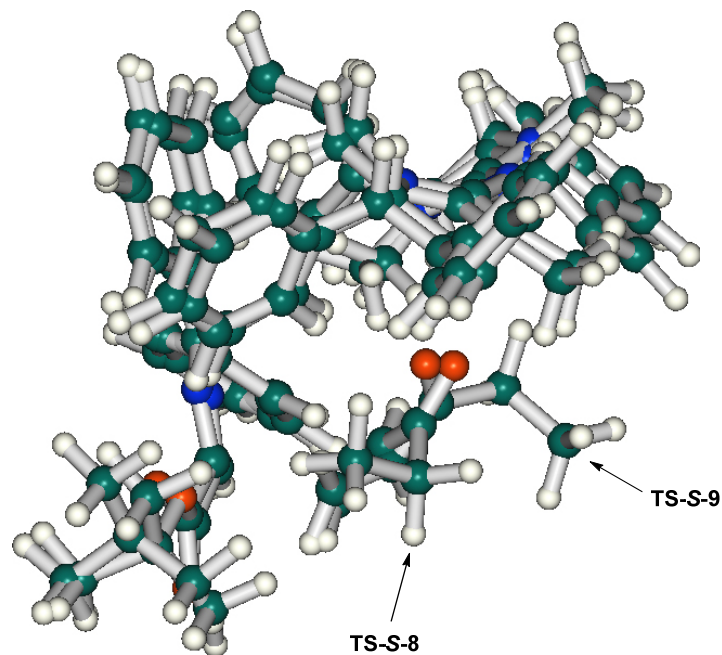SUPPLEMENTARY MATERIAL

Pentanidium-Catalyzed Asymmetric Phase-Transfer Conjugate Addition: Prediction of Stereoselectivity via DFT Calculations and Docking Sampling of Transition States, and Origin of Stereoselectivity

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Fig. S1. Overlay of the optimized geometries of transition states **TS-*S*-8** and **TS-*S*-9**.

Multiwfn Calculations

The hydrogen bond interaction energies were extracted from the potential energy density of the bond critical point. The required number can be obtained from Multiwfn using the wfn file generated from Gaussian through the output=wfn keyword. Details on how to perform these calculations can be found in the manual of Multiwfn at https://multiwfn.codeplex.com/. Once the potential energy density of a particular hydrogen bond is obtained from Multiwfn, the corresponding hydrogen bond strength is half the value of the potential energy density (E. Espinosa, E. Molins, C. Lecomte, *Chem. Phys. Lett*. **1998**, *285*, 170-173.). The resulting value is in Hartrees and can be converted to other units by multiplying by the appropriate constant (for e.g. 627.509 for conversion to kcal/mol).

AutoDock Vina Calculations

Vina charge calculation is hard coded as part of its program, so it does not read the partial charge supplied by the users. The detail of how to setup a Vina calculation can be found in its website (http://vina.scripps.edu/tutorial.html). The initial structures were loaded into AutoDockTools (ADT) and then converted to the PBDQT format, which could be used directly for subsequent docking calculation in Vina.

Characterization of Non-covalent Interaction Using QTAIM

From the topology analysis of electron density in the quantum theory of atoms in molecules (QTAIM), each bond is associated with a critical point (where the first derivatives are 0). The first number "3" refers to rank of the diagonal Hessian matrix (the matrix which contains the 2nd derivatives of the electron density). The rank indicates how many non-zero curvatures or 2nd derivatives. For equilibrium structure, the rank is generally 3. The second number "−1" is the signature which is defined as the algebraic sum of the signs of the curvatures. In $(3,-1)$ the number of positive curvatures or 2nd derivatives in the diagonal Hessian is 1 and the number of negative curvature is 2, therefore $1 - 2 = -1$. Bond critical point is used to characterize both covalent and non-covalent interaction. The IUPAC definition of hydrogen bond includes the presence of a $(3,-1)$ bond critical point (see *Pure Appl. Chem.*, **2011**, *83*,

1619). A good introduction to QTAIM is C. F. Matta and R. J. Boyd, in *The Quantum Theory of Atoms in Molecules*, Wiley-VCH Verlag GmbH & Co. KGaA, 2007, Chapter 1, pp. 1-34.

Table S1. Total energies, number of imaginary frequencies and Cartesian coordinates of M06-2X/6-31G* optimized geometries of all calculated transition states.

Transition state	No. of imaginary frequency	Electronic energy (Hartrees)
TS-*R*-1	1	-2801.772130
TS-*R*-2	1	-2801.770364
TS-*R*-3	1	-2801.773989
TS-*R*-4	1	-2801.768362
TS-*R*-5	1	-2801.764756
TS-*R*-6	1	-2801.767955
TS-*R*-7	1	-2801.768756
TS-*R*-8	1	-2801.742040
TS-*R*-9	1	-2801.758815
TS-*S*-1	1	-2801.746089
TS-*S*-2	1	-2801.765309
TS-*S*-3	1	-2801.75742
TS-*S*-4	1	-2801.757805
TS-*S*-5	1	-2801.771972
TS-*S*-6	1	-2801.753785
TS-*S*-7	1	-2801.748794
TS-*S*-8	1	-2801.771523
TS-*S*-9	1	-2801.771971

TS-*R*-1

N	1.142394	-3.584375	0.619966	H	-8.432847	-1.009804	-2.405544
N	0.661956	-1.492108	1.170495	C	-6.440292	-1.253418	-1.640130
N	-3.078974	-2.577842	-0.717249	H	-6.163223	-0.214258	-1.798660
N	-2.750093	-1.501325	1.191967	C	-4.539723	0.236170	1.085237
C	0.149175	-2.656571	0.719692	C	-5.583560	0.503425	1.969904
C	2.400894	-3.078326	1.141234	H	-6.077728	-0.321021	2.477685
H	2.566421	-3.467020	2.157712	C	-6.000377	1.812393	2.196565
C	2.129376	-1.558277	1.186101	H	-6.813090	2.010467	2.887784
H	2.485898	-1.097496	0.251458	C	-5.376777	2.860438	1.527165
C	0.905651	-5.004476	0.496394	H	-5.701775	3.882623	1.692183
H	0.898075	-5.494193	1.478903	C	-4.333048	2.597608	0.640956
H	1.698650	-5.445499	-0.112065	H	-3.850680	3.420507	0.120902
H	-0.057770	-5.155127	0.011392	C	-3.900759	1.291806	0.425119
C	0.080810	-0.156661	1.048394	H	-3.075789	1.083253	-0.259050
H	-0.857016	-0.190071	0.499807	C	3.427060	2.366783	-2.039772
H	0.779730	0.482803	0.492698	O	3.885707	2.647394	-3.141184
H	-0.063624	0.273587	2.040958	O	3.963446	1.366498	-1.263506
C	3.592240	-3.420569	0.278792	C	5.095911	0.624833	-1.779031
C	3.472965	-3.430662	-1.112485	C	4.667111	-0.193858	-2.996989
H	2.499826	-3.248085	-1.563902	C	6.282429	1.541357	-2.087397
C	4.589670	-3.661849	-1.908439	C	5.480512	-0.311429	-0.638406
H	4.490324	-3.662243	-2.989525	C	2.240819	2.990849	-1.515943
C	5.833627	-3.879756	-1.318716	N	1.730155	2.692932	-0.302520
H	6.705910	-4.056611	-1.939857	C	0.646211	3.261670	0.153707
C	5.956301	-3.864888	0.067789	C	-0.091026	4.359545	-0.553275
H	6.924382	-4.027563	0.530414	C	0.508323	5.617347	-0.690160
C	4.836997	-3.638893	0.865250	C	-0.158282	6.664269	-1.320270
H	4.930443	-3.616448	1.948177	C	-1.444715	6.476647	-1.819482
C	2.769434	-0.834119	2.345027	C	-2.055938	5.232383	-1.689878
C	3.530343	0.306502	2.094998	C	-1.381081	4.186374	-1.065676
H	3.581967	0.711623	1.084288	C	0.219244	2.920473	1.529081
C	4.187189	0.947628	3.145437	C	1.182881	2.546040	2.477746
H	4.782962	1.832048	2.941315	C	0.815815	2.114708	3.746324
C	4.065995	0.468548	4.445683	C	-0.531483	2.062268	4.109950
H	4.579904	0.968377	5.260854	C	-1.498033	2.485347	3.197470
C	3.265888	-0.645145	4.704209	C	-1.123649	2.926040	1.931419
H	3.148572	-1.008483	5.720205	C	0.872996	1.918680	-3.164755
C	2.620342	-1.292131	3.657184	C	-0.310442	1.448995	-2.666018
H	1.991777	-2.155561	3.863398	C	-0.476675	0.133391	-2.118396
C	-2.203941	-2.338289	0.286377	O	-1.558892	-0.267870	-1.646599
C	-4.164282	-1.603524	-0.661115	C	0.711096	-0.823127	-2.154641
H	-3.874935	-0.745373	-1.283453	C	0.912746	-1.427991	-3.550248
C	-4.135443	-1.193297	0.826723	H	5.487978	-0.846237	-3.314516
H	-4.797992	-1.863204	1.398682	H	3.816314	-0.831392	-2.726623
C	-2.650628	-3.073317	-2.013153	H	4.385745	0.461100	-3.822064
H	-2.344197	-2.232028	-2.642620	H	7.175406	0.929333	-2.251788
H	-3.480175	-3.614435	-2.472997	H	6.470259	2.194136	-1.229226
H	-1.806970	-3.746622	-1.864548	H	6.094577	2.156844	-2.964124
C	-2.333049	-1.354647	2.572030	H	6.317958	-0.945604	-0.943110
H	-1.339460	-1.781235	2.708610	H	4.645574	-0.965222	-0.369195
H	-3.041909	-1.871860	3.230691	H	5.777602	0.259003	0.246693
H	-2.300460	-0.293626	2.835539	H	1.964369	3.897605	-2.046683
C	-5.508856	-2.133054	-1.089104	H	1.510797	5.764875	-0.297701
C	-5.861987	-3.467550	-0.882433	H	0.326999	7.630411	-1.419870
H	-5.132099	-4.149966	-0.454027	H	-1.964594	7.292726	-2.311326
C	-7.131406	-3.917665	-1.231481	H	-3.054564	5.071195	-2.086576
H	-7.396232	-4.958801	-1.076596	H	-1.844763	3.207360	-0.983710
C	-8.060240	-3.034785	-1.777965	H	2.225136	2.587193	2.186121
H	-9.050125	-3.386360	-2.050145	H	1.586289	1.815221	4.451441
C	-7.713717	-1.701447	-1.978932	H	-0.821461	1.722266	5.099609
				H	-2.552898	2.475419	3.463859

H	-1.888317	3.260510	1.242569
H	1.721792	1.270248	-3.350329
H	0.909458	2.867218	-3.687298
H	-1.194415	2.075853	-2.668345
H	1.619877	-0.299067	-1.827142
H	0.493479	-1.628701	-1.447842
H	0.013054	-1.964782	-3.866438
H	1.121608	-0.656502	-4.294266
H	1.747691	-2.136134	-3.554462

TS-*R*-2

N	-3.735670	1.890037	0.270349
N	-2.770409	0.749220	-1.367724
N	0.373138	3.543447	-1.101298
N	0.401841	1.362786	-0.662514
C	-2.618409	1.762162	-0.487818
C	-4.627461	0.754802	0.059232
H	-4.424232	-0.011795	0.821826
C	-4.142269	0.233179	-1.315349
H	-4.728627	0.726693	-2.107184
C	-3.801857	2.675445	1.485783
H	-3.768265	2.024197	2.365314
H	-4.732376	3.248254	1.500916
H	-2.949693	3.354097	1.504725
C	-1.977241	0.578756	-2.579796
H	-1.487036	1.522133	-2.836756
H	-2.660495	0.308991	-3.389528
H	-1.236922	-0.216969	-2.454543
C	-6.093007	1.106979	0.083880
C	-6.552705	2.300280	-0.477343
H	-5.834802	3.003284	-0.893347
C	-7.913391	2.587459	-0.493564
H	-8.264520	3.520335	-0.922888
C	-8.824983	1.678700	0.041213
H	-9.886581	1.903026	0.027637
C	-8.371373	0.485570	0.595849
H	-9.077554	-0.224344	1.013750
C	-7.007996	0.202962	0.622350
H	-6.648012	-0.728125	1.052394
C	-4.256831	-1.263340	-1.455632
C	-5.478662	-1.816372	-1.846239
H	-6.312384	-1.164252	-2.096817
C	-5.627100	-3.198186	-1.911196
H	-6.578640	-3.624012	-2.213616
C	-4.553466	-4.031846	-1.601377
H	-4.669939	-5.109310	-1.661391
C	-3.331717	-3.480783	-1.225906
H	-2.478003	-4.110419	-0.991018
C	-3.185243	-2.098084	-1.144398
H	-2.213636	-1.686567	-0.886820
C	-0.361212	2.470202	-0.726917
C	1.735999	3.154231	-1.440814
H	1.841368	3.108530	-2.535287
C	1.813787	1.720384	-0.851286
H	2.285127	1.770511	0.139165
C	-0.199887	4.774934	-1.599168
H	-0.286509	4.757645	-2.692967
H	0.443545	5.608153	-1.308167
H	-1.187465	4.902723	-1.157430
C	0.121618	0.257263	0.255317
H	-0.890466	-0.113858	0.093332
H	0.270930	0.558020	1.298273
H	0.804781	-0.558716	0.020049
C	2.793981	4.063436	-0.861190
C	2.596229	4.682766	0.374424
H	1.644458	4.559323	0.885517
C	3.610392	5.443382	0.947300

H	3.447625	5.925634	1.906036
C	4.836255	5.574610	0.298430
H	5.630538	6.160219	0.749951
C	5.038287	4.955128	-0.932105
H	5.991024	5.055471	-1.441818
C	4.016567	4.210084	-1.515130
H	4.173488	3.721672	-2.473476
C	2.612780	0.787408	-1.725972
C	3.999765	0.776405	-1.565330
H	4.452685	1.356084	-0.765140
C	4.797505	0.016095	-2.415141
H	5.872655	0.000411	-2.265269
C	4.213188	-0.736038	-3.431475
H	4.832426	-1.334319	-4.092745
C	2.828245	-0.731297	-3.586761
H	2.364979	-1.326605	-4.368143
C	2.025226	0.025297	-2.735162
H	0.945176	-0.009097	-2.830259
C	-0.095674	-1.978100	3.283551
O	-0.895885	-2.776875	3.752523
O	-0.277965	-0.623400	3.359052
C	-1.507552	-0.092581	3.880687
C	-2.672083	-0.524755	2.987568
C	-1.725452	-0.493101	5.340359
C	-1.300212	1.417868	3.787019
C	1.055749	-2.358616	2.491337
N	1.976120	-1.398151	2.197734
C	3.108716	-1.598109	1.602099
C	3.544692	-2.906669	1.020348
C	3.724727	-4.044853	1.809077
C	4.074307	-5.262137	1.226739
C	4.272091	-5.349049	-0.147747
C	4.123381	-4.210099	-0.939662
C	3.759166	-3.000872	-0.360326
C	4.042903	-0.448414	1.524079
C	3.639780	0.817704	1.987199
C	4.497253	1.908883	1.932472
C	5.798632	1.764897	1.445124
C	6.226390	0.507324	1.026374
C	5.360929	-0.583886	1.059495
C	-0.246677	-3.134002	0.862209
C	0.417699	-3.605377	-0.255090
C	0.402395	-2.925338	-1.511389
O	-0.184769	-1.843648	-1.723479
C	1.116883	-3.588231	-2.683204
C	0.366137	-3.375299	-3.993164
H	-2.484166	-0.184245	1.959838
H	-3.608313	-0.078205	3.342930
H	-2.773810	-1.610763	2.989089
H	-0.830808	-0.250476	5.921209
H	-2.567671	0.071548	5.753737
H	-1.923288	-1.559787	5.426839
H	-0.409315	1.706304	4.351177
H	-1.164691	1.724415	2.743471
H	-2.163919	1.949062	4.199918
H	1.358718	-3.393098	2.624409
H	3.586654	-3.974632	2.884305
H	4.197429	-6.142360	1.850547
H	4.546976	-6.296777	-0.600434
H	4.278834	-4.267141	-2.013630
H	3.615351	-2.114414	-0.977861
H	2.639697	0.907071	2.402659
H	4.155750	2.880660	2.277877
H	6.465312	2.620776	1.405413
H	7.241519	0.371337	0.663893
H	5.711325	-1.552986	0.719466
H	-0.866161	-2.245070	0.755740

H	-0.563586	-3.806530	1.651517
H	0.966948	-4.541552	-0.197623
H	1.275527	-4.651140	-2.476765
H	2.114711	-3.133026	-2.747303
H	0.924695	-3.771043	-4.846128
H	-0.611313	-3.866576	-3.964863
H	0.185621	-2.308319	-4.148400

TS-*R*-3

N	-2.568902	0.377584	-1.579333	H	5.810025	2.192969	-2.034854
N	-2.089531	-1.781375	-1.715535	C	6.824796	0.290344	-1.933027
N	1.837920	-0.645382	-2.667841	H	7.816518	0.725730	-1.862530
N	0.936718	-1.510006	-0.833837	C	6.668383	-1.094277	-1.920946
C	-1.620344	-0.523505	-1.870216	H	7.536623	-1.740374	-1.839770
C	-3.747242	-0.276902	-1.009462	C	5.397646	-1.653000	-2.018212
H	-3.717274	-0.120649	0.078910	H	5.271486	-2.733081	-2.004118
C	-3.506869	-1.774269	-1.345530	C	2.752620	-3.014764	-0.055903
H	-4.098177	-2.045489	-2.232771	C	3.538074	-3.045413	1.094452
C	-2.334849	1.799639	-1.333383	H	3.865918	-2.113449	1.546856
H	-2.483075	2.031457	-0.274677	C	3.891870	-4.266658	1.664209
H	-3.027042	2.393340	-1.934645	H	4.503205	-4.278135	2.560913
H	-1.312417	2.058661	-1.604640	C	3.456326	-5.457319	1.092164
C	-1.464213	-2.973945	-2.245278	H	3.728912	-6.408359	1.538661
H	-0.751673	-2.699573	-3.026770	C	2.660160	-5.429417	-0.053331
H	-2.239792	-3.609757	-2.681746	H	2.311153	-6.357123	-0.495781
H	-0.945290	-3.538854	-1.464133	C	2.309726	-4.212002	-0.624474
C	-5.060851	0.224912	-1.559100	H	1.680813	-4.184262	-1.512267
C	-5.152174	0.744180	-2.850919	C	-1.406990	0.629150	2.316253
H	-4.251771	0.839000	-3.452440	O	-1.334027	-0.345280	3.045705
C	-6.383992	1.147056	-3.357169	O	-2.622452	1.156883	1.932281
H	-6.446294	1.562888	-4.357656	C	-3.743878	1.167531	2.855429
C	-7.533972	1.021191	-2.581742	C	-4.362165	-0.219676	3.005601
H	-8.493203	1.340208	-2.976127	C	-3.310217	1.703633	4.219243
C	-7.448890	0.491767	-1.297098	C	-4.723063	2.126633	2.187476
H	-8.341415	0.393935	-0.687688	C	-0.312849	1.419278	1.745957
C	-6.215520	0.097204	-0.786479	N	0.934284	0.921151	2.010787
H	-6.145650	-0.310384	0.219322	C	2.068782	1.291969	1.506396
C	-3.815129	-2.743977	-0.230006	C	2.271393	2.181633	0.322941
C	-4.696934	-3.801003	-0.448582	C	3.354936	3.071696	0.227830
H	-5.184507	-3.900921	-1.415289	C	3.570887	3.818329	-0.925010
C	-4.956240	-4.723019	0.563218	C	2.702820	3.711180	-2.014107
H	-5.647985	-5.539957	0.385288	C	1.616337	2.843561	-1.929540
C	-4.324978	-4.595700	1.796701	C	1.415285	2.084235	-0.781346
H	-4.520651	-5.316552	2.583989	C	3.268155	0.624142	2.113600
C	-3.445446	-3.537809	2.022318	C	4.513722	0.533507	1.471272
H	-2.955429	-3.419410	2.983620	C	5.577446	-0.155710	2.051648
C	-3.194308	-2.612293	1.015882	C	5.425841	-0.773283	3.289383
H	-2.528440	-1.776579	1.225220	C	4.189705	-0.701886	3.934662
C	0.697091	-0.786318	-1.951549	C	3.128295	-0.017924	3.356815
C	2.905383	-1.463751	-2.102609	C	-0.474705	3.141908	2.709885
H	2.945209	-2.427941	-2.636794	C	0.332026	4.107661	2.103059
C	2.385741	-1.688228	-0.666839	C	-0.066052	4.583546	0.819036
H	2.756112	-0.876911	-0.024424	O	-1.012112	4.083492	0.177270
C	1.853031	-0.217478	-4.049453	C	0.725284	5.736493	0.207455
H	1.847461	-1.078486	-4.730526	C	0.199370	6.153602	-1.157412
H	2.751642	0.374821	-4.233190	H	-4.667015	-0.621015	2.034224
H	0.970106	0.395081	-4.229857	H	-3.647613	-0.908719	3.456728
C	0.100545	-1.541600	0.360453	H	-5.253497	-0.155652	3.637866
H	-0.627138	-0.729751	0.332042	H	-2.906739	2.714915	4.127983
H	0.720781	-1.371217	1.244487	H	-2.554593	1.055025	4.666989
H	-0.417044	-2.501082	0.451581	H	-4.178317	1.737712	4.884315
C	4.274802	-0.829988	-2.113656	H	-4.261131	3.109700	2.062236
C	4.431295	0.555879	-2.114684	H	-5.628637	2.230098	2.792426
H	3.558079	1.201396	-2.152327	H	-5.007622	1.754788	1.197079
C	5.705547	1.112269	-2.036030	H	-0.564830	1.949961	0.826787
				H	4.026647	3.179290	1.074351
				H	4.411476	4.505466	-0.967368
				H	2.863871	4.308784	-2.905849
				H	0.919945	2.747503	-2.759432
				H	0.578719	1.399693	-0.737610
				H	4.658867	0.983460	0.495871
				H	6.521450	-0.215828	1.517625
				H	6.255442	-1.304115	3.746249
				H	4.053574	-1.181046	4.899855
				H	2.159957	0.028361	3.842998
				H	-0.252343	2.823323	3.726931

H	-1.532458	3.195472	2.459762
H	1.275676	4.425430	2.533472
H	1.776600	5.429051	0.146725
H	0.700853	6.578749	0.910606
H	-0.834086	6.500542	-1.081593
H	0.200952	5.299746	-1.838995
H	0.807992	6.952990	-1.590374

TS-*R*-4

N	3.138809	0.131370	-0.286405
N	3.619259	-0.994268	1.560656
N	1.635966	3.231357	1.817568
N	0.469027	1.571641	0.937644
C	3.053051	0.124031	1.065186
C	3.980612	-0.970711	-0.765076
H	3.463090	-1.513830	-1.563264
C	4.105421	-1.877539	0.498854
H	5.161952	-2.105493	0.685298
C	2.892346	1.316726	-1.094362
H	3.442180	1.209712	-2.031644
H	3.259444	2.213948	-0.581059
H	1.824056	1.423357	-1.307187
C	3.403466	-1.468708	2.911838
H	4.332695	-1.894502	3.300363
H	2.613797	-2.227136	2.935011
H	3.103518	-0.619943	3.525916
C	5.316471	-0.479599	-1.280589
C	6.103033	0.372201	-0.499028
H	5.742238	0.695269	0.475720
C	7.336870	0.808975	-0.965501
H	7.942721	1.470334	-0.354624
C	7.795463	0.400268	-2.217726
H	8.758070	0.744048	-2.581686
C	7.014906	-0.443281	-3.000520
H	7.365165	-0.760320	-3.977325
C	5.776010	-0.878745	-2.533125
H	5.161545	-1.533685	-3.145611
C	3.344739	-3.182254	0.397238
C	3.983112	-4.376527	0.729229
H	5.014146	-4.353837	1.074102
C	3.314496	-5.592720	0.611003
H	3.822304	-6.515877	0.871197
C	2.002525	-5.618811	0.149271
H	1.476382	-6.562227	0.043348
C	1.355353	-4.429183	-0.180776
H	0.330515	-4.447467	-0.537875
C	2.019293	-3.214148	-0.044168
H	1.498985	-2.288222	-0.287494
C	1.625134	1.917627	1.500141
C	0.454752	3.902094	1.242640
H	0.014314	4.551785	2.007209
C	-0.485349	2.700230	0.961237
H	-0.952422	2.767844	-0.024714
C	2.839586	3.947998	2.173394
H	2.588098	4.743722	2.879976
H	3.321324	4.397260	1.296764
H	3.525077	3.247494	2.650483
C	0.036160	0.195335	0.762861
H	0.469279	-0.224690	-0.149699
H	-1.050418	0.182184	0.657302
H	0.317326	-0.401013	1.637718
C	0.838685	4.743594	0.039280
C	0.890887	4.207189	-1.250296
H	0.569502	3.185329	-1.440648
C	1.317445	4.998297	-2.314496

H	1.340258	4.577773	-3.315258
C	1.694853	6.322139	-2.106381
H	2.020800	6.934096	-2.941362
C	1.634947	6.863527	-0.825195
H	1.911642	7.899094	-0.654989
C	1.205252	6.076239	0.238996
H	1.145549	6.502824	1.238210
C	-1.549346	2.495470	2.019698
C	-2.836185	2.124684	1.639293
H	-3.090058	1.957853	0.596406
C	-3.826228	1.923841	2.600831
H	-4.807681	1.609436	2.264235
C	-3.528212	2.093302	3.948179
H	-4.296101	1.939716	4.700251
C	-2.235284	2.448687	4.337710
H	-1.997227	2.570689	5.390327
C	-1.248328	2.641383	3.379215
H	-0.239037	2.906280	3.687837
C	-5.011212	-0.090335	-0.686633
O	-5.115503	0.878495	0.055479
O	-5.912057	-0.344265	-1.684482
C	-7.020289	0.550262	-1.919638
C	-7.946540	0.593974	-0.704729
C	-6.521959	1.943212	-2.304900
C	-7.737140	-0.095092	-3.102386
C	-3.942574	-1.063969	-0.725465
N	-3.156605	-1.150270	0.370490
C	-2.380731	-2.156405	0.666993
C	-2.179912	-3.343420	-0.214163
C	-2.387616	-4.646089	0.260486
C	-2.190362	-5.749527	-0.564575
C	-1.793132	-5.574302	-1.889602
C	-1.592282	-4.284967	-2.378211
C	-1.775017	-3.184012	-1.546126
C	-1.704282	-2.131033	1.985005
C	-0.663312	-3.013135	2.314708
C	0.003742	-2.917786	3.534229
C	-0.345272	-1.935432	4.456427
C	-1.391873	-1.063184	4.148756
C	-2.065865	-1.163194	2.940239
C	-3.014305	0.344264	-2.473504
C	-1.860243	-0.099480	-3.058560
C	-0.569507	0.401136	-2.675222
O	-0.391167	1.326560	-1.865554
C	0.661178	-0.218118	-3.329930
C	1.389461	0.805171	-4.204415
H	-8.858751	1.142815	-0.958861
H	-7.455953	1.079164	0.137871
H	-8.225263	-0.424213	-0.417811
H	-7.372489	2.569596	-2.592181
H	-5.996105	2.410633	-1.472969
H	-5.844905	1.874057	-3.162496
H	-8.612340	0.496740	-3.384955
H	-8.062865	-1.105314	-2.840928
H	-7.064266	-0.160660	-3.962030
H	-4.083405	-1.908131	-1.400524
H	-2.704287	-4.786816	1.290286
H	-2.356539	-6.749332	-0.174479
H	-1.641628	-6.434582	-2.534173
H	-1.278952	-4.135044	-3.407607
H	-1.600561	-2.177704	-1.915187
H	-0.361487	-3.780259	1.612177
H	0.797805	-3.626107	3.759549
H	0.174332	-1.860377	5.406972
H	-1.693089	-0.298633	4.858928
H	-2.877412	-0.485969	2.699436
H	-3.979072	0.121368	-2.913856

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H	-2.967792	1.172200	-1.770858
H	-1.896887	-0.862383	-3.831365
H	1.321882	-0.553836	-2.516623
H	0.390125	-1.102531	-3.914034
H	1.576290	1.720642	-3.636181
H	2.345756	0.417165	-4.567287
H	0.779113	1.071279	-5.071794

TS-*R*-5

N	2.595847	3.284102	-0.808637
N	1.606840	1.576019	0.177043
N	4.055661	-1.075643	-1.663047
N	4.318395	-0.201709	0.342064
C	2.562360	1.941416	-0.676905
C	1.437168	3.905588	-0.143590
H	1.792305	4.742420	0.468824
C	0.918640	2.750035	0.750154
H	-0.155585	2.598097	0.611492
C	3.342534	3.974456	-1.837222
H	3.721787	4.917864	-1.434762
H	2.711977	4.189607	-2.706221
H	4.178611	3.345122	-2.140397
C	1.214259	0.227366	0.540619
H	1.405183	-0.449141	-0.297125
H	0.141173	0.242837	0.736117
H	1.743277	-0.138469	1.428863
C	0.425199	4.424463	-1.145673
C	-0.430188	3.543436	-1.813578
H	-0.421983	2.481054	-1.581312
C	-1.355366	4.033473	-2.730115
H	-2.040118	3.342702	-3.212507
C	-1.416971	5.398950	-3.003323
H	-2.143072	5.779110	-3.714743
C	-0.554348	6.276963	-2.354031
H	-0.601828	7.341525	-2.559583
C	0.361930	5.789266	-1.424869
H	1.024162	6.476227	-0.902121
C	1.225064	2.828281	2.228729
C	0.343053	2.196796	3.107225
H	-0.563261	1.734071	2.718183
C	0.630083	2.143545	4.468694
H	-0.064252	1.646111	5.138411
C	1.795152	2.726268	4.959598
H	2.015520	2.692209	6.021821
C	2.679919	3.356835	4.085826
H	3.588422	3.812485	4.467320
C	2.398310	3.403122	2.723432
H	3.097931	3.883848	2.042014
C	3.847574	0.023386	-0.903239
C	4.891540	-2.043252	-0.962710
H	4.507408	-3.055323	-1.127032
C	4.667737	-1.622217	0.512105
H	5.603804	-1.687017	1.076552
C	3.781619	-1.160010	-3.080565
H	3.267472	-2.100577	-3.299382
H	4.709978	-1.117699	-3.660403
H	3.142246	-0.321419	-3.355432
C	4.390596	0.762894	1.418036
H	4.495421	1.764582	0.994032
H	5.281699	0.544851	2.012319
H	3.512028	0.744059	2.072133
C	6.348546	-1.977620	-1.380558
C	6.919986	-0.787873	-1.834381
H	6.304602	0.101346	-1.949851
C	8.273756	-0.739422	-2.155852
H	8.708571	0.187878	-2.514674
C	9.066329	-1.875935	-2.022563
H	10.120533	-1.837233	-2.276278
C	8.500151	-3.065469	-1.570791
H	9.110810	-3.957206	-1.473567
C	7.146390	-3.115466	-1.254724
H	6.703343	-4.046002	-0.907735
C	3.561271	-2.356307	1.242229
C	3.574906	-2.375521	2.637531
H	4.425045	-1.956718	3.172238
C	2.504461	-2.916029	3.346058
H	2.520220	-2.918681	4.431200
C	1.413709	-3.446060	2.662039
H	0.564415	-3.841063	3.210155
C	1.400034	-3.448071	1.267852
H	0.546022	-3.846519	0.724544
C	2.469491	-2.905350	0.563180
H	2.420934	-2.885691	-0.522584
C	-6.220517	-1.868369	-1.452091
O	-6.748585	-2.224677	-2.494889
O	-6.878984	-1.188098	-0.474690
C	-8.267304	-0.836118	-0.638857
C	-8.587185	-0.097387	0.657774
C	-8.447455	0.099397	-1.834111
C	-9.135405	-2.087951	-0.760180
C	-4.805542	-2.036031	-1.166314
N	-4.318951	-1.747202	0.037207
C	-3.055406	-1.846238	0.368736
C	-2.033430	-2.555839	-0.474003
C	-0.953299	-1.892513	-1.068394
C	-0.020935	-2.586592	-1.835860
C	-0.140154	-3.963330	-2.018259
C	-1.209421	-4.637167	-1.430361
C	-2.143219	-3.939045	-0.666839
C	-2.676618	-1.413763	1.723243
C	-1.345183	-1.421792	2.167970
C	-1.003025	-0.994715	3.449737
C	-1.985133	-0.549186	4.329074
C	-3.317698	-0.543399	3.904280
C	-3.660592	-0.968162	2.630382
C	-4.354978	0.122128	-2.115402
C	-3.081070	0.442588	-1.748594
C	-2.722794	1.011878	-0.472631
O	-1.528602	1.227122	-0.168342
C	-3.808660	1.487738	0.470753
C	-4.284813	2.883897	0.049885
H	-9.629618	0.234036	0.660513
H	-8.421092	-0.754371	1.515679
H	-7.937436	0.776490	0.761805
H	-9.483356	0.451306	-1.873837
H	-8.204773	-0.412739	-2.764769
H	-7.795084	0.972036	-1.722680
H	-10.192728	-1.806069	-0.726559
H	-8.930328	-2.759452	0.078839
H	-8.930617	-2.611752	-1.693032
H	-4.251346	-2.584559	-1.928866
H	-0.865743	-0.818695	-0.934959
H	0.796857	-2.042087	-2.306247
H	0.582953	-4.505497	-2.620905
H	-1.319541	-5.708413	-1.570471
H	-2.980991	-4.463386	-0.215042
H	-0.566706	-1.785102	1.506414
H	0.041883	-1.016110	3.755328
H	-1.727658	-0.234355	5.336375
H	-4.098282	-0.211246	4.583164
H	-4.693975	-0.974422	2.298786
H	-5.210728	0.456352	-1.537730

H	-4.575936	-0.257123	-3.108203
H	-2.250214	0.189608	-2.402582
H	-3.368204	1.520244	1.471139
H	-4.639653	0.774839	0.493820
H	-4.756709	2.855147	-0.936884
H	-3.437762	3.575450	-0.004884
H	-5.008969	3.283559	0.764636

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N	1.350960	-3.510568	1.300976
N	0.839057	-1.379651	0.961289
N	-2.293117	-2.214142	-0.272677
N	-2.986881	-1.880158	1.793179
C	0.349412	-2.600769	1.243506
C	2.621246	-2.903712	0.876326
H	3.414559	-3.211880	1.567413
C	2.315819	-1.395261	1.042661
H	2.725704	-0.802465	0.216314
C	1.126846	-4.936979	1.213767
H	1.902782	-5.457001	1.781547
H	1.158476	-5.285688	0.174533
H	0.151274	-5.158101	1.646302
C	0.142254	-0.136244	1.266004
H	-0.827321	-0.104152	0.770452
H	0.739788	0.674195	0.842319
H	0.045426	0.016579	2.347965
C	3.000860	-3.319973	-0.529260
C	2.279465	-2.852032	-1.632760
H	1.462614	-2.150689	-1.486279
C	2.630049	-3.244967	-2.919144
H	2.076895	-2.857515	-3.768887
C	3.704731	-4.111312	-3.116987
H	3.985430	-4.407520	-4.122314
C	4.425129	-4.581672	-2.024245
H	5.268040	-5.248699	-2.173441
C	4.071447	-4.187642	-0.734898
H	4.642560	-4.543992	0.119237
C	2.789468	-0.804456	2.357227
C	3.230958	0.518738	2.380574
H	3.235675	1.094351	1.454749
C	3.653105	1.086382	3.581465
H	4.005026	2.113911	3.593161
C	3.621628	0.348029	4.760172
H	3.954952	0.793604	5.692405
C	3.156702	-0.965686	4.742996
H	3.122234	-1.543948	5.660987
C	2.741322	-1.539364	3.546343
H	2.374686	-2.563315	3.537802
C	-1.974109	-2.323067	1.029960
C	-3.576943	-1.532305	-0.453793
H	-3.377934	-0.503801	-0.777720
C	-4.161885	-1.544090	0.987584
H	-4.897589	-2.357171	1.082767
C	-1.362452	-2.369234	-1.371903
H	-0.858693	-1.419440	-1.586783
H	-1.923414	-2.692642	-2.251470
H	-0.634841	-3.145044	-1.120264
C	-3.029006	-1.943626	3.234743
H	-2.055120	-2.278397	3.590556
H	-3.801061	-2.647098	3.567324
H	-3.250291	-0.952944	3.640865
C	-4.478324	-2.221336	-1.449573
C	-4.543829	-3.615226	-1.512498
H	-3.899793	-4.208858	-0.867871
C	-5.413948	-4.237100	-2.400730

H	-5.453519	-5.320587	-2.450011
C	-6.233247	-3.470045	-3.227468
H	-6.912840	-3.954751	-3.920880
C	-6.173691	-2.081078	-3.166046
H	-6.806230	-1.479379	-3.810526
C	-5.294444	-1.458689	-2.283371
H	-5.237893	-0.374005	-2.238342
C	-4.805876	-0.243441	1.403774
C	-6.082558	-0.239840	1.962201
H	-6.617762	-1.178652	2.081150
C	-6.674211	0.957022	2.359771
H	-7.670509	0.951044	2.789843
C	-5.986431	2.156273	2.202472
H	-6.444897	3.090565	2.510127
C	-4.708547	2.156690	1.645420
H	-4.167543	3.090607	1.518576
C	-4.115440	0.962241	1.248625
H	-3.123540	0.970580	0.795984
C	3.686640	1.321637	-1.858513
O	4.167219	1.201538	-2.979240
O	4.217790	0.676804	-0.772124
C	5.533147	0.073398	-0.903964
C	5.564649	-1.024144	-1.970230
C	6.565241	1.164099	-1.182863
C	5.788786	-0.548915	0.465173
C	2.505494	2.116391	-1.621894
N	1.961654	2.348525	-0.413770
C	0.978207	3.186174	-0.177406
C	0.498899	4.290613	-1.054709
C	-0.771877	4.875015	-0.890304
C	-1.197159	5.940575	-1.677523
C	-0.359234	6.487100	-2.644093
C	0.927832	5.971013	-2.777126
C	1.351129	4.904045	-1.995208
C	0.437550	3.107409	1.218158
C	-0.896890	2.779549	1.503804
C	-1.330445	2.624325	2.819118
C	-0.441502	2.791681	3.878082
C	0.887573	3.107560	3.609329
C	1.317229	3.262730	2.295405
C	0.931110	0.504663	-2.418676
C	-0.137781	1.224166	-2.854935
C	-1.345130	1.430605	-2.083635
O	-1.641252	0.789493	-1.062411
C	-2.316928	2.452113	-2.653252
C	-3.523482	2.708868	-1.766773
H	6.440882	-1.660663	-1.803604
H	4.671295	-1.647833	-1.882304
H	5.599456	-0.607648	-2.974518
H	7.568028	0.725823	-1.198326
H	6.529595	1.923058	-0.395674
H	6.370834	1.634521	-2.147000
H	6.803359	-0.956032	0.501108
H	5.674253	0.191067	1.260673
H	5.086820	-1.369513	0.652652
H	2.230356	2.668383	-2.512334
H	-1.441681	4.500469	-0.126392
H	-2.193528	6.346716	-1.525956
H	-0.691405	7.313910	-3.263454
H	1.619550	6.410624	-3.489718
H	2.373936	4.562981	-2.091518
H	-1.578183	2.575388	0.680572
H	-2.362522	2.348731	3.017698
H	-0.780479	2.669526	4.902114
H	1.594145	3.227923	4.425468
H	2.355742	3.497515	2.078694
H	1.747828	0.230670	-3.080054

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H	0.878504	0.010567	-1.448822
H	-0.078596	1.745390	-3.807389
H	-2.627563	2.087458	-3.642060
H	-1.761744	3.380421	-2.835861
H	-3.211772	3.120184	-0.801978
H	-4.072326	1.785720	-1.557668
H	-4.207175	3.423107	-2.232263

TS-*R*-7

N	0.685299	3.622767	-0.126324
N	0.342423	1.548629	0.563650
N	4.043805	0.715367	-1.365092
N	3.406923	0.349427	0.715783
C	1.197237	2.379625	-0.052219
C	-0.582449	3.714049	0.593839
H	-0.401678	4.177255	1.576509
C	-0.951449	2.223937	0.768717
H	-1.592622	1.911862	-0.063051
C	1.431791	4.803181	-0.489374
H	1.739761	5.365244	0.401640
H	0.802716	5.444560	-1.110918
H	2.314023	4.497994	-1.050427
C	0.328683	0.103945	0.375087
H	0.888335	-0.166696	-0.522726
H	-0.709987	-0.202021	0.230533
H	0.729018	-0.414989	1.247953
C	-1.628409	4.513370	-0.144333
C	-1.942143	4.190371	-1.468512
H	-1.426493	3.361163	-1.950705
C	-2.918514	4.916055	-2.141483
H	-3.165512	4.661550	-3.167271
C	-3.588022	5.958570	-1.500761
H	-4.354375	6.517275	-2.028618
C	-3.277978	6.277318	-0.182959
H	-3.799348	7.084691	0.321048
C	-2.295282	5.556677	0.492572
H	-2.052021	5.798577	1.524136
C	-1.608069	1.887860	2.081659
C	-2.856670	1.275026	2.076485
H	-3.336393	0.982068	1.147905
C	-3.502360	0.983531	3.276972
H	-4.465681	0.485673	3.234755
C	-2.895897	1.302503	4.486637
H	-3.395375	1.078007	5.424462
C	-1.632109	1.897610	4.497889
H	-1.148332	2.130356	5.441820
C	-0.989526	2.184038	3.300317
H	0.000194	2.637663	3.310257
C	3.184783	1.101689	-0.385093
C	5.094603	-0.142958	-0.841717
H	5.273058	-0.976684	-1.528896
C	4.434413	-0.670196	0.465263
H	5.159029	-0.648598	1.286807
C	4.166207	1.373944	-2.646876
H	4.294018	0.620580	-3.428867
H	5.026787	2.052756	-2.657330
H	3.253509	1.938346	-2.833658
C	2.968970	0.593382	2.076455
H	3.795135	1.012348	2.663162
H	2.645728	-0.351792	2.525154
H	2.126161	1.282173	2.090486
C	6.389808	0.603014	-0.587799
C	6.377752	1.918721	-0.118450
H	5.431671	2.442375	0.002118
C	7.572918	2.568376	0.174421

H	7.556039	3.592197	0.533863
C	8.788289	1.909827	0.001511
H	9.719375	2.419026	0.227536
C	8.805455	0.600501	-0.470241
H	9.750040	0.086301	-0.614829
C	7.609765	-0.048733	-0.764970
H	7.622083	-1.070512	-1.136130
C	3.861001	-2.063486	0.325482
C	4.262259	-3.084792	1.182176
H	4.955335	-2.867968	1.991880
C	3.783888	-4.383423	1.002142
H	4.098457	-5.172319	1.678032
C	2.906656	-4.662992	-0.040276
H	2.520533	-5.667514	-0.180996
C	2.492875	-3.641792	-0.897158
H	1.786437	-3.855996	-1.693633
C	2.966551	-2.349503	-0.711555
H	2.647471	-1.553938	-1.380419
C	-4.804635	-1.249679	-0.060113
O	-5.043750	-0.492128	0.869485
O	-5.759595	-1.634181	-0.957040
C	-7.108340	-1.125218	-0.863376
C	-7.757798	-1.556384	0.450781
C	-7.126832	0.393151	-1.036496
C	-7.809872	-1.796478	-2.040756
C	-3.513254	-1.806354	-0.434515
N	-2.589861	-1.804377	0.558443
C	-1.542115	-2.567330	0.666211
C	-1.109241	-3.550732	-0.364707
C	-0.794323	-4.874357	-0.025525
C	-0.421835	-5.794547	-1.000949
C	-0.358786	-5.414388	-2.341128
C	-0.670413	-4.102096	-2.693477
C	-1.033038	-3.180466	-1.714771
C	-0.761614	-2.439286	1.924323
C	0.542706	-2.937088	2.066770
C	1.269300	-2.718187	3.236320
C	0.717607	-1.989104	4.286354
C	-0.582805	-1.496682	4.158807
C	-1.313461	-1.725009	3.001951
C	-3.288653	-0.089488	-2.000730
C	-2.317884	-0.257870	-2.963468
C	-1.045220	0.397421	-2.918053
O	-0.688412	1.202061	-2.037876
C	-0.046304	0.087368	-4.029775
C	1.229705	-0.501892	-3.427081
H	-7.660761	-2.639478	0.571011
H	-7.284968	-1.061498	1.297987
H	-8.823083	-1.305630	0.431814
H	-6.611189	0.884507	-0.212128
H	-8.162991	0.744254	-1.073302
H	-6.641005	0.668493	-1.978179
H	-8.856788	-1.483572	-2.087013
H	-7.318315	-1.523341	-2.978598
H	-7.770221	-2.883664	-1.933654
H	-3.534146	-2.583870	-1.199533
H	-0.853767	-5.180761	1.015210
H	-0.192876	-6.817672	-0.716040
H	-0.073973	-6.134735	-3.101910
H	-0.627620	-3.789227	-3.733509
H	-1.269068	-2.155853	-1.989148
H	1.006775	-3.479961	1.251826
H	2.274538	-3.123732	3.318107
H	1.283776	-1.819356	5.197516
H	-1.036570	-0.935013	4.969897
H	-2.323444	-1.346811	2.895493
H	-3.147390	0.665441	-1.230634

H	-4.312301	-0.362014	-2.229394
H	-2.513161	-0.914823	-3.806370
H	0.190732	1.028273	-4.539802
H	-0.477787	-0.595663	-4.767301
H	1.017125	-1.464458	-2.946630
H	1.613429	0.185976	-2.665700
H	2.003653	-0.661930	-4.183818

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N	-3.619304	2.181763	0.446978
N	-2.331417	1.515378	-1.231544
N	0.453383	4.387299	0.077851
N	0.549501	2.164588	0.025323
C	-2.428687	2.346291	-0.174110
C	-4.247449	0.950032	-0.033639
H	-3.924572	0.115446	0.607541
C	-3.587911	0.783849	-1.421990
H	-4.191550	1.313789	-2.175536
C	-3.828312	2.616931	1.817263
H	-3.404056	1.895031	2.524198
H	-4.902512	2.703993	1.990167
H	-3.354557	3.588571	1.951760
C	-1.378316	1.645603	-2.318068
H	-1.021100	2.677509	-2.383607
H	-1.884931	1.382375	-3.249973
H	-0.529273	0.969425	-2.184277
C	-5.751348	0.998909	-0.092497
C	-6.426027	2.189686	-0.367875
H	-5.857916	3.108228	-0.492344
C	-7.813366	2.198124	-0.473604
H	-8.333278	3.128196	-0.679478
C	-8.533422	1.015859	-0.316538
H	-9.615252	1.023626	-0.399997
C	-7.862889	-0.174719	-0.050066
H	-8.419139	-1.098259	0.072702
C	-6.475624	-0.182144	0.066510
H	-5.943302	-1.106951	0.271258
C	-3.415432	-0.656464	-1.824794
C	-4.369900	-1.243957	-2.658448
H	-5.184109	-0.640021	-3.052070
C	-4.287039	-2.596797	-2.972067
H	-5.033003	-3.047727	-3.618494
C	-3.242448	-3.365757	-2.462760
H	-3.170770	-4.419555	-2.714184
C	-2.282049	-2.778914	-1.642304
H	-1.442599	-3.347101	-1.251439
C	-2.369250	-1.427998	-1.317821
H	-1.605944	-1.007642	-0.665867
C	-0.266063	3.236565	0.089087
C	1.839916	4.100838	-0.272887
H	1.963667	4.217935	-1.361326
C	1.955718	2.598863	0.077706
H	2.308718	2.493061	1.114152
C	-0.140127	5.660429	-0.281850
H	-0.208074	5.775587	-1.371481
H	0.483512	6.459973	0.121712
H	-1.138281	5.718941	0.150116
C	0.226062	0.818817	0.489136
H	-0.832753	0.729686	0.732219
H	0.795685	0.604671	1.399571
H	0.491964	0.066219	-0.261502
C	2.865042	4.948099	0.435975
C	2.621076	5.474209	1.704795
H	1.652789	5.314053	2.172247
C	3.612702	6.197044	2.361545

H	3.417454	6.610654	3.345671
C	4.855351	6.384072	1.760611
H	5.629416	6.942806	2.276186
C	5.104390	5.850335	0.499064
H	6.072819	5.989087	0.030098
C	4.109925	5.138585	-0.164407
H	4.300028	4.715903	-1.147883
C	2.878884	1.853266	-0.848969
C	4.101648	1.382932	-0.382216
H	4.352424	1.473846	0.670815
C	4.987881	0.741794	-1.248100
H	5.914301	0.329414	-0.859277
C	4.647828	0.579195	-2.585268
H	5.324974	0.061157	-3.256926
C	3.421998	1.053181	-3.061500
H	3.152681	0.912496	-4.104200
C	2.541083	1.688034	-2.197415
H	1.583851	2.054716	-2.563633
C	1.553061	-3.258920	-1.115981
O	2.206179	-4.185276	-1.557793
O	0.893783	-2.372886	-1.919666
C	0.994941	-2.505364	-3.362717
C	0.243187	-1.280625	-3.875992
C	2.447037	-2.437253	-3.835792
C	0.322301	-3.790433	-3.841661
C	1.512447	-2.904273	0.310027
N	0.322069	-2.373010	0.784107
C	-0.014929	-2.376120	2.038161
C	0.720809	-2.964305	3.194530
C	2.117283	-2.932836	3.313316
C	2.755854	-3.500170	4.412564
C	2.017948	-4.112511	5.419420
C	0.628225	-4.153145	5.318169
C	-0.010352	-3.584461	4.224551
C	-1.376804	-1.850398	2.370422
C	-2.507986	-2.394859	1.754696
C	-3.789285	-1.990639	2.122706
C	-3.963014	-1.015083	3.102974
C	-2.841463	-0.459772	3.721303
C	-1.563131	-0.882007	3.366238
C	2.897299	-1.468155	0.325563
C	4.184373	-1.751519	0.816943
C	5.327873	-2.159589	0.060851
O	6.474656	-2.165765	0.530766
C	5.158626	-2.626584	-1.382382
C	5.437208	-4.127663	-1.472689
H	0.222108	-1.282483	-4.969718
H	-0.785177	-1.275608	-3.502382
H	0.755668	-0.372512	-3.537564
H	2.998337	-3.339459	-3.572929
H	2.460501	-2.309419	-4.923661
H	2.943292	-1.574064	-3.382103
H	-0.735300	-3.795145	-3.566649
H	0.818706	-4.660319	-3.411623
H	0.389550	-3.847359	-4.932819
H	2.011201	-3.671332	0.902662
H	2.718079	-2.460509	2.549509
H	3.839102	-3.459072	4.471328
H	2.517700	-4.556048	6.274838
H	0.039444	-4.634853	6.092985
H	-1.093048	-3.630320	4.156523
H	-2.368548	-3.167427	1.006807
H	-4.652448	-2.461211	1.659792
H	-4.961678	-0.701013	3.393136
H	-2.966143	0.287216	4.500543
H	-0.692101	-0.481427	3.878867
H	2.788396	-1.192345	-0.726076

H	2.293594	-0.833411	0.974802
H	4.397110	-1.576347	1.869368
H	5.891909	-2.081186	-1.990536
H	4.160443	-2.412770	-1.768183
H	5.412772	-4.476426	-2.509817
H	6.421974	-4.339020	-1.048296
H	4.678179	-4.681825	-0.915484

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N	-1.122706	3.192370	0.206604
N	-0.201178	2.280942	-1.589869
N	3.522081	2.982577	0.236555
N	2.376139	1.116050	-0.110962
C	0.019304	2.862450	-0.381304
C	-2.289820	2.788323	-0.584473
H	-2.764450	1.939407	-0.080090
C	-1.635130	2.331339	-1.922035
H	-1.780315	3.111967	-2.684418
C	-1.245879	3.626988	1.586282
H	-2.240481	3.342050	1.935882
H	-1.126146	4.710917	1.663102
H	-0.487960	3.129619	2.194202
C	0.808894	2.261654	-2.633550
H	1.478247	3.124067	-2.535690
H	0.304369	2.311548	-3.600708
H	1.406054	1.344177	-2.601454
C	-3.296745	3.909265	-0.705503
C	-2.967554	5.110113	-1.339150
H	-1.971767	5.246313	-1.756859
C	-3.901417	6.135470	-1.426653
H	-3.641378	7.065855	-1.921411
C	-5.172209	5.966762	-0.876954
H	-5.903040	6.766033	-0.948341
C	-5.498585	4.778003	-0.232219
H	-6.482431	4.649719	0.207409
C	-4.562211	3.749231	-0.139482
H	-4.787940	2.825262	0.388305
C	-2.211378	1.023197	-2.421755
C	-3.601124	0.922864	-2.541097
H	-4.224708	1.788455	-2.329108
C	-4.192180	-0.289818	-2.875991
H	-5.273293	-0.362163	-2.935710
C	-3.400726	-1.412654	-3.111256
H	-3.861356	-2.367231	-3.343979
C	-2.016299	-1.308938	-3.035315
H	-1.388762	-2.175328	-3.216761
C	-1.425517	-0.093579	-2.695985
H	-0.344743	-0.048847	-2.606127
C	2.281101	2.448329	0.061018
C	4.545915	1.992280	-0.085214
H	4.861251	2.126923	-1.132751
C	3.761766	0.666137	0.046961
H	3.884796	0.267047	1.064640
C	3.783175	4.392217	0.027736
H	3.979126	4.609621	-1.031018
H	4.656473	4.681381	0.615520
H	2.913563	4.958914	0.358268
C	1.297086	0.162404	0.084035
H	0.465362	0.629819	0.613873
H	1.668107	-0.678713	0.679671
H	0.938229	-0.226851	-0.873015
C	5.764699	2.048301	0.802719
C	5.669503	2.476338	2.127295
H	4.710881	2.817279	2.509430
C	6.795279	2.469584	2.945300

H	6.717138	2.810782	3.972441
C	8.017816	2.023818	2.448417
H	8.894641	2.017637	3.087432
C	8.113146	1.587149	1.129934
H	9.062891	1.236818	0.739330
C	6.990350	1.604326	0.307590
H	7.061084	1.265806	-0.723238
C	4.117676	-0.406604	-0.951956
C	4.463451	-1.681138	-0.512219
H	4.485636	-1.904097	0.552464
C	4.745670	-2.686246	-1.437211
H	5.002025	-3.678769	-1.082920
C	4.670390	-2.424457	-2.799808
H	4.876859	-3.211566	-3.517885
C	4.309629	-1.151586	-3.245438
H	4.239183	-0.946095	-4.309035
C	4.033875	-0.148869	-2.324688
H	3.741759	0.840508	-2.670482
C	-3.240667	-2.656122	1.501942
O	-3.184945	-2.478761	2.706120
O	-4.412545	-2.704037	0.796827
C	-5.680560	-2.555709	1.465682
C	-5.891300	-3.683259	2.475695
C	-5.792520	-1.180014	2.116368
C	-6.685142	-2.677876	0.322457
C	-2.127858	-2.766198	0.581482
N	-0.895547	-2.992857	1.076202
C	0.163132	-3.269880	0.366563
C	0.166930	-3.550398	-1.101075
C	-0.743565	-4.458616	-1.662875
C	-0.716773	-4.756457	-3.021585
C	0.220543	-4.150088	-3.857200
C	1.135648	-3.248956	-3.315525
C	1.111803	-2.956941	-1.953765
C	1.444058	-3.408572	1.099189
C	1.625325	-2.761083	2.335517
C	2.802632	-2.909740	3.057518
C	3.828701	-3.729225	2.581729
C	3.654303	-4.393328	1.369642
C	2.487684	-4.222494	0.629915
C	-1.901384	-0.504540	0.463850
C	-1.729499	0.060767	1.701786
C	-2.781028	0.798913	2.361822
O	-3.764662	1.266106	1.766444
C	-2.599981	1.082669	3.846797
C	-2.615172	-0.184577	4.707717
H	-6.905680	-3.626082	2.883457
H	-5.170643	-3.605913	3.289573
H	-5.771244	-4.652958	1.982955
H	-6.821765	-1.013979	2.452116
H	-5.119867	-1.100295	2.970242
H	-5.520800	-0.398607	1.401539
H	-7.707048	-2.587398	0.701674
H	-6.510694	-1.888932	-0.414678
H	-6.576449	-3.646282	-0.173890
H	-2.384378	-2.922133	-0.465972
H	-1.466502	-4.942696	-1.013197
H	-1.425373	-5.471468	-3.428851
H	0.240273	-4.381473	-4.917556
H	1.879182	-2.774887	-3.950203
H	1.856738	-2.280157	-1.537603
H	0.801555	-2.163293	2.716041
H	2.916604	-2.397736	4.008871
H	4.741617	-3.858581	3.154605
H	4.430869	-5.058194	0.999406
H	2.367760	-4.748258	-0.313177
H	-2.834135	-0.333718	-0.073213

H	-1.060774	-0.836835	-0.134141
H	-0.834348	-0.164216	2.278052
H	-1.636341	1.595512	3.978741
H	-3.391894	1.774717	4.146954
H	-1.879416	-0.910844	4.356330
H	-2.411236	0.061231	5.753959
H	-3.584949	-0.682382	4.647241

TS-*S*-1

N	-3.429633	2.280090	0.588327
N	-2.104161	1.675612	-1.085999
N	0.730698	4.341015	0.456668
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C	-2.207281	2.426546	0.037469
C	-4.155761	1.187375	-0.052142
H	-4.017174	0.277539	0.550013
C	-3.390616	1.028983	-1.388662
H	-3.899955	1.616800	-2.167373
C	-3.794322	2.746934	1.912089
H	-3.890957	1.901429	2.600779
H	-4.749014	3.275669	1.861198
H	-3.015483	3.420397	2.267189
C	-1.187240	1.962662	-2.177670
H	-0.902312	3.019741	-2.164034
H	-1.707067	1.748983	-3.114864
H	-0.287155	1.343384	-2.136662
C	-5.629924	1.441970	-0.233542
C	-6.097941	2.706000	-0.598341
H	-5.391042	3.525482	-0.708083
C	-7.456821	2.913685	-0.808146
H	-7.817266	3.899540	-1.083476
C	-8.353854	1.856660	-0.664480
H	-9.414105	2.019307	-0.828176
C	-7.889450	0.594342	-0.307300
H	-8.585652	-0.229770	-0.192806
C	-6.529759	0.388042	-0.087434
H	-6.162266	-0.594814	0.197161
C	-3.262128	-0.405566	-1.829456
C	-3.903728	-0.854543	-2.980845
H	-4.454809	-0.152495	-3.602122
C	-3.858245	-2.206364	-3.320607
H	-4.362820	-2.553823	-4.216640
C	-3.180867	-3.107390	-2.505431
H	-3.156564	-4.161437	-2.763494
C	-2.532218	-2.659753	-1.354315
H	-2.014797	-3.352115	-0.695449
C	-2.562797	-1.310037	-1.026448
H	-2.060606	-0.976758	-0.119631
C	-0.019952	3.219855	0.360305
C	2.130044	4.075640	0.149690
H	2.356345	4.470729	-0.851198
C	2.179750	2.521862	0.115351
H	2.661914	2.146009	1.026483
C	0.191347	5.680931	0.365442
H	0.235589	6.056105	-0.664902
H	0.776619	6.342113	1.008198
H	-0.844205	5.662844	0.702310
C	0.403341	0.758011	0.453846
H	-0.460696	0.727222	1.121255
H	1.243796	0.274366	0.960432
H	0.178952	0.188929	-0.454702
C	3.101496	4.676321	1.138213
C	2.759240	4.824388	2.482610
H	1.761732	4.547792	2.814597
C	3.690736	5.323196	3.388005

H	3.419006	5.440434	4.431935
C	4.970323	5.665274	2.957011
H	5.696285	6.051526	3.664773
C	5.316518	5.510908	1.617394
H	6.312582	5.775459	1.278189
C	4.382180	5.022227	0.708863
H	4.647905	4.901071	-0.338551
C	2.885180	1.963323	-1.095666
C	3.941549	1.071207	-0.942407
H	4.245507	0.751216	0.051017
C	4.606503	0.570295	-2.060940
H	5.425450	-0.128619	-1.926717
C	4.199542	0.944987	-3.336270
H	4.705781	0.537975	-4.205580
C	3.132659	1.830103	-3.498612
H	2.810184	2.118876	-4.493973
C	2.481601	2.340100	-2.382289
H	1.650289	3.032103	-2.506530
C	0.057868	-1.973911	1.827054
O	0.707702	-1.566767	2.765865
O	-1.297480	-2.016570	1.803550
C	-2.093729	-1.692117	2.970515
C	-2.012633	-0.182764	3.192976
C	-1.680358	-2.469502	4.215826
C	-3.498470	-2.109031	2.546272
C	0.560726	-2.528563	0.554437
N	1.917958	-2.331903	0.317739
C	2.390227	-2.402810	-0.880263
C	1.504977	-2.404363	-2.093488
C	0.908954	-3.562966	-2.597701
C	0.020321	-3.489296	-3.668193
C	-0.281646	-2.260345	-4.249561
C	0.325890	-1.103820	-3.767797
C	1.219575	-1.177373	-2.701993
C	3.855834	-2.421070	-1.081176
C	4.414609	-2.686020	-2.338095
C	5.796871	-2.722040	-2.508337
C	6.643974	-2.480702	-1.430381
C	6.094211	-2.216256	-0.172344
C	4.717904	-2.196304	0.004319
C	0.354767	-4.373578	0.748532
C	-0.361745	-4.854529	1.878138
C	0.208543	-5.037204	3.163210
O	-0.442089	-5.414595	4.157159
C	1.710238	-4.751717	3.352429
C	2.001563	-4.282223	4.772513
H	-0.121035	-2.310213	-0.271652
H	-2.680251	0.119392	4.006569
H	-2.318679	0.345540	2.278434
H	-0.990037	0.104465	3.448921
H	-2.403456	-2.248020	5.009189
H	-1.674967	-3.547904	4.035991
H	-0.686463	-2.178439	4.554129
H	-4.223382	-1.854044	3.324591
H	-3.521323	-3.188714	2.379103
H	-3.785702	-1.613950	1.611664
H	1.139566	-4.519711	-2.138319
H	-0.443057	-4.396141	-4.045464
H	-0.987445	-2.205419	-5.072426
H	0.115542	-0.142985	-4.231243
H	1.709366	-0.279796	-2.327655
H	3.761403	-2.870666	-3.185713
H	6.212195	-2.940247	-3.487889
H	7.720980	-2.507410	-1.562634
H	6.747642	-2.037946	0.676633
H	4.274333	-2.018855	0.979291
H	1.417208	-4.614707	0.695264

H	-1.435359	-5.011555	1.803971
H	2.260094	-5.680321	3.142916
H	2.063743	-4.003693	2.634820
H	1.563851	-3.291547	4.932104
H	1.548579	-4.969725	5.488586
H	3.077518	-4.212054	4.960159
H	-0.121735	-4.565757	-0.216421

TS-*S*-2

O	0.521536	-0.527791	3.475411
O	-1.582386	-1.101311	2.822453
C	-2.228270	-0.196692	3.737190
C	-1.856330	-0.508442	5.186163
C	-3.713000	-0.471322	3.511842
C	-1.885264	1.242835	3.351537
C	0.152202	-2.048142	1.644123
N	1.482686	-2.171483	1.370727
C	1.951603	-2.576766	0.234332
C	1.199158	-2.558563	-1.066434
C	1.762373	-1.815951	-2.119547
C	1.116338	-1.685727	-3.343706
C	-0.125069	-2.290457	-3.543733
C	-0.707041	-3.008451	-2.503329
C	-0.054004	-3.147200	-1.276820
C	3.410354	-2.879471	0.192509
C	4.232077	-2.495770	1.265382
C	5.588909	-2.789808	1.265015
C	6.162655	-3.488338	0.199417
C	5.355899	-3.885384	-0.863239
C	3.995575	-3.583569	-0.868300
C	-0.197919	-3.838992	2.600380
C	0.244842	-4.938909	1.870369
C	-0.624858	-5.630462	0.975082
O	-1.778710	-5.260482	0.682346
C	-0.057814	-6.872084	0.292118
C	0.781909	-6.474839	-0.927401
H	-0.597596	-2.135128	0.860842
H	-2.035143	-1.568998	5.385679
H	-0.808449	-0.285174	5.379241
H	-2.487393	0.080021	5.859927
H	-3.983522	-0.294369	2.465827
H	-4.322722	0.173148	4.151381
H	-3.939363	-1.515728	3.741675
H	-2.113550	1.397568	2.287246
H	-0.826204	1.444611	3.518650
H	-2.484927	1.944972	3.940244
H	2.726854	-1.341464	-1.967820
H	1.586966	-1.111544	-4.137840
H	-0.634690	-2.198105	-4.498609
H	-1.679319	-3.474299	-2.632762
H	-0.525581	-3.735190	-0.495877
H	3.765816	-1.977612	2.097366
H	6.204745	-2.483646	2.105947
H	7.221588	-3.727632	0.205352
H	5.783634	-4.442429	-1.691842
H	3.377734	-3.907306	-1.700593
H	-1.273519	-3.687390	2.677017
H	0.371369	-3.538676	3.476942
H	1.261122	-5.300270	1.991405
H	-0.899570	-7.499488	-0.013647
H	0.561272	-7.437265	0.997006
H	1.228494	-7.350260	-1.407900
H	0.162285	-5.956653	-1.665053
H	1.586212	-5.792056	-0.631900
N	-0.810566	3.291261	-0.375590

N	1.298772	4.195040	-0.628182
N	1.249288	2.047532	-0.115018
N	-3.060331	2.830526	-0.138956
N	-1.894105	1.284614	-1.213424
C	0.499831	3.125432	-0.391167
C	2.710426	3.838350	-0.625776
H	3.099653	3.896977	-1.651282
C	2.684035	2.352995	-0.161004
H	3.080572	2.274169	0.859499
C	0.848576	5.449674	-1.185577
H	1.059747	5.502531	-2.260723
H	1.365447	6.270508	-0.682273
H	-0.224651	5.536481	-1.022096
C	0.826604	0.811746	0.526497
H	-0.256432	0.804756	0.656908
H	1.296004	0.711603	1.511553
H	1.123228	-0.040463	-0.088954
C	3.552026	4.732374	0.256171
C	3.069441	5.172885	1.489933
H	2.062797	4.900621	1.798205
C	3.869331	5.959818	2.311735
H	3.488414	6.302943	3.268094
C	5.157542	6.306600	1.908360
H	5.780652	6.920629	2.550236
C	5.642834	5.865798	0.680923
H	6.644987	6.134056	0.363139
C	4.839513	5.083121	-0.144673
H	5.214975	4.736950	-1.104356
C	3.451665	1.410554	-1.062644
C	4.346294	0.492831	-0.516560
H	4.462544	0.423549	0.562123
C	5.085639	-0.352100	-1.343682
H	5.761957	-1.077620	-0.902417
C	4.932950	-0.277689	-2.724346
H	5.507853	-0.935756	-3.367868
C	4.017846	0.619103	-3.278110
H	3.880676	0.663876	-4.354066
C	3.272587	1.450054	-2.449618
H	2.549841	2.138128	-2.885033
C	-1.818498	2.462451	-0.566741
C	-3.980794	1.704529	-0.257903
H	-3.977750	1.139268	0.687999
C	-3.294410	0.854290	-1.345995
H	-3.659202	1.170460	-2.335705
C	-3.266726	3.834390	0.887345
H	-3.212967	3.393913	1.890291
H	-4.252423	4.281731	0.745937
H	-2.496600	4.597656	0.786802
C	-0.893852	0.650324	-2.056492
H	0.019278	1.242928	-2.088766
H	-1.293659	0.548262	-3.070989
H	-0.665469	-0.349668	-1.675931
C	-5.397431	2.074910	-0.612363
C	-5.681201	3.200865	-1.386381
H	-4.867622	3.851141	-1.698261
C	-6.994072	3.485822	-1.748989
H	-7.211917	4.368091	-2.342276
C	-8.027114	2.639658	-1.352778
H	-9.050701	2.862375	-1.636014
C	-7.744963	1.508529	-0.591261
H	-8.546475	0.845325	-0.283053
C	-6.433781	1.228959	-0.217819
H	-6.205803	0.346244	0.374936
C	-3.486867	-0.629188	-1.177028
C	-4.199902	-1.370668	-2.116013
H	-4.618466	-0.876504	-2.989594
C	-4.374606	-2.742937	-1.931408

H	-4.926178	-3.317281	-2.669463
C	-3.822337	-3.375148	-0.820193
H	-3.896156	-4.449081	-0.682981
C	-3.118355	-2.630606	0.126962
H	-2.662632	-3.147429	0.965320
C	-2.956252	-1.262744	-0.051733
H	-2.387093	-0.696164	0.683450

TS-*S*-3

O	-1.734683	-0.990596	1.869996	N	-3.768873	1.441089	0.797357
O	0.264797	-0.943416	2.957147	N	-2.846797	1.361450	-1.210388
C	-0.159827	-0.034788	3.987967	N	-0.187190	4.335830	0.002150
C	-1.367582	-0.577855	4.750405	N	0.097512	2.172805	-0.398970
C	-0.413309	1.341237	3.370392	C	-2.812943	1.951382	0.000531
C	1.050929	0.022002	4.915457	C	-4.328411	0.224507	0.199736
C	0.146103	-2.166378	0.990494	H	-3.785808	-0.631336	0.626759
N	1.519122	-1.955089	0.892213	C	-3.958974	0.402530	-1.291168
C	2.192679	-2.238653	-0.158849	H	-4.793921	0.889785	-1.817931
C	1.616531	-2.785613	-1.431082	C	-3.793116	1.598880	2.240334
C	1.430350	-1.918325	-2.513427	H	-3.322437	0.727567	2.708358
C	0.946147	-2.398923	-3.726392	H	-4.831401	1.685092	2.568284
C	0.664696	-3.756525	-3.871035	H	-3.247021	2.505120	2.501564
C	0.853645	-4.622963	-2.795809	C	-2.227820	1.870725	-2.416491
C	1.322777	-4.146258	-1.569855	H	-1.984516	2.929119	-2.292344
C	3.654228	-1.965306	-0.148129	H	-2.940664	1.766953	-3.239218
C	4.203483	-1.139103	0.843229	H	-1.319609	1.313925	-2.667827
C	5.564334	-0.868058	0.865507	C	-5.811057	0.061736	0.418437
C	6.410204	-1.429680	-0.094863	C	-6.660596	1.169839	0.426946
C	5.876347	-2.262624	-1.073474	H	-6.236747	2.165847	0.321252
C	4.507038	-2.522035	-1.106653	C	-8.031981	0.999601	0.582965
C	-0.121234	-3.924010	1.852842	H	-8.685895	1.865585	0.598512
C	0.892855	-4.282274	2.750509	C	-8.564302	-0.281013	0.719276
C	2.057696	-4.940950	2.273113	H	-9.634305	-0.414692	0.841317
O	2.227001	-5.368390	1.112617	C	-7.720957	-1.388280	0.703765
C	3.226570	-5.081744	3.243722	H	-8.131576	-2.386701	0.812606
C	4.235876	-3.970529	2.941368	C	-6.346696	-1.217582	0.558547
H	-0.418342	-2.322059	0.069497	H	-5.683400	-2.078394	0.553469
H	-1.149990	-1.595221	5.088619	C	-3.568415	-0.859391	-2.013284
H	-2.258237	-0.609686	4.125226	C	-4.152688	-1.183318	-3.234574
H	-1.557896	0.044788	5.630357	H	-4.932046	-0.545855	-3.645540
H	0.507141	1.711233	2.903484	C	-3.740888	-2.322848	-3.924195
H	-1.193443	1.285241	2.610350	H	-4.201779	-2.575509	-4.873804
H	-0.720424	2.056143	4.140630	C	-2.735795	-3.126760	-3.396769
H	1.251814	-0.969576	5.328222	H	-2.398803	-4.006281	-3.936517
H	0.868848	0.721460	5.736608	C	-2.150419	-2.805833	-2.171326
H	1.934841	0.345520	4.359731	H	-1.358777	-3.430557	-1.765545
H	1.692745	-0.866906	-2.402668	C	-2.571467	-1.678976	-1.477375
H	0.801233	-1.716972	-4.559573	H	-2.133273	-1.433443	-0.511319
H	0.304063	-4.137629	-4.822342	C	-0.787602	3.113498	-0.011650
H	0.643410	-5.682386	-2.910860	C	1.113309	4.255557	-0.661444
H	1.501914	-4.807551	-0.719920	H	0.988270	4.492847	-1.731258
H	3.530627	-0.734012	1.593994	C	1.438514	2.758114	-0.504021
H	5.974831	-0.226099	1.639655	H	1.952423	2.607794	0.458230
H	7.476251	-1.225934	-0.070510	C	-0.954906	5.563934	-0.045927
H	6.527402	-2.717509	-1.813999	H	-1.219803	5.829350	-1.078227
H	4.098862	-3.176949	-1.869913	H	-0.358137	6.369897	0.385380
H	-1.124271	-3.715174	2.226772	H	-1.865309	5.428507	0.536617
H	-0.115373	-4.479586	0.914912	C	0.001439	0.746565	-0.128076
H	0.869638	-3.930614	3.777252	H	-0.907429	0.523101	0.425655
H	2.886916	-5.016939	4.283227	H	0.862605	0.434934	0.474937
H	3.688400	-6.061732	3.087136	H	0.010795	0.164380	-1.056150
H	3.759134	-2.991498	3.061155	C	2.166699	5.158544	-0.071762
H	5.112033	-4.017410	3.595804	C	2.188262	5.433480	1.296736
H	4.568082	-4.048393	1.901919	H	1.407888	5.026033	1.934773
N	-2.041652	2.969748	0.368798	C	3.198455	6.225230	1.833125
				H	3.206989	6.441546	2.896451
				C	4.198102	6.736601	1.008454
				H	4.986054	7.353076	1.428525
				C	4.183892	6.456293	-0.354923
				H	4.961527	6.850142	-1.000941
				C	3.167937	5.672313	-0.894124
				H	3.154142	5.449845	-1.958198
				C	2.253454	2.118494	-1.597869
				C	3.428035	1.445212	-1.272526
				H	3.766865	1.412319	-0.241023
				C	4.159909	0.779991	-2.254615

H	5.054666	0.233155	-1.972555	N	-1.868956	-1.613539	-0.064519
C	3.715549	0.794290	-3.572717	N	2.181736	-3.322530	-0.218487
H	4.272677	0.266425	-4.339749	N	1.419972	-1.496374	-1.215350
C	2.539197	1.467709	-3.907094	C	-1.346576	-2.759024	-0.522978
H	2.187786	1.469803	-4.934109	C	-3.656159	-3.028950	-0.642430
C	1.806972	2.122469	-2.923118	H	-4.310342	-3.060327	-1.520347
H	0.876390	2.625099	-3.178953	C	-3.319019	-1.553847	-0.286551
				H	-3.800368	-1.269384	0.655531
				C	-2.156166	-4.951744	-1.333441
				H	-2.839956	-5.213218	-2.144940
TS-*S*-4				H	-2.363468	-5.597366	-0.472611
O	-0.994189	1.047421	3.536374	H	-1.128608	-5.101399	-1.660532
O	1.077835	0.509782	2.770242	C	-1.191442	-0.475191	0.526759
C	1.339712	-0.425470	3.839933	H	-0.150488	-0.719887	0.746689
C	0.345205	-1.585890	3.785374	H	-1.694504	-0.204646	1.460270
C	1.325246	0.284174	5.192014	H	-1.231234	0.386208	-0.148047
C	2.744519	-0.926994	3.521978	C	-4.293642	-3.809383	0.487317
C	-0.032765	2.201796	1.656050	C	-3.630792	-3.952374	1.710490
N	-1.257249	2.661906	1.228889	H	-2.652508	-3.496878	1.854314
C	-1.525325	3.068183	0.031016	C	-4.219076	-4.671310	2.744065
C	-0.632065	2.903802	-1.157865	H	-3.701858	-4.775555	3.692176
C	-1.179476	2.353040	-2.330643	C	-5.473943	-5.253846	2.565109
C	-0.399369	2.137832	-3.460495	H	-5.932938	-5.812531	3.374102
C	0.961254	2.446056	-3.437958	C	-6.136110	-5.115646	1.350397
C	1.525279	2.966796	-2.277494	H	-7.112301	-5.567123	1.206826
C	0.738056	3.204577	-1.149680	C	-5.544057	-4.397482	0.313368
C	-2.879195	3.657282	-0.178108	H	-6.058732	-4.289667	-0.637987
C	-3.882237	3.442658	0.781056	C	-3.691390	-0.555327	-1.360925
C	-5.144696	4.000131	0.628734	C	-4.401848	0.594771	-1.026942
C	-5.435369	4.802538	-0.477505	H	-4.655008	0.794779	0.010874
C	-4.443690	5.037126	-1.425496	C	-4.786984	1.499736	-2.015012
C	-3.179935	4.468485	-1.279722	H	-5.325081	2.400071	-1.734008
C	0.698561	3.736081	2.672097	C	-4.456862	1.254060	-3.344250
C	2.100395	3.831586	2.658035	H	-4.753901	1.958135	-4.114972
C	2.890000	4.652713	1.802040	C	-3.724496	0.114795	-3.683879
O	4.129990	4.550659	1.734579	H	-3.457820	-0.072461	-4.719407
C	2.234672	5.769818	0.975892	C	-3.339923	-0.784598	-2.696153
C	3.005447	6.032211	-0.312886	H	-2.778414	-1.679404	-2.960780
H	0.766180	1.997042	0.942486	C	1.067640	-2.649409	-0.620460
H	0.357952	-2.040324	2.785827	C	3.361770	-2.476787	-0.352532
H	-0.664580	-1.241450	4.008988	H	3.566356	-1.984262	0.609653
H	0.634159	-2.353264	4.510818	C	2.879640	-1.410010	-1.361189
H	1.992793	1.150165	5.158372	H	3.140443	-1.729397	-2.381997
H	0.320526	0.620780	5.444626	C	2.139363	-4.348200	0.805411
H	1.682888	-0.399252	5.968388	H	2.220641	-3.908521	1.808205
H	2.743352	-1.451884	2.560009	H	2.973007	-5.035924	0.649811
H	3.088934	-1.619371	4.295252	H	1.196056	-4.886264	0.721010
H	3.442028	-0.087523	3.454233	C	0.599878	-0.618333	-2.029922
H	-2.234018	2.094391	-2.346563	H	-0.441883	-0.938808	-2.028207
H	-0.855219	1.717530	-4.353237	H	0.972496	-0.624595	-3.060285
H	1.579722	2.272625	-4.313714	H	0.665696	0.402786	-1.644768
H	2.588176	3.184080	-2.236509	C	4.604700	-3.193799	-0.815304
H	1.200196	3.628729	-0.262158	C	4.531323	-4.329253	-1.622755
H	-3.630588	2.841093	1.649197	H	3.557430	-4.737539	-1.880979
H	-5.906035	3.820702	1.382384	C	5.696768	-4.930646	-2.088653
H	-6.419432	5.246762	-0.590469	H	5.636012	-5.819132	-2.709019
H	-4.649249	5.673622	-2.281089	C	6.939065	-4.392587	-1.762032
H	-2.413840	4.670466	-2.021683	H	7.847285	-4.860917	-2.127211
H	0.127034	4.487458	2.130142	C	7.014303	-3.252477	-0.966002
H	2.676231	3.188805	3.322136	H	7.979900	-2.827819	-0.711669
H	1.181933	5.561081	0.763617	C	5.850358	-2.656737	-0.489695
H	2.244262	6.672822	1.599936	H	5.901789	-1.764353	0.129398
H	4.051833	6.230764	-0.075902	C	3.447616	-0.043635	-1.088616
H	2.980379	5.154361	-0.967974	C	4.348342	0.538051	-1.978085
H	2.589212	6.879035	-0.865392	H	4.594377	0.026808	-2.905887
N	-0.110100	-3.221396	-0.467606	C	4.944556	1.761189	-1.667751
N	-2.337983	-3.555559	-0.998826	H	5.647844	2.206858	-2.364749

C	4.641039	2.403080	-0.469187
H	5.078481	3.359411	-0.197237
C	3.735023	1.819865	0.419992
H	3.504901	2.324085	1.351056
C	3.135901	0.606651	0.108199
H	2.418602	0.174535	0.805436
H	0.205547	3.458052	3.604030

TS-*S*-5

O	3.352182	-4.108365	-2.976282
O	4.152825	-3.188559	-1.063510
C	5.525955	-3.416509	-1.460068
C	5.855915	-2.639075	-2.734225
C	5.802659	-4.912149	-1.609994
C	6.330735	-2.857169	-0.289964
C	1.807396	-3.271485	-1.422050
N	1.595607	-2.859262	-0.157098
C	0.464046	-2.938638	0.494164
C	-0.771295	-3.559847	-0.068267
C	-1.265190	-3.199597	-1.331773
C	-2.377647	-3.830761	-1.880385
C	-3.024296	-4.847909	-1.180471
C	-2.541217	-5.224884	0.071278
C	-1.434717	-4.585392	0.621902
C	0.468599	-2.480931	1.905637
C	1.694529	-2.195786	2.534659
C	1.748263	-1.666888	3.815735
C	0.573846	-1.433176	4.534813
C	-0.647409	-1.748684	3.946688
C	-0.704319	-2.264973	2.652973
C	1.838282	-1.400836	-2.936434
C	0.648371	-0.773884	-3.199668
C	0.289517	0.502970	-2.643113
O	0.982976	1.150452	-1.840355
C	-1.017839	1.116108	-3.139338
C	-0.839264	1.741557	-4.527766
H	1.045989	-3.793195	-2.001683
H	5.562640	-1.591528	-2.608587
H	6.935167	-2.673444	-2.914916
H	5.330701	-3.055859	-3.592606
H	5.516125	-5.433794	-0.691912
H	6.873144	-5.069183	-1.775650
H	5.243416	-5.328319	-2.446523
H	6.001499	-3.320597	0.645413
H	6.197597	-1.774362	-0.212241
H	7.394843	-3.066147	-0.431987
H	-0.748791	-2.423500	-1.891069
H	-2.732200	-3.534940	-2.863770
H	-3.885007	-5.349983	-1.611700
H	-3.022575	-6.031158	0.618172
H	-1.061235	-4.891313	1.595304
H	2.601258	-2.400452	1.980673
H	2.715882	-1.440715	4.255691
H	0.613793	-1.026464	5.540654
H	-1.574068	-1.591679	4.491073
H	-1.677267	-2.488856	2.220030
H	2.194721	-2.201524	-3.574597
H	2.573812	-0.893915	-2.315536
H	-0.047673	-1.215602	-3.909699
H	-1.326607	1.879964	-2.416563
H	-1.797609	0.344268	-3.184980
H	-0.534246	0.986440	-5.256800
H	-0.064288	2.513255	-4.505764
H	-1.767799	2.201078	-4.876970
N	-1.389031	3.006536	0.045546

N	0.764151	3.741817	-0.360493
N	0.568176	2.232290	1.250092
N	-3.653574	2.565553	0.030750
N	-2.346305	0.796074	0.292404
C	-0.089269	2.925369	0.304270
C	2.140283	3.365422	-0.048235
H	2.466217	2.620773	-0.787261
C	1.967649	2.671961	1.318002
H	2.049413	3.423102	2.119997
C	0.468706	4.239501	-1.691271
H	0.753469	3.484124	-2.431737
H	1.031981	5.160860	-1.853380
H	-0.599323	4.444326	-1.761753
C	0.014101	1.494909	2.372300
H	0.232560	2.028597	3.304568
H	0.471626	0.500628	2.420923
H	-1.063669	1.385640	2.262906
C	3.109753	4.517526	0.004817
C	2.700642	5.796494	0.385481
H	1.649803	5.976361	0.598335
C	3.629099	6.828490	0.482408
H	3.303076	7.822944	0.770261
C	4.974029	6.586112	0.212349
H	5.697886	7.390937	0.289700
C	5.386995	5.309268	-0.158979
H	6.433426	5.114861	-0.370608
C	4.457227	4.279287	-0.266878
H	4.773091	3.280746	-0.558114
C	2.956032	1.564670	1.561858
C	3.891687	1.690398	2.587193
H	3.873210	2.568827	3.227513
C	4.854229	0.702336	2.778074
H	5.585309	0.805359	3.573824
C	4.875599	-0.411854	1.943683
H	5.623707	-1.185210	2.091704
C	3.933122	-0.546682	0.923194
H	3.914766	-1.432058	0.291897
C	2.970547	0.439361	0.733595
H	2.235162	0.335900	-0.064256
C	-2.363858	2.136658	0.143352
C	-4.594833	1.489577	0.305005
H	-4.970120	1.586577	1.335160
C	-3.694054	0.233687	0.196613
H	-3.810234	-0.217786	-0.800215
C	-4.046123	3.945060	0.219441
H	-4.298114	4.148386	1.268321
H	-4.919928	4.153757	-0.401890
H	-3.217836	4.584674	-0.082274
C	-1.241994	-0.098946	-0.010003
H	-1.426249	-0.582812	-0.974477
H	-1.186304	-0.865602	0.761184
H	-0.298752	0.438314	-0.069231
C	-5.772452	1.451627	-0.639274
C	-5.623010	1.810276	-1.980009
H	-4.656749	2.164882	-2.331347
C	-6.703091	1.717520	-2.851528
H	-6.583594	2.003909	-3.891442
C	-7.935090	1.256208	-2.391684
H	-8.776423	1.183717	-3.073046
C	-8.084561	0.890225	-1.057201
H	-9.041502	0.529271	-0.694770
C	-7.006420	0.991978	-0.182308
H	-7.118697	0.707279	0.860956
C	-3.950915	-0.817455	1.250742
C	-4.194698	-2.138955	0.885636
H	-4.170302	-2.429786	-0.161809
C	-4.440366	-3.101560	1.864529

	x	y	z
H	-4.624237	-4.127861	1.566696
C	-4.429869	-2.749615	3.209570
H	-4.616541	-3.500009	3.970815
C	-4.163948	-1.431390	3.580487
H	-4.141871	-1.154590	4.630048
C	-3.917741	-0.472906	2.605571
H	-3.687805	0.549583	2.898069

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	x	y	z
O	0.195059	-1.008925	3.052937
O	-1.918487	-0.853860	2.228833
C	-2.382016	0.031162	3.270048
C	-2.204409	-0.578238	4.659356
C	-3.866304	0.175010	2.948173
C	-1.652116	1.368266	3.135669
C	-0.503391	-2.291410	1.142972
N	0.767376	-2.730335	0.864605
C	1.063373	-3.258851	-0.279667
C	0.095495	-3.246943	-1.426782
C	-0.998576	-4.116236	-1.478005
C	-1.943349	-4.007659	-2.495068
C	-1.809241	-3.030238	-3.478727
C	-0.717640	-2.167622	-3.446551
C	0.227626	-2.280549	-2.428585
C	2.381999	-3.902497	-0.454914
C	2.720208	-4.576803	-1.637005
C	3.931599	-5.255309	-1.749114
C	4.830292	-5.270898	-0.686696
C	4.508775	-4.587842	0.488417
C	3.304602	-3.909770	0.604077
C	-1.433351	-3.917506	2.028619
C	-2.752254	-4.150922	1.638300
C	-3.862468	-3.741902	2.443557
O	-3.785089	-3.053830	3.471936
C	-5.245028	-4.251568	2.019302
C	-5.682629	-3.747232	0.643765
H	-1.221200	-2.172726	0.335951
H	-2.771965	0.017131	5.382806
H	-2.604533	-1.594602	4.641655
H	-1.155007	-0.594383	4.951335
H	-4.338295	0.888430	3.630580
H	-4.342598	-0.804167	3.050904
H	-3.998657	0.524518	1.916543
H	-2.094058	2.111110	3.808748
H	-1.745931	1.732711	2.102799
H	-0.593161	1.250601	3.375533
H	-1.112414	-4.869009	-0.703593
H	-2.795102	-4.681674	-2.511487
H	-2.557253	-2.934389	-4.259357
H	-0.600293	-1.411112	-4.218231
H	1.088325	-1.615793	-2.396289
H	2.016997	-4.591132	-2.464888
H	4.165695	-5.785968	-2.667726
H	5.768336	-5.811829	-0.768658
H	5.203139	-4.591449	1.324138
H	3.033770	-3.390873	1.517650
H	-1.288550	-3.596428	3.059168
H	-0.645579	-4.562174	1.642719
H	-2.959228	-4.730015	0.741047
H	-5.949519	-3.924653	2.788303
H	-5.232562	-5.348385	2.016731
H	-6.684261	-4.105568	0.386893
H	-5.696855	-2.652782	0.618075
H	-4.993542	-4.090212	-0.135798
N	0.645759	3.458804	-0.128612
N	-1.655551	3.651654	0.043926
N	-0.929295	2.065991	-1.325462
N	2.959177	3.501076	-0.120236
N	2.031144	1.486771	0.039636
C	-0.561896	3.030706	-0.449778
C	-2.868125	2.933036	-0.341493
H	-3.132786	2.226598	0.459962
C	-2.376408	2.137554	-1.570834
H	-2.542385	2.742612	-2.476990
C	-1.634701	4.523141	1.203940
H	-1.890155	3.968837	2.112945
H	-2.362266	5.323565	1.055637
H	-0.634994	4.943989	1.301262
C	-0.102278	1.538721	-2.394473
H	0.951297	1.584454	-2.123746
H	-0.264217	2.111166	-3.316834
H	-0.383113	0.495324	-2.565562
C	-4.053550	3.811690	-0.644200
C	-3.892824	5.050163	-1.268521
H	-2.890662	5.407418	-1.494615
C	-5.005900	5.820622	-1.588294
H	-4.875637	6.787446	-2.063771
C	-6.285449	5.351492	-1.297649
H	-7.153607	5.952287	-1.548151
C	-6.448759	4.112524	-0.684371
H	-7.443405	3.743318	-0.457317
C	-5.334729	3.345441	-0.353927
H	-5.455869	2.377512	0.126253
C	-3.042351	0.797452	-1.720098
C	-3.951630	0.581809	-2.752591
H	-4.129586	1.363073	-3.487636
C	-4.645588	-0.624500	-2.824970
H	-5.360090	-0.789148	-3.625329
C	-4.429845	-1.608418	-1.865437
H	-4.979492	-2.543443	-1.914576
C	-3.510100	-1.401263	-0.835948
H	-3.339702	-2.164369	-0.076740
C	-2.813638	-0.200238	-0.768847
H	-2.110115	-0.039446	0.046906
C	1.789402	2.806721	-0.097358
C	4.075676	2.575275	-0.271522
H	4.289517	2.436194	-1.344244
C	3.463211	1.267265	0.278491
H	3.630682	1.217948	1.364658
C	3.050911	4.849507	-0.642291
H	3.171910	4.847607	-1.733259
H	3.913716	5.341837	-0.189772
H	2.141312	5.388224	-0.380680
C	1.059714	0.495354	0.498768
H	0.263867	0.980524	1.070182
H	1.559425	-0.221285	1.155265
H	0.622756	-0.060653	-0.338521
C	5.335963	2.994786	0.439809
C	5.278349	3.630544	1.681722
H	4.309538	3.868456	2.114051
C	6.451337	3.956625	2.354356
H	6.399958	4.454491	3.317217
C	7.688210	3.640600	1.795816
H	8.602229	3.893151	2.323129
C	7.748891	3.001196	0.561103
H	8.709716	2.752318	0.122633
C	6.575366	2.683374	-0.117382
H	6.619251	2.179603	-1.079653
C	4.036276	0.043735	-0.382607
C	5.178163	-0.542637	0.163051
H	5.582248	-0.162720	1.098015
C	5.794508	-1.605759	-0.488581

H	6.675803	-2.067177	-0.054908
C	5.264807	-2.099416	-1.677014
H	5.724146	-2.952018	-2.163950
C	4.113996	-1.529719	-2.213130
H	3.679704	-1.936518	-3.121180
C	3.509698	-0.450954	-1.575020
H	2.617338	0.005659	-1.996572

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O	-1.370160	-2.458857	-4.267290
O	0.099606	-2.217018	-2.551202
C	1.217945	-2.097276	-3.445075
C	1.079116	-0.846016	-4.312994
C	1.405018	-3.361323	-4.283973
C	2.394908	-1.934950	-2.487332
C	-2.194476	-2.315684	-2.052025
N	-1.851595	-2.528483	-0.758335
C	-2.696685	-2.652767	0.222010
C	-4.177257	-2.794729	0.047202
C	-5.077310	-1.938738	0.690700
C	-6.448803	-2.062319	0.502934
C	-6.950103	-3.058330	-0.333493
C	-6.068426	-3.928437	-0.967281
C	-4.695494	-3.800941	-0.774018
C	-2.114842	-2.755276	1.584750
C	-2.895373	-2.935426	2.738662
C	-2.310207	-3.014239	4.001450
C	-0.931287	-2.916697	4.152608
C	-0.137881	-2.752064	3.014621
C	-0.716167	-2.689736	1.755556
C	-2.268154	-0.183127	-2.028649
C	-3.151044	0.271814	-1.069007
C	-4.447452	0.783648	-1.449587
O	-4.847296	0.843156	-2.612939
C	-5.283922	1.420699	-0.339004
C	-6.729659	1.641645	-0.756537
H	-3.198002	-2.489167	-2.435653
H	1.996651	-0.687299	-4.891107
H	0.913123	0.028688	-3.671941
H	0.237164	-0.943906	-4.997359
H	2.355981	-3.307673	-4.823954
H	0.589895	-3.474880	-4.996606
H	1.428722	-4.236500	-3.628058
H	3.335477	-1.849532	-3.043226
H	2.254643	-1.028047	-1.884423
H	2.460564	-2.791661	-1.809872
H	-4.685142	-1.159369	1.338907
H	-7.125592	-1.373523	1.000692
H	-8.019844	-3.152880	-0.490780
H	-6.449271	-4.708547	-1.619208
H	-4.008376	-4.478001	-1.273899
H	-3.971318	-3.034920	2.648845
H	-2.943968	-3.163330	4.871349
H	-0.476795	-2.978675	5.136974
H	0.942534	-2.683820	3.114645
H	-0.109216	-2.601984	0.857302
H	-2.572355	-0.055698	-3.066986
H	-1.196323	-0.191032	-1.853362
H	-2.914420	0.223947	-0.009167
H	-5.218416	0.813503	0.570818
H	-4.803063	2.382652	-0.100736
H	-7.218029	0.684232	-0.959415
H	-7.294342	2.166857	0.018883
H	-6.762174	2.221715	-1.680830
N	1.859151	2.414223	-0.607883

N	3.766259	1.228462	-1.200745
N	3.036341	0.920085	0.875912
N	0.186692	3.768042	0.307901
N	-0.103254	1.589499	0.509520
C	2.801402	1.547473	-0.309221
C	4.632563	0.173099	-0.691208
H	4.317608	-0.787462	-1.119762
C	4.299151	0.178242	0.824967
H	5.067597	0.754257	1.362026
C	3.676049	1.507226	-2.621524
H	3.400050	0.604680	-3.176899
H	4.642244	1.869025	-2.980550
H	2.915311	2.271981	-2.772955
C	2.565165	1.408813	2.164938
H	2.161620	2.418459	2.064527
H	3.415633	1.443892	2.852108
H	1.795555	0.763297	2.598484
C	6.099785	0.377139	-0.975149
C	6.665129	1.653592	-0.974411
H	6.027366	2.519240	-0.810462
C	8.029394	1.813038	-1.193856
H	8.462156	2.808218	-1.203833
C	8.838563	0.697840	-1.402224
H	9.902394	0.823986	-1.574581
C	8.279469	-0.576678	-1.394263
H	8.905335	-1.447515	-1.559751
C	6.912097	-0.735949	-1.186096
H	6.469674	-1.729095	-1.186431
C	4.214548	-1.213862	1.400473
C	5.279101	-1.731039	2.135574
H	6.142856	-1.104912	2.345487
C	5.239961	-3.046938	2.593091
H	6.071537	-3.443208	3.166753
C	4.136444	-3.848662	2.317538
H	4.104564	-4.872273	2.675820
C	3.069309	-3.335400	1.580899
H	2.200949	-3.951374	1.365879
C	3.108207	-2.021837	1.125576
H	2.277290	-1.620544	0.550157
C	0.714861	2.549579	0.065381
C	-1.185466	3.653926	0.818343
H	-1.310776	4.331623	1.669393
C	-1.204333	2.179554	1.298256
H	-2.137899	1.699419	0.997304
C	0.675474	4.999354	-0.275351
H	0.624586	5.797838	0.469750
H	0.068356	5.281096	-1.141811
H	1.709111	4.851682	-0.584959
C	0.077040	0.153205	0.404352
H	0.636750	-0.086914	-0.504558
H	-0.901726	-0.325129	0.318223
H	0.584547	-0.260310	1.281098
C	-2.232849	3.977534	-0.225061
C	-2.237594	3.306180	-1.450467
H	-1.473480	2.565643	-1.669205
C	-3.252531	3.536694	-2.373270
H	-3.287591	2.958478	-3.289861
C	-4.257935	4.456873	-2.083448
H	-5.058797	4.620634	-2.796884
C	-4.244934	5.148976	-0.875149
H	-5.027080	5.866391	-0.648749
C	-3.235121	4.906704	0.053840
H	-3.234242	5.431110	1.006624
C	-0.935199	1.955542	2.773814
C	-1.352148	0.758531	3.361948
H	-1.914406	0.026061	2.782159
C	-1.046148	0.486531	4.693816

H	-1.381391	-0.447568	5.130248
C	-0.316070	1.402256	5.445621
H	-0.082375	1.190147	6.484016
C	0.110922	2.593535	4.863629
H	0.679585	3.312270	5.445366
C	-0.197103	2.867982	3.534538
H	0.151245	3.796629	3.088571

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O	3.395915	-4.620242	-2.443466
O	4.070413	-3.148269	-0.851230
C	5.471814	-3.404998	-1.107391
C	5.849760	-3.053907	-2.546626
C	5.814759	-4.856974	-0.775885
C	6.177073	-2.466799	-0.132794
C	1.755780	-3.538616	-1.157146
N	1.493015	-2.882963	0.000355
C	0.328000	-2.887332	0.585831
C	-0.855618	-3.660121	0.092596
C	-1.439339	-4.627709	0.922759
C	-2.475070	-5.434921	0.466714
C	-2.970555	-5.278254	-0.827322
C	-2.416658	-4.307524	-1.657571
C	-1.367941	-3.510526	-1.202400
C	0.225622	-2.268016	1.930685
C	-1.003908	-1.874282	2.486702
C	-1.058587	-1.270073	3.740207
C	0.106511	-1.042874	4.470308
C	1.330426	-1.449190	3.939143
C	1.383207	-2.070969	2.698557
C	1.439961	-2.184351	-2.953007
C	0.862170	-0.965800	-2.667906
C	1.557826	0.282863	-2.589187
O	1.025614	1.314810	-2.123511
C	2.974673	0.403225	-3.137868
C	4.036446	0.210259	-2.053158
H	1.054885	-4.275624	-1.547428
H	5.529322	-2.034524	-2.780885
H	6.938093	-3.102465	-2.656595
H	5.384852	-3.744875	-3.248063
H	5.328513	-5.537023	-1.474496
H	6.898928	-4.997637	-0.829904
H	5.486413	-5.092267	0.240895
H	5.884765	-2.710634	0.893376
H	5.906024	-1.425163	-0.332976
H	7.261966	-2.572858	-0.222724
H	-1.054756	-4.754201	1.930881
H	-2.894741	-6.192796	1.122225
H	-3.775119	-5.912688	-1.186841
H	-2.790817	-4.178535	-2.669039
H	-0.923152	-2.769511	-1.859204
H	-1.923754	-2.039497	1.929619
H	-2.021310	-0.970319	4.143199
H	0.059291	-0.568534	5.445957
H	2.249539	-1.291364	4.496192
H	2.324071	-2.424470	2.295744
H	2.478428	-2.241938	-3.269234
H	0.828764	-3.012582	-3.294932
H	-0.202285	-0.909713	-2.464488
H	3.136151	-0.314446	-3.946567
H	3.053375	1.409055	-3.563032
H	5.042598	0.291536	-2.476569
H	3.933210	-0.773424	-1.582513
H	3.937332	0.963346	-1.266706
N	-1.601441	3.175317	-0.268557
N	0.596681	3.807792	-0.609065
N	0.259215	2.409845	1.081554
N	-3.858335	2.683056	-0.346571
N	-2.505427	0.955715	0.021643
C	-0.315903	3.074586	0.054649
C	1.942792	3.454581	-0.165893
H	2.318280	2.676148	-0.843689
C	1.656522	2.837599	1.221272
H	1.694771	3.634953	1.981929
C	0.391097	4.280742	-1.967512
H	0.720208	3.509265	-2.670209
H	0.966246	5.198827	-2.105269
H	-0.669604	4.487337	-2.104476
C	-0.418428	1.945661	2.279413
H	-0.464472	2.747289	3.028206
H	0.144391	1.102142	2.689884
H	-1.426454	1.601875	2.050000
C	2.901531	4.614669	-0.097185
C	2.465389	5.894626	0.250563
H	1.405229	6.065471	0.421742
C	3.377507	6.938430	0.367261
H	3.030535	7.932805	0.629828
C	4.734163	6.707575	0.148802
H	5.446190	7.521260	0.241565
C	5.173967	5.431347	-0.191324
H	6.229315	5.246637	-0.363624
C	4.259722	4.389204	-0.319075
H	4.597045	3.391276	-0.587869
C	2.619676	1.742833	1.593750
C	3.621724	2.006918	2.529601
H	3.647971	2.971674	3.030636
C	4.592310	1.048447	2.801349
H	5.372633	1.258415	3.526239
C	4.563952	-0.174520	2.134554
H	5.329165	-0.917998	2.336260
C	3.559289	-0.447748	1.208493
H	3.516934	-1.401093	0.683979
C	2.580487	0.507893	0.945380
H	1.801974	0.296838	0.211724
C	-2.562447	2.292096	-0.171922
C	-4.769260	1.588670	-0.049621
H	-5.137178	1.689485	0.983400
C	-3.835356	0.359060	-0.148690
H	-3.900545	-0.060156	-1.163429
C	-4.286936	4.055011	-0.177069
H	-4.544720	4.266935	0.868949
H	-5.165423	4.231927	-0.801362
H	-3.475814	4.711831	-0.488383
C	-1.319527	0.141649	-0.247572
H	-0.666019	0.637658	-0.972446
H	-1.661401	-0.816983	-0.648326
H	-0.759928	-0.069993	0.666363
C	-5.955290	1.498565	-0.979229
C	-5.849634	1.886919	-2.315485
H	-4.912405	2.303619	-2.675628
C	-6.936720	1.743630	-3.171729
H	-6.851417	2.053690	-4.208217
C	-8.130771	1.201537	-2.701191
H	-8.977261	1.090003	-3.370878
C	-8.236186	0.805603	-1.370847
H	-9.164193	0.382910	-0.999865
C	-7.152149	0.957982	-0.511055
H	-7.229730	0.650436	0.529017
C	-4.137793	-0.725976	0.855315
C	-4.360832	-2.033722	0.429932
H	-4.293269	-2.279208	-0.626728
C	-4.655844	-3.033653	1.355442

H	-4.818105	-4.047993	1.009958
C	-4.727565	-2.730017	2.710519
H	-4.954268	-3.508199	3.431934
C	-4.499230	-1.424252	3.142551
H	-4.547322	-1.185355	4.200521
C	-4.197468	-0.429623	2.220388
H	-3.992723	0.581835	2.565155

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O	3.351882	-4.108376	-2.976386
O	4.152654	-3.188545	-1.063682
C	5.525758	-3.416589	-1.460283
C	5.855715	-2.639226	-2.734484
C	5.802361	-4.912254	-1.610157
C	6.330622	-2.857261	-0.290229
C	1.807189	-3.271580	-1.422018
N	1.595485	-2.859248	-0.157092
C	0.463983	-2.938636	0.494275
C	-0.771359	-3.559965	-0.068015
C	-1.265315	-3.199898	-1.331552
C	-2.377738	-3.831208	-1.880063
C	-3.024309	-4.848308	-1.180006
C	-2.541181	-5.225089	0.071780
C	-1.434706	-4.585464	0.622297
C	0.468619	-2.480817	1.905710
C	1.694588	-2.195641	2.534647
C	1.748398	-1.666700	3.815703
C	0.574023	-1.432963	4.534842
C	-0.647267	-1.748472	3.946793
C	-0.704256	-2.264801	2.653097
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