

Electronic Supplementary Information

A substrate-dependent mechanism for nickel-catalyzed *N*-allylation with allylic alcohols: nucleophilic attack vs. reductive elimination

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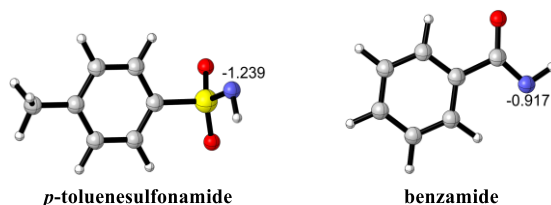


Fig. S1 The NBO charge of *p*-toluenesulfonamide and benzamide

To test the accuracy of our calculations, a larger basis set 6-311+G(2d,2p) + lanl2tz (BSII) was employed to calculate all intermediates and transition states in **Figs. 1** and **2**, and the results are shown in **Fig. S2**. Calculations demonstrate that the relative free energies of these structures under basis set 6-311+G(2d,2p) + lanl2tz (BSII) are similar as those under level of 6-31G(d,p) + lanl2dz (BSI).

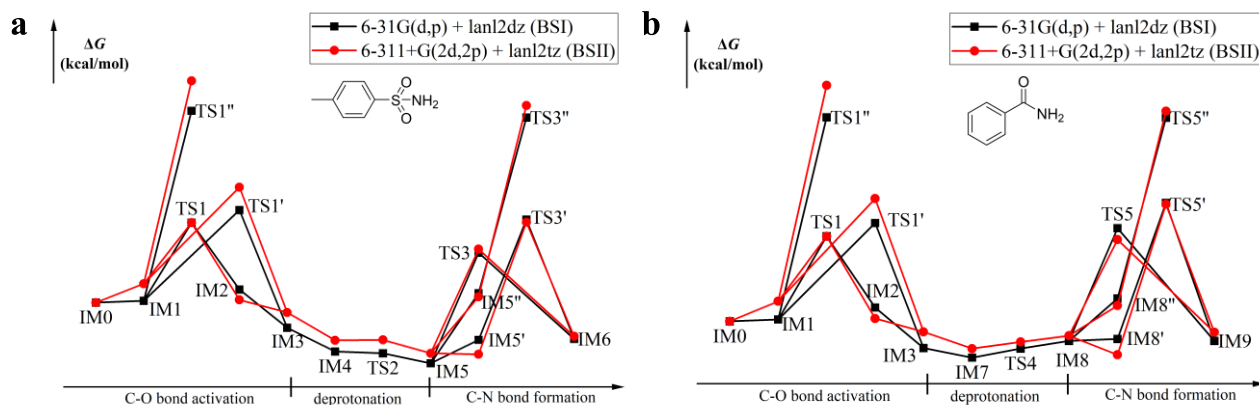


Fig. S2 Free energy profiles of *N*-allylation of *p*-toluenesulfonamide (a) and benzamide (b) at the M06-L/BSI (black line) and M06-L/BSII (red line) levels of theory.

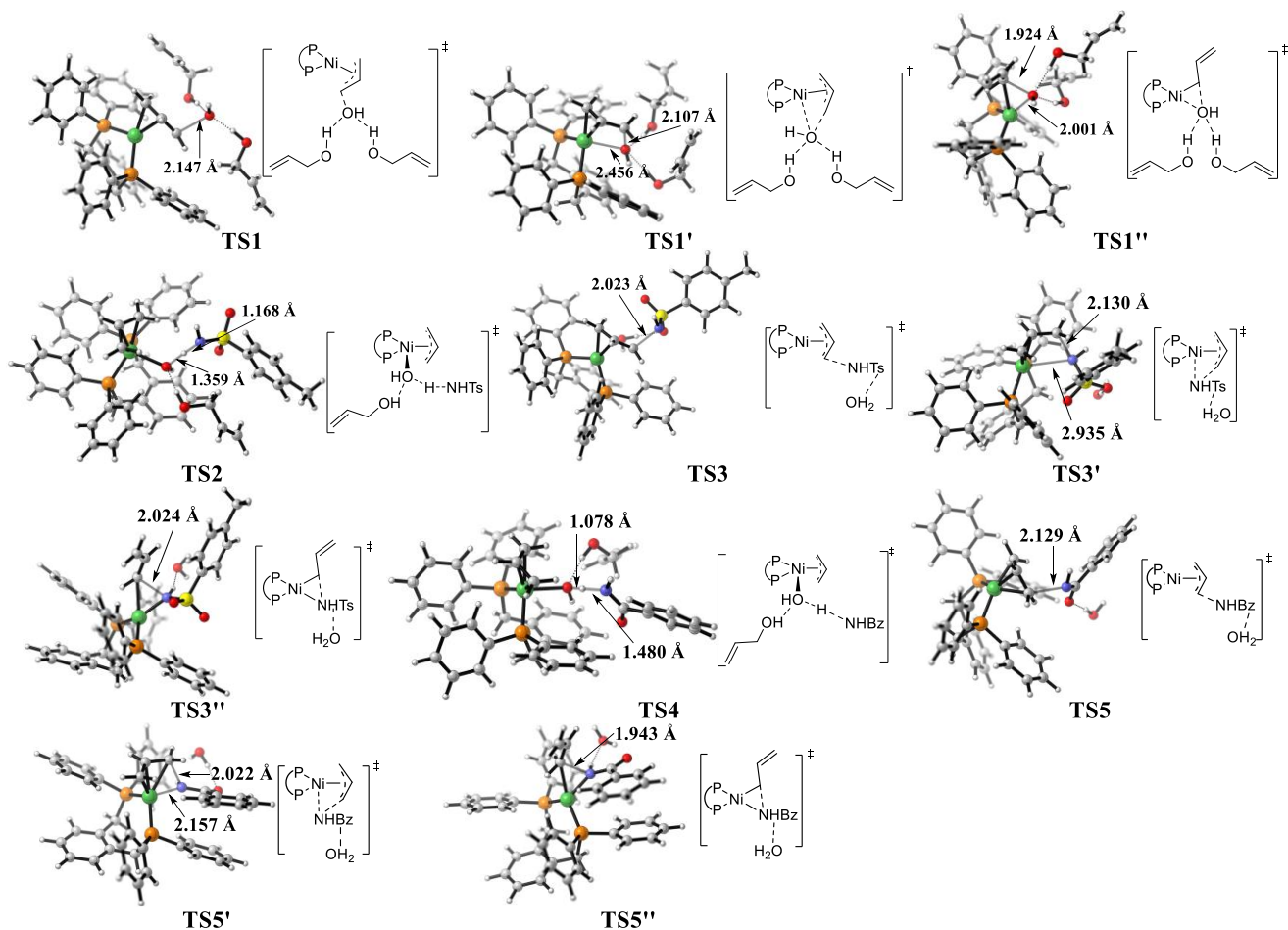


Fig. S3 3D structures of transition states in **Figs. 1** and **2**

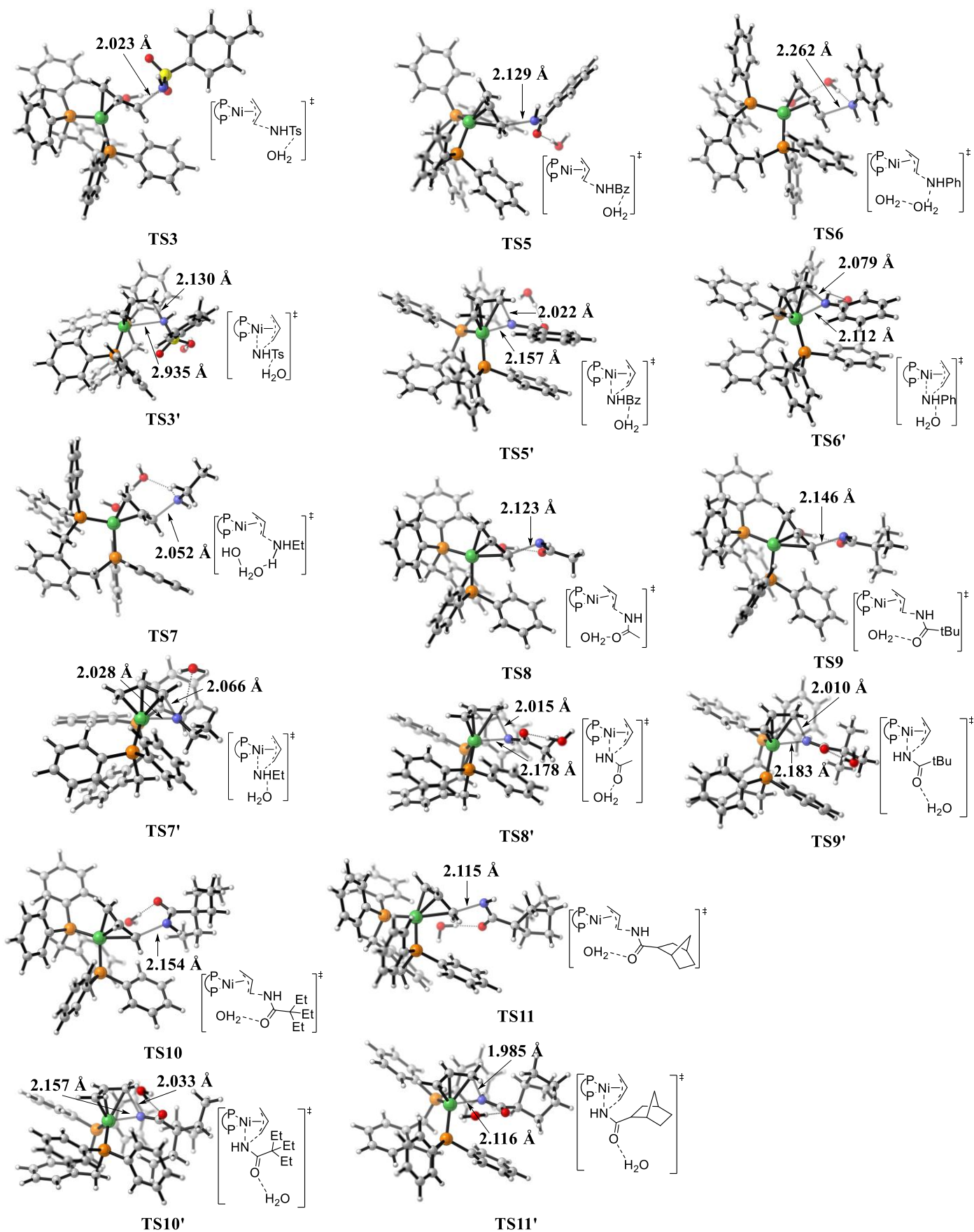


Fig. S4 3D structures of transition states in **Figs. 3** and **4**

Cartesian coordinate of all species

IM0	C	-5.436681	-0.195109	1.399498	H	-3.184192	0.662337	2.523395			
Ni	-0.122497	-0.119267	1.144356	H	-3.892733	1.291211	1.234981	C	1.169927	0.490087	3.802767
P	1.654817	0.294062	-0.041170	C	-5.047067	-2.264554	0.230197	C	0.936541	-0.618565	4.610365
P	-1.720047	0.113993	-0.322385	H	-3.196067	-2.415197	-0.844410	C	-0.318079	-1.220570	4.600228
C	1.451471	0.072057	-1.883773	C	-5.858863	-1.474754	1.041170	C	-1.315966	-0.704549	3.780948
C	-1.476729	-0.586587	-2.047034	H	-6.063090	0.428633	2.032021	C	-1.092448	0.401254	2.951036
H	-2.436066	-0.975492	-2.404175	H	-5.364942	-3.265420	-0.051184	C	0.181154	1.012520	2.959003
H	-1.237024	0.273284	-2.682782	H	-6.813635	-1.854509	1.394563	H	2.139865	0.983535	3.834888
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IM3

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C 1.988729 -5.027360 1.181266
H -0.140139 -4.712152 1.231784
C 3.326718 -3.169771 0.409148
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H 1.919673 -6.045152 1.556309
H 4.295668 -2.726652 0.188827
H 4.138011 -5.061384 1.043355
C -1.857865 -2.966837 -0.268102
C -3.187884 -2.825070 0.150745
C -1.566738 -3.886050 -1.287818
C -4.197960 -3.585949 -0.432339
H -3.447564 -2.113286 0.930802
C -2.579255 -4.642965 -1.869271
H -0.539505 -4.019674 -1.621404
C -3.898318 -4.494590 -1.444349
H -5.223383 -3.464052 -0.092266
H -2.335295 -5.353450 -2.654651
H -4.688435 -5.085708 -1.899240
C -1.186952 3.109434 -0.013590
C -1.934772 3.806907 -0.971585
C -0.104491 3.749370 0.600605
C -1.609452 5.121274 -1.296511
H -2.780464 3.325034 -1.458247
C 0.214285 5.065711 0.277262
H 0.509427 3.215214 1.319423
C -0.536254 5.755315 -0.672160
H -2.200625 5.652800 -2.037733
H 1.060561 5.544240 0.765448
H -0.286799 6.781893 -0.926231
C -3.324429 1.205719 0.072511

C -3.778788 0.305755 -0.896398
C -4.256795 1.970253 0.788993
C -5.142999 0.164819 -1.145382
H -3.051085 -0.291972 -1.444523
C -5.617563 1.825806 0.541414
H -3.915800 2.684047 1.536790
C -6.061797 0.923228 -0.425978
H -5.485775 -0.539537 -1.898974
H -6.334496 2.419888 1.101843
H -7.126063 0.814057 -0.617122
H 0.260468 1.620765 -2.651401
H -1.582844 1.571370 -2.698793
C 4.178220 -0.421346 -1.839971
H 3.643974 -1.384147 -1.953078
C 6.138988 -1.747474 -2.641911
C 5.617687 -0.614013 -2.174364
H 6.257568 0.255803 -2.011655
H 7.192443 -1.836956 -2.894325
H 5.521907 -2.631983 -2.797520
O 4.061311 0.096687 -0.534510
H 3.115897 0.421801 -0.427755
H 3.722803 0.271525 -2.575647
H 1.547158 1.642824 -0.929759
C 3.318862 3.559612 -1.053553
C 3.841057 3.126718 -2.202000
H 2.402662 4.155011 -1.061017
H 3.397699 3.366176 -3.165765
H 4.749803 2.526149 -2.216507
C 3.908281 3.290571 0.293482
H 4.310469 4.227086 0.707484
H 4.762719 2.601849 0.183161
O 2.966711 2.814496 1.237833
H 2.451739 2.085222 0.800198

TS1'

Ni -0.478842 0.009987 -0.852774
P -1.297152 -1.626895 0.275385
P -1.094696 1.780924 0.352594
C -0.330378 -0.916363 -2.588534
C 0.055642 0.452329 -2.764412
C 1.366502 0.850184 -2.474670
C -1.598434 -1.263421 2.074548
C -1.020227 1.684571 2.220302
H -0.685373 1.214100 -3.010832
O 1.867346 0.608164 -0.442745
H 0.453148 -1.678049 -2.609050
H -1.293997 -1.252049 -2.972833
H -0.772540 2.677115 2.612082

H -2.046063 1.470337 2.541653
H -2.423757 -0.544314 2.124844
H -1.930502 -2.185098 2.567415
C 1.135944 1.076626 3.341784
C 2.060133 0.168478 3.848776
C 1.778010 -1.193047 3.803594
C 0.576777 -1.624854 3.250466
C -0.351983 -0.724337 2.715504
C -0.065273 0.657540 2.759516
H 1.345498 2.143150 3.402842
H 2.990792 0.527325 4.280043
H 2.483283 -1.917055 4.202312
H 0.347104 -2.688854 3.223301
C -0.150940 -3.047499 0.373532
C -0.551213 -4.317101 0.809671
C 1.201990 -2.808910 0.107234
C 0.390393 -5.329625 0.971439
H -1.600041 -4.513472 1.026368
C 2.145098 -3.818481 0.286556
H 1.513441 -1.816433 -0.220550
C 1.739188 -5.079974 0.715041
H 0.072697 -6.314006 1.305671
H 3.196202 -3.610999 0.096996
H 2.472575 -5.870369 0.852108
C -2.868442 -2.355645 -0.297976
C -4.103357 -1.957760 0.230429
C -2.853537 -3.254261 -1.376138
C -5.292582 -2.452227 -0.301163
H -4.147503 -1.257424 1.061014
C -4.042611 -3.750854 -1.900174
H -1.902862 -3.573497 -1.800080
C -5.266365 -3.349428 -1.365587
H -6.241874 -2.133789 0.122000
H -4.013061 -4.452564 -2.729704
H -6.194731 -3.735968 -1.776910
C -0.206203 3.334172 -0.030049
C -0.603940 4.137727 -1.108536
C 0.979727 3.652293 0.644443
C 0.159585 5.238912 -1.487008
H -1.518100 3.902029 -1.651039
C 1.743545 4.752480 0.262333
H 1.327424 3.025869 1.462452
C 1.335028 5.550425 -0.804093
H -0.165792 5.857036 -2.319878
H 2.662750 4.978184 0.798808
H 1.929035 6.409321 -1.103821
C -2.845247 2.220119 0.056363

C -3.613207 1.389934 -0.767106
C -3.446794 3.336860 0.653378
C -4.963408 1.660825 -0.983703
H -3.135652 0.524625 -1.230912
C -4.793034 3.608928 0.433346
H -2.855986 3.994716 1.288540
C -5.552993 2.769965 -0.383166
H -5.551979 1.004629 -1.620119
H -5.253180 4.476181 0.899834
H -6.605168 2.984534 -0.550974
H 2.183396 0.153537 -2.629424
H 1.639768 1.901952 -2.509307
C 4.110022 -1.592677 -1.685308
H 3.204359 -2.159602 -1.971884
C 5.272468 -3.761100 -2.125740
C 5.295478 -2.494997 -1.711690
H 6.229052 -2.048110 -1.363805
H 6.168513 -4.375527 -2.151673
H 4.348697 -4.228012 -2.466303
O 3.990056 -1.022110 -0.398994
H 3.264397 -0.345833 -0.442650
H 4.242621 -0.804861 -2.451957
H 1.816513 1.560302 -0.290284
C 4.516072 2.381696 -0.860750
C 5.110117 1.826605 -1.917159
H 3.715895 3.112228 -1.002938
H 4.835382 2.087286 -2.936452
H 5.906515 1.092655 -1.797112
C 4.888857 2.100844 0.557734
H 5.415752 2.967849 0.979612
H 5.590616 1.252194 0.596370
O 3.769169 1.893047 1.408796
H 3.213019 1.212139 0.989596

TS1''

Ni 0.146685 0.534503 0.167927
P -0.796621 -1.138199 1.161105
P 2.311152 0.374543 0.129647
C 0.408119 -2.169054 2.172115
C 3.040796 -0.965884 1.208554
C 2.575366 -2.338355 0.816678
C 1.371165 -2.904045 1.289619
C 1.034699 -4.203411 0.883578
C 1.832856 -4.931900 0.010633
C 3.011212 -4.366810 -0.470507
C 3.373559 -3.089393 -0.058631
H 0.112504 -4.640728 1.262052
H 1.537165 -5.934353 -0.288254

H	3.652441	-4.920825	-1.151195	H	-2.177499	0.695193	5.548160	H	0.133782	-1.190334	-2.635478
H	4.303548	-2.650866	-0.417362	H	-5.373278	-0.057557	2.774688	H	-1.407918	-2.206049	-2.652700
H	2.754115	-0.728267	2.239525	H	-4.596672	0.789369	4.981111	H	2.625875	-2.114321	-2.375182
H	4.135248	-0.908101	1.153159	C	-0.787896	2.371438	1.263624	H	1.106556	0.027607	0.306840
H	0.920389	-1.474148	2.845541	C	-0.362883	3.747724	1.381026	H	2.213272	-0.898524	-1.238442
H	-0.163183	-2.873190	2.789093	C	0.807897	4.099541	1.937652	H	-1.369260	2.757735	2.370650
C	3.063952	-0.066006	-1.485870	H	-1.037193	4.510628	0.992996	H	-2.419957	1.372493	2.626487
C	4.442961	0.001069	-1.724565	H	1.109314	5.139524	2.024538	H	-2.585257	-0.591311	2.494303
C	2.225145	-0.556360	-2.492877	H	1.495547	3.349447	2.326739	H	-1.824578	-2.164269	2.732348
C	4.968767	-0.424984	-2.940911	O	-0.650258	2.179481	-0.645835	C	0.900750	1.484351	2.588760
H	5.108163	0.383976	-0.951703	H	-2.129374	3.191962	-0.915195	C	2.036499	0.728196	2.871658
C	2.750946	-0.991712	-3.707608	H	0.108434	2.742951	-0.860827	C	1.935959	-0.658453	2.951710
H	1.149953	-0.591960	-2.310018	H	-1.348278	1.105475	-1.968978	C	0.706870	-1.277909	2.734743
C	4.124155	-0.928307	-3.931001	C	-3.240283	3.715871	-2.425708	C	-0.439785	-0.530103	2.449638
H	6.040230	-0.369860	-3.116846	H	-2.772433	4.588958	-2.911000	C	-0.341361	0.876724	2.379205
H	2.088419	-1.376745	-4.478518	H	-2.816893	2.818140	-2.906451	H	0.967835	2.569778	2.535051
H	4.537770	-1.266487	-4.877477	C	-3.072123	0.333513	-1.592642	H	2.993261	1.221602	3.030763
C	3.310701	1.829107	0.625553	H	-2.766061	-0.229699	-0.696877	H	2.810341	-1.262044	3.177778
C	3.934888	1.941579	1.875292	H	-3.453148	1.307335	-1.238831	H	0.629936	-2.362764	2.786900
C	3.329555	2.943011	-0.231389	O	-2.963819	3.689322	-1.030338	S	3.923422	-2.287783	-0.608686
C	4.555562	3.131414	2.256228	O	-1.964873	0.533507	-2.466232	O	3.231879	-2.512429	0.668983
H	3.941077	1.099597	2.563291	C	-4.712837	3.739878	-2.649027	O	4.461687	-3.451677	-1.330084
C	3.956496	4.124615	0.145489	C	-5.343949	4.615201	-3.430338	C	5.252505	-1.157013	-0.278494
H	2.847147	2.877737	-1.206609	H	-5.277222	2.959004	-2.134786	C	5.386045	-0.594734	0.987087
C	4.568068	4.226159	1.396741	H	-6.417522	4.571876	-3.593905	C	6.128388	-0.817346	-1.310195
H	5.034581	3.198484	3.230056	H	-4.802434	5.407201	-3.945583	C	6.397305	0.333965	1.213625
H	3.965002	4.972008	-0.535718	C	-4.145548	-0.402124	-2.312241	H	4.690574	-0.864446	1.776202
H	5.052015	5.152107	1.695826	C	-4.705069	-1.523609	-1.859919	C	7.139241	0.101363	-1.064643
C	-1.608930	-2.474510	0.203839	H	-4.477908	0.039252	-3.254383	H	6.010621	-1.257840	-2.296678
C	-2.462343	-3.429796	0.772783	H	-5.512421	-2.023178	-2.388980	C	7.287646	0.696087	0.197377
C	-1.266516	-2.594275	-1.147919	H	-4.374244	-1.979231	-0.925563	H	6.492780	0.792417	2.195695
C	-2.962657	-4.475371	0.000726	H	-1.852418	2.151098	1.250107	H	7.821895	0.373554	-1.866268
H	-2.732732	-3.359835	1.825167	H	-0.184376	1.661045	1.849499	C	8.377665	1.688647	0.447546
C	-1.756732	-3.645391	-1.918198	IM4				H	8.483360	2.388812	-0.386711
H	-0.605285	-1.848152	-1.588537	Ni	-1.225856	0.030517	-0.982392	H	8.198349	2.263491	1.359910
C	-2.607692	-4.587162	-1.343840	P	-1.973755	-1.566723	0.374671	H	9.346346	1.187980	0.561131
H	-3.626427	-5.209499	0.450606	P	-2.006985	1.716929	0.260398	C	-1.203525	-3.210852	0.180328
H	-1.479075	-3.725035	-2.966070	C	-0.953995	-1.219444	-2.601379	C	-1.881074	-4.394460	0.498865
H	-2.996343	-5.407426	-1.941942	C	-1.692116	-0.073050	-2.952164	C	0.123442	-3.271319	-0.259254
C	-2.036526	-0.680670	2.427300	C	-1.106510	1.180433	-2.685145	C	-1.238845	-5.622324	0.365718
C	-1.613084	-0.192523	3.674367	C	-1.745200	-1.219349	2.184591	H	-2.911703	-4.356639	0.846345
C	-3.405601	-0.611853	2.118854	C	-1.541582	1.719536	2.072428	C	0.764775	-4.501907	-0.382866
C	-2.527824	0.329556	4.586104	H	-2.753509	-0.152251	-3.186129	H	0.641338	-2.342073	-0.495204
H	-0.557687	-0.216127	3.939847	H	-1.693104	2.090253	-2.791163	C	0.082399	-5.677529	-0.076981
C	-4.317493	-0.091077	3.031610	H	-0.024557	1.298865	-2.735464	H	-1.771588	-6.538267	0.607206
H	-3.761556	-0.974908	1.155249	O	0.936603	0.074126	-0.642425	H	1.798141	-4.542813	-0.719663
C	-3.883370	0.382253	4.269882	N	2.989676	-1.462678	-1.684157	H	0.579697	-6.638005	-0.182097

C	-3.760952	-1.890102	0.181255	C	-0.789155	-1.555783	-2.342684	C	-1.600872	-4.459022	0.845007
C	-4.708095	-1.669912	1.188177	C	-1.594530	-0.532449	-2.875973	C	0.364720	-3.232796	0.150150
C	-4.205165	-2.306397	-1.084252	C	-1.110567	0.787254	-2.774848	C	-0.857641	-5.636343	0.853079
C	-6.066110	-1.855858	0.932251	C	-1.711781	-1.243572	2.370572	H	-2.654301	-4.481749	1.115874
H	-4.403174	-1.351386	2.180995	C	-2.144429	1.638962	1.919932	C	1.109354	-4.409381	0.177763
C	-5.558732	-2.500867	-1.333094	H	-2.636408	-0.730871	-3.126706	H	0.833832	-2.289577	-0.128109
H	-3.481756	-2.479354	-1.879433	H	-1.745597	1.629901	-3.038298	C	0.496275	-5.612628	0.520985
C	-6.495321	-2.270221	-0.324939	H	-0.036270	0.966436	-2.815165	H	-1.337040	-6.573614	1.122746
H	-6.788650	-1.674419	1.723658	O	0.878280	0.308890	-0.382387	H	2.165215	-4.381398	-0.078508
H	-5.884022	-2.827725	-2.317092	N	2.800406	-0.835453	-1.556740	H	1.073693	-6.533177	0.531286
H	-7.554533	-2.412257	-0.521161	H	0.295358	-1.457488	-2.351351	C	-3.633896	-2.056057	0.285011
C	-1.433013	3.368865	-0.265452	H	-1.172072	-2.570333	-2.266336	C	-4.660925	-1.466799	1.032984
C	-2.289257	4.438462	-0.541987	H	2.682583	-1.181012	-2.503023	C	-3.974694	-2.857894	-0.816065
C	-0.049948	3.537187	-0.410388	H	0.956113	-0.019550	0.523540	C	-5.995270	-1.687898	0.698814
C	-1.762621	5.663524	-0.951162	H	1.894578	-0.334625	-1.015771	H	-4.430559	-0.818017	1.874612
H	-3.365867	4.320079	-0.442847	H	-2.310735	2.668543	2.254077	C	-5.307831	-3.074753	-1.147864
C	0.470522	4.761269	-0.816017	H	-2.975176	1.035894	2.301789	H	-3.189671	-3.319434	-1.412415
H	0.617267	2.695446	-0.234000	H	-2.671714	-0.868008	2.734605	C	-6.322912	-2.490456	-0.390734
C	-0.386232	5.828428	-1.086533	H	-1.518151	-2.182091	2.898005	H	-6.779183	-1.224708	1.292320
H	-2.434161	6.490131	-1.167824	C	0.250771	2.008505	2.565990	H	-5.554135	-3.703734	-1.999031
H	1.545900	4.873047	-0.935046	C	1.510283	1.550961	2.944627	H	-7.364191	-2.658628	-0.651435
H	0.017776	6.783551	-1.411032	C	1.718484	0.189518	3.148254	C	-1.681861	3.277238	-0.383534
C	-3.827316	1.831501	0.267604	C	0.660952	-0.702733	2.979772	C	-0.416567	3.421025	-0.959270
C	-4.523242	1.313719	-0.832309	C	-0.609734	-0.254722	2.603975	C	-2.438568	4.420810	-0.095255
C	-4.549019	2.407891	1.321060	C	-0.817880	1.125111	2.391166	C	0.093014	4.688615	-1.232968
C	-5.913220	1.366430	-0.879322	H	0.089465	3.071100	2.390208	H	0.167279	2.532564	-1.180383
H	-3.962268	0.848813	-1.641519	H	2.330905	2.255474	3.057212	C	-1.933078	5.684871	-0.382195
C	-5.940686	2.447834	1.278068	H	2.700845	-0.181635	3.430999	H	-3.426731	4.324494	0.350873
H	-4.027827	2.835028	2.174810	H	0.820123	-1.768931	3.131966	C	-0.665365	5.820838	-0.948591
C	-6.623810	1.927075	0.180500	S	3.773935	-1.768849	-0.681285	H	1.085287	4.785812	-1.665398
H	-6.440843	0.955210	-1.735922	O	3.295139	-1.764158	0.713019	H	-2.529271	6.566257	-0.161484
H	-6.491788	2.891000	2.103044	O	3.991004	-3.069722	-1.347394	H	-0.271641	6.809967	-1.166539
H	-7.709738	1.956772	0.152540	C	5.363867	-0.958423	-0.664161	C	-4.075233	1.658759	-0.225548
H	1.863593	1.294420	-1.208989	C	5.945837	-0.577622	0.539605	C	-4.571009	1.155796	-1.435313
O	2.561270	1.974086	-1.453107	C	6.005051	-0.694656	-1.876567	C	-4.979790	2.150822	0.725859
C	3.562673	1.826591	-0.464418	C	7.172675	0.083233	0.526722	C	-5.938520	1.145858	-1.692473
H	3.307731	0.966770	0.180791	H	5.435072	-0.785357	1.475710	H	-3.876364	0.756677	-2.170811
H	4.535648	1.589131	-0.927552	C	7.226058	-0.036790	-1.873692	C	-6.348817	2.136220	0.468156
C	3.700512	3.043432	0.390196	H	5.545004	-0.991065	-2.816415	H	-4.621348	2.544216	1.674127
C	4.851101	3.674391	0.626933	C	7.829549	0.367654	-0.672782	C	-6.830422	1.632710	-0.738477
H	2.774953	3.404799	0.846631	H	7.624104	0.390857	1.467727	H	-6.307962	0.744617	-2.632426
H	4.913916	4.543588	1.276643	H	7.723749	0.174658	-2.817719	H	-7.040189	2.516730	1.215244
H	5.780969	3.337047	0.168975	C	9.142066	1.085077	-0.687983	H	-7.899381	1.615545	-0.932942
TS2				H	9.474032	1.341837	0.320994	O	2.445974	2.511463	-0.049865
Ni	-1.239620	-0.118845	-0.929381	H	9.924026	0.475953	-1.154508	C	3.702466	1.948132	0.277557
P	-1.877252	-1.654463	0.558277	H	9.083182	2.011770	-1.269060	H	3.585884	1.018909	0.860917
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H -8.365529 -1.496276 -0.131413
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IM5'

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TS3'

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C 0.578048 -0.856037 2.604166
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H 0.705132 1.243812 3.094261
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C 1.386794 2.443316 -1.749798
C 1.495738 3.820378 -1.515165
C 2.727155 4.421612 -1.275328
C 3.883789 3.645705 -1.279504
C 3.789849 2.277636 -1.509372
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H 4.854608 4.102103 -1.105089

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C 2.735878 -5.150377 -1.181916
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IM8''

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H 4.455816 1.789039 -1.646172
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H 1.080691 -2.670112 -1.935703
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H 1.371655 -5.105781 -2.139027
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H 3.005224 -6.296406 -0.687330
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C -2.519946 0.142943 -1.560432
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C 0.468732 0.171996 3.863967
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H -1.398767 -5.239932 -0.852823
H 0.767894 -2.666965 2.041358
H 2.045739 -1.413247 2.297676

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H 3.572481 -2.431752 1.364342
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C	0.444298	-5.316109	1.069892	H	-5.840210	-1.056375	0.749359	C	2.271554	-3.130161	0.354975
H	0.185378	-4.636801	-0.951482	C	-6.543229	2.065840	-0.430943	C	2.647418	-4.052071	-2.239970
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H	0.195397	-1.584834	2.089353	H	-7.279592	0.091624	-0.894095	C	2.467205	-4.486361	0.124168
C	0.539446	-4.951966	2.413194	H	-7.173515	2.568708	-1.159390	H	2.121650	-2.768169	1.372308
H	0.508345	-6.362256	0.783027	TS6'				C	2.655286	-4.952884	-1.177460
H	0.522167	-3.323012	3.824059	Ni	0.059009	-0.027432	0.956777	H	2.793049	-4.408024	-3.256778
H	0.681487	-5.715392	3.173218	P	-1.200593	1.131222	-0.450886	H	2.467210	-5.182303	0.959031
C	-1.601137	-2.074024	-1.655133	P	1.973521	-0.456975	-0.275162	H	2.801890	-6.013501	-1.362297
C	-1.910975	-1.360965	-2.823055	C	0.003842	-1.390123	2.799070	C	-2.145967	2.646120	-0.018474
C	-2.552836	-2.956575	-1.130269	C	0.846429	-0.242215	2.807031	C	-3.052225	3.220653	-0.923700
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H	-1.195222	-0.648619	-3.231732	C	-0.336541	1.764503	-1.987262	C	-3.696298	4.414777	-0.621845
C	-3.783319	-3.126578	-1.762277	C	2.312901	0.417062	-1.890397	H	-3.255491	2.729515	-1.873603
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C	3.927932	-0.053401	2.550465	C	0.847455	3.907977	-1.475122	C	-3.809405	0.115935	-1.039813
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C	4.990833	2.001266	1.860019	C	3.239617	4.041919	-1.250290	H	-0.862065	-1.117837	-2.203675
H	4.041944	3.068599	0.248925	C	3.325336	2.675072	-1.496899	C	-4.674684	-0.822300	-1.599417
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H	3.894357	-0.931058	3.190802	H	1.910536	5.727693	-1.040051	C	-4.174745	-1.856211	-2.386859
H	5.793559	2.726747	1.962723	H	4.143524	4.619425	-1.074632	H	-2.399009	-2.763812	-3.207491
H	5.731121	0.728499	3.431625	H	4.298073	2.185047	-1.505453	H	-5.742566	-0.746393	-1.409837
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C	1.518006	4.906264	-2.652817	H	-1.060520	2.385419	-2.526841	C	-2.949532	-3.282557	1.059604
H	1.804128	2.838789	-3.142494	C	3.527688	-0.007230	0.599435	C	-4.366353	-1.174097	2.199853
C	1.302312	5.431648	-0.310975	C	4.715312	-0.742958	0.503848	H	-2.503607	-0.078533	2.111855
H	1.406806	3.767803	1.047352	C	3.527745	1.177056	1.349548	C	-4.305481	-3.412869	1.330097
C	1.339451	5.846238	-1.642251	C	5.871542	-0.305530	1.146114	H	-2.397441	-4.107397	0.612087
H	1.544856	5.220470	-3.692700	H	4.741506	-1.661847	-0.078388	C	-5.031070	-2.365951	1.905042
H	1.162163	6.159789	0.483398	C	4.686202	1.620720	1.981655	H	-4.910458	-0.345736	2.650095
H	1.226837	6.898539	-1.888754	H	2.606782	1.756134	1.418546	H	-4.803177	-4.352162	1.095477
C	-4.896276	0.746440	1.483380	C	5.860317	0.876324	1.884822	H	-6.089641	-2.479595	2.122110
C	-4.848359	2.154046	1.300089	H	6.785339	-0.889036	1.065974	H	-0.477576	-2.760258	0.793037
C	-5.796468	0.028846	0.651383	H	4.670258	2.544595	2.554304	O	-0.675667	-4.082427	-1.294335
C	-5.655976	2.791614	0.368329	H	6.764055	1.215035	2.384758	H	0.146590	-3.930286	-1.777012

H -1.019490 -3.189810 -1.157566

TS7

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P 1.530560 1.112376 -0.546595

P -0.820677 -1.440716 -0.562670

O -1.898934 2.546438 3.452577

C -1.261331 2.514178 0.021714

C -2.312801 1.597780 -0.214798

C -2.892701 0.832724 0.826869

C 2.271791 0.193942 -2.000826

C 0.289109 -2.084415 -1.921229

H -2.722105 1.484653 -1.218758

H -3.533537 -0.002765 0.557588

H -2.382815 0.757909 1.777011

O -0.334643 0.743348 2.305944

N -4.343424 1.951757 1.750444

H -3.736456 2.355665 2.469684

H -1.117930 2.913105 1.025055

H -0.931437 3.159952 -0.790504

H -5.043643 1.365220 2.194984

H 0.586550 0.993177 2.437942

H -1.256829 1.891018 3.024852

H -0.123752 -3.043050 -2.256291

H 0.178925 -1.382718 -2.755136

H 1.533509 0.225382 -2.810071

H 3.153354 0.755245 -2.332409

C 2.164085 -3.507858 -1.089668

C 3.489348 -3.737428 -0.736179

C 4.418224 -2.706620 -0.853396

C 4.001117 -1.459314 -1.302686

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C 1.728098 -2.254522 -1.539603

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H -6.614744 3.509704 2.157744

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C -0.388799 -2.532847 1.960256

C -0.835900 -5.181253 1.207586

H -1.255610 -4.403157 -0.751207

C -0.247726 -3.559257 2.895019

H -0.236151 -1.488694 2.246613

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H -1.014889 -6.212616 0.914067

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H -0.356317 -5.680933 3.248156

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C -2.662980 -1.118292 -2.647653

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H -1.864069 -0.564093 -3.138427

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H -4.047807 -0.784069 -4.256060

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H -5.908522 -2.003781 -3.145049

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C 1.982738 5.179427 -0.322625

H 1.851853 3.529019 1.049783

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C -0.197139 -1.907948 -2.490364

C 0.363091 -0.642681 -2.788991

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C -1.452449 0.550201 1.878181

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H 1.443851 -0.537741 -2.894747

N -0.185166 -2.614354 0.262890

H -0.943074 -3.244142 0.018080

H 0.157625 -3.883578 -1.661635

H 1.589245 -2.757025 -1.599799

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H 2.412063 3.227827 2.000259

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H -2.511857 2.967303 2.106825

H -0.887577 -0.295282 2.288157

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H 1.214609 -0.129360 2.490784

H 2.595920 0.955595 2.299153

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C -1.985418 2.513041 -1.200538

C -4.619197 3.101709 -0.538542

H -4.649415 1.191155 0.446305

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H -0.949983 2.280285 -1.447380

C -3.862773 4.023168 -1.262919

H -5.649595 3.330024 -0.277722

H -1.944323 4.441162 -2.154443

H -4.303963 4.967560 -1.570995

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C -4.172734 -1.310378 -0.639805

C -4.145164 -2.997046 1.572780

H -2.430096 -1.888348 2.224294

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 H 1.933379 3.950625 -2.924158
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 H 2.360943 -3.959386 0.097919
 O -2.429240 -4.336206 -1.222333
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TS8

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 C 0.551631 -0.052210 -2.738953
 C 1.770624 -0.451189 -2.155950
 C -2.185051 -0.099610 1.984546
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 H 2.567835 0.274552 -2.034982
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 N 3.015593 -1.682428 -3.355773
 H -0.519714 -1.903241 -2.400507
 H -1.541591 -0.533875 -3.076738

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 H -3.190873 -0.402001 2.294836
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 C -1.140944 -0.987052 2.589370
 C 0.172776 -0.528375 2.823309
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 H 1.535588 -3.411930 4.044689
 H -0.779248 -4.225652 3.607370
 H -2.476339 -2.664286 2.696282
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 C -4.575371 -1.542318 0.118095
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 C -5.387268 -2.660878 -0.034946
 H -5.005825 -0.607191 0.472423
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 H -1.597666 -2.900621 -0.811179
 C -4.839820 -3.866616 -0.474199
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 H -3.047493 -4.890624 -1.087331
 H -5.474936 -4.741028 -0.589139
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 C -2.633181 2.536387 0.097126
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 H -4.251451 0.295907 -1.888570
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 C 3.240089 -0.668096 0.727215
 C 5.188610 1.305881 0.953859
 H 3.564602 2.713882 0.941663
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 H 2.481039 -1.438695 0.607458
 C 5.562489 -0.035080 0.897427

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 H 6.613345 -0.309841 0.931501
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 C 0.794225 3.319914 -0.880345
 C 0.948455 5.165296 1.198003
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 H 0.711753 2.588520 -1.684021
 C 0.756049 5.604759 -0.110475
 H 1.006866 5.884087 2.011096
 H 0.528597 5.018133 -2.172390
 H 0.658704 6.667119 -0.317983
 C 3.697238 -2.535972 -2.601360
 O 3.201928 -3.152827 -1.609843
 C 5.161273 -2.796067 -2.904039
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 H 5.443587 -2.526539 -3.925570

TS8'

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 C 0.180917 -1.134855 2.665049
 C -0.557887 0.066418 2.784840
 C -0.512860 1.528457 -1.978609
 C 1.938463 -0.232507 -1.990865
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 H -0.081437 0.963994 3.174106
 H -1.636831 0.008627 2.935759
 N -1.278972 -2.276770 0.341334
 H 0.087606 -3.203793 2.032205
 H -1.513289 -2.467503 2.552891
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H -0.780102 -2.895089 -0.292917
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H 4.486107 0.015650 1.927618
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H -1.842552 6.227942 0.995570
H -1.267173 4.606803 -2.943775
H -1.993055 6.470695 -1.469160
C 4.339100 -1.339581 -1.475063
O 3.910477 -1.851202 -0.392423
C 5.879660 -1.362201 -1.660796
C 6.505164 -0.571099 -0.509602
H 6.227169 -1.000075 0.457765
H 7.599149 -0.580467 -0.584084
H 6.179677 0.476285 -0.521620
C 6.338487 -0.763393 -2.986117

H 7.429095 -0.827212 -3.073037
H 5.910441 -1.294488 -3.843917
H 6.068310 0.295423 -3.073357
C 6.337507 -2.819784 -1.582207
H 5.919814 -3.412390 -2.404740
H 7.429931 -2.889140 -1.642762
H 6.016356 -3.277790 -0.642343

TS9'

Ni 0.065597 -0.107671 -0.862474
P 0.170432 1.738706 0.267722
P -1.351784 -1.472479 0.229856
C 1.207104 -1.547087 -2.314298
C 0.052318 -0.818079 -2.735479
C 0.131769 0.595182 -2.780304
C -0.522044 1.693960 2.001950
C -1.876914 -1.003776 1.953197
H -0.885012 -1.344851 -2.908062
H -0.716374 1.177492 -3.135165
H 1.107636 1.063662 -2.917195
N 1.839949 -1.300273 -0.422920
H 1.131900 -2.629672 -2.235627
H 2.178739 -1.173064 -2.631405
C -2.648182 0.282588 1.970097
C -2.014165 1.542323 2.013125
C -2.810030 2.695481 2.033043
C -4.197666 2.627714 1.984209
C -4.821833 1.384304 1.923457
C -4.047337 0.229374 1.924148
H -2.317756 3.665923 2.076639
H -4.786293 3.541263 1.994239
H -5.905502 1.311637 1.886408
H -4.530610 -0.746041 1.891621
H -0.965527 -0.926267 2.555646
H -2.479273 -1.819170 2.371158
H -0.024865 0.864548 2.516855
H -0.225345 2.622280 2.504760
C -2.981345 -1.794418 -0.544395
C -3.799248 -2.861623 -0.149449
C -3.451943 -0.900271 -1.511093
C -5.062244 -3.025671 -0.709879
H -3.444323 -3.566047 0.601239
C -4.720587 -1.058408 -2.066423
H -2.808729 -0.075720 -1.821606
C -5.525927 -2.121687 -1.666185
H -5.688295 -3.858224 -0.399273
H -5.077573 -0.354201 -2.813303
H -6.513853 -2.249806 -2.100537

C -0.691852 -3.162363 0.469476
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C -0.690271 -4.053476 -0.616483
C 0.628266 -4.771997 1.725447
H 0.008807 -2.870320 2.497766
C -0.049289 -5.284905 -0.527953
H -1.204731 -3.781183 -1.537215
C 0.614472 -5.649005 0.643879
H 1.144831 -5.043881 2.642885
H -0.067624 -5.962782 -1.377558
H 1.118939 -6.609025 0.711145
C -0.679207 3.226856 -0.375828
C -0.313961 4.522971 0.010234
C -1.815190 3.052541 -1.173311
C -1.065668 5.619659 -0.403074
H 0.560871 4.673708 0.640277
C -2.574149 4.148272 -1.577591
H -2.110984 2.043154 -1.458102
C -2.197806 5.433732 -1.195478
H -0.770394 6.621252 -0.101151
H -3.459432 3.996921 -2.189725
H -2.785944 6.290870 -1.512385
C 1.885227 2.299684 0.546925
C 2.604477 1.894878 1.678536
C 2.552711 3.023824 -0.453257
C 3.956474 2.210223 1.808512
H 2.114777 1.328775 2.467822
C 3.900076 3.336910 -0.320828
H 2.010241 3.339648 -1.342849
C 4.608226 2.927936 0.809754
H 4.500622 1.889329 2.693774
H 4.404505 3.893361 -1.106457
H 5.665553 3.161301 0.904270
O 6.111121 1.138848 -1.681018
H 5.282788 0.699451 -1.411651
H 6.160657 0.945244 -2.622097
C 3.147918 -0.994841 -0.416349
O 3.617240 -0.110795 -1.168652
C 4.057311 -1.834656 0.506811
H 1.623693 -2.137443 0.112230
C 3.549980 -1.789965 1.950610
H 2.518990 -2.152146 2.042968
H 4.176330 -2.422028 2.590714
H 3.585214 -0.771005 2.352815
C 4.030105 -3.281128 -0.004133
H 4.333938 -3.338121 -1.056052
H 4.719751 -3.903182 0.577643

H 3.032317 -3.729174 0.080821
C 5.482921 -1.301413 0.457729
H 5.530665 -0.259972 0.793603
H 6.129378 -1.898300 1.110432
H 5.895013 -1.337906 -0.554780

TS10

Ni 0.651849 0.071919 -0.610229
P 2.256242 1.392517 0.054947
P 0.986344 -1.741817 0.619477
C -0.095076 1.240229 -2.032185
C -0.511123 -0.093481 -2.274318
C -1.415300 -0.745030 -1.414460
C 2.902772 1.169806 1.789725
C 1.717716 -1.509955 2.322094
H -0.082002 -0.658447 -3.101233
H -1.492623 -1.826460 -1.439593
H -1.757092 -0.256592 -0.510638
O -1.648668 1.526731 1.040678
N -3.469367 -0.531480 -2.028199
H -0.765705 1.907049 -1.488417
H 0.574557 1.730095 -2.737062
H -4.063989 -1.354634 -2.107429
H -2.177394 1.749921 1.815052
H -2.289918 1.557847 0.297032
H 1.497747 -2.401225 2.918632
H 2.804557 -1.475585 2.186384
H 3.576001 0.307901 1.784366
H 3.507295 2.047594 2.040672
C 0.133552 -0.374517 3.897963
C -0.391848 0.749802 4.528160
C 0.164567 2.001880 4.279582
C 1.240295 2.113891 3.403775
C 1.773249 0.993154 2.758380
C 1.205696 -0.275828 3.004596
H -0.291125 -1.356830 4.097181
H -1.224456 0.645146 5.218891
H -0.231162 2.887361 4.770138
H 1.686922 3.088408 3.210822
C 2.095995 3.211245 -0.006562
C 3.219917 4.048477 -0.053494
C 0.824558 3.781219 0.126574
C 3.070419 5.429794 0.009210
H 4.216295 3.618910 -0.136932
C 0.679987 5.165732 0.200980
H -0.048147 3.134945 0.201106
C 1.799570 5.990548 0.136131
H 3.947542 6.069909 -0.033822

H	-0.310866	5.598279	0.310741	C	-4.877560	0.005234	1.444764	H	-2.890408	1.004671	1.566697
H	1.685081	7.069965	0.188954	H	-5.025180	-0.643039	2.314576	C	-4.485225	4.010803	1.619240
C	3.688089	0.970215	-0.998134	H	-3.799824	0.054905	1.249126	H	-3.785919	5.790639	0.625621
C	4.409413	-0.200967	-0.724647	H	-5.200168	1.010315	1.739527	H	-4.925722	2.093555	2.500307
C	3.987772	1.688572	-2.163985	C	-7.594712	1.835645	-0.365853	H	-5.368721	4.493011	2.029643
C	5.419103	-0.630266	-1.579907	H	-7.897456	2.868868	-0.166477	C	0.445428	3.146761	-0.439456
H	4.170558	-0.798932	0.153415	H	-8.261357	1.452466	-1.146766	C	1.059416	3.412131	-1.671576
C	5.000200	1.257591	-3.017509	H	-7.798561	1.261722	0.545559	C	0.930528	3.807012	0.703582
H	3.430379	2.591592	-2.403706	C	-6.412670	0.353769	-3.469404	C	2.122456	4.310883	-1.758289
C	5.720423	0.100296	-2.727681	H	-6.953747	-0.236220	-4.216063	H	0.713151	2.918632	-2.576184
H	5.966676	-1.540810	-1.349429	H	-6.901065	1.332912	-3.415763	C	1.986232	4.707653	0.613874
H	5.226918	1.830972	-3.912503	H	-5.396676	0.512051	-3.849433	H	0.466575	3.615628	1.670975
H	6.509575	-0.233257	-3.396056	TS10'				C	2.590298	4.959665	-0.618842
C	-0.470345	-2.791430	0.992830	Ni	-0.137041	-0.023951	0.938548	H	2.587455	4.498967	-2.723219
C	-0.490425	-4.169151	0.748663	P	-0.667884	-1.728724	-0.340402	H	2.340813	5.212624	1.508928
C	-1.614710	-2.179036	1.526984	P	-0.824398	1.848325	-0.212328	H	3.421649	5.656290	-0.688051
C	-1.627499	-4.921153	1.038920	C	1.187609	0.755004	2.683287	C	-2.009829	-2.827320	0.268125
H	0.381740	-4.662500	0.326018	C	-0.225075	0.656668	2.835521	C	-2.028104	-4.208524	0.039058
C	-2.741735	-2.937025	1.830231	C	-0.846912	-0.611455	2.764532	C	-3.110886	-2.236652	0.901802
H	-1.622901	-1.102464	1.697124	C	-1.326823	-1.351766	-2.049909	C	-3.114509	-4.979186	0.448349
C	-2.752699	-4.309304	1.584073	C	-1.483603	1.658617	-1.942545	H	-1.193160	-4.689722	-0.465455
H	-1.629590	-5.989430	0.838345	H	-0.816668	1.569588	2.889873	C	-4.201556	-3.004123	1.299878
H	-3.617043	-2.453096	2.255819	H	-1.923064	-0.683106	2.910622	H	-3.115231	-1.159001	1.062004
H	-3.637500	-4.896975	1.813183	H	-0.278252	-1.501589	3.032719	C	-4.202663	-4.379987	1.079072
C	2.157181	-2.874295	-0.201833	N	1.954934	0.489344	0.819300	H	-3.110833	-6.051286	0.268676
C	3.023058	-3.726065	0.495134	H	1.643932	1.738102	2.755688	H	-5.050354	-2.526144	1.782274
C	2.198982	-2.853567	-1.602221	H	1.809332	-0.064589	3.033988	H	-5.049994	-4.982875	1.394748
C	3.919295	-4.534515	-0.200244	C	-2.707229	0.793574	-1.985177	C	0.672995	-2.917338	-0.732438
H	2.998022	-3.763098	1.582038	C	-2.630581	-0.613004	-2.050556	C	1.127713	-3.188816	-2.028966
C	3.087795	-3.670015	-2.295146	C	-3.820302	-1.351399	-2.100463	C	1.304044	-3.551993	0.346522
H	1.533179	-2.178368	-2.140255	C	-5.065390	-0.735428	-2.048763	C	2.189584	-4.069161	-2.236912
C	3.953112	-4.507477	-1.593367	C	-5.140022	0.652112	-1.958834	H	0.662689	-2.716818	-2.889952
H	4.591212	-5.189411	0.348224	C	-3.968511	1.401581	-1.939124	C	2.359635	-4.432003	0.138325
H	3.112925	-3.644214	-3.381264	H	-3.757030	-2.436333	-2.169357	H	0.978582	-3.335686	1.362995
H	4.655828	-5.138066	-2.131613	H	-5.969992	-1.337020	-2.077852	C	2.808313	-4.692143	-1.156514
C	-4.070743	0.474856	-1.413214	H	-6.104592	1.151289	-1.916192	H	2.532106	-4.265002	-3.250023
O	-3.451377	1.533317	-1.082549	H	-4.021789	2.488087	-1.885311	H	2.840141	-4.907131	0.990586
C	-5.574295	0.361805	-1.028959	H	-0.671390	1.235189	-2.545121	H	3.637480	-5.375260	-1.321241
C	-5.646617	-0.513421	0.242803	H	-1.705638	2.655679	-2.341892	O	1.834769	-2.605056	3.530686
H	-6.704155	-0.648568	0.509743	H	-0.538025	-0.798404	-2.573127	H	2.216028	-2.129144	2.763731
H	-5.276183	-1.515658	-0.018908	H	-1.449531	-2.312889	-2.563026	H	2.323224	-3.434958	3.537670
C	-6.391150	-0.347432	-2.123727	C	-2.207968	2.773003	0.556107	C	3.034186	-0.294432	0.754468
H	-7.418837	-0.478375	-1.757972	C	-2.465396	4.125512	0.298243	O	3.156014	-1.341847	1.434060
H	-6.008792	-1.369298	-2.250586	C	-3.100643	2.054737	1.360274	C	4.133781	0.071240	-0.275036
C	-6.131447	1.772703	-0.767210	C	-3.595215	4.740309	0.830936	H	2.049905	1.372434	0.330765
H	-5.971750	2.381365	-1.666247	H	-1.783435	4.698046	-0.328180	C	3.707311	-0.570138	-1.619795
H	-5.518937	2.251608	0.002829	C	-4.237398	2.666006	1.883997	H	4.561413	-0.507391	-2.308123

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 H 3.361254 2.038735 -0.777200
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 H 6.177756 -0.474366 -0.666889
 C 2.480589 0.017148 -2.297198
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 H 1.592615 -0.018170 -1.650290
 H 2.635120 1.062911 -2.589977
 C 5.408432 2.041798 -1.343405
 H 5.426014 3.133196 -1.431430
 H 6.396987 1.727255 -0.991643
 H 5.276525 1.637159 -2.353760
 C 6.055475 -0.028369 1.434488
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 H 6.945409 -0.591753 1.732291
 H 6.358200 1.019499 1.327290

TS11

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 P -2.633160 -1.081357 -0.045028
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 C -3.160527 -0.932862 1.734414
 C -1.410249 1.366280 2.427974
 H 0.105180 0.613257 -3.120500
 H 1.740185 1.312564 -1.406837
 H 1.624746 -0.323757 -0.574588
 O 1.215867 -2.099344 0.929024
 N 3.381881 -0.320071 -1.998362
 H 0.187515 -2.149742 -1.698502
 H -1.067285 -1.590197 -2.918920
 H 3.836130 0.310317 -2.656293
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 C -1.684431 -2.363995 3.160836
 C -1.986662 -1.097733 2.649214

C -1.152243 -0.006006 2.976241
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 H 1.088559 -1.629913 4.977167
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 H -2.333459 -3.199698 2.904060
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 C -1.705601 -3.692365 -0.211364
 C -4.211170 -4.855308 -0.583659
 H -4.991850 -2.853368 -0.523673
 C -1.824231 -5.077551 -0.308396
 H -0.731163 -3.235763 -0.045242
 C -3.074368 -5.659114 -0.503650
 H -5.189097 -5.307116 -0.727091
 H -0.937080 -5.700897 -0.235204
 H -3.165724 -6.738657 -0.588410
 C -3.976049 -0.270199 -0.980440
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 C -4.349318 -0.733116 -2.250959
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 H -4.230366 1.338274 0.450520
 C -5.260378 -0.019272 -3.024149
 H -3.928941 -1.660225 -2.635260
 C -5.805011 1.172719 -2.548498
 H -5.846256 2.578613 -0.915180
 H -5.545271 -0.397113 -4.002656
 H -6.514231 1.729155 -3.155210
 C 0.959357 2.298433 1.123965
 C 1.286722 3.651926 0.986485
 C 1.947705 1.399420 1.550855
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 H 0.538447 4.363460 0.644253
 C 3.230679 1.846376 1.847915
 H 1.715562 0.337862 1.619678
 C 3.548600 3.196887 1.709869
 H 2.820190 5.148071 1.159842
 H 3.987047 1.131975 2.164016
 H 4.554533 3.545511 1.929027
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 C -1.841987 3.080987 -1.323827
 C -3.004445 5.008474 0.315889
 H -2.086805 3.965351 1.956599
 C -2.604833 4.101195 -1.885272
 H -1.402468 2.307552 -1.954935
 C -3.190671 5.062881 -1.064619
 H -3.459985 5.758416 0.957118

H -2.754703 4.135858 -2.961140
 H -3.796945 5.852931 -1.499887
 C 4.120557 -0.490769 -0.906585
 O 3.702790 -1.098593 0.126527
 C 5.524089 0.106113 -0.828168
 C 6.517334 -0.676863 0.049738
 C 6.309046 0.285205 -2.157662
 H 5.379292 1.096526 -0.369273
 C 7.842379 -0.026233 -0.358249
 C 6.678831 -2.096046 -0.516937
 C 7.674693 -0.346945 -1.849767
 H 8.719553 -0.507951 0.090252
 H 7.879131 1.048887 -0.146877
 H 7.222914 -2.733948 0.188323
 H 5.710057 -2.572727 -0.696415
 C 7.496134 -1.869787 -1.813179
 H 8.477439 -0.010238 -2.512882
 H 8.467841 -2.374113 -1.761975
 H 6.985599 -2.242461 -2.708432
 H 6.406496 1.342363 -2.428405
 H 5.818544 -0.220058 -2.998317
 H 6.265335 -0.651849 1.113237

TS11'

Ni 0.338720 -0.010888 0.862695
 P 0.889713 1.749856 -0.339338
 P 1.024898 -1.841937 -0.439145
 C -1.205194 -0.725396 2.413540
 C 0.181616 -1.018158 2.599538
 C 1.107728 0.033781 2.783377
 C 1.845146 1.394632 -1.910603
 C 1.942299 -1.593363 -2.046129
 H 0.515518 -2.053162 2.533286
 H 2.149245 -0.212298 2.981723
 H 0.764780 0.956229 3.250108
 N -1.732604 -0.304707 0.546305
 H -1.903644 -1.558206 2.440234
 H -1.588974 0.212395 2.811675
 C 3.172456 -0.772071 -1.797655
 C 3.116504 0.634652 -1.695500
 C 4.288864 1.337574 -1.389877
 C 5.497305 0.680922 -1.181235
 C 5.554161 -0.705975 -1.292169
 C 4.399135 -1.417704 -1.600938
 H 4.245660 2.424047 -1.327486
 H 6.391485 1.251651 -0.945289
 H 6.493331 -1.232447 -1.143018
 H 4.437254 -2.503029 -1.685176

H	1.261818	-1.104689	-2.750683	H	-3.882249	4.049670	-2.495904
H	2.199337	-2.573849	-2.462427	O	-0.839696	2.791768	2.540895
H	1.161811	0.858170	-2.575024	H	-1.545200	2.341992	2.026276
H	2.050830	2.364023	-2.379458	H	-0.040249	2.384935	2.181725
C	2.163857	-3.041484	0.349401	C	-2.813139	0.499922	0.511250
C	2.225638	-4.392464	-0.017912	O	-2.901279	1.575412	1.142649
C	3.091367	-2.549283	1.275992	H	-1.914607	-1.193924	0.087468
C	3.188695	-5.230576	0.535735	C	-3.980173	-0.042562	-0.300847
H	1.518624	-4.788343	-0.744488	C	-4.684595	-1.214263	0.435804
C	4.062696	-3.385573	1.822266	C	-5.139939	0.940411	-0.575696
H	3.058435	-1.494779	1.547466	H	-3.576158	-0.435380	-1.244544
C	4.109825	-4.728127	1.455127	C	-6.025620	-1.249372	-0.300989
H	3.225871	-6.276944	0.244095	C	-5.115788	-0.754281	1.835524
H	4.781689	-2.987297	2.533207	C	-6.363110	0.216863	0.004682
H	4.863694	-5.383994	1.882575	H	-6.736172	-1.960287	0.136592
C	-0.414277	-2.856051	-0.918576	H	-5.922435	-1.459013	-1.372577
C	-1.147354	-2.563172	-2.079731	H	-5.478329	-1.610401	2.414822
C	-0.964920	-3.763737	0.003343	H	-4.296679	-0.305957	2.407659
C	-2.377263	-3.172972	-2.319712	C	-6.259125	0.246649	1.537312
H	-0.762713	-1.846488	-2.802517	H	-7.318228	0.584521	-0.381345
C	-2.189653	-4.377121	-0.242258	H	-7.198026	-0.075761	2.000811
H	-0.425735	-3.993063	0.921179	H	-6.042313	1.253967	1.909778
C	-2.902540	-4.083481	-1.404797	H	-4.093684	-2.137038	0.430859
H	-2.927715	-2.931868	-3.225873	H	-5.255665	1.113284	-1.651422
H	-2.591194	-5.083067	0.480117	H	-4.963098	1.911117	-0.101420
H	-3.864411	-4.553950	-1.590907				
C	1.930064	3.107081	0.325027				
C	2.145325	4.303227	-0.375795				
C	2.634523	2.886621	1.512494				
C	3.032467	5.256721	0.113155				
H	1.620841	4.488938	-1.311546				
C	3.528915	3.838363	1.999076				
H	2.486798	1.949958	2.045623				
C	3.726755	5.025480	1.301474				
H	3.187741	6.181274	-0.437001				
H	4.072112	3.648013	2.920978				
H	4.422405	5.770632	1.677917				
C	-0.572257	2.578058	-1.065463				
C	-1.323820	1.865909	-2.012243				
C	-1.044150	3.823294	-0.633177				
C	-2.502550	2.393981	-2.528953				
H	-0.999203	0.875061	-2.329709				
C	-2.227413	4.348717	-1.147546				
H	-0.492049	4.379137	0.120586				
C	-2.957133	3.639875	-2.098853				
H	-3.069807	1.828135	-3.264336				
H	-2.580015	5.316377	-0.800071				