C	1.142328	0.048186	-0.278350
H	1.553007	-0.945171	-0.048384
N	0.643617	0.609652	1.006342
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H	-0.727517	-0.705614	-1.027339
C	0.755383	-0.655733	-2.600904
H	0.033505	-0.752057	-3.417307
H	1.564285	-0.000376	-2.948401
H	1.181710	-1.647072	-2.398741
C	-0.494843	1.315586	-1.716625
H	-1.164829	1.221623	-2.577126
H	-1.063609	1.763686	-0.896387
H	0.312051	2.003015	-2.004556
H	1.450107	0.688386	1.632303
H	0.250219	1.563223	0.891125
O	-1.237456	2.681337	1.304542
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H	-1.631301	1.748366	1.208269
<b>TS<sub>1-H2O</sub></b>			
C	-2.594308	-2.620786	2.437556
C	-2.800631	-2.708630	3.937156
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H	-3.811768	-3.077533	4.125884
H	-2.080358	-3.366597	4.427118
C	0.865239	-5.142408	2.709996
C	2.111579	-5.526460	3.470871
H	2.035198	-6.589857	3.706545

H	3.031023	-5.325070	2.919598
H	2.126790	-4.976678	4.416570
N	1.072561	-4.486209	1.532815
H	2.049419	-4.346577	1.275284
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H	-1.133167	-4.008189	2.671782
O	-3.329592	-1.949472	1.720995
O	-0.250256	-5.410987	3.149458
C	3.302592	2.498395	2.141377
C	3.792341	2.474170	3.570692
H	4.855240	2.221662	3.572832
H	3.643303	3.422348	4.088755
H	3.261477	1.678627	4.101159
C	0.794432	5.808103	2.576789
C	-0.275823	6.376956	3.478820
H	-1.205111	6.556605	2.935663
H	-0.464329	5.675235	4.297436
H	0.102432	7.302681	3.911903
N	0.325435	5.137884	1.496526
H	-0.686759	5.122385	1.343855
N	2.807421	3.671538	1.721347
H	2.759887	4.470664	2.368226
O	3.353785	1.474252	1.440805
O	1.990372	5.939414	2.843983
C	-3.386192	4.832947	1.840610
C	-3.715016	5.382515	3.217052
H	-2.914134	5.109352	3.910383
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H	-4.657495	4.996320	3.609373
C	-5.228631	1.141424	2.732891
C	-5.251511	0.065807	3.795603
H	-4.880962	-0.887140	3.415153
H	-4.632464	0.381345	4.641035
H	-6.276296	-0.036107	4.154663
N	-4.434550	0.864606	1.674096
H	-3.907673	-0.012428	1.680961
N	-4.067675	3.709179	1.538294
H	-4.784536	3.382871	2.196005
O	-2.554715	5.379433	1.114340
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C	-1.707270	0.781547	5.149595
C	1.448683	-1.328781	3.304909
C	1.212881	-1.287591	6.091423
C	2.294170	-1.955525	5.512464
C	2.440608	-1.933459	4.085925
C	3.602780	-2.556539	3.510952
C	4.495187	-3.225404	4.303507
C	4.311172	-3.295720	5.713324
C	3.254124	-2.664078	6.300246
H	1.523691	-1.407019	2.223757
H	-2.385406	1.197438	3.113756
H	-0.857497	0.156110	7.007517
H	-2.503261	1.357644	5.612171
H	1.109287	-1.286894	7.174108
H	5.356725	-3.698525	3.842901
H	5.031954	-3.836961	6.316605
H	3.120565	-2.688297	7.378032
C	-0.654597	-0.084557	1.571444
H	-0.475025	-1.130238	1.272881
O	-1.766756	0.419499	1.000932
C	-3.116593	1.388514	-5.433934
H	-4.109629	1.719154	-5.122359
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H	-3.334181	2.303855	-7.380372
H	-2.131660	1.015789	-7.367508
C	-2.878291	0.038088	-4.768208
C	-3.503343	-0.229914	-3.547331
C	-3.295675	-1.423026	-2.869874
H	-3.827041	-1.640627	-1.953060
C	-2.461094	-2.383754	-3.424012
C	-1.850907	-2.188454	-4.667649
C	-2.063896	-0.960871	-5.302790
H	-1.598247	-0.789869	-6.269265
C	-1.029908	-3.305174	-5.295030
H	-1.429799	-4.238839	-4.892104
C	-1.165956	-3.358542	-6.820364
H	-2.220016	-3.415716	-7.103802
H	-0.733904	-2.484095	-7.314697
C	0.428995	-3.248098	-4.865306
C	0.902746	-4.075984	-3.845678

C	2.244823	-4.102017	-3.508032
H	2.595836	-4.803053	-2.763878
C	3.127985	-3.205195	-4.092126
C	2.694979	-2.309979	-5.072863
C	1.350345	-2.379666	-5.450781
H	0.993108	-1.688815	-6.211256
C	3.636607	-1.275450	-5.673858
H	4.650070	-1.596206	-5.421689
C	3.529405	-1.205877	-7.199404
H	2.529211	-0.928628	-7.542878
H	4.233122	-0.468711	-7.594474
C	3.433616	0.076104	-4.999234
C	4.127750	0.360927	-3.820110
C	4.023794	1.594630	-3.194590
H	4.659081	1.840969	-2.353810
C	3.160015	2.549213	-3.712491
C	2.430587	2.313831	-4.881369
C	2.591433	1.070344	-5.499477
H	2.053246	0.878469	-6.423294
C	1.549501	3.415366	-5.450510
H	1.980238	4.357596	-5.104662
C	1.539394	3.440703	-6.982135
H	2.560219	3.515114	-7.365826
H	1.082588	2.548840	-7.419297
C	0.144264	3.349173	-4.870888
C	-0.234126	4.173330	-3.809806
C	-1.525400	4.152522	-3.304439
H	-1.809224	4.813034	-2.493995
C	-2.459303	3.268972	-3.829993
C	-2.125530	2.405518	-4.879779
C	-0.819147	2.472117	-5.367179
H	-0.533754	1.796015	-6.169269
C	-3.898170	2.740874	-2.048616
C	-3.826781	3.523420	-0.904939
H	-3.620328	4.583645	-0.979001
C	-4.034769	2.949048	0.354627
C	-4.314099	1.580403	0.453615
C	-4.415978	0.814618	-0.703829
H	-4.682761	-0.231272	-0.613068
C	-4.217376	1.382756	-1.946456
C	-1.527711	-3.755044	-1.710974
C	-1.933883	-3.373710	-0.435753
H	-2.893019	-2.896586	-0.287118
C	-1.124753	-3.625172	0.680550



C	0.126569	-4.247966	0.491435
C	0.503257	-4.646678	-0.791464
H	1.439012	-5.179452	-0.922299
C	-0.311864	-4.419889	-1.890832
C	4.513688	-2.687454	-2.349558
C	4.351564	-3.518899	-1.257843
H	4.296702	-4.593974	-1.384513
C	4.218087	-2.920065	0.000432
C	4.260859	-1.520231	0.112600
C	4.524758	-0.676339	-0.965333
H	4.604946	0.394724	-0.832733
C	4.661833	-1.285392	-2.199245
C	2.417253	3.993086	-1.969899
C	1.197047	4.679141	-2.039191
C	0.543229	5.030439	-0.872885
H	-0.381486	5.595100	-0.920615
C	1.069314	4.700973	0.376228
C	2.259614	3.967516	0.447774
C	2.935632	3.637693	-0.731481
H	3.892751	3.133881	-0.666245
O	-3.746844	3.287263	-3.310767
O	-4.444109	0.674984	-3.102409
O	-2.358841	-3.618935	-2.800655
O	0.028835	-4.895464	-3.143669
O	4.447321	-3.191615	-3.638937
O	5.007453	-0.585069	-3.331684
O	3.130005	3.806925	-3.133340
O	0.692816	5.056478	-3.264554
H	-3.846843	0.605057	-7.315173
H	0.969663	4.304533	-7.332789
H	3.764605	-2.181300	-7.631709
H	-0.649857	-4.240378	-7.207407
H	3.911540	-0.318161	1.825385
H	1.932248	0.800485	-0.539620
C	1.106897	0.146282	-0.234437
H	1.532879	-0.838316	0.008502
N	0.557974	0.706401	1.029905
C	0.092469	0.007857	-1.361680
H	-0.749078	-0.609610	-1.020607
C	0.792355	-0.685785	-2.528021
H	0.100085	-0.799651	-3.367197
H	1.637542	-0.077765	-2.874838
H	1.174895	-1.679308	-2.257578
C	-0.438558	1.362761	-1.813545

H	-1.126822	1.219835	-2.652024
H	-0.964833	1.911501	-1.026860
H	0.393497	1.982290	-2.174760
H	1.331295	0.753086	1.697375
H	0.109482	1.725321	0.962342
O	-1.036731	2.681227	1.140353
H	-1.049140	3.008488	2.047642
H	-1.609780	1.587195	1.075797

**2·H<sub>2</sub>O**

C	-2.892233	-2.755362	2.339981
C	-3.083708	-2.777184	3.844541
H	-2.902256	-1.772631	4.236624
H	-4.118059	-3.049736	4.062197
H	-2.410821	-3.475774	4.345461
C	0.730649	-5.048112	2.751768
C	1.982912	-5.387287	3.523465
H	1.905181	-6.435084	3.819924
H	2.897300	-5.221435	2.952180
H	2.009892	-4.785524	4.437032
N	0.922362	-4.402706	1.562850
H	1.896793	-4.259763	1.300856
N	-1.768797	-3.411575	1.941818
H	-1.329691	-4.006286	2.650130
O	-3.688150	-2.187277	1.596394
O	-0.379288	-5.338997	3.189791
C	3.264695	2.324233	2.118438
C	3.683206	2.265332	3.570110
H	4.753613	2.052744	3.618209
H	3.470459	3.185555	4.115868
H	3.156767	1.430268	4.042760
C	0.769871	5.720365	2.553355
C	-0.293605	6.350862	3.422814
H	-1.225815	6.507759	2.877688
H	-0.479804	5.705442	4.286802
H	0.093978	7.298913	3.796030
N	0.294638	5.055930	1.470270
H	-0.714756	5.084387	1.305214
N	2.703141	3.482626	1.728861
H	2.641653	4.265222	2.391311
O	3.420073	1.343292	1.379239
O	1.962519	5.796608	2.848638
C	-3.408746	4.716460	1.771207
C	-3.741655	5.291289	3.136008

H	-2.931727	5.051605	3.831213
H	-3.803877	6.377216	3.052854
H	-4.674569	4.897182	3.542966
C	-5.279804	1.012572	2.695218
C	-5.371862	-0.074833	3.740529
H	-5.251592	-1.063539	3.294360
H	-4.580096	0.069221	4.483795
H	-6.334585	0.012249	4.242767
N	-4.459735	0.716765	1.653790
H	-4.057984	-0.224953	1.635937
N	-4.070975	3.572265	1.496867
H	-4.785160	3.254429	2.160765
O	-2.589429	5.261312	1.030473
O	-5.880910	2.079168	2.819017
C	3.942373	-2.552697	2.110943
N	3.999084	-3.591717	1.302003
N	4.124410	-1.361621	1.469486
C	-1.576418	0.528221	3.707713
C	-0.551331	-0.145560	3.104082
C	0.492151	-0.717663	3.915315
C	0.402107	-0.620423	5.346006
C	-0.692863	0.095959	5.924658
C	-1.639783	0.665953	5.128110
C	1.588983	-1.375429	3.350788
C	1.371404	-1.241533	6.136289
C	2.452806	-1.922465	5.571497
C	2.587397	-1.947557	4.144206
C	3.730964	-2.604511	3.570927
C	4.620728	-3.266370	4.370713
C	4.454682	-3.283127	5.785501
C	3.417973	-2.614525	6.368141
H	1.669210	-1.462949	2.271805
H	-2.372436	0.942599	3.094778
H	-0.748740	0.175887	7.006540
H	-2.464321	1.217732	5.570445
H	1.276883	-1.202466	7.219115
H	5.465481	-3.773322	3.915264
H	5.174519	-3.816875	6.396670
H	3.301001	-2.603641	7.448057
C	-0.519706	-0.346533	1.593964
H	-0.326826	-1.413177	1.400663
O	-1.759841	-0.084858	1.003542
C	-3.111579	1.225267	-5.454448
H	-4.103545	1.563589	-5.147615

C	-3.088769	1.159511	-6.983470
H	-3.314753	2.143474	-7.401373
H	-2.119921	0.848234	-7.383452
C	-2.888722	-0.128064	-4.791083
C	-3.535657	-0.403675	-3.583529
C	-3.364682	-1.612291	-2.926360
H	-3.921423	-1.837556	-2.026518
C	-2.530186	-2.574662	-3.477758
C	-1.877246	-2.362626	-4.695912
C	-2.068578	-1.125428	-5.319488
H	-1.576162	-0.943342	-6.270619
C	-1.034673	-3.469599	-5.312600
H	-1.431695	-4.407236	-4.916177
C	-1.151619	-3.521675	-6.839615
H	-2.201329	-3.595621	-7.134977
H	-0.729340	-2.638788	-7.327296
C	0.418708	-3.402389	-4.862831
C	0.874491	-4.211047	-3.819447
C	2.212066	-4.242717	-3.466357
H	2.549782	-4.935289	-2.708046
C	3.109430	-3.365028	-4.057902
C	2.694391	-2.484403	-5.059604
C	1.353953	-2.552910	-5.453978
H	1.012449	-1.876575	-6.234298
C	3.650184	-1.462633	-5.661427
H	4.658661	-1.790733	-5.399042
C	3.555889	-1.400801	-7.188036
H	2.561673	-1.114645	-7.541507
H	4.270360	-0.673110	-7.581348
C	3.451461	-0.105700	-4.995278
C	4.140248	0.182742	-3.814168
C	4.025490	1.415467	-3.187354
H	4.652157	1.665975	-2.341687
C	3.154228	2.362644	-3.704969
C	2.438307	2.127274	-4.882149
C	2.610191	0.886459	-5.501898
H	2.079242	0.693168	-6.429628
C	1.562029	3.229801	-5.456324
H	1.995415	4.171934	-5.113336
C	1.553727	3.250403	-6.988027
H	2.575400	3.319933	-7.370335
H	1.094709	2.358633	-7.423023
C	0.155998	3.170476	-4.878943
C	-0.227785	4.004840	-3.827862

C	-1.521144	3.986769	-3.326218
H	-1.806959	4.653980	-2.521883
C	-2.452874	3.101735	-3.851660
C	-2.116365	2.233997	-4.896093
C	-0.806956	2.292273	-5.374945
H	-0.518742	1.610471	-6.171159
C	-3.899814	2.574105	-2.080353
C	-3.826151	3.359716	-0.939242
H	-3.618777	4.419185	-1.019054
C	-4.039870	2.796347	0.324074
C	-4.314902	1.424395	0.428522
C	-4.411570	0.651794	-0.727908
H	-4.671754	-0.395805	-0.631689
C	-4.220868	1.216292	-1.975261
C	-1.650390	-3.919838	-1.747030
C	-2.111624	-3.541667	-0.491499
H	-3.102001	-3.124089	-0.374546
C	-1.314554	-3.710305	0.646210
C	-0.019815	-4.252123	0.499326
C	0.408672	-4.660369	-0.764454
H	1.381403	-5.130309	-0.862094
C	-0.394946	-4.515422	-1.885837
C	4.497640	-2.844092	-2.310514
C	4.328347	-3.660605	-1.207632
H	4.251787	-4.735825	-1.322361
C	4.231588	-3.046675	0.047601
C	4.315556	-1.647269	0.141606
C	4.579708	-0.821045	-0.948601
H	4.690498	0.247966	-0.825675
C	4.678549	-1.444297	-2.177924
C	2.384518	3.815513	-1.969424
C	1.185234	4.534919	-2.056287
C	0.534966	4.923134	-0.899064
H	-0.369368	5.518712	-0.963473
C	1.038176	4.587608	0.357993
C	2.197302	3.804546	0.447286
C	2.875321	3.446670	-0.723582
H	3.807926	2.901801	-0.646242
O	-3.744544	3.121117	-3.339629
O	-4.464370	0.511031	-3.128042
O	-2.451528	-3.816301	-2.863120
O	-0.013120	-5.013574	-3.117151
O	4.424237	-3.360508	-3.595121
O	5.020943	-0.759900	-3.321927

O	3.107332	3.619038	-3.123944
O	0.691932	4.900209	-3.289621
H	-3.837715	0.447547	-7.339692
H	0.987581	4.115110	-7.342387
H	3.784343	-2.380932	-7.613324
H	-0.616554	-4.393875	-7.222844
H	4.012468	-0.414505	1.834164
H	1.935231	0.506472	-0.542946
C	1.087299	-0.122898	-0.242629
H	1.488763	-1.135855	-0.038196
N	0.532907	0.470172	0.980812
C	0.093269	-0.216491	-1.398122
H	-0.713822	-0.910255	-1.122428
C	0.825998	-0.765805	-2.617326
H	0.136808	-0.881444	-3.459456
H	1.613022	-0.066769	-2.926164
H	1.293632	-1.739153	-2.417333
C	-0.516791	1.139964	-1.734971
H	-1.074554	1.072552	-2.674876
H	-1.202885	1.509277	-0.967792
H	0.275490	1.888980	-1.870182
H	1.303454	0.615752	1.628694
H	-0.367560	2.099634	0.969132
O	-1.162957	2.620997	1.239920
H	-0.991670	2.832294	2.165572
H	-1.870668	0.885990	0.998497

**1'**

C	-1.191953	-0.254632	0.000000
C	0.062219	-0.863628	0.000000
C	1.224173	-0.087203	0.000000
C	1.125225	1.296966	0.000000
C	-0.131250	1.905501	0.000000
C	-1.290257	1.133003	0.000000
H	-2.087962	-0.870963	0.000000
H	-0.205715	2.988450	0.000000
H	-2.263959	1.611590	0.000000
C	0.161379	-2.343214	0.000000
H	-0.813215	-2.876681	0.000000
O	1.204102	-2.953498	0.000000
H	2.184883	-0.592785	0.000000
H	2.022430	1.907194	0.000000

**2'**

H	1.350300	-0.256100	-0.239400
C	0.825900	-0.151400	0.720200
H	1.081700	-1.041400	1.308000
N	1.377900	1.011400	1.405200
C	-0.686900	-0.150900	0.454100
H	-1.195400	-0.072700	1.427000
C	-1.102500	-1.465000	-0.204700
H	-2.183700	-1.506400	-0.364500
H	-0.617300	-1.573000	-1.181800
H	-0.816700	-2.326100	0.407100
C	-1.104100	1.042100	-0.403900
H	-2.181400	1.037200	-0.592400
H	-0.857100	1.992900	0.077400
H	-0.594400	1.009900	-1.374500
H	1.254600	1.844700	0.838300
H	0.872500	1.173700	2.272200

**3'**

C	-2.266092	0.700286	3.390682
C	-1.514458	-0.438876	3.099193
C	-0.518243	-0.866577	3.975895
C	-0.270554	-0.158401	5.146453
C	-1.022455	0.978816	5.437605
C	-2.019239	1.407956	4.561372
H	0.066040	-1.748221	3.724050
H	0.504647	-0.487641	5.830807
H	-3.035458	1.006887	2.688379
H	-0.831164	1.532714	6.351428
H	-2.602001	2.292901	4.796022
C	-1.768792	-1.198864	1.845886
H	-1.172939	-2.123513	1.729475
O	-2.575402	-0.856843	1.010707
H	1.869967	0.294547	-0.760086
C	1.192432	-0.486256	-0.369645
H	1.738715	-1.435121	-0.426368
N	0.808265	-0.278356	1.027199
C	-0.032056	-0.563789	-1.281646
H	-0.671324	-1.374382	-0.909177
C	0.405687	-0.882832	-2.710110
H	-0.459042	-0.981924	-3.372025
H	1.039624	-0.081731	-3.108158
H	0.975847	-1.816114	-2.756434
C	-0.842920	0.731069	-1.239240
H	-1.686308	0.679267	-1.933573

H	-1.261773	0.914468	-0.246134
H	-0.219627	1.586509	-1.529174
H	1.626856	-0.321419	1.627548
H	0.425966	0.656337	1.148369

**TS<sub>1</sub>'**

C	-2.270567	0.716405	3.454882
C	-1.498715	-0.375499	3.069796
C	-0.487729	-0.843127	3.910825
C	-0.241092	-0.213241	5.126548
C	-1.012604	0.883829	5.508167
C	-2.027883	1.344618	4.673914
H	0.102972	-1.709327	3.615600
H	0.544448	-0.579499	5.780247
H	-3.057323	1.035782	2.778788
H	-0.825323	1.372571	6.459188
H	-2.633242	2.193669	4.976156
C	-1.771633	-1.019841	1.720337
H	-1.688581	-2.123030	1.809861
O	-2.795751	-0.530834	1.008158
H	0.716919	-1.171114	-0.763983
C	-0.042147	-1.633938	-0.121878
H	0.465461	-2.360490	0.524264
N	-0.630934	-0.580456	0.727054
C	-1.084941	-2.334173	-0.997282
H	-1.882248	-2.716038	-0.347935
C	-0.411531	-3.509273	-1.706702
H	-1.135437	-4.055026	-2.316771
H	0.384462	-3.155900	-2.372615
H	0.029842	-4.213992	-0.995335
C	-1.718697	-1.374622	-2.004868
H	-2.359517	-1.927649	-2.697158
H	-2.343525	-0.632482	-1.503662
H	-0.948735	-0.865285	-2.596822
H	0.072504	0.025253	1.150058
H	-1.620354	-0.092194	0.340268

**4'**

C	-2.127343	0.595276	3.686116
C	-1.055105	-0.043826	3.069758
C	0.047591	-0.421893	3.841208
C	0.085578	-0.149021	5.203919
C	-0.983997	0.505717	5.811896
C	-2.088985	0.873539	5.051045



H	0.879216	-0.944358	3.371971
H	0.947069	-0.448528	5.792394
H	-2.992393	0.859372	3.088276
H	-0.956758	0.721675	6.875105
H	-2.928021	1.376391	5.521731
C	-1.077462	-0.356809	1.579388
H	-1.076774	-1.452958	1.452744
O	-2.273479	0.071216	0.960644
H	1.592774	-0.084411	-0.448271
C	0.631626	-0.539337	-0.176300
H	0.839599	-1.579776	0.132410
N	0.063650	0.239578	0.919672
C	-0.265828	-0.565166	-1.417504
H	-1.247183	-0.950541	-1.112809
C	0.330901	-1.504469	-2.463953
H	-0.298040	-1.545948	-3.357553
H	1.323963	-1.156731	-2.772456
H	0.436206	-2.522690	-2.076889
C	-0.454577	0.838695	-1.986415
H	-1.148080	0.830811	-2.832108
H	-0.839594	1.522165	-1.226419
H	0.503298	1.238551	-2.340458
H	0.770760	0.518756	1.587791
H	-2.116911	0.996918	0.730368

**5'**

C	-2.208531	0.430743	3.647601
C	-1.039764	-0.068943	3.072581
C	0.112841	-0.177780	3.852999
C	0.097145	0.210146	5.189086
C	-1.070171	0.712297	5.758619
C	-2.221087	0.821790	4.983893
H	1.019628	-0.559987	3.396526
H	1.000161	0.123995	5.785650
H	-3.099709	0.516192	3.037371
H	-1.081846	1.017617	6.800325
H	-3.134395	1.215078	5.419609
C	-1.021212	-0.533482	1.624706
H	-1.129020	-1.630236	1.598022
O	-2.147039	0.060395	0.983318
H	1.626213	-0.644380	-0.458301
C	0.580695	-0.893793	-0.232439
H	0.554112	-1.978169	-0.059639
N	0.248904	-0.240570	1.022099

C	-0.255086	-0.566968	-1.485540
H	-1.256173	-1.011323	-1.371240
C	0.393162	-1.225340	-2.702907
H	-0.209914	-1.075996	-3.602645
H	1.382044	-0.790089	-2.886542
H	0.523099	-2.302133	-2.555102
C	-0.403903	0.939319	-1.684534
H	-0.935488	1.162188	-2.614191
H	-0.954597	1.394452	-0.857408
H	0.584303	1.411654	-1.746168
H	0.399090	0.763551	0.990674
H	-2.324760	-0.424928	0.171377
<b>6'</b>			
C	1.351408	0.914041	2.851318
C	0.306128	-0.009331	2.798827
C	-0.200815	-0.530666	3.993133
C	0.311577	-0.112896	5.218995
C	1.340989	0.824637	5.265554
C	1.862475	1.331548	4.078548
H	-1.008668	-1.254107	3.952682
H	-0.093257	-0.522142	6.139441
H	1.753272	1.299159	1.920013
H	1.737836	1.152885	6.220819
H	2.673124	2.053242	4.106225
C	-0.267074	-0.457135	1.462410
H	0.199625	-1.407202	1.158115
O	-1.665159	-0.742235	1.726645
H	0.201861	0.915005	-1.555459
C	-0.262094	0.138816	-0.932725
H	0.272598	-0.796348	-1.151388
N	-0.011242	0.498080	0.448660
C	-1.729375	0.003416	-1.389013
H	-2.150715	-0.930090	-0.979494
C	-1.772312	-0.125667	-2.911125
H	-2.791881	-0.298136	-3.266232
H	-1.406094	0.795596	-3.377810
H	-1.145629	-0.952237	-3.261232
C	-2.571705	1.182990	-0.907713
H	-3.591934	1.121304	-1.297192
H	-2.621907	1.226110	0.183677
H	-2.133756	2.127799	-1.249652
H	-0.344775	1.432780	0.701320
H	-2.059696	-1.088803	0.918345

O	-0.844525	3.068560	1.606766
H	-0.097810	3.154958	2.209766
H	-1.548093	2.667459	2.156850
O	-2.541914	1.513966	3.131987
H	-2.409287	0.685274	2.635678
H	-2.046831	1.369543	3.947032

**TS<sub>2</sub>'**

C	1.331491	0.998000	2.954227
C	0.415261	-0.042016	2.776365
C	0.012057	-0.801945	3.878559
C	0.500382	-0.502628	5.144259
C	1.398732	0.548287	5.321380
C	1.815830	1.295723	4.224255
H	-0.715987	-1.590829	3.730254
H	0.176685	-1.089155	5.997975
H	1.680211	1.556269	2.091417
H	1.778913	0.777832	6.311797
H	2.529510	2.102873	4.353905
C	-0.047612	-0.381864	1.405492
H	-0.032949	-1.430720	1.112476
O	-2.023085	-0.723940	2.002650
H	0.154154	1.007440	-1.526333
C	-0.238111	0.178540	-0.926023
H	0.346894	-0.715723	-1.175244
N	-0.012142	0.520698	0.471177
C	-1.711315	-0.044427	-1.289704
H	-2.048611	-0.944917	-0.756314
C	-1.816033	-0.317489	-2.789534
H	-2.848217	-0.541314	-3.071340
H	-1.498513	0.562547	-3.359870
H	-1.190424	-1.162638	-3.093884
C	-2.579879	1.142957	-0.877063
H	-3.606876	1.001278	-1.227209
H	-2.606476	1.289137	0.206131
H	-2.196449	2.068052	-1.322071
H	-0.162308	1.595888	0.784431
H	-2.601608	-0.898065	1.250744
O	-0.657218	2.827790	1.250983
H	-0.053999	3.314842	1.820899
H	-1.461273	2.345863	1.906889
O	-2.327969	1.624498	2.495213
H	-2.208953	0.341804	2.285143
H	-2.405719	1.822684	3.432698

**7'**

C	1.306114	1.098245	2.923962
C	0.571574	-0.045232	2.592894
C	0.065566	-0.860664	3.608297
C	0.253637	-0.509642	4.942216
C	0.965065	0.644122	5.267942
C	1.500279	1.442400	4.256359
H	-0.528033	-1.729187	3.341001
H	-0.161044	-1.132434	5.727993
H	1.729655	1.698627	2.125060
H	1.112032	0.916097	6.308293
H	2.072893	2.328456	4.511124
C	0.286081	-0.380930	1.184355
H	0.068987	-1.434184	0.966193
O	-2.420601	-0.850987	1.930314
H	0.277160	0.830360	-1.775161
C	-0.092577	0.075687	-1.070923
H	0.400445	-0.876843	-1.312585
N	0.258823	0.509683	0.278175
C	-1.609635	-0.082449	-1.248450
H	-1.919264	-0.924533	-0.615988
C	-1.915988	-0.403231	-2.709896
H	-2.983193	-0.595839	-2.850623
H	-1.642361	0.440306	-3.353841
H	-1.365103	-1.284041	-3.055127
C	-2.365515	1.156541	-0.773555
H	-3.429955	1.069048	-1.014335
H	-2.270611	1.281823	0.307392
H	-1.984282	2.065151	-1.253422
H	-0.167150	2.212314	0.778593
H	-3.307693	-0.852769	1.557654
O	-0.583338	3.011628	1.180602
H	0.140305	3.560090	1.497672
H	-1.553710	2.217398	2.454470
O	-2.025398	1.634438	3.086592
H	-2.334973	0.030428	2.352915
H	-1.373170	1.435456	3.769490

**8'**

C	-0.486704	-1.063809	4.234107
C	-0.932815	-0.337894	3.128745
C	-1.455658	0.947073	3.312066
C	-1.527176	1.491896	4.586277

C	-1.079216	0.761790	5.688465
C	-0.559238	-0.516769	5.511863
H	-1.795683	1.494733	2.439146
H	-1.933709	2.488517	4.726142
H	-0.079244	-2.061464	4.089830
H	-1.137843	1.191194	6.683661
H	-0.211533	-1.086810	6.367365
C	-0.839581	-0.934140	1.781684
H	-0.405081	-1.947017	1.736851
H	-0.629992	-2.009636	-0.421359
C	-1.064616	-0.999494	-0.535091
H	-2.058229	-1.113079	-0.986540
N	-1.227435	-0.328286	0.737486
C	-0.182234	-0.176787	-1.481477
H	-0.653258	0.808396	-1.588406
C	-0.117479	-0.851113	-2.850266
H	0.483134	-0.261037	-3.548115
H	0.344393	-1.841873	-2.769486
H	-1.114021	-0.978231	-3.284027
C	1.214326	0.011754	-0.893398
H	1.850039	0.589730	-1.570338
H	1.171944	0.532685	0.066285
H	1.694015	-0.961492	-0.730920