

## **Supplementary Information:**

# **AFIR explorations of transition states of extended unsaturated systems: automatic location of ambimodal transition states**

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**Table SII.** Cartesian coordinates (in Å) of the optimized TS structures at the  $\omega$ B97X-D/D95V level. Energies in a.u. are also shown.

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TS0 -803.009923

C	1.206269891675	0.314667496489	-2.292677184385
C	0.258658373725	1.175809441375	-1.446083152651
C	0.638717113231	0.967212097527	-0.115056397402
C	1.607914990623	-0.119434482446	-0.059122545345
C	1.898390765100	-0.568958348081	-1.318900015538
H	1.999714094148	-0.508748869867	0.870745971488
O	1.345286242569	0.381969745614	-3.523133923543
C	0.112671793729	1.723650023370	1.009762432129
H	-0.167683247296	2.100192692399	-1.817398649599
H	2.570182423022	-1.365011300934	-1.601926455572
O	0.792155664964	1.474492898232	2.180679283008
O	-0.855240228249	2.508678372645	0.956524946516
C	0.332952571674	2.186137127423	3.369718445980
H	0.982723103785	1.843965824853	4.173303724385
H	0.426755631894	3.264949524256	3.223907699170
H	-0.712730973947	1.944366279272	3.578900141997
C	-1.399973388221	0.049985811617	-1.897109046058
C	-1.058275532788	-1.263543406791	-1.564805741782
C	-1.063250112910	-1.692356354495	-0.212774355761
H	-0.710332265472	-1.960842992649	-2.318693010783
H	-1.473356615576	0.311978438513	-2.948233696766
H	-2.025743544885	0.632174009836	-1.225788959166
O	-0.554818688434	-2.958701612933	0.092106097002
C	-0.544148168168	-3.073317428766	1.467621824156
C	-1.031489372335	-1.928033873826	2.048121400399
C	-1.368793245575	-1.034879350900	0.975832610631
H	-0.182268278736	-4.006081628159	1.864351488978
H	-1.835511791877	-0.066855031248	1.064248806073
H	-1.139424346591	-1.743486497972	3.103909534227

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TS1 -803.003778

C	0.664251451250	1.961821788656	-1.804694182593
C	-0.470388296266	1.212476503741	-1.088384393272
C	-0.050892404419	-0.131057416034	-1.002678016379
C	1.337688614791	-0.217253408741	-1.445356670059
C	1.793927216623	1.000879017316	-1.867487542483
H	1.898143679643	-1.142313767751	-1.425654608046
O	0.610405389547	3.132878738275	-2.212615614327
C	-0.911992085128	-1.260336890029	-0.692784178497
H	-1.508140623821	1.493506277874	-1.228335757182
H	2.772604821802	1.249169102263	-2.250217010059

O	-0.215142731139	-2.455841432565	-0.715720441939
O	-2.128187901260	-1.213816600563	-0.434182603391
C	-0.988076729011	-3.663338563847	-0.448243982773
H	-0.263276179169	-4.475646719525	-0.471830149334
H	-1.470664862265	-3.596996602010	0.530025985775
H	-1.753895098691	-3.801105739941	-1.215951242161
C	0.347666009806	-2.046716150041	2.880026525552
C	-0.448107999133	-1.043730356536	2.458606016993
C	0.040011507966	0.172203342013	1.830811162131
H	-1.528299946042	-1.113072629615	2.541999945455
H	-0.074289053814	-2.936587200671	3.333371217585
H	1.428499632933	-2.011837606622	2.778573817429
O	-0.915997482548	1.082450819288	1.444297980137
C	-0.243813382282	2.065046940424	0.682837278723
C	1.151247801127	1.949431365753	0.983942199409
C	1.318807038545	0.721826821968	1.635176673243
H	-0.799512517801	2.979280204426	0.532591654037
H	2.248714760762	0.257281484614	1.919251701405
H	1.914868134192	2.650605547167	0.690684010953

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TS2 -803.002063

C	1.767194529979	-0.493271026558	-2.341236967288
C	0.661224711134	-1.060150903993	-1.426906927261
C	-0.132492899903	0.043591444539	-1.073783088741
C	0.518715832425	1.275456718352	-1.546368068131
C	1.648169581624	0.987606099773	-2.253157886946
H	0.115351143927	2.259506132540	-1.346192199502
O	2.568830159905	-1.167306083713	-3.003214006173
C	-1.451415020547	-0.063238355222	-0.485928916575
H	0.253318820490	-2.048722904899	-1.596378730246
H	2.339644730519	1.672814062995	-2.719788884943
O	-2.086175004062	1.160434649587	-0.380751345283
O	-1.991456608415	-1.124309003011	-0.112726342669
C	-3.436329172836	1.145192484014	0.171482483834
H	-3.743994495748	2.189484580780	0.199892115613
H	-4.100876154869	0.560993871752	-0.470184169509
H	-3.432540213129	0.708739149884	1.173414502791
C	1.935189145483	-1.589449197242	0.052208703942
C	1.135623570831	-1.888289925884	1.157453715118
C	0.503474779544	-0.860623153765	1.883338599209
H	0.863841125606	-2.912251659382	1.389636517260
H	2.451110812430	-2.400896695920	-0.452257798300
H	2.463331103364	-0.635580108948	0.030741838173
O	-0.444924001576	-1.198338651758	2.853425271223
C	-1.044698680121	-0.027075332937	3.258355348037
C	-0.501572625107	1.050423335858	2.599901040669

C	0.497090168153	0.527155595286	1.713608340386
H	-1.807544431516	-0.120916316823	4.011921731569
H	1.174996578559	1.094770383409	1.098217928614
H	-0.778754330104	2.083595124338	2.724606916431

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TS3 -803.001583

C	-1.330740892340	0.393594060789	-2.275751461143
C	-0.481313278570	1.174403108557	-1.340596644220
C	0.588966839914	0.372198983043	-0.999040714316
C	0.418499902672	-0.967518621619	-1.496092425238
C	-0.833661030764	-1.052161033207	-2.123674703312
H	1.145709277684	-1.756042351537	-1.373799733795
O	-2.235675292279	0.787553275175	-3.025204252195
C	1.726446844281	0.830395847946	-0.171461574017
H	-0.612943804735	2.219186577677	-1.102984345662
H	-1.115710738032	-1.821023725346	-2.833643124899
O	2.679795429457	-0.143629527922	-0.026251002320
O	1.832924833039	1.952395996517	0.339931747822
C	3.840211953370	0.194374889643	0.794140469096
H	4.467048300097	-0.695237287667	0.781450371496
H	4.366467476403	1.051757661924	0.367793745608
H	3.520400823493	0.437839703673	1.810680571428
C	-2.270095129879	-1.368913193081	-0.734547275614
C	-2.159659853573	-0.335217148987	0.216353765555
C	-1.203255492864	-0.430465110541	1.265455611704
H	-2.811694898375	0.529536626012	0.189151304805
H	-3.120153519405	-1.347272218603	-1.410470878369
H	-1.930598685729	-2.365029015965	-0.467267479594
O	-1.063836844612	0.648565356303	2.140193536634
C	0.013990961539	0.376460874896	2.960722690907
C	0.560097088701	-0.841251739820	2.640071085812
C	-0.216793912997	-1.367769866658	1.549961315431
H	0.251510562813	1.125753459787	3.695198162276
H	-0.088792464495	-2.322885252629	1.068363861353
H	1.405810978195	-1.308503859569	3.116919097500

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TS4 -803.001182

C	-1.910779426330	-1.262521096034	-1.414832491121
C	-0.383976325187	-1.166459041518	-1.194124223423
C	-0.219392690962	-0.977825915856	0.192778085119
C	-1.543075006587	-0.832996157952	0.818829817692
C	-2.536864300502	-0.985576889640	-0.099449080531
H	-1.663799748852	-0.631098129721	1.874953123111
O	-2.455747779601	-1.512474235032	-2.500656687286
C	1.045389661769	-1.114926979003	0.877328913566
H	0.286184541765	-1.768786272422	-1.796431117731

H	-3.602897290140	-0.904991723847	0.048401922598
O	0.931260328718	-0.939725450647	2.245225313399
O	2.144997492004	-1.345847595009	0.331283165473
C	2.157437660842	-1.071872253590	3.022722093654
H	1.858673101265	-0.907480681701	4.056830922702
H	2.585717215984	-2.069099926764	2.893790469213
H	2.893503226187	-0.327681294422	2.706152705550
C	0.172426241552	2.865644531143	1.980036635191
C	-0.532445229973	2.454287238290	0.907240680314
C	0.048629232476	1.769060192109	-0.234248334728
H	-1.607429477989	2.599345092971	0.857089012276
H	-0.316770956240	3.363519972106	2.809438168712
H	1.243943033929	2.708976308996	2.063779678341
O	-0.816765581721	1.389233337564	-1.234034859319
C	-0.072825818819	0.576462466337	-2.116922782590
C	1.308437346680	0.827392316846	-1.855734992921
C	1.372520114052	1.521348936570	-0.647935946675
H	-0.552588774077	0.391054448614	-3.067806367942
H	2.261474166005	1.772272530969	-0.093863673585
H	2.133965710702	0.422664586060	-2.417511456327

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TS5 -803.001126

C	1.304434566936	-0.410189006158	0.473928714510
C	0.056787869314	-1.243036737419	0.787726925765
C	-0.387785795425	-1.741231106345	-0.443425612661
C	0.324914311226	-1.077199808565	-1.509217989480
C	1.268557230087	-0.215910453476	-0.993280979599
H	0.107346535262	-1.235974481237	-2.556652906846
O	2.136534739623	-0.000809287226	1.301268218554
C	-1.499190988960	-2.671841881306	-0.583931018815
H	-0.096948057879	-1.738662406411	1.738753571638
H	1.956308769614	0.418492722790	-1.532060377125
O	-1.701844152582	-3.055206258977	-1.890662417227
O	-2.215081927526	-3.080329686357	0.349415627275
C	-2.795802003844	-3.990514450401	-2.139846980021
H	-2.788651150923	-4.154921786322	-3.215911143039
H	-2.624530505159	-4.925203156795	-1.600387098230
H	-3.745824216306	-3.558410180899	-1.815438730804
C	-1.022827962998	0.455979591161	1.229754842860
C	-0.619434885963	1.469987764510	0.349871323329
C	0.338785600035	2.480210816338	0.675667637881
H	-1.092181452234	1.558732567925	-0.622669844418
H	-1.978024285044	-0.030688754807	1.067799348415
H	-0.704171631449	0.514328061208	2.267651058505
O	0.612392755708	3.431496966672	-0.314037334546
C	1.590455271327	4.269078085695	0.184443693251

C	1.948497550010	3.878333114561	1.451578109204
C	1.148302202138	2.731087731622	1.772060411827
H	1.906817880892	5.069205318385	-0.462035318057
H	1.178975837517	2.156996953922	2.683121764249
H	2.692392585742	4.342864796573	2.077371223058

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TS6 -802.997498

C	-2.056226374281	-0.538239899412	0.068171849125
C	-0.882044815861	0.084085899016	-0.719273557471
C	0.164151903486	-0.874969000706	-0.649472451701
C	-0.250980951289	-1.964213886749	0.218346125618
C	-1.518658662737	-1.756924098122	0.696757259363
H	0.389594386251	-2.807264026432	0.442125859863
O	-3.210784983312	-0.075756965885	0.116368429452
C	1.385151234746	-0.756606189873	-1.408704407846
H	-1.081941889437	0.630207800465	-1.635738249505
H	-2.086284047321	-2.384068844764	1.367083376300
O	2.164872601994	-1.892929235062	-1.382050654498
O	1.742997591877	0.280516630271	-2.014411096277
C	3.422995974749	-1.841581316892	-2.120104983258
H	3.874630212914	-2.822140069621	-1.979157391025
H	3.234228183093	-1.647444169932	-3.178684204490
H	4.068211704152	-1.053317389974	-1.723094513301
C	1.737637171422	0.049047472205	1.568519808473
C	0.602102505520	0.389829834513	2.247865356140
C	-0.370910224169	1.225841537085	1.646681978037
H	0.373689949100	-0.033277232016	3.219701972810
H	2.432427202543	-0.676923629810	1.976335348192
H	2.042233428805	0.558448068115	0.661668781402
O	-1.468774458909	1.656198303349	2.356584425384
C	-2.217434446205	2.487064336719	1.504862755635
C	-1.628923024948	2.582554555036	0.289098614170
C	-0.457913897841	1.691219815801	0.292814938806
H	-3.117640969396	2.892566522101	1.930572692009
H	0.428210706572	1.896947778949	-0.300367083900
H	-1.998666119476	3.137671850519	-0.556421103788

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TS7 -802.996497

C	-0.406866066594	-0.432434173355	2.415255217267
C	0.816766599051	-0.067347425189	1.534488566380
C	0.293732069685	1.063870142083	0.672157248637
C	-0.929360033743	1.475936681217	1.216757108247
C	-1.363182961342	0.623252905032	2.253692059311
H	-1.492127036917	2.319697578149	0.834704389197
O	-0.472136727032	-1.519446775396	3.064548581246
C	0.908105706213	1.501965813958	-0.522231395657

H	1.561747938912	0.339688732101	2.233865768885
H	-2.289139426870	0.700215130928	2.805128431828
O	0.428985639417	2.689549321162	-1.040080434844
O	1.810419035085	0.851324802110	-1.152235676726
C	0.967972923292	3.111950451422	-2.326774982333
H	0.439619740032	4.034711866336	-2.563704102901
H	2.043419318885	3.289485921685	-2.250853397613
H	0.786722268009	2.350377285917	-3.090645089362
C	1.473193259427	-1.307955303143	0.858718284841
C	1.020999793325	-1.429313449201	-0.550675800288
C	-0.313074455794	-1.629149348524	-0.875242653913
H	1.743176318620	-1.417712969890	-1.357716424274
H	2.558803004234	-1.230091028340	0.877305886344
H	1.159988711246	-2.177391201114	1.461691353208
O	-0.677207383623	-1.650821165605	-2.243376765359
C	-2.013074297174	-1.872829756083	-2.292342619796
C	-2.546927693302	-2.026369318106	-1.019770076625
C	-1.475476063460	-1.871014748518	-0.110899490053
H	-2.460862662234	-1.902305982159	-3.272067634031
H	-1.506381068627	-1.964701670540	0.965800869300
H	-3.578357517937	-2.222406825346	-0.781682522010

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TS8 -802.995476

C	-0.907851782296	-1.745708553478	-0.328117867547
C	-0.266700594081	-0.515900458924	-1.022515430570
C	1.073961381526	-0.453963472252	-0.398363879815
C	1.073905512169	-1.228621724138	0.762936123838
C	-0.189717602792	-1.828608004637	0.949061366410
H	1.901953886738	-1.276654742990	1.456794425729
O	-1.853758999766	-2.426592048570	-0.756609539742
C	2.099859708747	0.455978107942	-0.862737260968
H	-0.311980723942	-0.479329110363	-2.108968525248
H	-0.476952874004	-2.490156191021	1.754082579039
O	3.321532483266	0.267450225538	-0.258117040708
O	1.906310923765	1.356450031011	-1.708985691215
C	4.402594673099	1.157774564937	-0.671250179246
H	5.270873324158	0.831596404363	-0.101223645257
H	4.581615445737	1.062137701763	-1.745008148340
H	4.151606482011	2.196977439567	-0.442050591006
C	0.506936646427	1.667273020820	1.941729592304
C	-0.613184715494	0.923530215569	2.129906461800
C	-1.407420732636	0.433417150180	1.039253534846
H	-0.945248507205	0.650778046137	3.126493914613
H	1.112650685648	1.977125209455	2.786398567480
H	0.817603337632	2.017302906587	0.962959259559
O	-2.729748899145	0.132396197401	1.292891161800

C	-3.431402383183	0.202828222682	0.060887070580
C	-2.624118329856	0.570508599718	-0.945451344400
C	-1.211577742228	0.678263430989	-0.429288348424
H	-4.474832810422	-0.051417980861	0.122273277540
H	-0.702788180523	1.611296360307	-0.681710614899
H	-2.903250751896	0.673797611333	-1.981247904153

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TS9 -802.995432

C	-0.438777926561	1.071090397034	1.802161353240
C	-1.120027032337	-0.126236010734	1.099554979800
C	0.033364045044	-1.062134972327	0.859801154102
C	1.103246442760	-0.613456419544	1.662454115784
C	0.826524012626	0.615260791284	2.289633875072
H	2.033934698211	-1.160342597408	1.758038454295
O	-0.931056833796	2.245735017229	1.751392809470
C	-0.060023916165	-2.247223820206	0.082433716109
H	-1.793951857465	-0.603189459755	1.825734824447
H	1.510670380918	1.208859694132	2.877079782473
O	1.085136679696	-3.039338113813	0.111125693877
O	-1.042280078525	-2.563964103723	-0.649270833165
C	1.047609843976	-4.260798795978	-0.680216020121
H	2.019539342141	-4.728853924356	-0.526406869474
H	0.243419269701	-4.916926935853	-0.336731864162
H	0.887719136054	-4.035631983588	-1.738632353188
C	-2.042776293958	0.354036945531	-0.079058543664
C	-1.539389389013	1.648246888812	-0.588234771401
C	-0.345029647065	1.713253144139	-1.291191173559
H	-2.100109324119	2.564016787702	-0.440593385073
H	-3.060158631003	0.476415513886	0.290340973928
H	-2.023808516607	-0.446185434614	-0.830091148509
O	0.173571809974	2.973189947621	-1.658895669407
C	1.372088660546	2.748314232740	-2.253731600123
C	1.657983872989	1.391493736507	-2.315483385118
C	0.566895191896	0.723722119603	-1.709827574545
H	1.913213342565	3.618250162811	-2.587392684900
H	0.421784812568	-0.338392807241	-1.596211860332
H	2.539360051613	0.946075180069	-2.744173459102

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TS10 -802.994603

C	0.486573320232	1.854846810542	0.297025633600
C	1.277802416243	0.735085034614	-0.330125102753
C	0.463917215114	0.048872029125	-1.160678345653
C	-0.944590864432	0.603688078496	-1.089496295035
C	-0.878454731286	1.723351847064	-0.231534019449
H	-1.579945800248	0.573062475299	-1.968099118380
O	0.947956540753	2.708837382489	1.088777874582



C	0.883613871353	-1.089899405485	-1.996675224914
H	2.323715874105	0.544031460545	-0.134186435593
H	-1.631953133687	2.489540663120	-0.120266986211
O	-0.144273670396	-1.544527511011	-2.791650622961
O	2.013925486160	-1.594478662906	-2.020284563527
C	0.164734949144	-2.648199393887	-3.700727986375
H	-0.766103286340	-2.851130112465	-4.226855080360
H	0.951989940930	-2.350604511300	-4.397083930710
H	0.496211333875	-3.522624852366	-3.135658832821
C	-1.932130003031	-0.910716048117	-0.237868166199
C	-1.098850980116	-1.285328792991	0.836122933403
C	-0.933632434249	-0.399221982988	1.902229269287
H	-0.414665163170	-2.121809312789	0.746708656432
H	-2.027659583423	-1.604171227634	-1.068555866502
H	-2.828033752295	-0.330085303728	-0.035941052627
O	0.153108773870	-0.539946307023	2.784012651774
C	0.173145540962	0.586628196331	3.579227157012
C	-0.862088882808	1.432310671582	3.265527303454
C	-1.572787170214	0.822875091215	2.182211152083
H	0.967284418969	0.640299922317	4.303717495522
H	-2.512888368542	1.146229656496	1.769522275540
H	-1.064217346221	2.384890875378	3.723466739393

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TS11 -802.994035

C	0.659114822390	-0.495008663291	-1.858164067024
C	-0.366594669781	-0.488421716879	-0.714662509289
C	0.389498262400	-0.701090624607	0.474417808415
C	1.812190388631	-0.676082709949	0.136203615701
C	1.991935554154	-0.485379060089	-1.204031202566
H	2.588845061683	-0.789307701107	0.880814765176
O	0.398466915645	-0.514484963952	-3.072238892345
C	-0.172374898374	-1.234429181430	1.708467507074
H	-1.332268143300	-0.962179669445	-0.857232965585
H	2.923480662475	-0.409844661704	-1.745305053529
O	0.801631627476	-1.446568632868	2.670739318193
O	-1.370641506088	-1.486275525533	1.920313062304
C	0.353843237794	-2.033090764109	3.930003647381
H	1.254566378787	-2.131325641995	4.533864635883
H	-0.375594294482	-1.381066429103	4.417746252538
H	-0.105650292893	-3.008641050907	3.752691160772
C	-2.061412900344	1.638661700987	-2.966841452918
C	-2.139538693174	1.396533999270	-1.648700249416
C	-0.975495523674	1.341244144414	-0.737702081097
H	-3.090335683273	1.177907023242	-1.170681263488
H	-2.952456362541	1.625557311912	-3.584469597118
H	-1.118424704402	1.821776503021	-3.471650649107

O	-1.335036107126	1.399572035982	0.645386827180
C	-0.167512446873	1.658513657019	1.308551922475
C	0.777236036754	2.226020015314	0.431496167004
C	0.266890021026	2.082510942222	-0.853246050711
H	-0.199778289945	1.609944078222	2.384717882151
H	0.719440883600	2.389022339639	-1.782539447756
H	1.738664124899	2.619950550594	0.716451687360

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TS12 -802.993724

C	-0.382788486935	1.394392949704	-0.612695418787
C	-0.591860853232	-0.079295706909	-0.717682551569
C	0.508692067434	-0.587835663271	-1.398471271648
C	1.528166111267	0.406835980181	-1.534737182716
C	1.110534842445	1.569413132904	-0.880457685442
H	2.488195524114	0.232916494095	-1.997628025413
O	-1.210600753673	2.283093289244	-0.372092712227
C	0.613400981611	-1.991809890694	-1.845107403071
H	-1.522066859523	-0.589035106271	-0.512818657271
H	1.571551521676	2.545138339527	-0.968303847423
O	1.802011249572	-2.238403140222	-2.484721513412
O	-0.249860696487	-2.863128770007	-1.676249302210
C	2.008806434562	-3.593657400414	-2.993632516794
H	2.988786236291	-3.572084063532	-3.466152864393
H	1.984311190244	-4.313422460160	-2.171903803259
H	1.229902773722	-3.846825424129	-3.716748349023
C	1.347276708686	1.177813832934	1.186914432875
C	0.364174357792	0.233824523109	1.551854770428
C	-0.850398739104	0.587511163646	2.246547835985
H	0.606083888948	-0.822932674476	1.540482663971
H	2.373060468859	0.847741548808	1.086416260654
H	1.221847337196	2.213240151035	1.493405648947
O	-1.673519953520	-0.472519101167	2.633082783664
C	-2.794174232075	0.075823032534	3.232820983651
C	-2.704233510748	1.444264580654	3.231320958884
C	-1.456026003001	1.777347937226	2.597816088197
H	-3.527958081653	-0.622288186582	3.595699062695
H	-1.070338789815	2.766430278911	2.413979362205
H	-3.433629418939	2.133448508514	3.623598573337

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TS13 -802.993161

C	-1.645885974933	1.838064356207	-0.274487100592
C	-0.466303074549	0.860789316534	-0.041380765564
C	0.146039945977	1.291493957159	1.156326971678
C	-0.650807546062	2.365963977164	1.738794801327
C	-1.700459172893	2.700045924665	0.924270870546
H	-0.408769537480	2.824668264420	2.688886002035

O	-2.384814838528	1.836047912893	-1.274119605718
C	1.313422715642	0.651015151025	1.686764685431
H	0.121214073277	0.506565122748	-0.883508473815
H	-2.458706696750	3.450154559076	1.089520760288
O	1.835559612301	1.266869946672	2.802784670547
O	1.822408736334	-0.399395713090	1.211795097520
C	3.020435799413	0.656821275370	3.397039998918
H	3.259828390020	1.280529089498	4.256690264259
H	2.807385226663	-0.369921354845	3.705703522036
H	3.843931599457	0.650072480710	2.678601245956
C	-1.385465951046	-0.815406862146	0.343207741992
C	-1.604163953062	-1.391059702321	-0.916058371030
C	-0.553908217862	-2.039324204648	-1.613813555623
H	-2.540375719639	-1.238439948814	-1.443745760686
H	-2.249510411141	-0.456373505270	0.896129612389
H	-0.583199094882	-1.233723792110	0.945653564550
O	-0.831126027375	-2.618724770372	-2.859918106751
C	0.352570362917	-3.128401597199	-3.338400290673
C	1.377640836608	-2.883130601362	-2.450383340415
C	0.807155913176	-2.182923357125	-1.341577541629
H	0.306903367187	-3.621520470006	-4.294180956763
H	1.315729898676	-1.796422989464	-0.466011506057
H	2.410472288087	-3.161197060963	-2.578442947845

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TS14 -802.993023

C	-2.553256126175	-0.290597553647	-0.036000381652
C	-1.585519514065	-1.414332464820	-0.114461277555
C	-0.458724693881	-0.940125422941	-0.739366185923
C	-0.540441281088	0.484565717854	-0.992331062184
C	-1.757778693588	0.955955329190	-0.447830059791
H	0.163159827159	1.037083145537	-1.594471966684
O	-3.747423128822	-0.317457576452	0.300278054579
C	0.718187759369	-1.782969123068	-1.052807630428
H	-1.778357692650	-2.427689556084	0.204144957189
H	-2.278494739196	1.825121463682	-0.834263297763
O	1.693895724419	-1.071189493395	-1.698261232094
O	0.839830930371	-2.981547519835	-0.767294970538
C	2.908285782312	-1.794922494446	-2.069103631314
H	3.556420440988	-1.046659353337	-2.520625227083
H	3.372336935884	-2.235014596188	-1.182917544666
H	2.668737554369	-2.588664578587	-2.780697552986
C	3.249295812468	1.267061125894	0.545870942291
C	2.114431007834	1.994639898105	0.564735461450
C	0.836932145392	1.513050843542	1.064993347191
H	2.101450834505	3.008605528177	0.174986112397
H	4.171219420439	1.685415570296	0.157979684620

H	3.285303241298	0.243031758978	0.906486650086
O	-0.232400100006	2.396001057051	0.989684887433
C	-1.373089609799	1.624013113866	1.326238205767
C	-0.906235872609	0.488426153795	2.080235282383
C	0.469122864658	0.402885876806	1.845334083703
H	-2.255953393103	2.206072477404	1.550863340747
H	1.135556586413	-0.383245666060	2.162425637118
H	-1.522132826749	-0.175802181019	2.663468184471

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TS15 -802.992819

C	1.197103414197	-0.593046474425	-2.038566707991
C	0.470343897008	0.225929492978	-0.945580985196
C	-0.732291846500	-0.477535535800	-0.690656783720
C	-0.692000805031	-1.756334078765	-1.407737767149
C	0.444777782018	-1.864805938348	-2.158117001674
H	-1.483619814656	-2.490789818194	-1.333747211800
O	2.207235228655	-0.226069082269	-2.659108999379
C	-1.883700912151	0.138173760461	-0.068293146959
H	0.495053406375	1.309874559178	-0.973296475846
H	0.753913205965	-2.686910758863	-2.785795274547
O	-3.008958560077	-0.667202910309	-0.105896590527
O	-1.898255574195	1.272916925903	0.451122101476
C	-4.220094191769	-0.116323682800	0.491298757947
H	-4.981097508140	-0.882496833805	0.350602447170
H	-4.062333571714	0.087489351648	1.554109374457
H	-4.504185582143	0.812416646606	-0.009592680017
C	-0.360623937123	-1.489122887749	1.829900960405
C	0.132701094771	-0.304400465966	2.311222693563
C	1.213704040232	0.323828897806	1.657920992993
H	-0.368502967445	0.237283464012	3.104515123093
H	-1.269508949444	-1.920137614296	2.235288330767
H	0.190002205831	-2.101318251260	1.125125512687
O	1.702679280417	1.537760653434	2.087390898365
C	2.723103924733	1.915166318736	1.194506620410
C	2.876153191656	0.989557135024	0.216979227288
C	1.843424199555	-0.040538329060	0.429336856529
H	3.206097045623	2.850224299004	1.417610327728
H	2.018400063157	-1.085643299468	0.186068193574
H	3.560941457520	1.020829560179	-0.614317858180

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TS16 -802.991842

C	0.404968908584	-0.641562708319	-1.152304497806
C	-0.306872895632	-0.812535998994	0.205609240065
C	-1.675422288959	-0.982741883520	-0.107392349929
C	-1.862516295699	-0.749671323482	-1.521964386864
C	-0.657564345495	-0.518408491378	-2.151756616716

H	-2.835317253347	-0.771543941030	-1.995897118296
O	1.646987382888	-0.600359423820	-1.308262670793
C	-2.690359342987	-1.229203985860	0.887914463534
H	0.178239979270	-1.318786982871	1.031036203391
H	-0.484637431969	-0.331244039125	-3.200896595920
O	-3.941401798977	-1.444991841513	0.344815986645
O	-2.495515117019	-1.228242156650	2.123768261813
C	-5.026520740991	-1.702204511034	1.285524685618
H	-5.917846064314	-1.809693654281	0.669402749281
H	-4.829874483677	-2.617893124400	1.848927902945
H	-5.132208001841	-0.869217169632	1.985397245773
C	-0.160133879565	1.041613105075	0.869195163548
C	1.170690420457	1.271666220375	1.248765717277
C	2.195483835309	1.706139892663	0.382916855982
H	1.479325584382	1.024158100518	2.261201166736
H	-0.879393516325	0.913514284412	1.673498366710
H	-0.539478358936	1.532225808405	-0.026438414932
O	3.490255287512	1.802455284430	0.917407040183
C	4.320687153774	2.205042888203	-0.099402003208
C	3.611051624280	2.372032168466	-1.267590231452
C	2.253217981913	2.047656528653	-0.969802552970
H	5.360323918935	2.325910529128	0.152262410104
H	1.421379186889	2.065711921021	-1.654181165602
H	4.013427726674	2.668758279356	-2.221376176759

29

TS17 -802.991773

C	1.571844797864	1.033572872321	1.998277203062
C	0.603127811779	0.687061238508	0.839296312342
C	-0.659703015251	0.557288698470	1.439518076769
C	-0.513249145349	0.649020752019	2.895262810440
C	0.780253977622	0.922844954567	3.242494461522
H	-1.345124652685	0.515034908334	3.574564661797
O	2.767978651676	1.332779774952	1.849057711089
C	-1.822766922245	0.207102227353	0.681496186384
H	0.756327899249	1.130474694200	-0.141134171429
H	1.196651319104	1.040262873739	4.231220926755
O	-2.975979179994	0.096130048118	1.432506826940
O	-1.801488802554	-0.038332930588	-0.551371592144
C	-4.190145070868	-0.277814650306	0.715178086712
H	-4.972246038916	-0.297077839396	1.472348554365
H	-4.415783517522	0.458592676760	-0.060386173577
H	-4.072662643919	-1.260248117634	0.250385218666
C	1.315801649173	-1.097370730659	0.305417347043
C	0.641654738785	-1.421924375980	-0.874303460796
C	0.994209358123	-0.848627585040	-2.131054508839
H	-0.228459597691	-2.068002149667	-0.864908264262

H	1.096396018128	-1.672477431194	1.200092104739
H	2.338433956280	-0.731840016083	0.236476016876
O	0.249107993264	-1.222158962354	-3.250766794863
C	0.732287975273	-0.507528351070	-4.322172613725
C	1.763784005033	0.312090314380	-3.923515734956
C	1.937363131842	0.095556976447	-2.518547739013
H	0.254804021446	-0.686099544404	-5.269809618431
H	2.665206778115	0.566510459218	-1.875916550865
H	2.325763526356	0.982641627959	-4.552055445740

29

TS18 -802.991707

C	1.990923437855	-0.190875298414	0.492695838049
C	0.606056869901	-0.781198877431	0.111654253790
C	0.215894243508	0.032383637216	-1.058544049945
C	1.018684155053	1.179147692201	-1.109278722010
C	1.935732339203	1.180475718621	-0.043454976835
H	0.895359355320	1.967115107896	-1.839600550678
O	2.878473211557	-0.748386293028	1.154584831226
C	-0.795825147509	-0.380202723461	-2.020202953676
H	0.520638547883	-1.860924756102	0.017024092762
H	2.689891426701	1.929030195749	0.156031528714
O	-0.992950391367	0.562142250247	-3.013486093373
O	-1.424949252342	-1.451889958190	-1.993261851586
C	-1.951541681656	0.213309430985	-4.057367081642
H	-1.948679325752	1.060336993594	-4.741518592726
H	-1.641512631990	-0.701891053464	-4.567948842366
H	-2.944741502438	0.060577043558	-3.626804727976
C	0.806266793881	-1.386371540435	3.500165526271
C	-0.123378791546	-1.355395651291	2.535197333564
C	-0.226562676552	-0.314239469754	1.458450428106
H	-0.870113399430	-2.140037192082	2.448826923715
H	0.832328200884	-2.202894848545	4.213334473735
H	1.583102275035	-0.634389404005	3.593314215392
O	-1.632285307020	-0.232899386260	1.020490759015
C	-1.847970393044	1.075490246598	0.708911431465
C	-0.874895938096	1.919424492323	1.222893786632
C	0.156695187040	1.112069752519	1.743429196954
H	-2.784332654854	1.300868131429	0.222409130107
H	0.915344189982	1.410516857236	2.450096023812
H	-0.897260742988	2.995906382737	1.181939665053

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TS19 -802.991496

C	-0.199761094552	0.065356158208	-2.172639005990
C	-0.484322577087	0.490626722749	-0.721952464314
C	-0.748924461472	-0.722764148060	-0.028228745783
C	-0.528233571988	-1.859805782484	-0.948185225183

C	-0.166111693033	-1.420492541400	-2.180029520356
H	-0.647916665291	-2.888583644107	-0.635329757174
O	-0.067355267879	0.832478249698	-3.138358231592
C	-1.554476341690	-0.782697357737	1.181408134624
H	-1.045457685673	1.400605151963	-0.544446814700
H	0.095227583999	-2.004232412133	-3.049800919674
O	-1.831064839232	-2.080839639661	1.566045007730
O	-1.949924648125	0.198013609910	1.839629139256
C	-2.654196001239	-2.246633166258	2.759904466922
H	-2.770573244860	-3.322574180301	2.878571485332
H	-2.157860649734	-1.809064925690	3.630141618030
H	-3.623744966849	-1.761652553347	2.622590338080
C	1.878518986758	3.390584686246	-0.976345751205
C	1.847328053464	2.056786308358	-1.131074250428
C	1.318988763852	1.120930681071	-0.118716057202
H	2.188667407654	1.601400576757	-2.054618084193
H	2.240873772719	4.029652564770	-1.773377734007
H	1.541253382875	3.883751585443	-0.068967514470
O	1.890302800302	-0.185179786642	-0.152587085623
C	1.473703732743	-0.786061437670	1.006303113539
C	1.123089859524	0.203501295058	1.957290755564
C	1.042560782392	1.401485004100	1.270148471160
H	1.706657973336	-1.831752324522	1.122007371409
H	0.705718292208	2.350313920542	1.654604333864
H	0.862030820413	0.020617564829	2.986153797423

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TS20 -802.991365

C	-0.989264718763	-1.187150969936	1.403493877254
C	0.096822958312	-0.254822884534	1.888870294258
C	0.039274818372	0.874684837401	1.149732492709
C	-1.025622673533	0.762934019942	0.083908016792
C	-1.646048904209	-0.492332101869	0.275453368381
H	-1.558053966997	1.648340937176	-0.241493900637
O	-1.260409043664	-2.303683824968	1.889140470604
C	0.940657042626	2.031023178149	1.310249159236
H	0.787892377853	-0.480507370142	2.689119044506
H	-2.624029190012	-0.776539808453	-0.082940622422
O	0.721638786928	2.977423606288	0.335860308666
O	1.801371049528	2.166369504633	2.189388421203
C	1.537079203534	4.190578756857	0.402778757422
H	1.192937591710	4.811369632718	-0.422302164975
H	1.384549035721	4.691764375579	1.361443977049
H	2.595074626707	3.940615673413	0.292202177627
C	-1.538951574028	-3.858032855414	-1.315585044587
C	-1.621388838691	-2.652142440437	-1.911059126714
C	-0.715188214147	-1.547669660100	-1.622850892404

H	-2.413688877585	-2.429885973133	-2.620231872742
H	-2.252701142301	-4.640960838675	-1.545766561168
H	-0.787824222773	-4.082448159643	-0.564598722600
O	-0.977528306588	-0.329280693770	-2.240401193331
C	-0.034510979429	0.557612961119	-1.677865830404
C	1.089766593427	-0.229679307340	-1.267160552251
C	0.638376499883	-1.537417503849	-1.171365516706
H	-0.017888445802	1.544627419503	-2.114169805099
H	1.168136992213	-2.396645434907	-0.792602875123
H	2.049814417544	0.158856084411	-0.967454665798

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TS21 -802.989118

C	-0.470076217809	-1.762224540396	0.779269578421
C	0.229907207136	-0.804824382480	-0.220696568193
C	1.147824355221	0.010430390600	0.646476760853
C	1.189072561699	-0.622100691842	1.907048974713
C	0.277269377328	-1.685918243751	2.002298095230
H	1.846332007768	-0.297102368287	2.705408515765
O	-1.535565800916	-2.377131527509	0.481052463138
C	1.836420751255	1.141461997120	0.155358214321
H	0.837795667502	-1.425834239673	-0.893426246679
H	0.076369714742	-2.284834503978	2.878126183196
O	2.725001561085	1.726766197282	1.045212381805
O	1.635834765597	1.656930126589	-0.993213636594
C	3.431338739538	2.910927866556	0.575583166245
H	4.095370523700	3.188027820491	1.393763182517
H	4.002203552589	2.684494605091	-0.328689659614
H	2.728422479157	3.719241178169	0.354953957208
C	-1.649920621734	1.515743944038	1.438160532355
C	-2.523563378637	0.830055144276	0.662030989247
C	-2.117108149228	0.181676694954	-0.551531330167
H	-3.571066067840	0.734518396763	0.923791666328
H	-1.983068918009	1.974379002639	2.362936154865
H	-0.598312799006	1.612964877274	1.181334877487
O	-3.074513473741	-0.284061868109	-1.348764549397
C	-2.467304849456	-0.890407020649	-2.501318104278
C	-1.136398568224	-0.765298343562	-2.419568489596
C	-0.777423330709	-0.043369052858	-1.148544842070
H	-3.162639445114	-1.334601173045	-3.189713996252
H	-0.235795599106	0.907312359447	-1.362191307438
H	-0.409894222456	-1.121141635522	-3.132322134746

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TS22 -802.988944

C	1.084308241041	-1.746709440911	-0.165279978659
C	0.412976166189	-0.781613541295	0.843189921527
C	-0.938994434274	-0.673037448902	0.399979511348



C	-1.047569053821	-1.269616535796	-0.895657271823
C	0.152050259652	-1.849661327714	-1.280817813495
H	-1.960333244933	-1.255426256791	-1.476707751347
O	2.218770555312	-2.249782980318	-0.019386679492
C	-1.979802067533	-0.022340288863	1.158455246787
H	0.649025042947	-0.847201721732	1.901371777025
H	0.368369526245	-2.368028807538	-2.202568928769
O	-3.216141122473	-0.092957347627	0.545866305934
O	-1.820246552437	0.563348354298	2.251874951924
C	-4.333767108430	0.517299465909	1.256793761903
H	-5.202360083453	0.343102413799	0.623655151671
H	-4.464118740557	0.048136906724	2.235297349221
H	-4.160409519281	1.587669237392	1.396161929951
C	3.628678176571	-0.393824918218	-1.576941085404
C	2.518527399631	0.297469597174	-1.937872639812
C	1.568645836369	0.828533697544	-1.000419065655
H	2.295212488784	0.487446172169	-2.982890103624
H	4.298065198478	-0.790032622706	-2.332039615403
H	3.891974013513	-0.580255224014	-0.542837863524
O	0.634608412030	1.710558528088	-1.475401329163
C	0.052326967455	2.367059068531	-0.360283426415
C	0.578891650429	1.900824466508	0.791371066747
C	1.451499505117	0.757355554101	0.437652967675
H	-0.688010484091	3.107681608168	-0.604245286562
H	2.322760822992	0.493159750930	1.025685577373
H	0.289299653736	2.180085791047	1.790069230540

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TS23 -802.988379

C	-1.650954824849	1.196297316527	-0.231903094950
C	-0.778706683099	1.042658522613	-1.458710481109
C	-0.279860082813	-0.210224678132	-1.461966164134
C	-0.707957567084	-0.958566382930	-0.213702139014
C	-1.554484355821	-0.078880055666	0.504857702858
H	-0.861524002452	-2.029198890911	-0.270165935275
O	-2.327285540850	2.205887320995	0.048863890914
C	0.594923994303	-0.756391746735	-2.515448837564
H	-0.608416188678	1.819013261970	-2.191450186309
H	-2.263624991640	-0.352740035750	1.270761657566
O	1.041718085120	-2.021701797816	-2.200108911046
O	0.908167163524	-0.186097951238	-3.567706355547
C	1.891312073351	-2.685087205302	-3.189438422841
H	2.108803390794	-3.663654680900	-2.765580601306
H	1.359728677689	-2.778393804631	-4.139157904309
H	2.807867884822	-2.111276991596	-3.345554684313
C	-0.706410108032	2.462288531963	3.491874837496
C	-0.031390432498	2.045937754519	2.403546716810

C	0.214936491647	0.649624680217	2.076990237352
H	0.332259387785	2.762039564647	1.673061406072
H	-0.889369659525	3.517109726544	3.659699309118
H	-1.106098932740	1.771075623606	4.228727639000
O	1.072493985226	0.396837090256	1.021134695883
C	1.006551535840	-0.993856878242	0.815030360659
C	0.603407933002	-1.578896900653	2.062841047875
C	0.057118561817	-0.557014991606	2.821911566951
H	1.723581776223	-1.385421475148	0.108143707241
H	-0.447083552098	-0.637657999070	3.771600697175
H	0.609532506982	-2.634589622895	2.283447408326

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TS24 -802.988312

C	-1.739227702533	-0.305343232232	-1.756469426703
C	-1.254245461471	0.040506597702	-0.319854492766
C	-0.408487392486	-1.149297211411	0.064030958969
C	-0.642749826120	-2.141168429194	-0.892221254990
C	-1.444584186000	-1.682364756592	-1.966633796013
H	-0.217218310164	-3.135494838656	-0.822215816213
O	-2.211771994038	0.601616447029	-2.512699488078
C	0.465559430565	-1.161090148854	1.178801957938
H	-2.159825432977	0.051319269970	0.303945968015
H	-1.721883203786	-2.244845844647	-2.845795560480
O	1.042215812538	-2.389580466446	1.457848991369
O	0.765528532107	-0.135131315378	1.862451456463
C	1.996940149872	-2.426612805646	2.556345506928
H	2.348186891934	-3.457368472851	2.592109795975
H	2.827190185009	-1.738798348654	2.372007855742
H	1.511991544641	-2.150190148414	3.496233336516
C	1.409583706117	0.472179333750	-2.381765753540
C	1.766155551907	1.056275843312	-1.211683413944
C	0.793464789637	1.603972750815	-0.309278013469
H	2.803827445009	1.157066967544	-0.914354238451
H	2.168825554365	0.071159131127	-3.044665292361
H	0.378171820091	0.392382084731	-2.712811228814
O	1.216743207118	2.421114148875	0.643759577121
C	0.088762438132	2.853088530723	1.423203051599
C	-1.032522198052	2.333858266796	0.907761791373
C	-0.687872683576	1.490955486849	-0.289984184841
H	0.340894663256	3.470714516058	2.265186103077
H	-1.126008816613	1.923535032883	-1.224567647000
H	-2.035903099891	2.472622111755	1.276988165816

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TS25 -802.988189

C	0.306363457420	1.946202583373	0.170674759924
C	0.202473146550	0.437719543742	0.526432209816

C	1.434653716505	-0.132301266935	0.108311406476
C	2.210255416185	0.882235232114	-0.573995205776
C	1.566561532835	2.099137211782	-0.565055835546
H	3.176229766228	0.680080503882	-1.019566616631
O	-0.552732368523	2.796131076139	0.473953048593
C	1.692806048848	-1.528947457053	0.270585256827
H	-0.259770819821	0.155488650506	1.470748624193
H	1.905973202036	3.030106824794	-0.992714523548
O	2.954684748097	-1.928951814395	-0.112715417267
O	0.833961836781	-2.351584305109	0.693607385281
C	3.262300548739	-3.348772729356	0.020967779391
H	4.291975523867	-3.449000314716	-0.318902709540
H	3.163289120343	-3.663142445748	1.062994804344
H	2.587537484906	-3.946724407936	-0.597350392769
C	-2.544093845999	-1.047428211585	2.047234009726
C	-3.020452921004	-0.078726415390	1.225862892027
C	-2.387416868635	0.243312744246	-0.023602784543
H	-3.892364095605	0.509269580345	1.491839162582
H	-3.032005584489	-1.255369317631	2.993017611510
H	-1.677772080595	-1.655631915618	1.794488140914
O	-2.920889192471	1.220616438479	-0.804274467297
C	-2.127491412805	1.334579601065	-1.961668657327
C	-1.095530218488	0.455558327612	-1.905860849532
C	-1.174305241063	-0.237182872949	-0.605320794285
H	-2.443959751842	2.082548488875	-2.665570226101
H	-0.874582006610	-1.273519039109	-0.458650052179
H	-0.319195873270	0.323851380717	-2.640569775519

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TS26 -802.988176

C	0.379573051688	-1.971227860454	0.370845603342
C	0.364746245240	-0.514457737705	0.866788230254
C	-0.995230145918	-0.117923303991	0.832395849626
C	-1.744659712536	-1.107876435579	0.121501444028
C	-0.936255364480	-2.179459068070	-0.235295375642
H	-2.799820288078	-1.007995878397	-0.095998713439
O	1.359346627780	-2.743781166347	0.452380854422
C	-1.500088927173	1.112287229281	1.416535916975
H	1.066875147134	-0.171920141772	1.619302424209
H	-1.228918357342	-3.081932522440	-0.751151936957
O	-2.859577090565	1.262549120374	1.228898693005
O	-0.823310143108	1.957616277127	2.032582681567
C	-3.469583503139	2.456961280304	1.803717023849
H	-4.531153583134	2.370764629444	1.577649432867
H	-3.300842535953	2.488987353384	2.882969534477
H	-3.044085939305	3.355813656177	1.349895165446
C	0.430934220763	2.455153697947	-1.359181151933

C	1.113265565762	1.668019413041	-0.512536589076
C	1.280969256196	0.204704058557	-0.695369452351
H	1.542257991576	2.074972561639	0.397684295968
H	0.299957113190	3.509467456149	-1.142913657626
H	-0.016022348100	2.079822877995	-2.274895511744
O	2.624059022460	-0.242263398255	-0.425588378783
C	2.886555758913	-1.290386650902	-1.253236588401
C	1.870400203896	-1.468493493313	-2.181320750548
C	0.848261810029	-0.559256768369	-1.844532709692
H	3.812791080350	-1.813702507163	-1.088435896201
H	-0.086881377880	-0.410671336228	-2.358037021626
H	1.843054832731	-2.225213777767	-2.946566162384

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TS27 -802.987840

C	1.388030191815	2.017483162808	0.592767071787
C	0.174975574852	2.078900251183	-0.275381745452
C	-0.624106384993	1.036129789112	0.072015479877
C	0.001978858676	0.185257460181	1.103589166437
C	1.270807658948	0.727112401980	1.408795772277
H	-0.561089877108	-0.518431831237	1.695884155822
O	2.316283031678	2.836673607448	0.654465746241
C	-1.945714919607	0.763540927178	-0.537068212449
H	-0.001005747328	2.819153061193	-1.041140449220
H	1.725761734656	0.695002622386	2.391251727553
O	-2.656036473903	-0.150548594714	0.192953126863
O	-2.383120519970	1.285353312965	-1.571226212211
C	-3.966080953655	-0.533881407046	-0.327582205036
H	-4.361161257309	-1.246039119047	0.394187533531
H	-4.612165545908	0.343476846757	-0.409193751719
H	-3.853944288081	-0.993563289637	-1.312927460567
C	-1.004888880474	-2.681357537618	-1.559538377822
C	-0.093550124831	-1.689517959895	-1.553799270629
C	0.889910351293	-1.466204744504	-0.500183713944
H	-0.062398878813	-0.965482667457	-2.363983518752
H	-1.711184292516	-2.779615249581	-2.376498529027
H	-1.072874116902	-3.412547354772	-0.759044618231
O	1.845090481803	-0.492594129046	-0.759433656345
C	2.602529653728	-0.399213577436	0.421039103606
C	2.481158270864	-1.658345885166	1.100943479032
C	1.371554439902	-2.288785521620	0.558089620968
H	3.474209286361	0.236201248908	0.350761564308
H	0.911599460883	-3.208307827492	0.883940773340
H	3.062524737218	-1.962186309798	1.956708811004

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TS28 -802.987349

C	0.239771363149	-0.448614993643	-1.847190744602
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C	0.816539939213	-1.007394840256	-0.502909532568
C	-0.296635600585	-1.806204305227	0.040979703650
C	-1.445592172756	-1.617253827805	-0.773332303271
C	-1.167790575930	-0.818309988839	-1.876739742486
H	-2.404406020064	-2.066816797433	-0.546975130218
O	0.918945255068	0.151903979825	-2.715739372900
C	-0.180275677428	-2.541445679593	1.265118034958
H	1.755079167909	-1.537787587339	-0.669828579125
H	-1.847157381504	-0.539713731887	-2.668933096917
O	-1.330772300551	-3.233239837012	1.611997378991
O	0.844895027163	-2.564116313897	1.992788265568
C	-1.267790381746	-4.026587876717	2.832598813310
H	-2.250102886043	-4.488424037852	2.923187722298
H	-0.486636993789	-4.787417021921	2.754404653262
H	-1.055613641028	-3.389663069180	3.695736205481
C	1.139854439223	0.170075720911	0.585134106697
C	1.401434726761	1.412149006049	-0.117595642582
C	0.610596020217	2.554512849413	0.005597537578
H	2.189676841145	1.439046674226	-0.865514017114
H	1.996369710598	-0.224292081618	1.139811400812
H	0.302941265162	0.246235718419	1.280684538542
O	0.922869242016	3.665309435262	-0.801852721382
C	0.008797184675	4.639222725088	-0.526271619464
C	-0.892306798932	4.208684776122	0.434343236427
C	-0.514512932131	2.885800894341	0.779846228918
H	0.113578909365	5.564194364974	-1.067467660456
H	-0.999569472298	2.236472515352	1.490980173051
H	-1.717002449469	4.776475347487	0.831083037315

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TS29 -802.987151

C	2.097526220806	-1.472052252126	1.807393562775
C	1.263072416323	-0.719355836451	0.717598922589
C	0.939195040890	0.589439202031	1.363598895087
C	1.580751713348	0.621305226588	2.626896618208
C	2.284352669004	-0.551414675395	2.901050295737
H	1.511064526554	1.473755451998	3.291993636883
O	2.451732912813	-2.671122943139	1.670346757814
C	0.092370638788	1.580799103744	0.805128955540
H	1.912431677927	-0.604895419387	-0.158090309961
H	2.811542812968	-0.793332863467	3.812090920171
O	0.032578238723	2.755811031723	1.549947181354
O	-0.609957570506	1.453483716076	-0.241396539498
C	-0.862154774280	3.792115826240	1.062862645293
H	-0.728204121491	4.628157713431	1.748823139448
H	-0.599980671807	4.082246761846	0.041676141506
H	-1.900901152083	3.447468515832	1.075807753114

C	0.015712000171	-1.616603374134	0.315334123018
C	-0.219880335168	-1.563099493353	-1.126478795957
C	-1.347056412067	-1.100838234417	-1.778338764216
H	0.584003752917	-1.928807988985	-1.765548640299
H	0.348414703890	-2.637584034243	0.566550308729
H	-0.852494904544	-1.344055512951	0.915106743954
O	-1.382297926957	-1.211580010805	-3.190991981259
C	-2.554330111042	-0.668903221389	-3.604409471321
C	-3.294590003468	-0.195514940507	-2.526782147798
C	-2.531632916020	-0.460420373327	-1.369829705149
H	-2.741821737540	-0.677001325787	-4.665445705145
H	-2.752033386552	-0.173352814776	-0.355363730959
H	-4.249753339828	0.298140924863	-2.582160438233

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TS30 -802.986889

C	2.077770159460	-1.459262752062	1.751800493426
C	1.117442420524	-0.772673334531	0.722428353695
C	0.829520833881	0.575913388694	1.338563937464
C	1.672159972851	0.698601557520	2.463546584768
C	2.425177955916	-0.456309291168	2.713628565769
H	1.707323619412	1.600388946589	3.063847018817
O	2.379547939953	-2.680246022106	1.654832489675
C	-0.078661064794	1.526804832368	0.836519753193
H	1.721235436029	-0.647141090949	-0.190149593364
H	3.105541034036	-0.616916783239	3.536839431088
O	-0.081473802212	2.737606649465	1.530687225333
O	-0.880718357717	1.368602931729	-0.143861597818
C	-1.023628874889	3.746458834461	1.081983202463
H	-0.823980663999	4.618183466433	1.705229128028
H	-0.867529855556	3.982718270617	0.025657902014
H	-2.055289933223	3.406859672631	1.219045413485
C	-0.091799397330	-1.740982675505	0.438072286285
C	-0.281126787757	-1.785749674144	-1.017661960838
C	-1.296008248094	-1.194013409820	-1.724167919427
H	0.492622802985	-2.291702060930	-1.595336559523
H	0.255293213938	-2.727100664479	0.787520503904
H	-0.973161855366	-1.413912685345	0.988069959597
O	-1.271351184613	-1.269940441427	-3.145921174065
C	-2.316590124735	-0.542463287483	-3.592529251748
C	-3.042196022711	0.014736509871	-2.542452233653
C	-2.398889758504	-0.387474492608	-1.357039306387
H	-2.445973922478	-0.490048869547	-4.661664424627
H	-2.650797735134	-0.117103806107	-0.346398874184
H	-3.906797838094	0.648954440801	-2.633718982173

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TS31 -802.986675

C	-1.522448205578	2.243858287385	0.128443592681
C	-0.721568532077	1.861858052085	1.329975084186
C	-0.496227828245	0.519377481613	1.251893380825
C	-1.023879183293	-0.0511111656639	0.000487891041
C	-1.551286955755	1.003946209402	-0.772619989851
H	-1.170257661320	-1.108056140888	-0.153353164420
O	-2.066796432171	3.332228612016	-0.102623534310
C	0.189987980027	-0.254298993086	2.315144092063
H	-0.423807000255	2.535378704541	2.119655097109
H	-2.372487110186	0.877112763776	-1.467003992024
O	0.179789627283	-1.597820433626	2.052472213839
O	0.708636518629	0.228579600517	3.329732306251
C	0.794583816632	-2.473747312769	3.049393371390
H	0.668128037490	-3.480283764266	2.655752364982
H	1.852199780014	-2.226043078889	3.169530769910
H	0.288420967182	-2.361783163591	4.010952742972
C	-0.220971930426	1.707722784465	-2.091543762369
C	0.130374625382	0.620532883667	-2.909116279223
C	0.822058230448	-0.451076970066	-2.336638825234
H	-0.292900444232	0.502441166231	-3.900286896124
H	-0.776255211338	2.530711381438	-2.533759178677
H	0.480239756093	2.023271289624	-1.315730205791
O	0.928729452916	-1.674792435918	-3.016125935386
C	1.489779839071	-2.581828796441	-2.128976483775
C	1.738006574123	-1.992197587794	-0.919987295215
C	1.301023221833	-0.620483286214	-1.026154628683
H	1.647606563866	-3.575743779215	-2.511215270035
H	1.540920059702	0.176071553805	-0.341295817297
H	2.170614090671	-2.462666592438	-0.053200268708

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TS32 -802.986663

C	-0.517963984716	2.144808166474	0.644252604718
C	0.052689596397	0.723191233408	0.859134551979
C	1.512807443515	0.966414605724	1.116664822137
C	1.748397794469	2.337304363389	1.053312084867
C	0.563618432072	3.060669788026	0.750071930549
H	2.724376424510	2.781739033262	1.206014542670
O	-1.747539133977	2.327993204720	0.336167987072
C	2.449306859914	-0.095224965250	1.351697107299
H	-0.427364787440	0.226490409162	1.707602391585
H	0.477185539920	4.131184128286	0.632727446346
O	3.725907071964	0.348826836800	1.662271081843
O	2.187913791046	-1.323571904500	1.284951972724
C	4.728837990747	-0.677678701355	1.908433033416
H	5.644208842740	-0.132655139151	2.136096628041
H	4.432948938800	-1.309273013644	2.750388487866

H	4.860943816292	-1.307283940441	1.024003987371
C	-0.232165071828	-0.066873519003	-0.439317848558
C	-1.688092849440	-0.238901089369	-0.671859740648
C	-2.208093829595	-1.159466952912	-1.571170913397
H	-2.363986570556	0.403218206091	-0.104644723935
H	0.173119677137	0.537836431570	-1.268933623186
H	0.307389781854	-1.021770168442	-0.449290862006
O	-3.612581973937	-1.255230209114	-1.701785202306
C	-3.868908188210	-2.208320335939	-2.633853071661
C	-2.689402223456	-2.755348302156	-3.124033919792
C	-1.633661571799	-2.092903437497	-2.455571492020
H	-4.905656516721	-2.399252009569	-2.855298845700
H	-0.575259996730	-2.259780409725	-2.581001236907
H	-2.610351472550	-3.529957738400	-3.867906635589

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TS33 -802.986506

C	-1.068085608139	-2.349605031937	-0.432429380437
C	-0.388569325674	-1.137097046528	0.287847449560
C	-1.212588865397	-0.011891129719	-0.038450433925
C	-2.216119243898	-0.434554716763	-0.985221548640
C	-2.141912888594	-1.786118997865	-1.246680292289
H	-2.938048885724	0.251798974463	-1.409925610947
O	-0.681964470137	-3.528067133740	-0.304800590626
C	-1.029079686849	1.284711943593	0.531712240629
H	-0.046088721510	-1.283142447103	1.312448739816
H	-2.765191036661	-2.368255746597	-1.908037634674
O	-1.966621385685	2.216186735572	0.117425892003
O	-0.101598074288	1.593555730720	1.324322256249
C	-1.827336883892	3.562844013554	0.655703516084
H	-2.657465532326	4.125387101402	0.230345133567
H	-1.887016719875	3.547544336390	1.747147254668
H	-0.869360493079	3.997826706483	0.357933668614
C	2.723139125843	-0.617016897742	2.151144034384
C	2.482524852702	0.318183375660	1.204435275527
C	1.890013530444	-0.007369329146	-0.065009511485
H	2.698957306070	1.365464076260	1.374531760237
H	3.146929082688	-0.338774110923	3.108943472702
H	2.507425009810	-1.670994984145	1.998841658240
O	1.814650660687	0.948934234849	-1.020168528925
C	1.295530892563	0.359164025785	-2.202808392442
C	1.040884209694	-0.951197321189	-1.991315137247
C	1.259941233348	-1.206580413199	-0.551059692942
H	1.214597683291	1.024674376624	-3.043051551334
H	1.561519155717	-2.185085433996	-0.193062575336
H	0.651364007376	-1.660247299227	-2.701673381950

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TS34 -802.986207

C	-1.304274030275	1.267540705932	0.770220505670
C	-0.195810308975	2.125960531800	0.197591254980
C	0.364840728794	1.452292821014	-0.828680503253
C	-0.256665068591	0.071442443230	-0.965684511055
C	-1.274505054997	0.000792246011	0.010688545889
H	-0.355817835792	-0.371826339032	-1.948401320453
O	-2.083034430636	1.611633433469	1.681556505895
C	1.437752827949	1.990678673988	-1.689785634541
H	0.060600799902	3.114325443007	0.553044929737
H	-2.088227483958	-0.707836216286	0.034541366305
O	1.741112207821	1.135904228666	-2.721383255093
O	2.001556313602	3.082229251638	-1.538814657319
C	2.762940607132	1.582452312128	-3.669192874769
H	2.830270486660	0.787511794856	-4.409174600758
H	2.459124668202	2.524380157148	-4.131416089192
H	3.716561866465	1.724407704041	-3.155341429576
C	1.337298451360	-1.088549560591	-0.487355817312
C	0.818273781907	-2.324769312009	-0.067410923184
C	0.037655851424	-2.363863711089	1.088607324491
H	0.831279587064	-3.192025870577	-0.718740451773
H	1.918690303713	-1.052270300196	-1.403880075159
H	1.667721823395	-0.381164683976	0.271593739050
O	-0.751352677360	-3.486867755676	1.387880812679
C	-1.577522906564	-3.127702516921	2.442209695637
C	-1.356186932641	-1.832220360903	2.823780304557
C	-0.329722684921	-1.314822435578	1.952559949913
H	-2.244683703460	-3.894255498621	2.797830242255
H	0.225936642776	-0.404926294533	2.110273121170
H	-1.860075963679	-1.296238135324	3.610145082085

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TS35 -802.984935

C	0.295816172188	1.173243148169	-1.523891828858
C	1.345084866381	0.519811707117	-0.732306316327
C	0.985623893133	0.642805666506	0.617563784674
C	-0.362373090597	1.013264017346	0.757270929301
C	-0.942877701473	1.159001304987	-0.588561626901
H	-0.859545050447	1.238474275882	1.688109828273
O	0.331970937294	1.604202582875	-2.687885226707
C	1.895902143948	0.296508405860	1.730857070176
H	2.315424173356	0.231024668469	-1.109376751581
H	-1.687692416084	1.936973132362	-0.740130202121
O	1.355327251382	0.596447567415	2.953634660505
O	3.017146255552	-0.212771787542	1.600816454635
C	2.180460529523	0.316567561834	4.128150827455
H	1.596514829512	0.670437005869	4.975402263623

H	2.374703505283	-0.756058787107	4.205651639654
H	3.131308991269	0.849689243446	4.056111306413
C	-2.235621730341	-0.107187328035	-3.518097092620
C	-2.573637242975	-0.070563317910	-2.221016434237
C	-1.631186616609	-0.282480078693	-1.076727484148
H	-3.590814087619	0.158125673818	-1.913681668265
H	-2.973552518353	0.096887542654	-4.286233934229
H	-1.222672964522	-0.303113065896	-3.854443092799
O	-2.389774484551	-0.692016009036	0.114036842817
C	-1.490828178870	-1.424649104659	0.853932636975
C	-0.458401346578	-1.930899333528	0.066202615114
C	-0.514991809607	-1.279138986224	-1.172823586134
H	-1.786020656058	-1.671623529303	1.861530013649
H	-0.010101295791	-1.552573616265	-2.085511161395
H	0.287868073602	-2.636974168825	0.393060921920

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TS36 -802.984835

C	-1.301144227589	-0.531172213107	-1.752372709302
C	-1.074036240880	-0.067755499766	-0.287896536638
C	-0.146333125414	-1.103090428109	0.287153626324
C	0.079558103735	-2.055343860792	-0.713068246844
C	-0.579582325696	-1.738331917191	-1.924783705649
H	0.669954242714	-2.948674295460	-0.546550744262
O	-1.954806363413	0.195094531392	-2.576393708331
C	0.143879284486	-1.224978254832	1.681020633690
H	-2.028916984122	-0.031722411542	0.249350508305
H	-0.547622720288	-2.307271320179	-2.842218552371
O	0.972669538199	-2.301257162968	1.980862378559
O	-0.278995267038	-0.468830560381	2.596281957544
C	1.262498878619	-2.523012122343	3.389443914601
H	1.908607577091	-3.400232974956	3.411790061591
H	1.770210686408	-1.656208249558	3.821922084986
H	0.340307186075	-2.705780338952	3.947951024694
C	0.520332976730	1.468139965371	-3.368551944675
C	1.295784601738	1.534675775936	-2.253729265818
C	0.769408103627	1.636362797923	-0.925439167599
H	2.377551064072	1.586906875328	-2.323551503323
H	0.995002324500	1.428046058743	-4.344070880992
H	-0.567236648650	1.417616859214	-3.327856401292
O	1.625447931406	2.025494554896	0.014776929079
C	0.917488945054	2.232252905270	1.255012598561
C	-0.380686968401	1.958701671392	1.075160368803
C	-0.587279773743	1.450410922345	-0.326982519249
H	1.540329959037	2.515006551228	2.082911440230
H	-1.361598731160	1.952450351035	-0.923416075675
H	-1.139050612489	1.957582291020	1.838919344880

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TS37 -802.984828

C	-0.135964741671	0.156668873108	-1.679966395267
C	-1.283723914987	0.032652778577	-0.863384793735
C	-1.013130102602	-0.942883180004	0.167103054240
C	0.312911575995	-1.305593857508	0.170088827220
C	1.014117996886	-0.504967778840	-0.862902184837
H	0.778368520866	-2.009656238626	0.843293892919
O	0.068627561939	0.881202869235	-2.715919702264
C	-2.052801287314	-1.435124769370	1.095756757068
H	-2.248487649867	0.477770446225	-1.060111105118
H	1.807016270977	-0.993823056105	-1.426549044061
O	-1.575039061230	-2.386590871631	1.961166254652
O	-3.227974448472	-1.043773039502	1.117324813210
C	-2.531954163634	-2.957630659692	2.907243891385
H	-1.963215295693	-3.689590336163	3.477452391092
H	-2.931710970309	-2.177028296969	3.559306502370
H	-3.355951498552	-3.433379320345	2.370055887597
C	2.469891109108	0.363618785633	2.142986826981
C	2.697914016327	0.543820611136	0.833693295930
C	1.632738277301	0.828070182126	-0.188979651907
H	3.700119983631	0.463127007751	0.420482680549
H	3.282469127488	0.127750224759	2.821551211117
H	1.475697549233	0.431725922396	2.575482914575
O	2.279246523813	1.525332287693	-1.334277505085
C	1.424093953818	2.496962115477	-1.742090858942
C	0.475232732835	2.808627342945	-0.751459956092
C	0.502048795023	1.773183802255	0.170735896196
H	1.667015829777	3.000690482997	-2.662915150645
H	-0.083475907900	1.681278666945	1.071566366452
H	-0.243754980016	3.608198158344	-0.807833072238

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TS38 -802.983866

C	0.519480112795	1.948856564619	2.175614384352
C	0.055309007245	1.060016008194	0.987398101669
C	0.943596829131	-0.179612671078	1.078842562086
C	1.793664605910	0.008330163322	2.187066507570
C	1.580977303902	1.233464931418	2.832937410903
H	2.505035008900	-0.742852898292	2.508677227656
O	0.034765866280	3.092732501559	2.386728676720
C	0.697706506431	-1.415660897186	0.416574343780
H	-1.007067534385	0.810956166408	1.086959203075
H	2.084754977290	1.589018947030	3.720350413107
O	1.572649491628	-2.431036201183	0.799439997592
O	-0.207417913284	-1.655874508805	-0.437850671390
C	1.374855997616	-3.728794877584	0.175047760947

H	2.146022198381	-4.369580507112	0.602192916267
H	0.378868436242	-4.119905034388	0.400037532781
H	1.488914945415	-3.658109041731	-0.910742763046
C	0.280734137643	1.932392551126	-0.292623814311
C	0.235296651778	0.995190024180	-1.437340241184
C	-0.932358675611	0.569907009540	-2.036299919230
H	1.164787592368	0.568138844324	-1.804288609484
H	1.266335326879	2.397325639687	-0.225045710888
H	-0.481173839499	2.717088798634	-0.322589098972
O	-0.856224736176	-0.400826203506	-3.053709884922
C	-2.119395304539	-0.761667723156	-3.355131896107
C	-3.045022180858	-0.045449395870	-2.595761065283
C	-2.295582876792	0.805238336637	-1.762560370748
H	-2.239650718192	-1.517549438242	-4.113383406204
H	-2.668713342756	1.493067741339	-1.019820579313
H	-4.115815320102	-0.148048116353	-2.641237838339

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TS39 -802.983388

C	1.437760791173	-1.040773272370	0.703197174330
C	0.825104726124	0.190749593087	1.185020971238
C	0.735081329749	1.071015901370	0.091817338150
C	0.947066931875	0.407292054374	-1.121533145133
C	1.184062534154	-1.022375757055	-0.834911107971
H	0.978227351766	0.878576352497	-2.092914822312
O	1.999850356488	-1.955991024590	1.332636787011
C	0.373872075638	2.499098291128	0.229739885358
H	0.690653488185	0.450267040237	2.224547764961
H	1.925466135149	-1.532907429923	-1.449005541818
O	0.473504122323	3.177322421127	-0.958460880024
O	0.016145599606	3.044120264233	1.281822149997
C	0.149184140852	4.602217578483	-0.933217507086
H	0.296605597607	4.944975708071	-1.955544815209
H	-0.885979164450	4.748970393517	-0.614758044782
H	0.814211195085	5.128344876139	-0.244250682406
C	-1.954351532105	0.527164458297	-1.086207794147
C	-1.972583903495	-0.262571780107	0.035086327788
C	-1.152392805692	-1.408195454704	0.121326396556
H	-2.542250473622	0.020306253940	0.913293329232
H	-2.477468830092	1.477289137281	-1.104293493544
H	-1.510320220591	0.201921329322	-2.019265381531
O	-1.369980241922	-2.376577637187	1.083715774463
C	-0.644880744761	-3.526674167381	0.689983275547
C	-0.001070512006	-3.340466067268	-0.473646235243
C	-0.206502817325	-1.915094920247	-0.918710878781
H	-0.706271116833	-4.354191183231	1.374898805985
H	-0.563658159643	-1.813495573327	-1.944822361998

H	0.641364032036	-4.053428483301	-0.963733446324
29			
TS40 -802.982398			
C	-0.400404661418	0.891864288538	-1.677727023618
C	0.201614935246	0.596894344199	-0.278759957334
C	1.302445166595	-0.283449061704	-0.536779216549
C	1.229840803676	-0.704697183419	-1.906127654839
C	0.201007714503	-0.068592431089	-2.584592066716
H	1.923666903521	-1.416581242248	-2.334773409329
O	-1.244099277074	1.794180429999	-1.904355016083
C	2.300948687698	-0.667186296240	0.425121818970
H	0.260886532435	1.395965563100	0.454137590497
H	-0.055494882064	-0.165591147938	-3.628822393505
O	3.297985329576	-1.455031268691	-0.126282129958
O	2.312203459761	-0.359842607997	1.639834542574
C	4.370174457974	-1.872155602377	0.769210171338
H	5.040385805149	-2.467320905544	0.150670922550
H	4.886997857921	-0.999841010042	1.177222309008
H	3.971106653727	-2.466897026081	1.595288969156
C	-3.483025997768	0.515992021223	-1.552676705136
C	-3.423052266548	0.818382663586	-0.227728171992
C	-2.406323838776	0.337156987172	0.645870958707
H	-4.149470316784	1.489696812356	0.218028978707
H	-4.258265772860	0.941412160706	-2.179434742255
H	-2.802271888607	-0.179696697035	-2.029064121913
O	-2.514752687688	0.674365100821	1.967734971228
C	-1.498544927765	-0.006090041695	2.676868902189
C	-0.739878776606	-0.729274330257	1.825960733357
C	-1.214990596374	-0.451210349731	0.448415558217
H	-1.481534503967	0.166188279736	3.737872031813
H	-1.212923341397	-1.209814104639	-0.330664190918
H	0.136079567651	-1.299459524561	2.082868866714

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TS41 -802.978342

C	-0.240403041186	-0.556346275210	1.799664181460
C	0.518473529711	-1.179196917973	0.784335174298
C	-0.268861005685	-1.205996095281	-0.427716507382
C	-1.408392923290	-0.456683832714	-0.283412766701
C	-1.359164073009	0.222303123664	1.040517425683
H	-2.166116753294	-0.313290884767	-1.039648571822
O	0.028116189006	-0.397892255412	3.036711739598
C	0.146191422588	-1.946061799718	-1.637051986685
H	1.464375889176	-1.681833561555	0.923378599592
H	-2.309183310298	0.344715496190	1.560716505049
O	-0.756661387056	-1.821849205851	-2.664080728560
O	1.188363533022	-2.606127883438	-1.741666813948

C	-0.439503443724	-2.528278293119	-3.903699404422
H	-1.269133996277	-2.311947090615	-4.574147080364
H	0.503999642151	-2.161698807711	-4.315799355682
H	-0.355655305195	-3.601497841065	-3.716311868430
C	1.533503109313	1.374050811230	3.063754921785
C	1.845214089731	1.410939448370	1.720154841553
C	0.846056191477	1.501029558660	0.736981013361
H	2.858412905752	1.236776810207	1.375003857659
H	2.297113035694	1.135423326272	3.795270292681
H	0.591867561549	1.733250738099	3.455620329585
O	1.193865246536	1.766764207435	-0.581058509574
C	0.056652939745	2.349542835912	-1.204732876564
C	-1.003651486427	2.398341602599	-0.386157139101
C	-0.646229761254	1.683185211121	0.898779181758
H	0.220369406879	2.663590409947	-2.221459912002
H	-0.895944747569	2.229034016524	1.810432454293
H	-1.982146315547	2.780506124126	-0.629048360769

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TS42 -802.978105

C	-0.182800349480	-2.059832141035	-1.144579903896
C	-0.888897733946	-0.693237156274	-1.178224431177
C	0.133206515137	0.256578442245	-1.377376154867
C	1.439777230011	-0.425397731905	-1.328900935547
C	1.273143486966	-1.770360580669	-1.202081525765
H	2.380638491927	0.106111708064	-1.379433871902
O	-0.758549738142	-3.156654340881	-1.089424340165
C	-0.170257657491	1.622501653381	-1.256438352063
H	-1.881926813318	-0.611590194086	-1.602824155111
H	2.034537088669	-2.531021493621	-1.121516606687
O	0.878863853224	2.511998370027	-1.299738619659
O	-1.364746237139	2.011559439743	-0.990313759138
C	0.552750364379	3.929514581560	-1.186948784572
H	1.500966074557	4.447677391786	-1.319591118235
H	-0.161770400546	4.220696532595	-1.961322411908
H	0.125517980799	4.150444009504	-0.205059517077
C	-2.219130312651	0.853602909854	0.634597152533
C	-1.523781228433	-0.364470340716	0.738444206615
C	-0.321576972117	-0.416329701434	1.575455351675
H	-2.096733306059	-1.288350307273	0.681031554451
H	-3.193889131718	0.887315869704	0.163918971227
H	-1.936028436610	1.719537961303	1.220153698428
O	0.062636746264	-1.662038692116	2.053689722223
C	1.261969466898	-1.492476334394	2.730259941950
C	1.637970198087	-0.176207688775	2.684299995940
C	0.619789459706	0.520106720162	1.934187973283
H	1.687217265153	-2.377154827466	3.169998808105

H	0.604154090952	1.569485670760	1.684897738027
H	2.526036604941	0.250263583318	3.121174986373

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TS43 -802.977632

C	-0.817814403965	1.748526988374	0.081636556960
C	-0.147492693628	0.514326530825	-0.593649729331
C	-1.179879335688	-0.552081826397	-0.457111787682
C	-2.193543048044	-0.074932943479	0.393474863217
C	-1.966643228294	1.254060119154	0.790110102544
H	-3.045352072826	-0.674254846339	0.692198916399
O	-0.430244776539	2.940249442743	-0.114867975284
C	-0.966624094618	-1.845196900892	-1.009290598376
H	0.123848377660	0.724437940678	-1.629880449412
H	-2.618726315721	1.867112292147	1.394451175795
O	-2.004170529682	-2.741854026905	-0.804921862260
O	0.088132115859	-2.191654715690	-1.615806915202
C	-1.841778590620	-4.066917513672	-1.388631315183
H	-2.762814899311	-4.597120638905	-1.149272645445
H	-1.704746822908	-3.994199683049	-2.470721815557
H	-0.975580206471	-4.575887568598	-0.956721926569
C	2.133621473493	2.853633826133	-1.011010491226
C	2.594423549206	2.317512948442	0.152755050231
C	2.100194905895	1.096962507070	0.680390923824
H	3.249439831300	2.884396401266	0.804408176789
H	2.429198842077	3.854035830678	-1.307182472292
H	1.462043318054	2.332188670402	-1.677471810672
O	2.428753208881	0.840852842126	1.962954555053
C	1.746760742871	-0.346582864077	2.386426957559
C	0.999559087014	-0.823423779697	1.386080047662
C	1.193754511549	0.034782450366	0.154375580694
H	1.931020867737	-0.628665737923	3.407278689759
H	1.682404910836	-0.583123792623	-0.618849911456
H	0.366425409164	-1.694071677410	1.415971640117

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TS44 -802.977395

C	1.478915482564	-1.421621987399	0.695941472664
C	0.468667148695	-1.425948387708	-0.362661427861
C	0.194721098024	-0.122455827151	-0.843590359620
C	1.282815507694	0.824630016469	-0.275582122712
C	1.894627429682	-0.028855013050	0.760943104624
H	1.980261421171	1.178661601501	-1.038104886448
O	1.877510027086	-2.395586462571	1.400272356124
C	-0.381929200395	0.033757415569	-2.208539974614
H	-0.044787916707	-2.318526580574	-0.699237877855
H	2.587689322739	0.342921799726	1.508693674432
O	-0.153136764791	1.292690287120	-2.716502436363

O	-1.020190854925	-0.824160431885	-2.825977031529
C	-0.690099133297	1.572985839363	-4.049928229721
H	-0.416222201953	2.606012086389	-4.254720533119
H	-0.244786802159	0.895300759426	-4.781582927968
H	-1.774975223149	1.444277270866	-4.054040392659
C	0.314736315546	1.961096871621	0.232470556831
C	-0.877173550205	1.025851088572	0.244948076817
C	-1.115147373086	0.346496883410	1.488672945304
H	-1.742264904570	1.243169544784	-0.375660368847
H	0.218272164089	2.732812663505	-0.529476058676
H	0.585343561919	2.410847023764	1.186827329347
O	-2.063732480482	-0.673402916927	1.500982703471
C	-1.912132183928	-1.357072934403	2.695194339852
C	-0.904377654811	-0.800817322531	3.438588451246
C	-0.381390970562	0.292247228350	2.664786077528
H	-2.583488583660	-2.182152504342	2.857220060454
H	0.398046815816	0.973266276773	2.963276626770
H	-0.558136239587	-1.138888294900	4.400280559989

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TS45 -802.977030

C	-1.481580930333	-1.229208987405	-1.211444710913
C	-0.551995088114	-0.026796387709	-0.823816255976
C	-1.084790833061	0.445656693935	0.418274715659
C	-2.115746230601	-0.470684121324	0.866271798914
C	-2.355416622092	-1.456871109429	-0.056952731141
H	-2.626719051285	-0.348594879515	1.812919523765
O	-1.467386806595	-1.800767922528	-2.314888883000
C	-0.615567392874	1.616620061807	1.078423172553
H	-0.313325400578	0.667920730191	-1.630005960236
H	-3.066348658092	-2.266528183852	0.005253672530
O	-1.264364157866	1.887085627825	2.272518386146
O	0.327289552537	2.349488884285	0.666387140838
C	-0.851729474503	3.089854639915	2.983495648379
H	-1.505172150960	3.143029076688	3.853294767961
H	0.195576206246	3.016887696281	3.289597289499
H	-0.974994282315	3.971712472256	2.349375995623
C	1.066715542540	-1.675534037950	1.726793821127
C	1.009864475339	-1.876962546753	0.400969342371
C	1.119039190018	-0.781504768382	-0.601071571179
H	0.827340131724	-2.861520352117	-0.018215185667
H	0.933128324198	-2.501186316755	2.416420665004
H	1.226208153714	-0.693790547082	2.162816217076
O	1.383920373448	-1.295578287959	-1.930394516867
C	2.161060059441	-0.403060395288	-2.572237479237
C	2.583571347136	0.616029032502	-1.718074127187
C	1.999633096953	0.361514488507	-0.468699179575



H	2.348518753933	-0.589946745651	-3.617481991490
H	2.114098006831	0.947620634611	0.427560496606
H	3.228827583599	1.437468677883	-1.979659983432

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TS46 -802.976049

C	-0.025747864060	-0.847663291053	-0.593315804961
C	1.028012395323	-0.996448883219	0.386930373668
C	0.420730463713	-1.046569648244	1.644041770997
C	-0.992731319763	-0.883801580530	1.564373253003
C	-1.323980201170	-0.594458716601	0.216181801556
H	-1.666803154523	-0.928230751935	2.405979848324
O	0.040017336647	-0.872887157298	-1.851517240456
C	1.184155807176	-1.279203962715	2.893231616939
H	2.079123009862	-1.121886978103	0.176012657526
H	-2.286169181301	-0.828061933350	-0.225301651159
O	0.372201233607	-1.316865670309	3.997726281068
O	2.411994023928	-1.423269927488	2.963459246683
C	1.022713873932	-1.556765580628	5.284593909274
H	0.217943949713	-1.541390315395	6.016903665262
H	1.527026536985	-2.526104558518	5.276329954930
H	1.755729434996	-0.772579972250	5.489367204607
C	-1.305793372830	1.328701741111	0.067151017112
C	-1.702191512523	1.720446363359	-1.233997580810
C	-0.853357116863	1.765712701994	-2.349070159318
H	-2.753442852065	1.914751038100	-1.428634018152
H	-2.012504812043	1.563524325498	0.856157959504
H	-0.260198568283	1.473860185662	0.345768587204
O	-1.437767210885	2.044916090836	-3.598046835231
C	-0.430345283139	2.010920245555	-4.534048888992
C	0.777138190298	1.725289566338	-3.940914323015
C	0.518844607039	1.553516791323	-2.546434003322
H	-0.720128036098	2.204460982840	-5.552672330557
H	1.246439090773	1.350515159010	-1.779234287336
H	1.726591401766	1.626367814599	-4.439166605517

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TS47 -802.975973

C	-2.131920192707	-0.042738924588	-0.596408421532
C	-0.726097535110	-0.144963440738	0.093980640390
C	-0.435992766027	1.269061933286	0.459821550284
C	-1.422558697630	2.091366918028	-0.116292262974
C	-2.398074947615	1.349983379295	-0.798560796011
H	-1.423827531149	3.168834198724	-0.003896953142
O	-2.837925128018	-1.052655495790	-0.883490611145
C	0.618903606481	1.652616980991	1.339486459110
H	-0.710485186885	-0.843844086689	0.930641895103
H	-3.270906340746	1.733695128261	-1.305026930996

O	0.650801334846	3.017673791797	1.608145119222
O	1.475206556986	0.875193920204	1.837691690486
C	1.675333640155	3.470598411038	2.537617267177
H	1.501202954017	4.539827346502	2.653957009873
H	1.579867385334	2.955205561141	3.497035464674
H	2.674528201882	3.282823942623	2.134092701580
C	-1.436369390549	-3.391009366993	-1.641937213290
C	-0.187314828771	-3.352496300540	-1.107765278197
C	0.599969099162	-2.165846119662	-0.972651812710
H	0.311064512713	-4.264291323142	-0.793104784570
H	-1.963652459369	-4.337940185036	-1.704108129533
H	-1.964629131014	-2.503583293665	-1.971941503142
O	1.899774172165	-2.373939575511	-0.699109890838
C	2.586880721435	-1.116733213718	-0.693693272071
C	1.712231724811	-0.129152340377	-0.913520316410
C	0.325787338083	-0.704204402976	-1.048590990903
H	3.637938039629	-1.177671406890	-0.480426144820
H	-0.159094764603	-0.418524126482	-1.991518823355
H	1.927708730524	0.924803958292	-0.937884037185

29

TS48 -802.975711

C	1.536549700460	1.620910529105	0.426060456978
C	1.110044007605	0.147807925695	0.136208345335
C	-0.043874679257	-0.079225241066	1.092504845518
C	-0.176321757979	1.081870121409	1.880390322456
C	0.717607176931	2.090595694651	1.505507099737
H	-0.893285696181	1.155091916447	2.689490184335
O	2.463979290560	2.197058546907	-0.210302159219
C	-0.667650401430	-1.328373503589	1.274372523178
H	1.962377247497	-0.497830029608	0.382295649230
H	0.817356839279	3.066932119335	1.956033768920
O	-1.613455216716	-1.363397740040	2.294546205479
O	-0.458883684809	-2.364032018330	0.563530786018
C	-2.247759032487	-2.646269592235	2.551945556080
H	-2.935738443639	-2.461962440113	3.376684938181
H	-2.789758123284	-3.000132758451	1.669868856104
H	-1.502765559010	-3.396623981023	2.830094673482
C	-2.119239976793	-1.458380647752	-1.430795247424
C	-1.869847296735	-0.129609168421	-1.577435405191
C	-0.547832954551	0.372944629095	-1.801588409411
H	-2.675939480298	0.591095937353	-1.667884409532
H	-3.142011050095	-1.808518557977	-1.337922254117
H	-1.334559914114	-2.203184798399	-1.392405797955
O	-0.423436194378	1.433219670207	-2.590719287544
C	0.975630917637	1.614450149050	-2.932779239316
C	1.713373940533	0.698447181641	-2.293851628929

C	0.810437239746	-0.121588456895	-1.397931456549
H	1.166893933208	2.452884982078	-3.576073239195
H	0.877930029837	-1.207288275726	-1.526573048618
H	2.786145639631	0.621659886735	-2.317328249868

29

TS49 -802.975429

C	-1.226909874229	1.703890933739	1.252593240385
C	-0.270714416862	0.863859405425	0.314059910380
C	0.138535187374	-0.296114999735	1.210068753550
C	-0.497147520168	-0.115678518488	2.462375610044
C	-1.312281342810	1.011511519506	2.503291067862
H	-0.322060482106	-0.785353117302	3.295727301729
O	-1.803738450827	2.768942884710	0.894149874999
C	1.248792527258	-1.145290852928	1.003081486748
H	0.592279701611	1.477873965104	0.029463328285
H	-1.898904156393	1.362049509626	3.339158675771
O	1.558408678214	-1.949901469630	2.100574007854
O	1.923273269409	-1.270476186795	-0.071415883563
C	2.695159917301	-2.844428590848	1.953888318338
H	2.797381005182	-3.332089899332	2.923078196333
H	2.513125314270	-3.584904499876	1.168573308615
H	3.600124308821	-2.284525743712	1.704566046706
C	0.051266180743	-2.403213789018	-1.319639315598
C	0.088994625747	-1.478016230856	-2.318466916442
C	-0.392037604275	-0.160246495473	-2.135817172967
H	0.570369142567	-1.686627584306	-3.266219128219
H	0.486904862543	-3.385502134653	-1.463738568026
H	-0.454280274725	-2.210080035736	-0.376863149371
O	-0.288207403262	0.647034213105	-3.193308544616
C	-0.969087953099	1.892811710821	-2.915636059731
C	-1.492236620726	1.856870675943	-1.688500615111
C	-1.102596012021	0.553294113477	-1.006128104456
H	-0.930170655857	2.605038226165	-3.719761663589
H	-1.971107127849	-0.037835948345	-0.688236323694
H	-2.012776930004	2.640050768492	-1.158198402812

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TS50 -802.975102

C	-0.166381526113	-2.096623580989	0.222000004695
C	-0.557502532543	-0.580678846139	0.217852670352
C	0.299467367750	0.026751595181	1.185884115051
C	1.209902619192	-0.978218339434	1.684743260853
C	0.950829427601	-2.222415799936	1.147422884036
H	1.972567116659	-0.755655420291	2.420676176107
O	-0.711467988254	-2.957371880881	-0.501664781136
C	0.119128778971	1.365699929260	1.674056311977
H	-1.616310907219	-0.322291166872	0.216997132704

H	1.477560186911	-3.145723766508	1.332871605316
O	1.041828378329	1.705903813507	2.654385459204
O	-0.759431101306	2.174916702377	1.296877597635
C	0.917344705630	3.039539925864	3.226781853694
H	1.712261351199	3.106832579005	3.968479136026
H	1.040978632933	3.801671652772	2.452562895723
H	-0.062674558015	3.165956084249	3.694690962678
C	1.814853832879	-1.206142729233	-2.647881786834
C	1.320088193222	-0.385238877573	-1.709290103096
C	-0.129508945890	-0.101597472555	-1.517599254661
H	1.967664464331	0.120515078393	-0.997516148987
H	2.881287183212	-1.394342734513	-2.706918206592
H	1.183036741144	-1.721657414124	-3.364274252126
O	-0.396555386434	1.323588897928	-1.472634003404
C	-1.615407993338	1.533744420781	-1.994478723179
C	-2.151251235443	0.356519474024	-2.528531906313
C	-1.212834849168	-0.657311117570	-2.292573662644
H	-2.008071035439	2.534498448151	-1.917095407459
H	-1.310677019010	-1.710714687948	-2.504336619340
H	-3.113082755548	0.259779688621	-3.003662797730

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TS51 -802.974918

C	0.996495136707	-0.897574559650	-1.899498830538
C	0.264762307934	0.120391485452	-0.943621971843
C	-0.951028233092	-0.641764073882	-0.481496431282
C	-0.863488306363	-1.942993494689	-1.026892275979
C	0.286031520210	-2.142578704559	-1.793215246431
H	-1.629839275830	-2.689517553579	-0.857986438409
O	2.012693360215	-0.589021257573	-2.571987294548
C	-2.057031917764	-0.169672908343	0.285529394632
H	0.031774726009	1.057686805799	-1.456916640975
H	0.567220006745	-3.042213737033	-2.319985132852
O	-3.140574496264	-1.043066123034	0.257625625220
O	-2.135922360333	0.891036662773	0.976403339837
C	-4.303562901797	-0.668755452501	1.047531880916
H	-5.025277707338	-1.468515733489	0.883687960325
H	-4.047250235263	-0.590246113521	2.108337697749
H	-4.704864533629	0.290106541560	0.710394691354
C	3.775876674366	1.186710417280	0.151799711396
C	2.562328835285	1.217559620773	-0.417660219391
C	1.363600332229	0.510804659020	0.154549152792
H	2.390475261037	1.765540951897	-1.336427531536
H	4.609254378116	1.716789897872	-0.295628413484
H	3.984265043930	0.625087962272	1.059276972899
O	0.612983966323	1.491515291257	1.045524827152
C	0.202716193560	0.836674140954	2.096940365606

C	0.786985254495	-0.471013998620	2.193860010896
C	1.566262979752	-0.637019333091	1.077752409516
H	-0.468270332667	1.344032619103	2.773158631497
H	2.154948773097	-1.499191180732	0.800703128732
H	0.619769889906	-1.164029728696	3.001100956857

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TS52 -802.974739

C	-1.098542498171	1.660546172388	0.425268511746
C	0.135238923665	0.857721556193	-0.058598960036
C	-0.332224108024	0.102076256846	-1.182732232248
C	-1.749211887769	0.259391514974	-1.274078661925
C	-2.225014348818	1.151682201350	-0.318349947554
H	-2.349766176083	-0.240670930512	-2.023300954984
O	-1.051387379202	2.513571276476	1.355298701507
C	0.544607032958	-0.576639581721	-2.106220283973
H	1.101045316387	1.347676143447	-0.106091169980
H	-3.248503418703	1.453354708805	-0.155526952161
O	-0.144789280335	-1.206495892868	-3.129663827639
O	1.791841480092	-0.613359403517	-2.038351091232
C	0.662639757789	-1.886598323927	-4.134538664499
H	-0.052668908172	-2.281957534579	-4.854439854241
H	1.349819622309	-1.183893710376	-4.612827302188
H	1.241951789233	-2.693181946826	-3.677002687282
C	1.717389278061	-2.307147041874	0.865883201478
C	0.548878255360	-1.653275616788	0.918068213967
C	0.373693748333	-0.277961096088	1.452767701860
H	-0.363419189702	-2.087271230029	0.518942710730
H	1.779881281769	-3.289324466646	0.411665074292
H	2.643526384887	-1.881429748140	1.238813091165
O	-0.872798764243	-0.170530799908	2.194733063057
C	-0.695644542515	0.748145552196	3.166778773176
C	0.657865375936	1.115560833583	3.270928216412
C	1.334071512113	0.450889981566	2.256529106279
H	-1.563585039836	1.035743485073	3.735180128585
H	2.381975278651	0.528915630373	2.010661248346
H	1.058676587469	1.822788298806	3.976987023188

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TS53 -802.973631

C	-0.605994315702	1.824158592968	0.786238488117
C	-0.689813308139	0.423004296356	0.060013323420
C	-0.306088428925	-0.554405266856	1.168622561896
C	-0.220312628898	0.179781453818	2.364042679368
C	-0.388888317054	1.555035060539	2.173160951938
H	-0.026325273933	-0.295857302039	3.317673152418
O	-0.733146894831	2.931331468290	0.187955465072
C	-0.128222120875	-1.955339281648	1.034998494194

H	-1.727175815400	0.281945948362	-0.266929249780
H	-0.351913016895	2.324044978894	2.930266199301
O	0.055253391816	-2.611877038310	2.248213459677
O	-0.075630702131	-2.611752981689	-0.049274528806
C	0.268722097882	-4.049799062996	2.183567050416
H	0.381962235962	-4.365037454713	3.220541625253
H	-0.587479049620	-4.545695619552	1.718871719353
H	1.167729991660	-4.285081560572	1.606570480177
C	-0.711008370280	-0.356648676377	-3.495612497395
C	-0.309302939789	-0.677664753521	-2.257720041916
C	0.201789490269	0.315748030574	-1.235803689660
H	-0.350138730759	-1.685843206670	-1.852857221823
H	-1.088357390747	-1.132664092277	-4.153380909991
H	-0.703236816000	0.658215719678	-3.878862497256
O	0.257206380950	1.676320515544	-1.888944188759
C	1.426628242179	2.196277427612	-1.658673730461
C	2.324735882978	1.296129750427	-1.006262943937
C	1.623713127838	0.133524817370	-0.805565519819
H	1.590960184321	3.211001766416	-1.993680188416
H	1.964842031941	-0.795760083401	-0.372938596974
H	3.348087563802	1.513792473714	-0.751681615061

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TS54 -802.972466

C	-1.362323387848	0.463366114753	-0.134739245769
C	-0.153834207969	0.861775733458	0.568071062524
C	1.086242652231	0.530884173981	-0.187912381365
C	0.536976875209	-0.436454097548	-1.256767134381
C	-0.863633835564	-0.309178853414	-1.278941717208
H	1.106600709346	-0.650597030092	-2.155513428699
O	-2.566413017370	0.685525713389	0.186290155443
C	1.766305661148	1.796183562147	-0.680213544602
H	-0.153387620807	1.437004665802	1.486970135728
H	-1.524693534232	-0.769402263401	-2.003153037237
O	1.304522367598	2.203187810055	-1.893893224402
O	2.639119000228	2.396391186449	-0.042907247181
C	1.817791021584	3.473358281581	-2.413148020200
H	1.313968468850	3.610147702138	-3.367337379295
H	1.574493299330	4.282385794739	-1.720887823387
H	2.901120183146	3.416056777319	-2.541997838193
C	2.087023596050	-0.480139842031	0.483240476102
C	1.299595036417	-1.683398896065	0.006910143045
C	0.249969407947	-2.089311447792	0.886700073679
H	1.755202651843	-2.432705280656	-0.632189519883
H	3.065359394925	-0.407172273490	0.005053208583
H	2.211886675384	-0.363842106694	1.558151005286
O	-0.687353813234	-3.007797049532	0.419598218844

C	-1.770174751439	-2.962431999643	1.286215140145
C	-1.547752545378	-2.054393843470	2.285451377720
C	-0.254866853857	-1.474896552852	2.031693910185
H	-2.585786678596	-3.626102980129	1.058009256934
H	0.272786214326	-0.784783664715	2.668060830443
H	-2.226662996111	-1.802153486222	3.081715371294

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TS55 -802.972049

C	-0.847997447701	0.736757532127	1.581054793733
C	-0.738504591608	-0.700805286919	1.220299134213
C	0.586163620103	-0.874959859814	0.727599470083
C	1.105048419959	0.321891403361	0.246248965895
C	0.125865164462	1.447912119087	0.616358058686
H	2.131013936245	0.473609449408	-0.060082361107
O	-1.574499510051	1.276136819556	2.422615118049
C	1.207690433726	-2.201126957002	0.556359424291
H	-1.312518890686	-1.481515573498	1.702667238219
H	0.562813377152	2.355951653673	1.030810052665
O	2.481483698008	-2.119952455696	0.054013533673
O	0.659388304043	-3.281207784636	0.818147388437
C	3.198704568874	-3.381081921319	-0.132089785156
H	4.161945068892	-3.100073381152	-0.553177797092
H	3.323039998095	-3.886304562898	0.828636052128
H	2.646246836511	-4.033289179019	-0.812759051699
C	-0.077020037755	3.627610820806	-2.248008349760
C	-0.703511887955	3.121916991611	-1.175244606882
C	-0.649731461591	1.694090702185	-0.731042388784
H	-1.303834978482	3.760243815969	-0.530603486367
H	-0.154171531332	4.682162419395	-2.490558396282
H	0.521229088765	3.016485436229	-2.917806671238
O	-2.052040485777	1.217993640391	-0.513942993437
C	-1.979085208508	-0.163355909130	-0.737547628241
C	-0.954769373592	-0.454763117490	-1.662692172285
C	-0.059577326829	0.607798122498	-1.648111521139
H	-2.892032667162	-0.706843603230	-0.545032917649
H	0.765161112443	0.763866356207	-2.328352786200
H	-0.804422745191	-1.414913846734	-2.131438287233

29

TS56 -802.971982

C	2.382588666077	2.349461687063	-0.110285373402
C	0.977499070785	2.068336189738	-0.483231163192
C	0.816980378225	0.753378277487	-0.896279604636
C	2.191445116242	0.069427772158	-0.932945413296
C	3.074252407792	1.110957538993	-0.391624934250
H	2.459922471898	-0.295166975027	-1.927941775166
O	2.839556013178	3.433507564817	0.358120318164

C	-0.320403639204	0.200509494496	-1.644165668993
H	0.182592574488	2.799841715349	-0.405310781415
H	4.121142821723	0.951606898115	-0.159880980351
O	-1.469405417914	0.917229624643	-1.468995918570
O	-0.273840618124	-0.844005948556	-2.319501967073
C	-2.677375844152	0.402410985150	-2.113291565493
H	-3.448812708839	1.136710182813	-1.891092422015
H	-2.521475130467	0.308064416281	-3.190289597963
H	-2.932258850718	-0.574713069063	-1.694633125421
C	1.939690426185	-1.179574682872	0.026968897814
C	0.786954502531	-0.622476910902	0.789620027966
C	-0.466651955090	-1.281561496011	0.916840632450
H	0.998548144299	0.155158557761	1.519012332239
H	2.813259412988	-1.418854162830	0.631900867047
H	1.654039833032	-2.044914069710	-0.572976929762
O	-1.413518408702	-0.695448515501	1.768955221520
C	-2.561071106728	-1.445181795031	1.680877260979
C	-2.385980376334	-2.487254821056	0.796733929038
C	-1.045447760061	-2.386999374897	0.305496577054
H	-3.386257176812	-1.129441041779	2.295587065795
H	-0.568602611521	-3.029157170861	-0.416394813027
H	-3.118321521498	-3.233379678868	0.536923274654

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TS57 -802.970984

C	-1.028043014473	1.682495798089	0.213204688158
C	-0.659451703299	0.193002152472	0.350314583620
C	-1.624034679359	-0.498614711364	-0.410083467989
C	-2.464886866392	0.469932795055	-1.133946372731
C	-2.118132755038	1.743677770709	-0.799884124416
H	-3.234689484425	0.172735100824	-1.833838040358
O	-0.528026162256	2.610839672886	0.862833660385
C	-1.473322317366	-1.882637154218	-0.603592213188
H	-0.265991257883	-0.179622575287	1.287918269351
H	-2.537964096440	2.667969401251	-1.167283374307
O	-2.386679155238	-2.515464733850	-1.411924901725
O	-0.439970866698	-2.491957285466	-0.148254714733
C	-2.212820264676	-3.950290205056	-1.616723294099
H	-3.061077563430	-4.252175937996	-2.228585074064
H	-1.271111601386	-4.154350982542	-2.132845326922
H	-2.218205111516	-4.475174112187	-0.657931832743
C	1.310983608493	-1.368903133866	-0.814419698803
C	1.164483726255	0.003997574516	-0.536533628862
C	2.035230645160	0.627610644122	0.477346152949
H	0.929523755006	0.655784456821	-1.377285215270
H	1.034407734216	-1.767225923799	-1.781976072642
H	1.938311746332	-1.998764606536	-0.194864779681



O	2.473438145170	1.912887746673	0.197027985955
C	3.244606769738	2.328945644394	1.272219633228
C	3.303425640960	1.334387958427	2.211451840422
C	2.519889230395	0.233476607434	1.700569353946
H	3.650914993546	3.322464454647	1.207535829491
H	2.335301444418	-0.711684138041	2.186748884736
H	3.825346435974	1.375255645275	3.153457477029

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TS58 -802.969168

C	-0.688684232824	0.226956030245	-1.032997599788
C	0.249432164535	-0.133787192285	-2.053756051357
C	1.039098283830	-1.199743041009	-1.556620907453
C	0.738931415881	-1.505699615043	-0.227316582207
C	-0.223591085794	-0.508755310352	0.271814061225
H	1.209717661621	-2.282408277933	0.357688437235
O	-1.710623059010	0.967603689615	-1.096310068183
C	2.043625219953	-1.907641324193	-2.387181811205
H	0.286955533312	0.274869016219	-3.051945112183
H	-1.046533989104	-0.863238201779	0.890643477608
O	2.673011630795	-2.914505233796	-1.698259173030
O	2.308466500280	-1.642736248397	-3.566684885367
C	3.673622346454	-3.687336478376	-2.431419396438
H	4.042076031759	-4.422399492989	-1.718329831880
H	3.215086031215	-4.174538968445	-3.295433221923
H	4.479557108743	-3.033506700734	-2.773849212317
C	0.658148490205	0.606336529872	1.123173078610
C	0.007551516803	1.105316186973	2.329490379435
C	-1.183552992315	1.824530210437	2.394220727054
H	0.447872841228	0.851230868012	3.291111381994
H	1.613776590245	0.150883722922	1.379742907349
H	0.848690560059	1.381492092249	0.364329252457
O	-1.692232726190	2.099372926458	3.689138412210
C	-2.848015105598	2.813376325121	3.523474715875
C	-3.111850772053	3.017132770863	2.181842823837
C	-2.055043493980	2.405600867350	1.453416036602
H	-3.360330927165	3.109640113519	4.423376902471
H	-1.943663781550	2.331574674735	0.380222648916
H	-3.955547869295	3.546924509661	1.772498484147

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TS59 -802.969008

C	0.889323626069	0.916961287373	-1.787146343827
C	0.132069069507	0.806354868575	-0.402268194120
C	-1.061676987756	-0.021030881026	-0.721928930612
C	-1.023660698055	-0.338525069847	-2.093113698973
C	0.102937952991	0.192029414324	-2.738699772723
H	-1.809994574571	-0.904188309056	-2.579133205328

O	1.968617236998	1.562001896410	-1.931939698225
C	-2.094119913356	-0.261910868517	0.230604286345
H	-0.133392239913	1.813502148778	-0.063849935963
H	0.356552750949	0.095829925748	-3.783664006910
O	-3.156927137136	-1.005135778339	-0.266417813156
O	-2.083682733447	0.137125073681	1.425738708717
C	-4.260972346062	-1.249308109190	0.650365953304
H	-4.972088157562	-1.850787575473	0.084866555686
H	-3.914436719143	-1.786359933751	1.537634361001
H	-4.715362466851	-0.305840323419	0.965080746541
C	1.897931517900	1.888849954069	2.553066951590
C	0.923731672113	1.133486544364	2.026563928469
C	1.083768196104	0.261804013094	0.806875219504
H	-0.092153693920	1.117372040394	2.413866320578
H	1.693505763683	2.524960516167	3.407362281564
H	2.906368904899	1.921775563562	2.150276308080
O	0.621902624739	-1.111565597606	1.206749924314
C	1.492584771262	-1.988954742551	0.756004536932
C	2.634728498161	-1.385111072796	0.179657191520
C	2.432865691394	-0.020946065594	0.261379260426
H	1.257892451133	-3.033921381530	0.902098824768
H	3.081554902067	0.761613979539	-0.104090998349
H	3.477750286974	-1.902637418374	-0.245253909726

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TS60 -802.968780

C	-0.887423705295	0.900784915554	-0.881007332340
C	-1.733988044893	1.507836971436	0.137422868034
C	-1.067777260099	1.385864218230	1.350422995499
C	0.176471464429	0.689243785426	1.225769490220
C	0.287820300991	0.203581145368	-0.110296084915
H	0.870545777199	0.525242562288	2.035868217503
O	-1.009817847292	0.899067444147	-2.124751066154
C	-1.600093929860	1.949105648044	2.617809881830
H	-2.688520240417	1.980256509122	-0.034592700541
H	1.240476786701	0.182179478488	-0.634807430135
O	-0.754905218931	1.728597006917	3.673295682467
O	-2.675752816608	2.549042594648	2.734617147146
C	-1.170975934839	2.254926741508	4.973017428735
H	-0.368613196383	1.987000272598	5.657471347284
H	-1.294908429494	3.339058786370	4.917106596784
H	-2.116227436718	1.799604113990	5.278249276459
C	-0.236740355420	-1.543093090063	-0.159820816334
C	0.848090422162	-2.364484606868	-0.573913646832
C	1.420489494962	-2.271491907986	-1.861547143432
H	1.342016854845	-3.020788113183	0.136677734884
H	-0.622938135958	-1.756360760714	0.832641745824

H	-1.045759586871	-1.427867407645	-0.883189610177
O	2.518521040361	-3.097026066502	-2.157616450955
C	2.919171333827	-2.794484786663	-3.439865351411
C	2.125002610947	-1.801126544254	-3.969915896781
C	1.162049557570	-1.459963914604	-2.969453170876
H	3.754441437945	-3.354884023754	-3.823372183915
H	0.383663057981	-0.710275376113	-3.031672851555
H	2.217910954203	-1.368157744966	-4.952108661402

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TS61 -802.967682

C	-0.177914560153	2.931030777302	-1.249651984470
C	0.463246525499	1.704843650269	-1.829142614335
C	-0.282525461775	0.604463733203	-1.550385668686
C	-1.546819783265	0.992741388888	-0.783344511276
C	-1.369810103976	2.454333632783	-0.596286677197
H	-2.450524957726	0.716452008321	-1.337987471953
O	0.283457124334	4.106520322722	-1.329185958995
C	0.049982701885	-0.759343029499	-1.987093679183
H	1.396676378878	1.718108663974	-2.378188479756
H	-2.078553565651	3.094358607748	-0.085992714767
O	-0.957811439223	-1.655025185230	-1.683111085702
O	1.090529351171	-1.111481116469	-2.559990777743
C	-0.743324851308	-3.041734828006	-2.092175823652
H	-1.642480309129	-3.572085271996	-1.783016412687
H	-0.608993261705	-3.099309440116	-3.174803214733
H	0.143509582972	-3.449187896370	-1.600427878471
C	-1.606666850993	0.258858087956	0.603708939943
C	-0.261118458259	0.435639783957	1.195483572126
C	0.281345646991	-0.442067507439	2.139103600924
H	0.340827961775	1.284569903133	0.883018408791
H	-2.398561008836	0.743511477356	1.186584744047
H	-1.862518478925	-0.801331076780	0.493937633009
O	1.602611870119	-0.220186965009	2.573297934320
C	1.919276657144	-1.220551020926	3.448207935015
C	0.854819225798	-2.092298212903	3.599026699287
C	-0.193413756725	-1.597971464585	2.775354950661
H	2.904548031850	-1.186061393737	3.881000647144
H	-1.179406172039	-2.017159972779	2.654316147070
H	0.834886396546	-2.966232333109	4.228376272070

29

TS62 -802.967581

C	-1.141489830539	-1.387903237399	0.294853614848
C	-0.237386312651	-2.308431436439	0.969093686760
C	0.718470843605	-1.546726170679	1.641967754802
C	0.532886204069	-0.149719710790	1.450775688540
C	-0.518244992859	0.034439311101	0.491510608705

H	1.116623489692	0.622627271173	1.927893153173
O	-2.164965573947	-1.626685240777	-0.383771413112
C	1.774053864428	-2.155330560796	2.490568293337
H	-0.317863516025	-3.384512460825	0.962739281691
H	-1.198757003065	0.876286112450	0.584541606407
O	2.582343184508	-1.209590762819	3.066914142496
O	1.931865448261	-3.368949321378	2.672513752227
C	3.651430343838	-1.698796646971	3.936362987098
H	4.169244530137	-0.805042744857	4.278853037545
H	3.228223512900	-2.253454647928	4.777288052605
H	4.323189744428	-2.352846217052	3.375175947205
C	0.214908837752	0.226013751070	-1.120089040690
C	-0.822271248559	0.612764093982	-2.020043720298
C	-0.998567014994	1.936332898247	-2.480458085076
H	-1.604690575450	-0.102672277005	-2.257079241570
H	0.591134745278	-0.793204091441	-1.258837651055
H	1.021094033034	0.946182771353	-0.992647889745
O	-2.141088446724	2.205457689916	-3.250835511803
C	-2.113099507439	3.539014252250	-3.580665933574
C	-0.994765430482	4.141809549274	-3.044648892736
C	-0.277325819808	3.125065361520	-2.343615196456
H	-2.928367423684	3.899850538437	-4.183585303377
H	0.652347346508	3.242228495767	-1.810091803951
H	-0.722584721870	5.179432710522	-3.144616722599

29

TS63 -802.966954

C	-1.140926463472	1.997045419943	-0.488700271765
C	-0.164728774574	2.361493197522	-1.488651133246
C	0.375866804021	1.176164984569	-2.021460570049
C	-0.114179825671	0.026776990597	-1.382196962720
C	-0.984231213137	0.448198846449	-0.273773670538
H	0.124581717449	-0.987620379634	-1.666161541244
O	-1.943591723599	2.697166993741	0.170404872431
C	1.357088066013	1.174977955388	-3.135610898455
H	0.095411588572	3.369000298459	-1.775869112230
H	-1.936078340967	-0.072520980656	-0.162242407802
O	1.719761855561	-0.095139905181	-3.506464930314
O	1.814191013216	2.185294499307	-3.684204899235
C	2.671188435156	-0.211183069088	-4.610272877785
H	2.819948480115	-1.280699713589	-4.745650528483
H	2.257373219788	0.244792788949	-5.512958324890
H	3.609434908439	0.287058584058	-4.354198270504
C	-0.232251758046	0.407502876223	1.162857767936
C	0.100262690666	-0.955393473150	1.537589269533
C	-0.336130650665	-1.566210234266	2.719151319810
H	0.684662424034	-1.561370892661	0.849796069760

H	0.650994902430	1.041229697721	0.984353749297
H	-0.878556101427	0.912993708142	1.885796573770
O	-0.019981578934	-2.925352438608	2.912404836233
C	-0.573790587741	-3.309661850089	4.108136718322
C	-1.238032041664	-2.250729252555	4.695976765244
C	-1.087672034260	-1.135505138995	3.823305859667
H	-0.413811129709	-4.332545462353	4.403011907513
H	-1.469934392095	-0.138692999381	3.974194562251
H	-1.760683214299	-2.273280740468	5.637700989419

29

TS64 -802.966751

C	0.003081172828	2.004427086890	0.514479789259
C	0.274165608672	0.484727945118	0.619585928207
C	1.637986600861	0.344498604033	0.037056052191
C	2.080446100787	1.594298762874	-0.465008799112
C	1.103264676054	2.565436084081	-0.289473553568
H	3.033982283419	1.732752622104	-0.957469703024
O	-0.954142859085	2.608175068910	1.032941589614
C	2.322944504782	-0.928184065441	0.021835062278
H	0.142530410319	0.092866317545	1.628202089593
H	1.150617142325	3.601503168303	-0.593737215786
O	3.578607683361	-0.878207468850	-0.536065177876
O	1.813182128699	-1.991261417894	0.444677987299
C	4.312396372515	-2.139474809043	-0.612541737174
H	5.275638277188	-1.880911482059	-1.048385308258
H	4.435287838239	-2.567857023411	0.385164873347
H	3.775522650333	-2.851369377776	-1.244562368479
C	-0.377395617058	0.150413610553	-1.727915075018
C	-0.680534160325	-0.312155945385	-0.364756545928
C	-2.142745138886	-0.304833084607	-0.062491218431
H	-0.317924627467	-1.353347329471	-0.227314814258
H	0.438839281829	0.816617148456	-1.964617112140
H	-1.029564587760	-0.160538559418	-2.541994381482
O	-2.666798498416	-1.451425719926	0.529744294408
C	-4.018568500647	-1.224902158481	0.730871440103
C	-4.354116835084	0.025144750403	0.280058107662
C	-3.142795947377	0.619583696326	-0.230293301465
H	-4.570181696601	-2.024804279328	1.192666416248
H	-3.018263313404	1.617858940593	-0.617859824357
H	-5.331394340412	0.477377327360	0.317713418158

29

TS65 -802.965901

C	1.222229998489	0.459553541267	0.804474129355
C	1.520617436914	-0.542076586667	-0.189372467182
C	1.066252448743	-0.072842751051	-1.436710057429
C	0.472273864819	1.195813303864	-1.351903091317

C	0.399497281412	1.581361539234	0.064384438418
H	0.065899773282	1.749929064294	-2.185778489245
O	1.557608727266	0.506638036571	2.018052830879
C	1.242348364226	-0.841175410943	-2.694005936186
H	2.035056415178	-1.473375880961	-0.007482022244
H	0.756828182917	2.578157684881	0.330977549181
O	0.778383010280	-0.159273870638	-3.791846955521
O	1.743626783386	-1.969774937981	-2.778100043671
C	0.930675688075	-0.818343892194	-5.087181396602
H	0.522929549150	-0.116517865476	-5.812296768879
H	1.986449003715	-1.018202641449	-5.286012045285
H	0.379015946744	-1.761722632052	-5.099446339201
C	-1.186515113763	1.526451047825	0.502109640048
C	-1.279596668730	1.154858023394	1.907162069298
C	-1.791418973438	-0.057360332395	2.368825206251
H	-0.796804900409	1.786140735873	2.647495602091
H	-1.700512370552	0.823140298786	-0.155291882009
H	-1.555318704140	2.535602179560	0.299443501286
O	-1.706368828650	-0.314551856614	3.750505672440
C	-2.237776973866	-1.554698355368	3.970666083954
C	-2.669700335279	-2.117402883043	2.781803505487
C	-2.392381094963	-1.172520265669	1.759164804911
H	-2.242746955711	-1.901279053376	4.989895600439
H	-2.574636867264	-1.289073348311	0.702965720202
H	-3.119897388678	-3.089050031919	2.666009610254

29

TS66 -802.965028

C	-1.685971617535	-0.663519115341	-1.492518914753
C	-0.877970236433	-0.177717596389	-0.120010152914
C	-0.086259641290	-1.398320898240	0.245963205954
C	-0.341225100854	-2.394623235232	-0.683074461221
C	-1.240047518050	-1.985190975185	-1.703318873102
H	0.086922062557	-3.386914715737	-0.609231080787
O	-2.486640609922	0.100324180600	-2.093347247580
C	0.651698352188	-1.516214903377	1.477349463284
H	-1.649604269856	0.097729101275	0.602986955804
H	-1.636290798180	-2.612252192701	-2.488692781587
O	1.353071501246	-2.714521240106	1.561627633898
O	0.678119652522	-0.683363288893	2.408182576790
C	2.064990927515	-2.958262567411	2.808548910986
H	2.533326606860	-3.933882733621	2.682741038305
H	2.817946792358	-2.183973513621	2.978651773723
H	1.369424047034	-2.966409538153	3.652288454311
C	1.571255200442	1.683343938014	-2.299933164923
C	1.055259751871	0.759459192223	-1.464001764571
C	-0.146059863474	0.985589522280	-0.648154547600

H	1.503165931278	-0.223464219482	-1.360782044471
H	2.444810279628	1.457896894137	-2.901939767181
H	1.138849194296	2.674433501490	-2.412636804136
O	0.771308802043	1.943401386818	0.968515403485
C	0.140675177219	3.029723045015	0.983883500126
C	-0.891104823021	3.235443944453	-0.038903977868
C	-1.002154461643	2.174347582448	-0.868069977570
H	0.362371947944	3.785057526471	1.741139469650
H	-1.757658765552	2.040392366798	-1.648546160538
H	-1.500467106590	4.126569052437	-0.083041756276

29

TS67 -802.964959

C	-1.098609546197	-0.845473907934	1.590997427883
C	-0.105471509207	-0.829883098245	0.267777857266
C	1.219789359733	-0.461305649756	0.863165072589
C	1.083942973812	-0.296734368375	2.244634219722
C	-0.235070979150	-0.482967795446	2.681097953715
H	1.917919588961	-0.059796693928	2.893642057066
O	-2.281656848887	-1.200591081954	1.526624282728
C	2.382022346934	-0.298234214592	0.031938731782
H	-0.167117280221	-1.848071308764	-0.122422795998
H	-0.567977987438	-0.532883670455	3.708132488368
O	3.534411892344	-0.054614063296	0.755936926242
O	2.394509429277	-0.374354198932	-1.220923362248
C	4.770460625523	0.072993121334	-0.007124745751
H	5.539044016458	0.288307705877	0.733711345914
H	4.989471148707	-0.858717117317	-0.535111398323
H	4.690211158197	0.884433123985	-0.735116020006
C	-0.318360659272	2.493743141390	-1.481386753360
C	-0.234601419907	1.563993663910	-0.498297194828
C	-0.560311309386	0.170790991051	-0.682795028427
H	0.140403702190	1.836937620901	0.484029302347
H	-0.060289051181	3.529307528752	-1.289296949602
H	-0.619489687104	2.237987317567	-2.493286897045
O	-3.176157237002	1.212702655701	-0.226865310816
C	-3.502809734284	0.701646257581	-1.307857110772
C	-2.583718545090	-0.094397631305	-2.163724319668
C	-1.280749363768	-0.312063129856	-1.876109416191
H	-4.523990849874	0.824044427008	-1.702233403981
H	-0.693257484681	-0.963076273259	-2.521672923582
H	-3.016380668895	-0.548689990024	-3.049887094488

29

TS68 -802.963201

C	-1.108697484689	1.685695304660	-1.054928979144
C	-0.329189595370	0.363149096782	-1.304803533351
C	0.899342783685	0.513666461980	-0.572010564060

C	0.909394981536	1.816546262575	0.019021847251
C	-0.217745254116	2.557799861240	-0.325071467301
H	1.723512737495	2.170112470218	0.640008831755
O	-2.327835880097	1.811763198045	-1.335837166141
C	1.878893594847	-0.529081364673	-0.542653346087
H	-0.266390495451	0.027038485095	-2.339986194588
H	-0.481798450018	3.544687429973	0.021825184934
O	3.020342103365	-0.218473242995	0.164320966777
O	1.712560967347	-1.651178018682	-1.086049910775
C	4.028213897782	-1.267983985438	0.266922433652
H	4.830609638695	-0.834085112239	0.861716694057
H	3.609456250224	-2.149947375634	0.758305607272
H	4.387828039038	-1.550058844928	-0.725972280947
C	-2.536841306390	-0.783478440071	-1.348027639948
C	-1.359535089456	-0.930382977946	-0.588510697733
C	-1.441238730361	-0.752239402511	0.876764467355
H	-0.656242236596	-1.722172532787	-0.887058226460
H	-2.528608536374	-0.978947918482	-2.416088876148
H	-3.471148076561	-0.448561487406	-0.914263764105
O	-0.572533437373	-1.519136084552	1.641063990970
C	-0.772730685239	-1.165454164989	2.965712435800
C	-1.739733427347	-0.198434278271	3.047531698418
C	-2.170726723115	0.071970678189	1.696418744325
H	-0.168358718556	-1.681573555684	3.690486827788
H	-2.899846199022	0.800813578944	1.379461219803
H	-2.101076633432	0.270652943432	3.947808163267

29

TS69 -802.961997

C	-2.540460962059	0.419331475268	0.389375384876
C	-1.145392188733	0.413671180637	0.055639687159
C	-0.558981873099	-0.923468768905	0.378005439131
C	-1.730171520763	-1.713550367033	0.941847876268
C	-2.837338404670	-0.950826041605	0.969806659820
H	-1.625483240707	-2.742832630055	1.262865153011
O	-3.400267634284	1.336220307204	0.258714471923
C	-0.044576053360	-1.303185078564	-0.974613235185
H	-0.635159744412	1.196933021999	-0.484907485456
H	-3.821242607151	-1.230243700400	1.325294512305
O	-0.794355472562	-2.041906277432	-1.799366470148
O	1.132276725926	-0.900256923899	-1.275106995711
C	-0.403828943858	-2.103721724820	-3.213474664735
H	-1.140145921544	-2.756658839825	-3.675739549678
H	-0.445885048584	-1.100480990857	-3.643737768517
H	0.604498935554	-2.511816616396	-3.308786145149
C	0.731995145479	-1.001000424370	1.300131302948
C	1.897383821294	-0.469220336051	0.532237076788



C	2.158994558819	0.925243104408	0.534182347412
H	2.732119241152	-1.118231630726	0.290699412990
H	0.901657299193	-2.045495931546	1.576361132581
H	0.522838700680	-0.424329086636	2.201242291007
O	3.311840660203	1.379233438085	-0.122510594001
C	3.304015201404	2.748694685317	-0.044321867864
C	2.194241061440	3.189934988859	0.642878308617
C	1.457517432203	2.023730589901	1.020367580577
H	4.133879569413	3.257561006792	-0.504048808998
H	0.532866684758	1.982045126267	1.573810912945
H	1.939857155885	4.215009546069	0.853523076866

29

TS70 -802.961510

C	1.136954838424	-1.444647089298	-0.516023906360
C	0.115119025673	-1.900904921284	0.309834937608
C	-1.039723802526	-1.038668187786	0.135463678264
C	-0.819306573017	-0.026813126629	-0.764534888556
C	0.570803200746	-0.225896265617	-1.304517907855
H	-1.542426136046	0.700440132566	-1.103226508255
O	2.389972938500	-1.757680646359	-0.640827957125
C	-2.308556348847	-1.254228960340	0.869031377613
H	0.171756946504	-2.725825643128	1.003430204039
H	0.557587850937	-0.452012066111	-2.378840427579
O	-3.289113557344	-0.354333059793	0.514222679511
O	-2.502801834127	-2.131817004105	1.721368751494
C	-4.577044743795	-0.494884708834	1.186290790139
H	-5.206725653768	0.285435394996	0.761614514173
H	-4.999807510328	-1.484729486748	0.996043910729
H	-4.459543054349	-0.359002136941	2.264644982975
C	3.047581664953	-0.049443314706	1.511953342370
C	2.204479536476	1.022986553738	1.452454741717
C	1.661796269998	1.510691162466	0.229902103959
H	1.954344217691	1.597606755331	2.338386030544
H	3.445632573522	-0.356759110591	2.474520570170
H	3.293558764573	-0.652698580576	0.632957610682
O	1.087301066798	2.721629333584	0.259516224512
C	0.757168922742	3.118703628769	-1.081014923208
C	1.118547488122	2.154087832752	-1.939226050926
C	1.614280732295	0.967956967091	-1.157203182809
H	0.294025893005	4.085780406538	-1.158377816574
H	2.563707690389	0.507131482657	-1.463024697877
H	0.981581981967	2.162473875600	-3.008803983816

29

TS71 -802.961354

C	-0.780661809238	-0.982520590769	0.436326206531
C	-1.600737973456	0.041523582836	-0.164704278128

C	-0.950652561183	1.268854741416	0.018616425666
C	0.289021791681	1.140660137399	0.687207170148
C	0.540728320220	-0.261487644755	0.896409967145
H	0.930834236134	1.962989167505	0.965354530779
O	-0.974643734165	-2.215975144012	0.560642564035
C	-1.540784142146	2.555809480978	-0.429183800890
H	-2.556264942772	-0.114553590969	-0.640483239321
H	0.961394565633	-0.598770543533	1.846735142431
O	-0.754506659135	3.631075253813	-0.099974848849
O	-2.613795729176	2.678425487011	-1.033854673343
C	-1.258360487892	4.951625246837	-0.472361864540
H	-0.506390245042	5.653349278519	-0.116320104628
H	-1.377400685623	5.019601696290	-1.556693730373
H	-2.223753753106	5.134351431122	0.006088170756
C	3.040175654479	-2.357847028823	2.193858651965
C	2.455245882198	-2.989139563670	1.143968673203
C	1.924428392109	-2.298415533169	0.008764199424
H	2.344036788272	-4.068334458808	1.136511461628
H	3.408969055371	-2.919869107875	3.044029390156
H	3.178059028624	-1.280589390223	2.222733541132
O	1.381677337695	-3.029556833762	-0.995530539766
C	0.926376353024	-2.149617666448	-1.994593100870
C	1.140839900866	-0.866280873487	-1.622582235845
C	1.732453098782	-0.877916737968	-0.250386555625
H	0.468302465199	-2.618324847171	-2.846337088265
H	2.572824066529	-0.223515742195	-0.034482434179
H	0.874913556087	0.020078933834	-2.173388412626

29

TS72 -802.960836

C	-1.597784435649	-1.168230405204	0.745706639698
C	-1.623650990012	-1.014225626966	-0.659379671270
C	-1.220486165386	0.324793379176	-0.951020574245
C	-1.010715984982	1.089201097839	0.189926201348
C	-1.376291818853	0.253418792909	1.369329265042
H	-0.778311878187	2.144728826901	0.199579683663
O	-1.594317845013	-2.218814597488	1.472811312789
C	-1.057324068446	0.823214180463	-2.337480951050
H	-1.748095718419	-1.804154999543	-1.384028212545
H	-2.359348081738	0.598810665005	1.727533781152
O	-0.739609027967	2.160986980047	-2.386037799972
O	-1.178383597879	0.139211390275	-3.362865404481
C	-0.569678055821	2.745426977714	-3.713329625911
H	-0.354088616822	3.797502967148	-3.534852201629
H	0.256477756365	2.259477366372	-4.239029485136
H	-1.484821761156	2.626939203012	-4.298911153605
C	-0.535243071692	0.157328557385	2.719484850505

C	0.919410572423	0.351798029397	2.617282231204
C	1.769165856576	-0.404248586835	1.836132808932
H	1.370128471046	1.210131468248	3.111021179705
H	-0.937684533195	0.856814672398	3.453364674663
H	-0.783875826475	-0.872566320776	3.035459433217
O	3.123361785718	0.014709677945	1.732131653521
C	3.748324303450	-0.858473187594	0.897152027636
C	2.872542646212	-1.840071031238	0.451842347958
C	1.620090765871	-1.566643283706	1.044315091903
H	4.792900509924	-0.676735119683	0.705566278213
H	0.702294149604	-2.130683271444	0.949141887890
H	3.112844023539	-2.650937350627	-0.214732878438

29

TS73 -802.960773

C	0.281960276493	-1.027755986589	-0.459919711913
C	-0.975646024767	-0.643892147776	-0.914877785219
C	-1.840731383524	-0.095119538994	0.076735864820
C	-1.322716055261	-0.052329574411	1.351512866980
C	0.012994370436	-0.635963268664	1.438158214490
H	-1.781973789841	0.487153273134	2.170555585761
O	1.245685652133	-1.708167925537	-0.824229414329
C	-3.185755733702	0.412810416585	-0.293764726653
H	-1.286350732824	-0.848224376574	-1.930625051609
H	0.121573950453	-1.714603577486	1.555935760396
O	-3.851181176596	0.964683263783	0.772255452913
O	-3.678845860156	0.359563298022	-1.428110596577
C	-5.189376013560	1.490155067595	0.511065452465
H	-5.529127350231	1.888691651356	1.465213477663
H	-5.146540348984	2.274213441613	-0.248932037338
H	-5.848004218093	0.690185311044	0.164147585116
C	1.067883806038	0.178905520513	2.196683660440
C	1.428829431147	0.703886092429	0.855510729625
C	2.644402813834	0.397589877468	0.197365668347
H	0.807671815933	1.491555007421	0.441103754141
H	0.648222360074	0.909093795289	2.886470390786
H	1.839603992000	-0.416205375654	2.680923669214
O	2.835382020457	0.933856931131	-1.080473655312
C	4.001539410839	0.406503710576	-1.571303479797
C	4.564431267202	-0.454639693565	-0.656415291258
C	3.691908553637	-0.467950116723	0.475516560228
H	4.295507719103	0.730386649316	-2.554704282099
H	3.811391242654	-1.050666141381	1.374644315636
H	5.474429187340	-1.016292282804	-0.784659056473

29

TS74 -802.960731

C	-0.779647857233	-0.701638861350	-1.584205072886
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C	0.486183173681	-1.296628183933	-1.633117882917
C	1.340267354014	-0.572192509392	-0.721663017131
C	0.704922074070	0.485437853254	-0.094692595726
C	-0.640886505319	0.614697787673	-0.749977324497
H	1.173149123234	1.202735610673	0.562900345373
O	-1.965416494560	-1.055832698628	-1.945678234841
C	2.749585380602	-0.963414569286	-0.482238961486
H	0.756343404489	-2.206033665346	-2.146157576459
H	-0.572790647876	1.435892996331	-1.479386129548
O	3.398593989373	-0.109018701460	0.378414764401
O	3.311604382717	-1.947882529678	-0.980913702490
C	4.800281618249	-0.405750993280	0.661908372363
H	5.125407067355	0.381051383570	1.340321209607
H	4.894071524799	-1.389432755977	1.129259777851
H	5.383635108296	-0.392809033899	-0.262237457501
C	-0.776204505264	-1.556456829897	1.626477990372
C	-1.610985846840	-0.616745607341	2.157741481184
C	-2.156522154186	0.440457430245	1.382094559877
H	-1.831407774666	-0.596039503775	3.219606496045
H	-0.319069509248	-2.296283030054	2.276527899392
H	-0.578922945785	-1.661732857411	0.564434964752
O	-2.904733087136	1.362006892840	2.029218958156
C	-3.236669012641	2.406944520209	1.112800284907
C	-2.704663435731	2.136180638370	-0.090238373935
C	-2.011799803237	0.809297905537	-0.030850585066
H	-3.832299084351	3.199555309515	1.528550339971
H	-2.586000791088	0.057888079960	-0.709268883375
H	-2.792535185287	2.732630040211	-0.984615487548

29

TS75 -802.959772

C	-1.538737643333	-0.114510750305	0.685828867227
C	-0.547699352171	-0.565274550322	1.610634751246
C	0.607335068197	0.206944662391	1.408309937402
C	0.448786693774	1.145635192133	0.363071125559
C	-0.837766911987	0.941583168904	-0.223983100709
H	1.177646538508	1.888864182458	0.080201285199
O	-2.717967813306	-0.538260282847	0.487778412709
C	1.827100932384	0.056845144636	2.238136142935
H	-0.670221905959	-1.356622229897	2.333716078406
H	-1.412621503492	1.778523287533	-0.606124782952
O	2.827591776637	0.911414671162	1.847631347044
O	1.960541267557	-0.739238947002	3.176453338635
C	4.073894177179	0.856402191518	2.608959881783
H	4.712962660437	1.616017911475	2.162722241843
H	3.883090425482	1.073740577805	3.662712036729
H	4.524839907061	-0.135362841550	2.523107859091

C	0.870203590309	0.886867205081	-3.489436914414
C	0.642619997259	0.191821213163	-2.363927269124
C	-0.706254196448	-0.112728275610	-1.815444247546
H	1.461333018716	-0.170040064868	-1.748038180845
H	1.883955169195	1.104152513695	-3.807668814963
H	0.067850901244	1.253513413396	-4.122716715167
O	-0.789292983365	-1.477571990240	-1.327172402998
C	-2.069640015822	-1.895208605581	-1.492871959409
C	-2.793469936790	-0.978428753082	-2.276676876549
C	-1.956084850339	0.100260371735	-2.519785312388
H	-2.328588513019	-2.853353860175	-1.077041860815
H	-2.203235445008	1.009396534047	-3.045614962646
H	-3.825411774284	-1.088602624669	-2.564317430654

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TS76 -802.959325

C	0.858451075604	1.222035946522	0.606412797024
C	0.031655469568	0.917467490562	1.689731692442
C	-0.456442609278	-0.429754638165	1.514743836610
C	0.034135426984	-1.033403341420	0.379171820343
C	0.955239644584	-0.056036901841	-0.278271039263
H	-0.112133778594	-2.065977340438	0.098419959019
O	1.385561405195	2.323300983311	0.183787087743
C	-1.366758016855	-1.075543260926	2.489816784739
H	-0.272465983908	1.593129445641	2.474205515538
H	1.983987005879	-0.441502931690	-0.299636910637
O	-1.677514192781	-2.370695933605	2.145805982534
O	-1.819537943583	-0.538541486364	3.509491825576
C	-2.563896107233	-3.093839266554	3.053073690842
H	-2.700893996765	-4.072465071964	2.596095236742
H	-2.103057945696	-3.184356576310	4.040083176505
H	-3.518025752077	-2.569799432475	3.150815305277
C	1.146416013120	-1.086114589814	-3.745120620507
C	0.425869341722	-0.790928358558	-2.652887004621
C	0.650747451771	0.398437161647	-1.743018223481
H	-0.393945522589	-1.427434889610	-2.330437172225
H	0.927071207445	-1.978478577023	-4.321666812264
H	1.967974153575	-0.468359517234	-4.095363450944
O	-0.647320111224	1.167793243808	-1.712142239193
C	-0.403548860174	2.401699557022	-2.154662720383
C	0.930165459189	2.600464699534	-2.547650969855
C	1.609822108367	1.440868698209	-2.229217863358
H	-1.241304138107	3.082894674882	-2.168215300257
H	2.668750791086	1.260311935855	-2.336764198550
H	1.346035964119	3.529970628362	-2.895864457491

29

TS77 -802.959023

C	2.711654364722	-1.145705206101	0.561633960909
C	1.431606871022	-1.655868624766	1.010788981240
C	0.322097423821	-0.855582371320	0.507647926553
C	1.024708328753	0.337013450638	-0.177910576432
C	2.379032145364	0.114506643869	-0.151555932588
H	0.553032663300	1.299905821703	-0.316304041099
O	3.860586622260	-1.638662965482	0.734823730405
C	-0.738296312575	-0.479323261900	1.528179775901
H	1.307624553084	-2.605651971665	1.516891038737
H	3.138825339942	0.767099759291	-0.563480669579
O	-0.369867199223	0.614040164799	2.248705383637
O	-1.804505077372	-1.082358056078	1.709581134858
C	-1.259035386422	1.034200733712	3.333780009732
H	-0.778637478670	1.908725342289	3.766452458300
H	-2.245945843913	1.281864638837	2.935668557880
H	-1.352991396013	0.233155591438	4.070235348554
C	-0.395895585024	-1.604170097837	-0.767631482061
C	-0.198578619525	-0.566434845913	-1.789590381253
C	-1.189044816929	0.444745113616	-1.993837827795
H	0.554612799232	-0.689255597504	-2.559436288344
H	0.128933848927	-2.529158741668	-0.986955069816
H	-1.429916572728	-1.821693899438	-0.496888424869
O	-0.939062443972	1.410154677416	-2.972970533809
C	-1.994088287766	2.300217979847	-2.949952629151
C	-2.899413845584	1.936148294392	-1.981420734170
C	-2.387286077528	0.747019790095	-1.362709488910
H	-1.957514614994	3.101161709977	-3.667625321545
H	-2.845578261181	0.177926175162	-0.568288327018
H	-3.818842477803	2.445712635450	-1.745168532226

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TS78 -802.958764

C	1.658698781797	2.080559590049	-0.804193115769
C	1.515748333371	0.823740529248	-1.507416355870
C	0.334257272203	0.105126764635	-1.056323318663
C	-0.309601776748	1.062308378544	-0.044818019224
C	0.463233663576	2.164050950087	0.097882855758
H	-1.268032724057	0.862304903097	0.414430500222
O	2.571758124015	2.943898195137	-0.903989234527
C	-0.517386678670	-0.366226779729	-2.218828342183
H	2.197656819155	0.460927410798	-2.264724429704
H	0.286298190373	3.001848495103	0.759533229643
O	-1.692409210616	0.322772014954	-2.303441329958
O	-0.193844091022	-1.260924035600	-3.008698012771
C	-2.540191174225	0.049482902980	-3.466984737608
H	-3.411055657502	0.688114046169	-3.335980881932
H	-2.003362180646	0.301711648716	-4.384103607134

H	-2.821722098066	-1.005903003443	-3.489170306735
C	0.680524752725	-1.301510696914	-0.194213123611
C	0.867431475007	-0.832825655749	1.165065863622
C	0.025359110083	-1.187830761874	2.242699911782
H	1.713678771816	-0.189087434275	1.387175258925
H	1.554789415838	-1.721078222576	-0.685828389770
H	-0.166469218769	-1.983205531895	-0.302954823724
O	0.240256780405	-0.540972090868	3.468395163148
C	-0.703260871625	-1.007706508856	4.351658356329
C	-1.518462488554	-1.934000962320	3.736123351027
C	-1.054455808676	-2.058736327021	2.390742576489
H	-0.663889446239	-0.606303395702	5.349506314994
H	-1.445507418495	-2.716596471756	1.631230903127
H	-2.337878778317	-2.463299678752	4.193224191585

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TS79 -802.958683

C	1.444028935258	1.312190007574	-1.765703394601
C	0.166887456886	0.713184683751	-2.071195165923
C	-0.266406554575	-0.214067966659	-1.017300789179
C	0.882097910108	-0.143043626636	-0.001035407561
C	1.837360554910	0.718444724446	-0.451959034283
H	0.952397419192	-0.812190184562	0.846190104814
O	2.107058195645	2.158848025659	-2.428343176941
C	-0.583573272243	-1.582364131150	-1.594465363180
H	-0.418786216638	0.934338159093	-2.954298426874
H	2.760404205501	0.977057028353	0.051545192051
O	0.452381655143	-2.455867651419	-1.444631475272
O	-1.647391844081	-1.874927441555	-2.153388866299
C	0.319521104457	-3.763665781089	-2.091516682372
H	1.254441507437	-4.277579361620	-1.879041194380
H	-0.533622036358	-4.304314481018	-1.675074261060
H	0.178585813536	-3.633110551554	-3.166700311457
C	-1.565181161443	0.285789128423	-0.182397664987
C	-0.929301305296	1.120493977241	0.847509291330
C	-1.059162519687	0.880812780589	2.236275874933
H	-0.453613244663	2.047774719485	0.543083588613
H	-2.238692467233	0.803876164150	-0.861767056848
H	-2.079414781046	-0.582272895938	0.237494734715
O	-0.341509761780	1.716285639035	3.103973876029
C	-0.580784943553	1.281197700593	4.385285816245
C	-1.427504291160	0.193461710276	4.371349159023
C	-1.739948161779	-0.064948646876	3.000888033527
H	-0.101170140020	1.832369327502	5.175579229207
H	-2.396423921689	-0.831854798573	2.622135769519
H	-1.786818282942	-0.344050001229	5.233007979569

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TS80 -802.958593

C	-0.632007639768	1.761967629812	-1.870571070497
C	-0.504456604088	1.947420569374	-0.446264794222
C	-0.806903672905	0.693062549418	0.281355077902
C	-1.109643591450	-0.294953001298	-0.847497832551
C	-0.999916498682	0.316297353571	-2.049051166110
H	-1.399647271667	-1.319976066346	-0.654555662155
O	-0.460216340596	2.597837236658	-2.801686080842
C	-1.922739323297	0.923038600315	1.290015382332
H	-0.282467164139	2.888654816591	0.039303506566
H	-1.141329651592	-0.132733173675	-3.023767709831
O	-3.136508725693	0.506888915994	0.832124334263
O	-1.757480216315	1.447945182850	2.398982640900
C	-4.301298543969	0.804574900112	1.668689148788
H	-5.149465599589	0.393792591750	1.125202482128
H	-4.192440538355	0.332666866864	2.648082948247
H	-4.402023493767	1.884936139327	1.794636274649
C	0.449984768011	0.149264777759	1.103024453779
C	1.403465463067	-0.294638635953	0.077360574171
C	2.217044018701	-1.428026232047	0.214887873361
H	1.508712505692	0.303357547513	-0.824171642829
H	0.788833397039	0.989164551657	1.716158951291
H	0.165130077717	-0.666325339341	1.778836043139
O	3.019204372063	-1.800928404178	-0.879426958236
C	3.688904652769	-2.941119201351	-0.526957278147
C	3.350202153053	-3.326124809311	0.757024623834
C	2.419427292980	-2.362643820425	1.238077055854
H	4.358795318082	-3.350933445870	-1.263350943345
H	1.960244318143	-2.334181830509	2.213340866845
H	3.732092828508	-4.184522453396	1.283899698369

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TS81 -802.957623

C	-2.409252206363	0.339843713854	2.115039369728
C	-1.164711354381	0.944917420731	2.711295260775
C	-0.266711867048	1.199649662231	1.733616927954
C	-0.805127853495	0.755403042588	0.371418730445
C	-2.153318353950	0.238073602631	0.702372860889
H	-0.801039936513	1.578368204955	-0.351032442737
O	-3.438457073346	0.011011103343	2.770349968540
C	1.043504048913	1.830072491390	1.951956885899
H	-1.038630218183	1.146952012148	3.767486205041
H	-2.908756058982	-0.064658281137	-0.010080412354
O	1.714027425903	2.050656266653	0.763144555400
O	1.527254458300	2.151614920159	3.046246328843
C	3.012403011027	2.715502105561	0.863019494218
H	3.363457660516	2.813026287032	-0.162916543239



H	2.897487755024	3.695731314180	1.331468535378
H	3.701236650337	2.113035502516	1.460316625199
C	0.146878841617	-0.370665284912	-0.229191422096
C	-0.553119155409	-1.202555683923	-1.212490112440
C	0.092425679041	-1.859419162608	-2.265107422689
H	-1.626554001205	-1.336429447481	-1.122996059056
H	0.401535799517	-0.964586781848	0.662349350887
H	1.080815480125	0.052096046125	-0.614947049129
O	-0.701830943897	-2.582223368769	-3.177839300388
C	0.135282917339	-3.102863127834	-4.126876490942
C	1.446177820007	-2.744962824819	-3.868488874843
C	1.428226544144	-1.961143450553	-2.681731016791
H	-0.324461215883	-3.693786129749	-4.900567031010
H	2.276330196767	-1.529125896536	-2.175054305976
H	2.306725449187	-3.021564753830	-4.454284771888

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TS82 -802.954624

C	-0.873125573151	1.616317566303	-1.058321878632
C	-1.263803887165	2.325277338887	0.119274751647
C	-1.132419493729	1.461716843089	1.255287292864
C	-0.671410593268	0.209504012586	0.900339922485
C	-0.361461972206	0.240433201009	-0.580527165410
H	-0.542556498912	-0.634096046943	1.564898152813
O	-0.855380710110	1.958769082670	-2.278329165938
C	-1.496613861130	1.884314476392	2.628227350808
H	-1.563861403440	3.362708354843	0.157838206385
H	0.730230445561	0.311544451571	-0.706464606757
O	-1.311377678959	0.882346032498	3.550355956538
O	-1.920197330911	3.004017384091	2.941407163336
C	-1.646243717304	1.198233945308	4.937238161440
H	-1.423334127644	0.291220495181	5.496251519617
H	-1.040657091595	2.036294944543	5.290912602687
H	-2.703987737112	1.459791712492	5.021031201828
C	-0.935643837472	-0.921843226410	-1.419813132989
C	0.051913982911	-1.428552339246	-2.410337690877
C	1.243341169614	-2.025328835579	-2.018500264335
H	-0.148963934726	-1.340370602664	-3.473732892376
H	-1.837270103043	-0.585356687680	-1.932269168098
H	-1.227974680167	-1.725143853149	-0.722121531710
O	2.150708110502	-2.456434236792	-3.009493923332
C	3.227860489974	-3.002920856887	-2.366577233947
C	3.057791425336	-2.952824373888	-0.992814537872
C	1.803161445159	-2.333931896435	-0.758697303147
H	4.019645178546	-3.378572885852	-2.992345941451
H	1.343546574979	-2.129589290543	0.195604508926
H	3.754154179973	-3.315406417988	-0.255287741967

29

TS83 -802.954395

C	-1.292913319401	-0.624704241261	1.265816647275
C	-0.318970277594	-1.611781979300	1.461929798155
C	0.879367582847	-1.205746131641	0.771320065308
C	0.767667301823	0.017371033113	0.138803827821
C	-0.591671070696	0.535848933503	0.450546063927
H	1.558918891050	0.541078132737	-0.376594397043
O	-2.543994476961	-0.523009575638	1.519994825519
C	2.105777816431	-2.040834255835	0.768044704813
H	-0.460522211524	-2.560445310867	1.955336883535
H	-0.551296649407	1.438308788576	1.075558910228
O	3.139275424702	-1.462622328916	0.066107144165
O	2.223534514218	-3.143666882210	1.318353249890
C	4.391895734630	-2.210320578181	0.013317857617
H	5.062210334087	-1.598407535681	-0.588009116207
H	4.791292772139	-2.353864015688	1.020595782908
H	4.232454501540	-3.187728585051	-0.449375680754
C	-2.063982331945	3.646565843356	0.531483742945
C	-1.569700635444	3.466507373101	-0.719874399778
C	-1.461625366607	2.159771194620	-1.305504440523
H	-1.259803812189	4.305214246074	-1.333668851768
H	-2.148295406523	4.641837271276	0.953694460646
H	-2.409925783377	2.819907704503	1.146859613630
O	-1.138394007624	2.059550792105	-2.603486027375
C	-1.181150195868	0.663501010452	-2.969568024714
C	-1.503766235715	-0.073421892887	-1.896159980674
C	-1.645006591188	0.836394296757	-0.714227650206
H	-0.947087139208	0.468949391924	-4.000414061671
H	-2.584630760533	0.700492567854	-0.128884286668
H	-1.587487033101	-1.146600460086	-1.837196534549

29

TS84 -802.954187

C	0.205016603210	3.451056973305	0.375712757060
C	-0.372323115478	2.141119313034	0.309644892909
C	0.698360822354	1.127216229720	0.135183515687
C	1.984811293134	1.946506962610	0.107453919119
C	1.702518680443	3.255741961790	0.221788743548
H	2.959152117479	1.483861729890	0.008009316543
O	-0.351896963536	4.576253445183	0.522753992943
C	0.510464138033	0.179182551979	1.298332174291
H	-1.422384001542	1.919391054073	0.441062606805
H	2.400569005724	4.083349869482	0.224109969265
O	1.279494015118	0.376966916759	2.383260684906
O	-0.351156446187	-0.734853406485	1.214238927678
C	0.938207159754	-0.365085880185	3.601928863271

H	1.652132854275	-0.019921097131	4.346141888259
H	-0.085746296796	-0.129106503130	3.900463570357
H	1.035749544531	-1.438976763382	3.427270135733
C	0.580820337124	0.190051727430	-1.151826680574
C	-0.630780112556	-0.635102280101	-1.027755048708
C	-0.680193876640	-2.007585309018	-1.349004549332
H	-1.578259127687	-0.129697363502	-0.866805413061
H	0.505892645671	0.889974666713	-1.987779427499
H	1.484382121373	-0.418275197875	-1.270938386423
O	-1.923219597277	-2.649356220706	-1.253568628289
C	-1.726746546184	-3.968311155970	-1.561719570988
C	-0.398078653562	-4.203175031200	-1.856140202930
C	0.273440946628	-2.952398720966	-1.724752596992
H	-2.596831727365	-4.601659118795	-1.537086132558
H	1.321732203038	-2.761622887897	-1.889270574641
H	0.035112440175	-5.149381277300	-2.133934752376

29

TS85 -802.953524

C	1.052484026190	1.407171607150	0.397703859169
C	1.660048078819	0.343293339484	1.141163092852
C	1.332232124239	-0.864779465266	0.496978133957
C	0.483580968715	-0.686849626114	-0.612666785253
C	0.115102460752	0.709754815992	-0.674943541658
H	0.129585354976	-1.475057178061	-1.258798552670
O	1.165570633143	2.656770131247	0.508944799564
C	1.870505962911	-2.174551726686	0.946482771009
H	2.301427329342	0.459103474483	2.000344988777
H	0.064226012267	1.209307610221	-1.641859487331
O	1.362732856656	-3.222506231140	0.218969614852
O	2.675875373573	-2.337539947500	1.871374356838
C	1.845796368771	-4.557894583333	0.565135476542
H	1.309013226076	-5.233962865770	-0.097632051110
H	2.924191349471	-4.622847937331	0.400924898306
H	1.629173020976	-4.779056106431	1.613223773223
C	-1.110268247175	3.898602729337	-1.230881704413
C	-2.180227513530	3.085643205763	-1.437267235720
C	-2.329722958505	1.789996098095	-0.844589675338
H	-2.988771516126	3.383722319211	-2.098080012593
H	-1.062803749959	4.859037188240	-1.734548451542
H	-0.278629677576	3.629162516464	-0.577138427538
O	-3.439215977056	1.080468025343	-1.225787871910
C	-3.409253755344	-0.167026743985	-0.548626415652
C	-2.305240786695	-0.256454487660	0.212280092408
C	-1.496402224352	0.985663133197	0.030989770349
H	-4.242609445980	-0.816303069584	-0.750498885151
H	-1.162540042026	1.458590776904	0.958752429910

H -1.999618229485 -1.097257117267 0.812987015144  
29

TS86 -802.953520

C	0.635949085389	-0.972819749637	-1.369542144401
C	0.200989391734	0.221291636518	-2.007726198815
C	-0.887825767866	0.742969653678	-1.254251011042
C	-1.127217230717	0.024180316554	-0.088617621713
C	-0.073644936943	-0.999431013672	0.044535099983
H	-1.902641876641	0.237134909970	0.631622241497
O	1.418844429556	-1.884642860426	-1.769236648632
C	-1.682898856660	1.912681246429	-1.702575677391
H	0.549554162002	0.592390539109	-2.958780347129
H	-0.372417896801	-1.992626597933	0.379388191479
O	-2.660930429884	2.257004996664	-0.799218480579
O	-1.508873511765	2.535010402874	-2.757593117533
C	-3.524248234424	3.378157865671	-1.163097108573
H	-4.245687621165	3.456298764770	-0.351744080789
H	-2.936507120554	4.295030020006	-1.255192548234
H	-4.024557579308	3.177563756858	-2.113638927832
C	2.887831195538	-3.110669216241	0.476345652152
C	2.493401052032	-2.654449992853	1.696076666116
C	1.769005680078	-1.445398171425	1.935186690773
H	2.741639394302	-3.206757469997	2.598066686148
H	3.416585066708	-4.056917285250	0.410211315556
H	2.650476226018	-2.595594168308	-0.454249089498
O	1.594911030374	-1.148601972649	3.257994393369
C	0.888925872120	0.081034951805	3.355054666172
C	0.586045318439	0.535785255495	2.131431019280
C	1.098710285572	-0.431556092287	1.098431178687
H	0.712878386138	0.427408652536	4.357844303416
H	1.771194198493	0.057437786249	0.370918162506
H	0.032677570374	1.428610143344	1.891490757652

29

TS87 -802.953228

C	1.848300124842	1.777733763643	-1.649045403926
C	0.823345163776	1.410623565995	-0.702811048201
C	0.238727407454	0.085038955232	-1.075271358884
C	0.989860161586	-0.282039721640	-2.354924998885
C	1.917226784021	0.648229471123	-2.647190301339
H	0.780107775132	-1.194968698521	-2.898674312600
O	2.568068442435	2.813676473801	-1.675924083636
C	-1.271887490478	0.222224912896	-1.200460424672
H	0.404877138695	2.097039347429	0.020498614357
H	2.619987285256	0.640759374702	-3.470289339491
O	-1.710787414172	0.322150184631	-2.482227363382
O	-2.028796884409	0.264769051032	-0.216446106713

C	-3.133570614624	0.609371792896	-2.680046584502
H	-3.257148222449	0.685728434501	-3.758097787355
H	-3.741887193385	-0.199296132302	-2.268176231895
H	-3.394553113214	1.548777957155	-2.187376878531
C	0.524982448472	-1.000081511846	0.026282972346
C	0.218604686110	-0.456334384894	1.362053066043
C	0.039491558202	-1.269138790476	2.486514081734
H	0.128631460729	0.613447868902	1.495940664408
H	1.601047110396	-1.189685846690	-0.087409077891
H	0.008735854231	-1.955171238908	-0.150681339860
O	-0.299040229603	-0.651910570632	3.705293127154
C	-0.452270462085	-1.641127137181	4.635595005157
C	-0.226228995532	-2.883011606593	4.069056314940
C	0.095332779104	-2.652254727759	2.703365084005
H	-0.710404074446	-1.327149995027	5.632591990750
H	0.348447062018	-3.392812547041	1.961521979487
H	-0.279273039976	-3.831732185574	4.576273794709

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TS88 -802.951944

C	1.253850638250	1.729542133568	0.105499733693
C	0.817149779561	1.667850688518	-1.236933262513
C	-0.329185543636	0.797016749699	-1.322900012649
C	-0.693140890879	0.271712053099	-0.103972175605
C	0.258111517011	0.871363711061	0.923567251579
H	-1.563647812655	-0.334646465606	0.102060575435
O	2.259055449935	2.263691917276	0.683538138892
C	-1.024614360484	0.528302949013	-2.604046433257
H	1.239765271979	2.214183443748	-2.067138301425
H	-0.268427790020	1.524769690619	1.627306552919
O	-2.085527845592	-0.335595577287	-2.458010980583
O	-0.712047456086	1.006690616988	-3.702306110745
C	-2.839891155861	-0.653860432825	-3.667198003402
H	-3.612776101336	-1.349549875316	-3.345037687263
H	-3.280365329284	0.253238511759	-4.088716275908
H	-2.185605905948	-1.112491394148	-4.413024093507
C	-0.957142348138	0.216862342226	4.060189407531
C	-0.718911463945	-0.973641002025	3.451261507566
C	0.256895716128	-1.146446364055	2.416691647148
H	-1.260023491681	-1.867090568349	3.745355060984
H	-1.698804019090	0.293593963811	4.847317914057
H	-0.417592369441	1.122891399871	3.802966719770
O	0.491195327957	-2.401558952558	1.996194409463
C	1.489230131002	-2.360229369029	0.964256732859
C	1.868911072006	-1.094389966895	0.746598304297
C	1.115169109389	-0.176168775868	1.682819986731
H	1.733766950291	-3.318259520169	0.542596414479

H	1.812665783367	0.406261171222	2.314637491763
H	2.582526512873	-0.739450597449	0.020485999294

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TS89 -802.951425

C	-1.037869291485	-2.523610127269	0.033336082968
C	-0.145881465529	-1.244955181187	0.036692869558
C	-0.709880065218	-0.404832699617	-0.984624519275
C	-1.838483648582	-1.085142426872	-1.546989182229
C	-2.002961494962	-2.365162592470	-1.022105234802
H	-2.446600429655	-0.649895373909	-2.330495001603
O	-0.942387920404	-3.405419971190	0.928028730069
C	-0.067539782989	0.763871777121	-1.535183855532
H	0.933022460723	-1.402179800250	0.017262921360
H	-2.783179052903	-3.074623033032	-1.249368657981
O	-0.813165166919	1.345784841839	-2.549046940777
O	1.037689434591	1.229157240110	-1.188701283397
C	-0.240090924464	2.529930939601	-3.175905061635
H	-0.970754124249	2.838921565794	-3.922114900795
H	-0.085133130608	3.316539149295	-2.432581197606
H	0.718206584935	2.290529299643	-3.644268279672
C	-0.013749842320	-1.790339970174	2.522803268510
C	-0.352012350990	-0.651966508772	1.742169488974
C	0.538997888582	0.537259574858	1.821662313651
H	-1.406375451679	-0.376455014897	1.767269854660
H	-0.762311119662	-2.426651365583	2.970221472891
H	1.026172646151	-2.031357222664	2.729456778082
O	-0.076876091371	1.747881083987	1.554249572861
C	0.897797887439	2.730453600374	1.648074949227
C	2.097423893540	2.162018049107	1.977211380936
C	1.866265126600	0.742046589497	2.092917120727
H	0.576190473365	3.737290462938	1.451286459285
H	2.602293985383	-0.009507582720	2.331221147062
H	3.034873117648	2.676275699396	2.109702547758

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TS90 -802.950922

C	-0.185647733199	1.266823005689	1.224031853253
C	-1.492430012011	1.148831396811	0.750822291899
C	-1.697397067599	-0.146415855178	0.141785647336
C	-0.575784129376	-0.933577653731	0.155693400590
C	0.512032079652	-0.168057840900	0.849523796184
H	-0.472984110665	-1.926838416042	-0.254259111311
O	0.477239950550	2.169924300934	1.835040220051
C	-3.007436481837	-0.550313748996	-0.421950072053
H	-2.265704446528	1.887840429872	0.896753939832
H	0.822206547865	-0.602652259538	1.804858204708
O	-2.979102442716	-1.808194938384	-0.977688219448

O	-4.033293481462	0.142995557901	-0.414157609510
C	-4.231545917539	-2.300001816638	-1.544876696886
H	-4.000366109850	-3.292628723499	-1.927356906467
H	-5.003492131330	-2.347664399157	-0.772672647624
H	-4.570071071158	-1.639459439869	-2.347265177877
C	2.263581247060	1.335460873760	-2.148387589670
C	1.402048576481	0.634430223362	-1.386774873292
C	1.667437363172	0.252018106152	0.018175492821
H	0.438516638612	0.313767387791	-1.770853600186
H	2.005461758525	1.606885285197	-3.166155345588
H	3.235233740349	1.662692105539	-1.786052835617
O	2.718313697978	-1.335901698358	-0.171550582452
C	3.787705359704	-1.043171866196	0.453619661477
C	3.871098774765	0.289251072272	1.018547697006
C	2.716772837660	0.968171759409	0.782672507298
H	4.569139306721	-1.795193698649	0.558142997024
H	2.411983503134	1.940697588013	1.180175363339
H	4.716210353255	0.645093290683	1.587603079916

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TS91 -802.948012

C	-0.635530970531	0.738333645142	-1.662697626719
C	-1.597421306186	0.534559062908	-0.669080472609
C	-1.090996684322	0.650589598801	0.662456927917
C	0.267184041382	0.816246259373	0.744633487332
C	0.881470544836	0.987184465357	-0.610412595110
H	0.809927544020	0.995947922080	1.664015476350
O	-0.510900894060	0.896737897256	-2.868863070117
C	-1.990941173413	0.512743407380	1.830997165585
H	-2.564048704497	0.114572600401	-0.909080582136
H	0.976966296688	2.036183864867	-0.922700295231
O	-1.311400552079	0.563426646251	3.023781020493
O	-3.216946921677	0.358669979115	1.770585088380
C	-2.112966173270	0.455640458930	4.241578295581
H	-1.398548221795	0.539850523083	5.058293932452
H	-2.850898371911	1.260486366622	4.280053095266
H	-2.630234747044	-0.506527782290	4.269669525417
C	3.480919654319	-0.159743335145	-3.024418871844
C	2.625365881533	0.610401040077	-2.316797229014
C	1.953243308620	0.181626595702	-1.088414454616
H	2.359471726250	1.593335449778	-2.695114004343
H	3.929058110413	0.204751158102	-3.942547694852
H	3.730952239510	-1.173958390637	-2.725518283301
O	-0.392854537979	-1.880077376354	-0.765210103325
C	0.222109801626	-1.967040980319	0.324099992222
C	1.676525497480	-1.764237803569	0.455573811306
C	2.436031855360	-0.959328896738	-0.346021912721

H	-0.294492358639	-2.314768434871	1.231466700642
H	3.512888588647	-1.112344236767	-0.361678887744
H	2.175851697412	-2.422424154067	1.164933189780

29

TS92 -802.947025

C	-0.700187308060	1.190992988610	1.154707587066
C	-0.319883170698	0.005997551717	1.821101819273
C	-0.336616134633	-1.083678930157	0.894937426963
C	-0.712573794404	-0.701007751070	-0.376040666377
C	-1.029928973570	0.789213189336	-0.330302928256
H	-0.864648929449	-1.346562278518	-1.228976256770
O	-0.757307428048	2.404687055309	1.576248039265
C	0.043795978064	-2.463895118188	1.278433214356
H	-0.074677355454	-0.068505236367	2.869575523324
H	-2.068127828514	1.049564993806	-0.557631488396
O	0.033006255083	-3.330739842664	0.208405720153
O	0.347639332598	-2.833976523699	2.419737413531
C	0.352484257639	-4.726700271370	0.495391266072
H	0.287876743973	-5.236201537541	-0.464517988940
H	1.357504260481	-4.809166255293	0.917207338827
H	-0.367108807508	-5.140135707510	1.206539971800
C	-0.243835116438	0.708610641193	-3.792803418334
C	-0.631547261733	1.498893735356	-2.781254737501
C	-0.071705270963	1.447773672951	-1.395286458997
H	-1.439660571005	2.214803477920	-2.906847952244
H	-0.730956785529	0.767752914996	-4.759746810564
H	0.550887659681	-0.024992387677	-3.693782722503
O	0.153919232218	2.870534965709	-0.915001696577
C	1.150959776808	2.807064432724	-0.063942948132
C	1.896599172973	1.584891871143	-0.164421684411
C	1.261273089476	0.807622828619	-1.111967911587
H	1.350751060080	3.682523049126	0.535915977910
H	1.614419441780	-0.106234963588	-1.560047390273
H	2.805915990652	1.375353083123	0.371886564482

29

TS93 -802.946877

C	2.556336785972	-0.168781475340	-0.657030959896
C	1.223392193406	0.579405790611	-0.443346612483
C	0.828479570790	0.209954276746	0.939827461704
C	1.677811914920	-0.789590932373	1.396653534465
C	2.678724972664	-1.086702068847	0.426385137225
H	1.576212837096	-1.275460886691	2.358042741635
O	3.212060632315	-0.068047217322	-1.747061715785
C	-0.293146713895	0.815371083209	1.630270753209
H	1.220386321255	1.646137477789	-0.658778491429
H	3.453937062509	-1.834605559687	0.512993125111



O	-0.508028178680	0.278173622244	2.882464789556
O	-1.006993318147	1.730098475820	1.171072069215
C	-1.621652369891	0.831732339222	3.644977010442
H	-1.620160180998	0.285729431598	4.587008444235
H	-1.473541451789	1.901510274163	3.813261135406
H	-2.561523216084	0.681939714000	3.106886129141
C	0.828378199532	0.144833350171	-2.889510108495
C	0.378504196069	-0.211022793810	-1.548911952551
C	-1.107214016985	-0.224286187311	-1.415541250595
H	0.730038780773	-1.257705778920	-1.340302029987
H	1.690843431883	0.782597757412	-3.042856645970
H	0.241490642725	-0.170901548236	-3.749939857823
O	-1.664929075384	-1.282652676228	-0.707414779734
C	-3.032811214244	-1.059399668282	-0.652402107078
C	-3.341401114908	0.102389411248	-1.308341190837
C	-2.097313790525	0.642679026977	-1.800239560282
H	-3.612685564027	-1.797838616178	-0.127396140429
H	-1.956588745252	1.576314220735	-2.320105964610
H	-4.322249684761	0.534409084900	-1.417959492348

29

TS94 -802.940798

C	-0.188828294626	1.052562766380	-1.739531987303
C	-1.058078897759	1.465091832185	-0.681885329802
C	-0.346153203180	1.260896890555	0.513881811579
C	1.014959882604	0.913945495629	0.308816086875
C	1.216454607560	0.788531150319	-1.097152889219
H	1.764795515371	0.875319547566	1.082567618254
O	-0.458284522197	0.734207322261	-2.932139470356
C	-0.977321205999	1.447714284971	1.847600777289
H	-2.114565409766	1.661415785891	-0.772317328944
H	2.062067225107	1.298127900310	-1.560834470113
O	-0.077987210548	1.306637450099	2.870039086213
O	-2.174038411405	1.699254425996	2.037297318425
C	-0.593081886444	1.469016656664	4.228492060684
H	0.271208019429	1.338823888241	4.876698490938
H	-1.030190531190	2.463115874788	4.350476647050
H	-1.355279184602	0.713333913710	4.433764352462
C	1.412998456892	-0.793540982423	-3.119584420018
C	1.575537835239	-0.937982567081	-1.724152462019
C	0.705836556307	-1.875660804054	-0.987862500847
H	2.601646465861	-0.933803526159	-1.353410800934
H	2.124845531555	-0.212737294082	-3.697902105473
H	0.615799840713	-1.279419073346	-3.664897523503
O	1.278699692086	-2.499362767996	0.113695289072
C	0.290341278488	-3.274244192519	0.704023437808
C	-0.878950883459	-3.146433694102	0.002818294270

C	-0.612841472842	-2.239287601206	-1.089466997277
H	0.581064160054	-3.829564048134	1.578113783681
H	-1.314470499013	-1.885276610726	-1.827883674366
H	-1.817086924920	-3.625653956261	0.229886902314

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TS95 -802.939983

C	-0.571261682777	1.145757395235	-0.777797049792
C	-1.230378002043	0.782832971890	0.498014165984
C	-1.638783389757	-0.549064143190	0.371849806998
C	-1.047242553812	-1.165153562405	-0.756217995621
C	-0.108458419954	-0.229579113528	-1.337213404730
H	-1.234157409160	-2.180121506108	-1.071595324553
O	-0.395485230513	2.247528328273	-1.304015743013
C	-2.532769545111	-1.219835836593	1.346059827326
H	-1.525131556148	1.478206012240	1.269371353741
H	0.192041469752	-0.290008778105	-2.378133856084
O	-2.811937620504	-2.509980785587	0.980407460791
O	-2.986686757794	-0.697174866146	2.370833669953
C	-3.699669653177	-3.268913567119	1.861587251889
H	-3.822196300377	-4.234954564627	1.376159475956
H	-3.243018416698	-3.379800171784	2.847985784158
H	-4.658510736725	-2.755305559514	1.963292041296
C	1.755662723825	-1.679360195789	-0.278869920991
C	1.335210648159	-0.336090481967	-0.347793017751
C	2.396589904991	0.654550762953	-0.648708872854
H	0.719750513499	0.078147874160	0.539450318795
H	1.046079875699	-2.493653036602	-0.376274944658
H	2.799974011891	-1.923957791133	-0.106425229298
O	2.397272509536	1.834350945520	0.085863528865
C	3.439799311541	2.611654926436	-0.384873146620
C	4.095704630960	1.952424155665	-1.391946868045
C	3.420069843391	0.689058462105	-1.564576516137
H	3.566349023872	3.571310613568	0.084096231065
H	3.648868296935	-0.078560808134	-2.286632746177
H	4.942721901304	2.317818994095	-1.948867559907

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TS96 -802.939390

C	-0.962191740169	-1.897216969584	-1.950146262435
C	0.370463633846	-2.044813176716	-1.264304374477
C	0.832092395933	-0.838877211097	-0.853201378607
C	-0.155581875822	0.260554668417	-1.246112535923
C	-1.227568360997	-0.490309485311	-1.960985527405
H	0.307845585245	1.113730436981	-1.745084336768
O	-1.638877517197	-2.863446712520	-2.409315022495
C	2.118456686944	-0.649740851676	-0.168702711999
H	0.870027067640	-2.995824230968	-1.123986539865

H	-2.065973474074	-0.027453101200	-2.459429363849
O	2.389463013970	0.679352395493	0.066904987283
O	2.899310445331	-1.551440261130	0.170068343384
C	3.681539359334	0.992972868014	0.672252487261
H	3.679594967672	2.074373293626	0.798073227548
H	3.789479214091	0.481264225736	1.632206756165
H	4.491439498151	0.679241799648	0.009504024968
C	-3.318171712938	1.670696191984	0.256916326928
C	-2.129263568277	1.667432826521	-0.367190807541
C	-1.002171160264	0.742097027131	-0.040826063883
H	-1.916820631606	2.375993189255	-1.163266281648
H	-4.089703294563	2.379386662380	-0.023344100021
H	-3.564101148659	0.958177322944	1.039285748064
O	-0.064666853460	1.988832372745	0.913449571940
C	0.079189734748	1.462286382472	2.075752074057
C	-0.558514721100	0.193106972288	2.265935138145
C	-1.084518894884	-0.236501626879	1.073556608240
H	0.707137278470	1.959755191701	2.811201207099
H	-1.483589718543	-1.226835695193	0.904905185327
H	-0.507056806753	-0.383125216692	3.176561539752

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TS97 -802.937410

C	0.716665205002	1.222208415187	1.293183049867
C	0.501232961367	2.053843774978	0.176399496426
C	-0.514884358630	1.479084888184	-0.669430017601
C	-0.995718803987	0.285154880809	-0.195837505520
C	-0.268544486062	0.008167227554	1.115285734103
H	-1.830446618468	-0.269360410340	-0.598591893227
O	1.514671742729	1.280809097863	2.281875186774
C	-0.995454990982	2.148103516819	-1.901851699177
H	0.960943121653	3.018336565771	0.021329269905
H	-0.955598114643	-0.031945483566	1.970753367857
O	-1.973265175336	1.425042214293	-2.549639877877
O	-0.587772127185	3.233119296845	-2.335483723697
C	-2.517685508314	2.013266749343	-3.769688053165
H	-3.260447578843	1.299654822572	-4.122736489645
H	-2.977654368836	2.980734241323	-3.552835632764
H	-1.726210964843	2.153369623581	-4.510478020242
C	2.142046138726	-1.785561511361	-0.839133199923
C	1.876873367787	-1.184133911594	0.329364589690
C	0.565346474108	-1.311789197249	1.058764086665
H	2.578964150754	-0.509799934223	0.808927876824
H	3.085763505965	-1.609905847515	-1.343339239329
H	1.436244033224	-2.439064327510	-1.344334992807
O	0.889982721013	-1.673830235935	2.509956683342
C	0.146199729868	-2.705451066339	2.848799763687

C	-0.665155511171	-3.185167134481	1.790245605729
C	-0.368012582684	-2.413898635853	0.684750089263
H	0.245882305061	-3.072610498895	3.860927236802
H	-0.761407947793	-2.523520797817	-0.314620161724
H	-1.346625708074	-4.017210067847	1.854408532419

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TS98 -802.937384

C	-2.819198102037	0.145922300074	1.032822815165
C	-2.135438072000	0.359250320277	-0.228192191315
C	-0.723471530478	0.193508709028	-0.030831451970
C	-0.531987451414	-0.056673013479	1.460000126996
C	-1.731189421819	-0.120783322705	2.060641264460
H	0.446096009720	-0.183903848277	1.903882837618
O	-4.047908934517	0.175549847809	1.284341198950
C	0.003743136583	1.308679918308	-0.711168883438
H	-2.622723474745	0.619975090955	-1.156486344154
H	-1.943249127340	-0.319134638361	3.102469503279
O	0.396042586668	2.336853851631	0.046650025019
O	0.204272798729	1.250829206110	-1.959443914408
C	0.928432899873	3.528477253484	-0.628069272376
H	1.155636610090	4.223758972385	0.175995967537
H	1.826622419480	3.266142560444	-1.191231475650
H	0.171570229935	3.936708877352	-1.300965957787
C	-0.001079989236	-0.756434331742	-2.285724863557
C	0.053224380146	-1.212419671379	-0.929341295707
C	1.402149278917	-1.472086299425	-0.385727502701
H	-0.683013183124	-1.956720816863	-0.636867112871
H	-0.961896337066	-0.690173265181	-2.784330985325
H	0.879112974664	-0.732882205072	-2.918647505445
O	1.518247274933	-2.477434328902	0.564234204108
C	2.843187282976	-2.502393944595	0.982032855315
C	3.553514562880	-1.535641950765	0.322515870530
C	2.624133883552	-0.865500951744	-0.558437115089
H	3.094313199940	-3.244451773740	1.718974326537
H	2.839804531171	-0.045790916679	-1.226188956838
H	4.602876279479	-1.321527291844	0.443000198592

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TS99 -802.936688

C	1.398931246682	2.952350020287	0.456038555759
C	0.141998090821	2.442825256734	1.102526252513
C	-0.260389065658	1.312152279945	0.478313037729
C	0.710342363284	0.936173363865	-0.641824726535
C	1.704812706131	1.996591985223	-0.597157999781
H	0.228010142869	0.722960987543	-1.597669301508
O	2.025458707115	3.991387841137	0.784164138944
C	-1.518304971122	0.584919615080	0.749274825523

H	-0.353039319923	2.934787863649	1.929383843347
H	2.538676284792	2.100921862362	-1.278982403692
O	-1.971234449261	-0.038573728442	-0.383651836743
O	-2.121504411411	0.548493200475	1.829811747179
C	-3.198318728840	-0.823009124890	-0.268335504067
H	-3.356833849292	-1.246186217237	-1.258011170937
H	-3.066600477006	-1.613066384540	0.475288217650
H	-4.030033779023	-0.178635038257	0.026378755095
C	1.949897563657	-0.306790960369	1.096296278427
C	1.470938415357	-0.500600094223	-0.261761954044
C	0.651730185255	-1.734069377309	-0.427672701884
H	2.245020442599	-0.497948152181	-1.039051485715
H	2.137960909653	0.683897585741	1.490213174400
H	2.120137829209	-1.156738168555	1.752666134835
O	0.549562746819	-2.235168289411	-1.719647690696
C	-0.275246639105	-3.348444585226	-1.665409521558
C	-0.684134768193	-3.559112785241	-0.374890327812
C	-0.090711116569	-2.512930686061	0.423936473048
H	-0.452391773323	-3.854601091900	-2.598039366649
H	-0.225796756429	-2.349920546073	1.482086250788
H	-1.325679027781	-4.353463632870	-0.029709846126

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TS100 -802.936002

C	-0.380587651853	-0.050577430176	2.845494224262
C	0.690736768882	0.797557595887	2.189564592740
C	0.949245673758	0.341155534091	0.944181028975
C	0.064527622349	-0.853216361131	0.634616965196
C	-0.715354372417	-1.059157097301	1.883919942598
H	0.628336263973	-1.688214278024	0.214726632795
O	-0.815724525261	0.141158484826	4.016601724784
C	1.987885991439	0.864725131963	0.045381172437
H	1.179313727429	1.629169120257	2.682596903435
H	-1.401129027850	-1.874230760773	2.066297080811
O	2.365199940099	-0.064675052992	-0.900399192799
O	2.516881645845	1.982540313067	0.119933988045
C	3.386147986292	0.358960177661	-1.854076531598
H	3.570133272453	-0.511393881898	-2.482249301217
H	3.020864895191	1.202250173417	-2.445951819174
H	4.295827258740	0.658202482857	-1.328209193815
C	-3.101468097904	1.035182587944	-0.526796399558
C	-1.892403994496	0.755285184654	-0.006599456259
C	-1.121587086495	-0.476936429708	-0.323787390195
H	-1.399481383329	1.457372477187	0.656279231622
H	-3.602167575634	1.965903490007	-0.285137622906
H	-3.628708249723	0.352496124509	-1.189070389119
O	-0.406627005120	-0.065122304234	-1.897881145141

C	-0.660390162578	-1.063476196759	-2.666052727748
C	-1.569135285868	-2.030370433536	-2.111843414339
C	-1.813575044334	-1.703113145303	-0.807342215316
H	-0.156844521591	-1.140798546673	-3.625710516602
H	-2.389571900141	-2.303339013848	-0.116344061057
H	-1.921091263894	-2.908411338047	-2.630726859768

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TS101 -802.935765

C	2.212290752550	-0.612261631176	0.468545649788
C	1.409766162364	-0.563905011717	1.635923479404
C	0.435154124356	0.484300852231	1.476329289622
C	0.473634959754	1.013668693306	0.204373800424
C	1.476442597248	0.255587041672	-0.584655399015
H	-0.157582235984	1.806968518882	-0.168038061741
O	3.180832493580	-1.377856785627	0.140348102841
C	-0.483027087298	0.896018407078	2.560983209887
H	1.552989326273	-1.152024865151	2.530934462854
H	2.093421362711	0.837605422552	-1.266773373392
O	-1.292703573685	1.938230806782	2.190153735203
O	-0.533925641479	0.374230159609	3.682504867820
C	-2.240448937566	2.424347754213	3.191294961400
H	-2.765121494091	3.246482834984	2.708412914186
H	-2.933038542644	1.627428724013	3.472916641669
H	-1.707058766642	2.768040217624	4.080877628142
C	1.813455633402	-1.735972914863	-2.090063834398
C	0.807005189132	-0.988575417924	-1.351221906402
C	-0.444146078377	-0.730612961994	-2.124762118714
H	0.514495388501	-1.595146265189	-0.441541245060
H	2.867928761639	-1.514688745415	-1.985311211197
H	1.496923215900	-2.486810421620	-2.810674446860
O	-1.644728593707	-0.820323623105	-1.430173013499
C	-2.659700539009	-0.502405082290	-2.319643710079
C	-2.127815252460	-0.220395033250	-3.549979650054
C	-0.696093481468	-0.367545739637	-3.424285015661
H	-3.660368863414	-0.528103842228	-1.925765343198
H	0.043440614258	-0.210592649614	-4.193368769001
H	-2.675840528037	0.057688255148	-4.435124443071

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TS102 -802.935070

C	1.344691083555	-1.761710195255	0.035709728105
C	2.279373652467	-0.792729298194	-0.442649943715
C	1.535732928410	0.358370022077	-0.777213111084
C	0.139597711040	0.166329000920	-0.684774342236
C	-0.084688164637	-1.168694656094	-0.195413086428
H	-0.608315744397	0.864155825250	-1.025360737030
O	1.535463730683	-2.836735791538	0.674283102467

C	2.187302187846	1.611995108018	-1.240768252694
H	3.353946523796	-0.865653358753	-0.385073289704
H	-0.754440059821	-1.801275461271	-0.781306185519
O	1.275779706240	2.566111846386	-1.606878494676
O	3.409590569920	1.796331243482	-1.298771504567
C	1.810930934761	3.838840241565	-2.087814044894
H	0.936706776868	4.439488986234	-2.330914314244
H	2.410070275799	4.313935709120	-1.307268271798
H	2.433838832462	3.675903796238	-2.970724290682
C	-0.718763232630	-2.655406856922	1.771686823183
C	-0.871511468292	-1.285827625983	1.405926568475
C	-2.253002506857	-0.789266803427	1.145835904484
H	-0.291096449337	-0.589615081256	2.010916027147
H	0.064749248327	-2.983734922660	2.436914429299
H	-1.397254756491	-3.414786016354	1.391275867848
O	-2.420570249696	0.585080399305	1.223809873624
C	-3.748287212772	0.858488143904	0.921334398223
C	-4.409112880307	-0.309769792332	0.653295693123
C	-3.444114826420	-1.376086976384	0.799628502652
H	-4.037018868389	1.894045645611	0.951320991063
H	-3.629882810169	-2.430518686138	0.671072773890
H	-5.449466989133	-0.411486542790	0.391434601728

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TS103 -802.934432

C	-0.473849939978	2.623273523930	0.653018611236
C	-1.452540843157	2.143669150549	-0.366587515671
C	-1.386779174013	0.788685571233	-0.483938390382
C	-0.380799852602	0.204859466733	0.505221832900
C	0.181668631023	1.420370082753	1.135768102352
H	-0.837959108802	-0.499282944846	1.208642072909
O	-0.266725694407	3.820533855244	0.986893039417
C	-2.261496163137	-0.013685450565	-1.361144867255
H	-2.104843966686	2.796827724032	-0.932308827047
H	0.913811438584	1.413160558867	1.932315653430
O	-2.097864719999	-1.361725756052	-1.140200093543
O	-3.058515082480	0.435795764488	-2.194066053507
C	-2.927264628000	-2.266751533541	-1.937230317484
H	-2.647789770575	-3.267106149512	-1.612819634487
H	-3.984536088950	-2.072152097419	-1.743798650071
H	-2.723692393165	-2.124945444674	-3.001247177162
C	1.071320794530	0.358642605102	-1.397793998108
C	0.731113447411	-0.566856331850	-0.302061611270
C	1.890621855493	-0.947366751789	0.576929709811
H	0.330537553847	-1.503170263650	-0.714356660980
H	1.538573893029	-0.012557921768	-2.307111502359
H	0.923980227462	1.428165968140	-1.300490775161

O	1.840143523670	-2.225704280824	1.123954876739
C	2.975869697386	-2.381322365912	1.909654277709
C	3.731961216179	-1.241703733040	1.860110457164
C	3.034040415759	-0.315458699978	0.995962195078
H	3.080883987774	-3.328027624090	2.409480634319
H	3.341374538979	0.682432196172	0.728550154107
H	4.668264824364	-1.073534639435	2.366414107405

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TS104 -802.934288

C	-1.290800672849	0.896379744485	-2.384359383428
C	-0.114345832356	0.645717699177	-1.611195053020
C	-0.487075745829	0.258678953897	-0.223721979665
C	-2.010835231147	0.354870805095	-0.213789159883
C	-2.457415543879	0.712582077921	-1.429847999617
H	-2.609643238062	0.115304939421	0.657051147758
O	-1.416144612495	1.220208335653	-3.599910438094
C	0.069049602135	-1.141390615449	-0.173210778266
H	0.903608334103	0.725663007929	-1.965161635863
H	-3.486573850770	0.845412469466	-1.739466861186
O	-0.664823597718	-2.143212391349	-0.686127107213
O	1.197793408700	-1.322976592173	0.385835565788
C	0.013756451663	-3.413235098352	-0.954463444746
H	-0.768123155818	-4.076665546551	-1.316666285328
H	0.778742453596	-3.260469500619	-1.719720736875
H	0.470717381487	-3.799324639703	-0.040525957182
C	-0.810475409338	-0.973907427472	3.125470132940
C	0.505830449249	-0.762032018243	2.916675027498
C	1.011438181710	0.128277322941	1.886032550198
H	1.261896915491	-1.266957126349	3.507687031550
H	-1.147281508724	-1.658526210105	3.895297659933
H	-1.580066596369	-0.470978865301	2.548229999490
O	2.294798649879	0.538922816005	2.021563103274
C	2.496518950278	1.636804615967	1.123592925776
C	1.351435810655	1.971088803969	0.517000398987
C	0.248463922967	1.044217242263	0.970644762192
H	3.507288330204	2.001767962696	1.081758364708
H	-0.542388064232	1.579653069120	1.507483279039
H	1.212034342668	2.736998317745	-0.227925996766

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TS105 -802.933644

C	-1.691505570444	-0.987265403490	0.456549559819
C	-1.750044516831	0.076854198809	1.397198839305
C	-0.430343969149	0.564819790236	1.646440156184
C	0.533309049340	-0.113410101787	0.927286134208
C	-0.171049234935	-1.232028010229	0.180248309104
H	1.594681889510	0.075012344760	0.953455180626



O	-2.593202165739	-1.694532857157	-0.080207502836
C	-0.157803331577	1.688172745128	2.574469270354
H	-2.645263860749	0.413605248876	1.898732795779
H	0.049388450149	-2.190063513881	0.679886239750
O	1.179034037254	2.004392502541	2.638725371613
O	-1.012148375395	2.295038912600	3.232529912446
C	1.547671573139	3.106147605496	3.523962219668
H	2.623923118916	3.218519565234	3.405340120180
H	1.023770533555	4.019426136237	3.230934181708
H	1.291077134254	2.863222433514	4.558181276846
C	-1.030032276977	-1.730357432278	-3.480315408014
C	-0.873706050864	-1.049698035262	-2.335687788932
C	0.206362626456	-1.349040798610	-1.320959839237
H	-1.512968587403	-0.207644455005	-2.093325385470
H	-1.807761107596	-1.454666382430	-4.183674367128
H	-0.417167225370	-2.589786523068	-3.740076351884
O	1.281251117451	-0.264242811289	-1.548475526513
C	2.436946796813	-0.875417538257	-1.782376796245
C	2.328275860099	-2.291647457552	-1.770367660562
C	1.009920451951	-2.601883317674	-1.526872487757
H	3.301661957891	-0.248961965256	-1.946305810592
H	0.560848986823	-3.580300071610	-1.437017377942
H	3.148302831072	-2.975503844046	-1.919276092488

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TS106 -802.933209

C	-1.738733694626	-0.568516016023	1.998193973357
C	-0.610390371220	0.411988496131	2.232093024814
C	-0.143597008472	0.870079030692	1.050566090051
C	-0.883403366012	0.206308071775	-0.097155736653
C	-1.899903842873	-0.644677642549	0.574155633251
H	-1.184572104280	0.895950069441	-0.885766260088
O	-2.377625741932	-1.150628680448	2.919166540249
C	0.923087896814	1.866806151956	0.880085411758
H	-0.259266898596	0.696582488555	3.216131795643
H	-2.703181779337	-1.170475888479	0.078588428245
O	0.899666077442	2.427076208844	-0.376559865646
O	1.745540586721	2.207411197984	1.742862549479
C	1.938318866488	3.408574715196	-0.673977859653
H	1.730674625804	3.746007015637	-1.687991382409
H	1.888311576394	4.239870608518	0.033278550204
H	2.924490382519	2.941722041496	-0.609758973966
C	0.442893835236	-2.901856026152	0.852361319232
C	0.834740936061	-1.771655600716	0.246219442852
C	-0.042406586265	-0.972040519235	-0.687527270008
H	1.820389587671	-1.353108233554	0.418961955828
H	1.107158278846	-3.413899305479	1.540655745720

H	-0.552731547484	-3.313766654829	0.723089670323
O	1.326207159405	-0.305699993784	-1.660199798106
C	1.075872412473	-0.636532785103	-2.877515366733
C	-0.052859144654	-1.502229893391	-3.047267239315
C	-0.693675776558	-1.641852248250	-1.844350561791
H	1.675680651367	-0.215489037652	-3.680315069343
H	-1.646075512481	-2.137884141460	-1.721876463618
H	-0.385487597258	-1.895557266690	-3.995305738678

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TS107 -802.932742

C	-2.539399426277	1.437980501828	-0.523596378020
C	-1.663129146430	1.058944610071	-1.690646217443
C	-0.765789584616	0.108730283896	-1.328910894034
C	-0.977752910324	-0.265479096869	0.139443744621
C	-2.101086288800	0.609509779527	0.559120833819
H	-1.134828323973	-1.341350423611	0.257106113375
O	-3.458421416528	2.307936181706	-0.572551315456
C	0.179407948329	-0.528077800572	-2.250475036372
H	-1.764004588419	1.490889819809	-2.679241432984
H	-2.483462280711	0.649697362259	1.567253292110
O	0.888164263448	-1.554809697864	-1.644793235023
O	0.349795710259	-0.237611925575	-3.441980684220
C	1.798472499741	-2.311781303121	-2.502760364855
H	2.250406683903	-3.058624864097	-1.851241473099
H	1.242402563787	-2.788651841894	-3.312899864037
H	2.555437774954	-1.650136776531	-2.931079201153
C	1.673738968741	2.100571518372	1.597353018446
C	0.592838004516	1.573951919805	0.978284817362
C	0.281339172799	0.142854581254	0.949956805366
H	-0.137600748168	2.213324255195	0.486812522086
H	1.870457996838	3.166043723535	1.549610481112
H	2.367130241476	1.497455467300	2.178394976236
O	-0.490327373078	-0.379232968810	2.659907379742
C	0.269827203370	-1.327756969828	3.045027615680
C	1.364430064988	-1.668416115776	2.167965648435
C	1.391616335816	-0.815581684409	1.103238861564
H	0.085352247837	-1.810480044292	4.004057461744
H	2.168797599189	-0.805268898609	0.350783468915
H	2.082080609775	-2.446873168665	2.378049322064

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TS108 -802.931562

C	-0.954633862433	1.644061224303	1.698879933128
C	-1.173841867727	1.107960570144	0.385822665681
C	-0.431109339593	-0.179180306050	0.225280212057
C	0.217403792772	-0.391169133577	1.592747063113
C	-0.079914943639	0.640382700037	2.409349199367

H	0.803515293076	-1.272223981060	1.817704247948
O	-1.369842507877	2.722760266228	2.210542508863
C	-1.285460625440	-1.331646164486	-0.267633091032
H	-1.810376728993	1.529271308146	-0.377668656726
H	0.245310480991	0.777121797026	3.433173515182
O	-1.545252157198	-2.223086742758	0.728373334841
O	-1.749936201987	-1.450587158402	-1.408596722842
C	-2.490907177749	-3.300329368397	0.426440104544
H	-2.597094002925	-3.848479375041	1.360102885301
H	-3.446170887441	-2.877913250121	0.107046707063
H	-2.091916034668	-3.938619678424	-0.365169574397
C	0.680360944165	1.730030426364	-2.834123210342
C	0.198687592619	0.666817373339	-2.169272546754
C	0.640118499896	0.290118752597	-0.788630462056
H	-0.550286769346	0.013577247522	-2.601849911425
H	0.330989154793	1.955192643103	-3.836177788194
H	1.403826825776	2.415909204750	-2.401407038381
O	1.617344133934	-1.164508551008	-1.288226260329
C	2.831427736646	-0.860555802559	-0.968620266209
C	3.013821076814	0.424682225156	-0.378072813032
C	1.783537621590	1.000417697522	-0.155505957146
H	3.610832160574	-1.608647327854	-1.092231164422
H	1.623500546817	1.888796969663	0.438312233048
H	3.959572732409	0.802156556363	-0.021897508378

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TS109 -802.930024

C	1.925053981551	-0.600662243300	0.292643740952
C	1.788560649374	0.057456831308	-0.954879691524
C	0.479295771425	-0.210936537672	-1.455810340507
C	-0.234632585798	-1.073856797199	-0.636647851270
C	0.635843623096	-1.453630159027	0.509832078341
H	-1.215589171268	-1.474059073881	-0.848130772369
O	2.847818609059	-0.510025628823	1.171162214443
C	-0.024880649781	0.366402170841	-2.725404640385
H	2.510733350274	0.723807839828	-1.401666655809
H	0.910378856768	-2.514243667744	0.444067362115
O	-1.270560703640	-0.103618219273	-3.056510064952
O	0.584658942003	1.186521663626	-3.424240889482
C	-1.860512738669	0.409512623302	-4.291254803341
H	-2.824094396912	-0.089638157465	-4.374226286838
H	-1.984654275829	1.493420756703	-4.227576775456
H	-1.220058685339	0.170477352376	-5.143771748079
C	1.009323407644	-1.295505063982	3.036738301452
C	0.012432716588	-1.278195040642	1.949804409631
C	-0.596256593365	0.079112982040	2.148312722865
H	-0.762975474636	-2.034566547276	2.095190694476

H	0.867324242709	-1.925335869445	3.912281772935
H	1.870045463090	-0.639504528010	2.973208740106
O	-1.591180597247	0.168822538222	3.128898967646
C	-2.039954695787	1.476830311178	3.129940418521
C	-1.360373900022	2.209205989686	2.190080848005
C	-0.430146152540	1.313140955706	1.554255916650
H	-2.823224158638	1.709589192450	3.830032439045
H	0.270590906511	1.548893232071	0.770058183551
H	-1.504791669690	3.253250912550	1.967183796042

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TS110 -802.929553

C	2.004085819017	-2.612169294617	-0.382107102743
C	1.240498895529	-2.210747527977	0.853903805437
C	0.245317529465	-1.369771724700	0.504057365538
C	0.309366710913	-1.041671552007	-0.991570909970
C	1.370086789522	-1.904736505129	-1.488209270581
H	-0.652529852411	-1.048639454885	-1.502163977895
O	2.963940715086	-3.418287543748	-0.416694713380
C	-0.786103784897	-0.855532074029	1.427635074537
H	1.454891235988	-2.580973908904	1.847511739600
H	1.585157155919	-2.133529492220	-2.521866253439
O	-1.845043559966	-0.322791001050	0.738266217686
O	-0.747194644339	-0.917690491786	2.662756483233
C	-2.942366268317	0.227486215050	1.529684913020
H	-3.618080691652	0.674818400110	0.803478646602
H	-3.435484522830	-0.569901495855	2.091202727101
H	-2.561395116419	0.979263873481	2.225019671008
C	1.519155957373	0.720712335469	-2.380569320457
C	0.841134447345	0.560278632460	-1.112130845945
C	-0.151013338147	1.631732753949	-0.834456884636
H	1.523466043498	0.504460040198	-0.248755597149
H	1.861045729478	-0.127404599586	-2.957492583085
H	1.678515525754	1.716533790071	-2.787986951902
O	-0.169491957474	2.162674837172	0.450029094096
C	-1.176058070403	3.112903286583	0.488046041942
C	-1.786364093998	3.193462074888	-0.736866603674
C	-1.124735963009	2.235763232645	-1.590723243248
H	-1.311169138170	3.625039733524	1.424661158248
H	-1.356642660687	2.011709220489	-2.619931624836
H	-2.599809223835	3.848373784546	-1.003448240854

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TS111 -802.928453

C	1.380094094297	-1.910379930986	-2.014104253167
C	0.313779666770	-1.940063425650	-1.016694806272
C	0.259575786282	-0.653546650784	-0.318470507673
C	1.433879293383	0.137799412222	-0.899473070961

C	2.025310632006	-0.556200492270	-1.889678525589
H	1.672511460324	1.134461612546	-0.553279251840
O	1.715430925307	-2.816120094827	-2.813419585210
C	0.185838244383	-0.803716655694	1.187207347352
H	-0.184349905023	-2.847524627305	-0.706798004176
H	2.842998480640	-0.236434407605	-2.521110077447
O	1.255774644334	-0.264245568660	1.825325342466
O	-0.760162400321	-1.348295827558	1.773839366625
C	1.292346957371	-0.386499727080	3.285221683853
H	2.220415486500	0.095707969077	3.583959344764
H	0.426615887168	0.117241838493	3.721328910887
H	1.285726589421	-1.440694803306	3.570743130305
C	-2.212342186454	-0.800070958177	-0.747603127015
C	-1.120374480538	0.155819570573	-0.751444100063
C	-1.416106614540	1.407139855364	0.001189018028
H	-0.788479655469	0.441644455555	-1.762149098199
H	-2.036482506018	-1.864468644906	-0.714148229854
H	-3.241605733019	-0.448315149608	-0.733019687299
O	-0.945937982060	2.604088630246	-0.534141978771
C	-1.306949428129	3.613952203717	0.343235457913
C	-1.984772792381	3.084790337229	1.410387009789
C	-2.050730146924	1.659370148353	1.192961930056
H	-1.013938836583	4.611666221795	0.066987465618
H	-2.487815879535	0.914265207610	1.838957019950
H	-2.384414476672	3.632561637561	2.247925633931

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TS112 -802.926804

C	1.949880888578	-0.505981302239	-0.298996693027
C	1.379760850766	0.787246902083	-0.485107781894
C	0.150879025593	0.640382175770	-1.184959972745
C	-0.128795650168	-0.692222867995	-1.459151404894
C	0.937410260919	-1.533252253835	-0.859293624978
H	-0.991018870065	-1.052958523107	-2.000715741802
O	3.003672810174	-0.852223729250	0.322356453885
C	-0.694976034281	1.794331153238	-1.570726793860
H	1.800547006752	1.719574794705	-0.138368145790
H	1.377098145222	-2.246687910764	-1.557474258260
O	-1.813777852096	1.409733105423	-2.261556598344
O	-0.443127280992	2.976990864239	-1.307390689216
C	-2.721051320740	2.473166369534	-2.690205540349
H	-3.530918692252	1.963360593428	-3.208232205429
H	-3.094008681095	3.021985517262	-1.822096350711
H	-2.201259073497	3.165090978422	-3.357280037291
C	1.517416180989	-3.194236726833	0.928167710212
C	0.425193438812	-2.349499432498	0.423160624703
C	-0.088244703161	-1.393696125702	1.485434157067

H	-0.437658191287	-2.973971150668	0.147719485386
H	1.294073711556	-4.158084780889	1.377866330260
H	2.547770609021	-2.873722618606	0.807796214628
O	-1.366631417659	-0.895297648839	1.261251245932
C	-1.652427571941	-0.023331075428	2.303893654722
C	-0.595053530358	0.019096321376	3.172598446928
C	0.412826637823	-0.874131629134	2.648956781480
H	-2.616404717933	0.452822208441	2.271909098725
H	1.387697186054	-1.075724839281	3.061699547606
H	-0.529974636848	0.609835259703	4.071550782449

29

TS113 -802.926180

C	-0.555944308119	1.093457024095	1.825707994909
C	-0.232664929936	-0.315703128021	1.885565003667
C	0.859482022536	-0.547157537309	1.042854308045
C	1.307405453113	0.626255212656	0.399977374069
C	0.422067316257	1.743472677170	0.793965533443
H	2.205156927704	0.696810204789	-0.197532943813
O	-1.454508868527	1.740777654774	2.410975203390
C	1.460915807641	-1.890420474070	0.849857890364
H	-0.783102849683	-1.063076458406	2.436954838938
H	0.935909347518	2.599659608362	1.237484094025
O	2.446344405881	-1.879214142648	-0.107247207618
O	1.130768489803	-2.917376383844	1.453390314933
C	3.120408769353	-3.150119369745	-0.369855087787
H	3.862013346994	-2.926023219059	-1.134216637269
H	3.595841659564	-3.519934996106	0.541714238465
H	2.400518597405	-3.891483257392	-0.725021953313
C	0.216983037508	3.059158330925	-1.433937215913
C	-0.474133210803	2.317987850959	-0.380474129690
C	-1.040618882242	1.211006042948	-1.233791666706
H	-1.294682238123	2.888626828676	0.063491332080
H	-0.190390631496	3.982031224142	-1.834999374221
H	1.118432394412	2.655686490838	-1.886824150001
O	-2.420987239266	1.116604057258	-1.333561141250
C	-2.698681639445	-0.035951942536	-2.059028064607
C	-1.530578211624	-0.648153432581	-2.431814882801
C	-0.452056201517	0.162181528377	-1.925369332890
H	-3.740385319255	-0.256592271643	-2.212415581885
H	0.600591202694	0.007588673656	-2.084182685775
H	-1.442028765269	-1.555862952290	-3.005348041244

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TS114 -802.925853

C	-0.205909898449	-0.390925840065	-2.149109628365
C	0.851474443265	0.431837804595	-1.575947184516
C	0.279649431644	1.284415302348	-0.632617954694

C	-1.113229180656	1.078932283326	-0.499252142830
C	-1.504768848912	-0.063135165700	-1.363391235920
H	-1.772413325879	1.718601463587	0.069170038172
O	-0.147456838613	-1.225798466395	-3.073994466141
C	1.067354204277	2.278297255396	0.139649455546
H	1.902598062162	0.353477076446	-1.812084756676
H	-2.334455029696	0.126447082706	-2.046815293644
O	0.292854403298	2.948242571463	1.050543299433
O	2.277235881376	2.490102395827	0.001585061184
C	0.961427154080	3.964339454673	1.863855334098
H	0.191701823145	4.344644201772	2.532349959693
H	1.784267559157	3.515301744904	2.424983713119
H	1.352836611137	4.758317761717	1.223473866691
C	-3.034811139063	-0.959842278915	0.383423248887
C	-1.899699525061	-1.317671785966	-0.473224691290
C	-0.718812390299	-1.734568741271	0.386842467165
H	-2.131140382756	-2.178924647519	-1.115012234413
H	-3.735136079513	-1.719411340373	0.718196052976
H	-3.166651299582	0.053176887338	0.749115989319
O	0.029424531293	-2.811052154807	-0.066283182152
C	1.089926857899	-2.974451280144	0.816166032663
C	1.007826451391	-2.040780298029	1.814828272115
C	-0.168835506496	-1.246480659662	1.547822521527
H	1.774630143932	-3.772867890867	0.590746066527
H	-0.545433272532	-0.424682695692	2.133000311053
H	1.692084485371	-1.927718009050	2.639716870751

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TS115 -802.924625

C	-0.878400847100	-2.594727183419	-0.821067624840
C	0.072187503853	-1.529490681328	-0.559450006485
C	-0.555648515639	-0.442007888371	0.231774200592
C	-1.998064459242	-0.919228749453	0.385163384377
C	-2.158571472124	-2.135126660529	-0.199881459396
H	-2.728893906259	-0.348566381917	0.942932062588
O	-0.698453199307	-3.671703298999	-1.448964586059
C	0.152164260023	-0.110188624122	1.538185230969
H	1.134092424217	-1.599163499929	-0.750030847602
H	-3.072498331685	-2.713162743508	-0.249326872148
O	-0.670597774011	0.612397060573	2.362237848272
O	1.315415586647	-0.391605642251	1.824396606381
C	-0.093126798835	1.080810828996	3.624504311347
H	-0.898551148725	1.616175474047	4.122973164157
H	0.242682690158	0.229701857991	4.220951223339
H	0.753242284512	1.740458147775	3.420277214213
C	-1.513769168368	0.534703416608	-1.758893424744
C	-0.628580679652	0.892051573038	-0.632957943097

C	0.740597597564	1.346583772814	-1.055920192347
H	-1.066317496630	1.716544390252	-0.053289377007
H	-1.989114867410	1.322542000515	-2.339028999957
H	-1.609659213351	-0.485706858210	-2.107486043111
O	1.304195747117	2.359447145172	-0.285956580260
C	2.568078523217	2.611003213251	-0.804677535361
C	2.799461416277	1.793496540323	-1.877264079596
C	1.617064984360	0.978719250244	-2.044663157008
H	3.143129201009	3.370564315204	-0.305313064723
H	1.447601321691	0.222591194511	-2.793476284275
H	3.693995467380	1.765273679137	-2.477351981048

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TS116 -802.924567

C	-1.881487715933	-1.481741843032	-1.021255162770
C	-1.562943458766	-1.322592621531	0.446252064489
C	-0.229555227099	-1.193852512327	0.607281063435
C	0.484512027269	-1.224505808433	-0.746676039854
C	-0.612281436019	-1.415439327141	-1.705191425959
H	1.275275510140	-1.978868931258	-0.777394890943
O	-3.037014585640	-1.646994246986	-1.498041524533
C	0.439573676948	-1.039985558609	1.907905004709
H	-2.310064796674	-1.328023320367	1.229320014519
H	-0.496762796173	-1.559410420711	-2.771438688980
O	1.814071515543	-1.022418329639	1.778283042525
O	-0.119675085778	-0.944149617212	3.008271962629
C	2.585497328898	-0.882872645226	3.012638542200
H	3.628497381209	-0.934913291562	2.705304212379
H	2.363181151100	0.075577112741	3.487706470325
H	2.339381722480	-1.692272111375	3.703656488674
C	1.794232628785	0.426247349465	-2.295809388545
C	1.267428214865	0.168555677916	-0.966934627951
C	0.291500988717	1.316378349111	-0.900888502040
H	2.022391647644	0.280544922335	-0.187582724499
H	2.782939791655	0.851512323789	-2.440449692343
H	1.173009457194	0.265462842500	-3.172657150709
O	0.524782839983	2.280712670613	0.070802124530
C	-0.562482602580	3.150744930956	0.045395816160
C	-1.449000326012	2.763444737185	-0.922962791547
C	-0.894494258061	1.592799366951	-1.559054726509
H	-0.539869600163	3.953305198756	0.761450141540
H	-1.300836056336	1.062545286673	-2.402355523253
H	-2.378557498822	3.248650592106	-1.169713061841

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TS117 -802.923557

C	2.386011681558	0.016332735617	0.521129243762
C	1.819355202638	-0.278447497967	-0.857045259222



C	0.669936941765	-0.991438171172	-0.734511429040
C	0.361721837384	-1.203737514107	0.737849055051
C	1.489895554374	-0.604711366990	1.435385618733
H	0.090523790457	-2.231153232358	0.995465056720
O	3.468622315696	0.655144296207	0.692107062506
C	-0.183673487319	-1.415520375131	-1.807520808624
H	2.284701073875	0.054461979389	-1.778158535064
H	1.623970118943	-0.616356865019	2.506946727201
O	-1.462737337345	-1.862369899174	-1.265562034602
O	-0.022688205241	-1.465847215176	-3.023264962636
C	-2.445933656243	-2.388490343169	-2.222415986669
H	-3.314301307058	-2.676210462335	-1.629526301331
H	-2.701400189108	-1.622016153836	-2.956229749588
H	-2.017137023084	-3.255753650341	-2.723813822751
C	-2.195840936701	-0.891560628879	0.242887492676
C	-1.119055423209	-0.357679544044	1.056219014105
C	-0.903159836174	1.105383914295	0.933406495006
H	-1.251698836936	-0.630342751864	2.106921247891
H	-2.708049988002	-1.787748666635	0.581109027413
H	-2.757800127763	-0.228275664670	-0.409288737591
O	-0.769912018978	1.793054514895	2.130598214052
C	-0.499958075592	3.117417565577	1.817016376201
C	-0.472132943191	3.274566637483	0.458278326553
C	-0.728835367612	1.973237849352	-0.115401956469
H	-0.350074549536	3.781905211832	2.649166054333
H	-0.749169859824	1.727844162218	-1.165407287874
H	-0.273498880652	4.189267591891	-0.075344539131

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TS118 -802.923282

C	-1.653951078384	1.525172144621	0.014879321800
C	-0.286585096636	1.242261990131	0.344321942318
C	-0.140594539226	-0.194023811224	0.714769899670
C	-1.553327601253	-0.750250589919	0.570785118342
C	-2.394884282246	0.209852012988	0.151087869208
H	-1.784420930418	-1.788273887008	0.776664950081
O	-2.187790843341	2.615148760623	-0.337931579169
C	0.467586738736	-0.226806692596	2.110325808706
H	0.482868215072	1.992213336568	0.475844690053
H	-3.453096948755	0.114165868727	-0.055870627542
O	-0.421177628365	-0.351697773206	3.119340689658
O	1.701244863929	-0.125060769523	2.291068422694
C	0.082928447980	-0.192981282161	4.486563671809
H	-0.794394888728	-0.299249028731	5.120483516086
H	0.825895734352	-0.963133681918	4.705842388913
H	0.533221193121	0.795531323216	4.602122745076
C	2.240584340166	-0.532081881495	-0.131501065514

C	0.870492943287	-1.027831604753	-0.142061595542
C	0.823871129845	-0.772857817678	-1.620044652657
H	0.804366923094	-2.099957280279	0.056748068609
H	3.089118721004	-1.208062644473	-0.165178712989
H	2.424213154461	0.535501374964	-0.149681481944
O	0.815303938487	-1.892287950552	-2.458850711580
C	0.553196805100	-1.430150092883	-3.737411258501
C	0.411068855888	-0.065444973741	-3.734840191330
C	0.608229354267	0.374061692480	-2.381095032351
H	0.509405277645	-2.178970489455	-4.509174436653
H	0.617862953734	1.384114576548	-2.010968942044
H	0.207326104121	0.557155436757	-4.589689269823

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TS119 -802.922538

C	1.875907138819	0.759372148618	-1.931792999134
C	2.468299350448	0.903406002392	-0.569646186943
C	1.710047227362	0.248704636402	0.348361364331
C	0.499190069970	-0.404786377432	-0.302672503000
C	0.699974827109	-0.079547317266	-1.745199112335
H	0.345331782968	-1.443224628368	-0.016290389813
O	2.317742846444	1.265980247887	-2.994446596873
C	2.100383278495	0.082539155287	1.760973167024
H	3.385769197986	1.440512449996	-0.366237134383
H	0.082746218197	-0.467100475289	-2.544087243109
O	1.220362293215	-0.735796521937	2.433277525620
O	3.092539302470	0.584233243951	2.304685386190
C	1.520012474906	-1.015513113462	3.838249403294
H	0.719598712568	-1.672098238495	4.173067239990
H	2.492113339464	-1.506407890416	3.922677453638
H	1.535835708014	-0.086312418108	4.413088596298
C	-0.758976161470	1.364055723115	1.027785325143
C	-0.789624224311	0.486693455547	-0.103324437456
C	-2.074480299642	-0.220530308607	-0.400851998753
H	-0.627530989465	1.161868764797	-1.047476861950
H	-1.306447395146	2.301713941303	0.999921410844
H	-0.174612792660	1.143311333688	1.910709091331
O	-2.251406517569	-0.721080245792	-1.687506609598
C	-3.487988999359	-1.353402396724	-1.714388590392
C	-4.084308355551	-1.256796994996	-0.486765052439
C	-3.171171639575	-0.524597923433	0.362322940553
H	-3.771767244309	-1.798961695050	-2.651507940100
H	-3.305143286334	-0.268427252062	1.400591678866
H	-5.047734081250	-1.653756009073	-0.212182005765

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TS120 -802.920117

C	1.606639970044	-0.318919536087	-1.089715426424
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C	1.101435785915	0.973893307069	-0.669671577819
C	-0.270103851163	1.053049733335	-0.975472907236
C	-0.738367352642	-0.126714843827	-1.566505145748
C	0.390034944796	-1.122575853488	-1.564921316329
H	-1.719509884583	-0.281200621643	-1.992425967898
O	2.776081032925	-0.774032623997	-1.042033879053
C	-1.094337588908	2.251910837970	-0.683996877566
H	1.690464022763	1.756904086249	-0.213630248157
H	0.580933609861	-1.626694573827	-2.513402735498
O	-2.381673103225	2.108832930075	-1.127149732497
O	-0.688143809511	3.269719616441	-0.110821998205
C	-3.291758578843	3.228806559059	-0.888874306129
H	-4.237133308551	2.924699172881	-1.333522213007
H	-3.400469805297	3.401746369769	0.184431807560
H	-2.906885984227	4.134353197308	-1.363740732520
C	0.131885931248	-3.524873078871	-0.782938721959
C	-0.062750683412	-2.129508030768	-0.465926753276
C	0.369784919407	-1.758160171783	0.938514874698
H	-1.184795006490	-1.924623378442	-0.393010726255
H	-0.249154159489	-4.290361005658	-0.112843444322
H	0.581207878672	-3.837636870935	-1.720161670554
O	-0.488079035957	-0.924380106197	1.650048229012
C	0.121545580210	-0.660069925454	2.868233455474
C	1.320031102298	-1.319676860628	2.938699809600
C	1.476840468688	-2.036686409537	1.695382084324
H	-0.418606459995	-0.015428303206	3.538768524245
H	2.317321198163	-2.634387945140	1.385116225493
H	2.014232526186	-1.297854865374	3.762644189751

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TS121 -802.918754

C	-0.561925916161	1.247415283594	-0.438517491210
C	-1.620723276676	0.331120410727	-0.787585521157
C	-1.038897814095	-0.793453351920	-1.392614836841
C	0.364591419764	-0.718843123104	-1.416247995511
C	0.791128245062	0.512271344311	-0.722024919790
H	1.018624895096	-1.498386614453	-1.780035971325
O	-0.632586043253	2.440134152977	-0.056063189282
C	-1.837914719659	-1.928460232693	-1.919464661101
H	-2.673308369258	0.486743080215	-0.604767552002
H	1.467760369111	1.173841624818	-1.265996825326
O	-1.046836625616	-2.913248036797	-2.452108562842
O	-3.072046231359	-2.002731276197	-1.891419343866
C	-1.731932468586	-4.079934131467	-3.007874515419
H	-0.938788577973	-4.719579460355	-3.389829962456
H	-2.303892025336	-4.587219580198	-2.227134496526
H	-2.409358143531	-3.772458462712	-3.808032586283

C	2.979113029341	-0.134874936083	0.432381922078
C	1.545444456379	0.059020444308	0.632062754586
C	1.536609312333	1.104735389169	1.726498875055
H	1.053335335543	-0.836169660567	1.017159920836
H	3.484579380304	-1.052136222691	0.718190210646
H	3.581686803250	0.692100529217	0.066873516057
O	1.533309751158	0.584281615559	3.022224814675
C	1.557186290049	1.665427508704	3.892454665394
C	1.588918769329	2.835194180334	3.180556667872
C	1.580547222471	2.478907816458	1.783016477902
H	1.531302031447	1.429329149547	4.941640997114
H	1.556433694117	3.149829214399	0.942730864472
H	1.597301332099	3.831919232595	3.589622880639

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TS122 -802.918370

C	1.690743877973	1.292715894694	2.118059474613
C	1.397533586261	1.041152691584	0.744027356047
C	0.068506862493	0.266699467477	0.623025314965
C	-0.308377865196	0.045946911893	2.094543152325
C	0.601798684874	0.603935115499	2.912029064451
H	-1.215781227207	-0.473407892537	2.380034862527
O	2.647728703092	1.934248355330	2.646511881092
C	-1.055308563388	1.055485948208	-0.044645064653
H	1.750351844629	1.726732238211	-0.015242885425
H	0.578970185072	0.615032242652	3.995301713688
O	-1.753428993256	0.266720664761	-0.955661237096
O	-1.358865866411	2.229052157050	0.154388794343
C	-2.862961115716	0.900207623208	-1.666518432416
H	-3.268072215177	0.126255547779	-2.316536684216
H	-3.612664514466	1.245433186619	-0.951226068394
H	-2.499593930840	1.752002901838	-2.246087426018
C	1.800960205300	0.431241392618	-2.463347136218
C	0.868035335092	-0.543807901888	-2.632370758644
C	0.236657696787	-1.229819138195	-1.550750621937
H	0.593546722373	-0.893709076943	-3.622168573761
H	2.295543887412	0.866058594873	-3.325416716926
H	2.106337740661	0.762500248471	-1.476976134990
O	-0.483969989290	-2.308914522679	-1.894125949215
C	-0.960041484526	-2.954819987185	-0.707761328079
C	-0.535013680943	-2.290776721783	0.372158539791
C	0.315710948568	-1.115856078419	-0.055648646940
H	-1.555729220917	-3.832204739043	-0.885256295137
H	1.388102843827	-1.261363933362	0.230269310271
H	-0.728652052850	-2.549125206050	1.399911285418

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TS123 -802.913544

C	-1.880410271780	0.858024365313	-1.856393622862
C	-1.231635844541	1.546472249946	-0.684684081878
C	-0.963600776016	0.640091419017	0.277833704649
C	-1.383638602863	-0.760276274702	-0.148726205989
C	-1.991653507832	-0.544788744049	-1.473743835247
H	-1.970964593552	-1.257943700459	0.621371081513
O	-2.258772363020	1.411327626697	-2.916601144046
C	-0.344913502418	0.939328198349	1.579080323875
H	-1.025502413634	2.607785764390	-0.647169775663
H	-2.499202129321	-1.301567286807	-2.057169754112
O	-0.344248707905	-0.169769808979	2.396106752737
O	0.113902061280	2.031560634193	1.935985126009
C	0.281765453522	-0.012011213722	3.706757788695
H	0.162815056650	-0.975759815679	4.198486912121
H	1.338196432690	0.242385353294	3.586810331536
H	-0.216114813920	0.780137979521	4.270682972054
C	-0.227567143704	-3.028883076276	-0.007649349703
C	-0.148592905315	-1.713283972914	-0.573150352530
C	1.162645618252	-0.972818470362	-0.463140322600
H	-0.267541273602	-1.810153174360	-1.695464978571
H	0.171910031017	-3.885377582744	-0.542032036236
H	-0.759243231198	-3.210742893137	0.921544180458
O	1.467197984972	-0.120743289740	-1.515378326455
C	2.676008403967	0.491231048496	-1.209113889809
C	3.134268385437	0.028810734842	-0.005155125604
C	2.158854701978	-0.924232845463	0.475035843535
H	3.047283432309	1.193992612987	-1.933495805487
H	2.189451803927	-1.491305750198	1.390551806516
H	4.046380100892	0.324481177449	0.486469413132

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TS124 -802.907797

C	0.118701690076	-2.155228296403	1.340736100554
C	-0.143121168455	-1.579158406256	0.014597367484
C	0.632886204794	-0.344378325490	-0.135240585504
C	1.081668130808	-0.005699943892	1.304106976944
C	0.843063588089	-1.063059525207	2.102271884744
H	1.583726952633	0.919116066995	1.555279012520
O	-0.243080103012	-3.250916503983	1.814363484780
C	1.951736434323	-0.461529760744	-0.928345624945
H	-1.091314026181	-1.750845786685	-0.471998876998
H	1.096831239079	-1.173526888715	3.147908230517
O	2.470430982816	0.785624343058	-1.186692955407
O	2.525524551687	-1.498770534899	-1.254353748639
C	3.778455859876	0.840745785392	-1.842488817338
H	3.992231899491	1.900968512254	-1.960606578260
H	4.528784988388	0.354259685313	-1.215343834882

H	3.735081056244	0.336968757341	-2.810900944817
C	-0.552673669286	-0.182266026703	-2.216901649163
C	-0.322824103959	0.633513595505	-1.022151109005
C	-1.544105049510	1.054362644242	-0.279190158831
H	0.311560479459	1.505050770498	-1.225567212744
H	0.253943128890	-0.346820789840	-2.924688710044
H	-1.545475679386	-0.502024024515	-2.515548087695
O	-1.382252260309	2.146658874190	0.565331199152
C	-2.600785391352	2.367243509891	1.193674656284
C	-3.515325389203	1.445272527388	0.763170169827
C	-2.832865700394	0.596649190067	-0.187941225688
H	-2.635732138033	3.188478905857	1.887372832775
H	-3.258665591064	-0.241593878268	-0.716198938804
H	-4.543091031282	1.367390220143	1.077432407281

**Figure S11.**

Variations in the four lowest transverse vibrational mode frequencies along the product side of the IRC path for the TSs which are shared by two AFIR paths.





















